



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 06:11 PM EDT

PDB ID : 2KLX  
BMRB ID : 16403  
Title : Solution structure of glutaredoxin from Bartonella henselae str. Houston  
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Deposited on : 2009-07-10

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

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A user guide is available at

<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>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.33

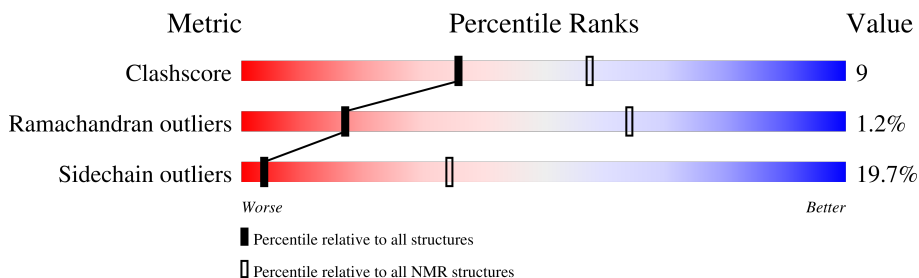
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 80%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	89	65% 27% • 6%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:2-A:85 (84)	0.63	18

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 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1401 atoms, of which 697 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Glutaredoxin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1401	439	697	126	134	5	0

There are 4 discrepancies between the modelled and reference sequences:

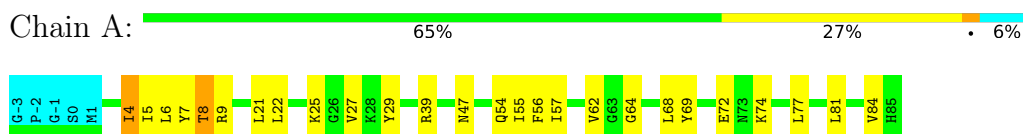
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q6G5J5
A	-2	PRO	-	expression tag	UNP Q6G5J5
A	-1	GLY	-	expression tag	UNP Q6G5J5
A	0	SER	-	expression tag	UNP Q6G5J5

## 4 Residue-property plots [i](#)

### 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: Glutaredoxin

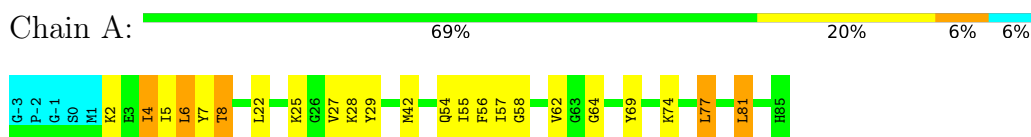


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

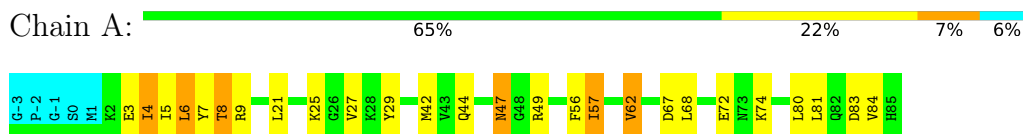
#### 4.2.1 Score per residue for model 1

- Molecule 1: Glutaredoxin



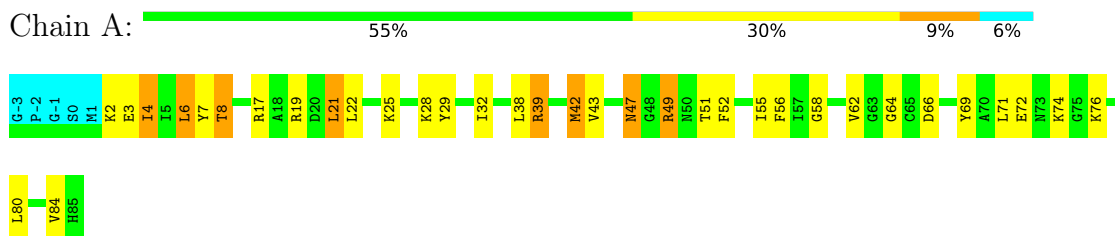
#### 4.2.2 Score per residue for model 2

- Molecule 1: Glutaredoxin



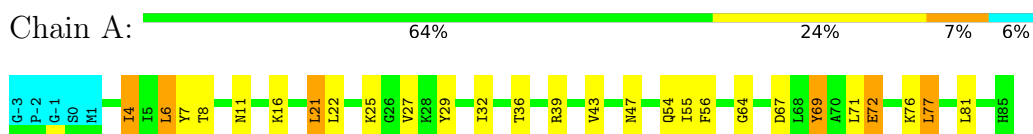
### 4.2.3 Score per residue for model 3

- Molecule 1: Glutaredoxin



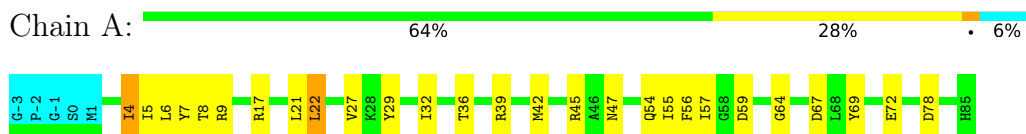
### 4.2.4 Score per residue for model 4

- Molecule 1: Glutaredoxin



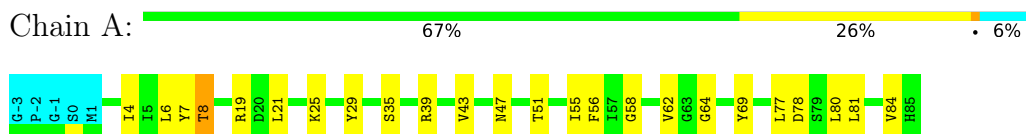
### 4.2.5 Score per residue for model 5

- Molecule 1: Glutaredoxin



### 4.2.6 Score per residue for model 6

- Molecule 1: Glutaredoxin



### 4.2.7 Score per residue for model 7

- Molecule 1: Glutaredoxin





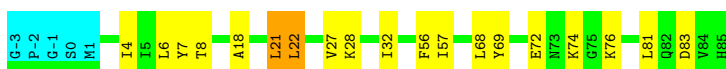
#### 4.2.8 Score per residue for model 8

- Molecule 1: Glutaredoxin



#### 4.2.9 Score per residue for model 9

- Molecule 1: Glutaredoxin



#### 4.2.10 Score per residue for model 10

- Molecule 1: Glutaredoxin



#### 4.2.11 Score per residue for model 11

- Molecule 1: Glutaredoxin



#### 4.2.12 Score per residue for model 12

- Molecule 1: Glutaredoxin





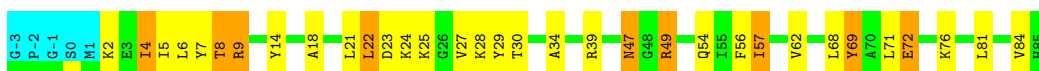
#### 4.2.13 Score per residue for model 13

- Molecule 1: Glutaredoxin



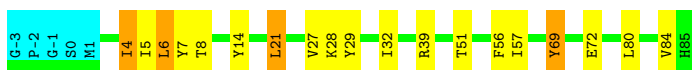
#### 4.2.14 Score per residue for model 14

- Molecule 1: Glutaredoxin



#### 4.2.15 Score per residue for model 15

- Molecule 1: Glutaredoxin



#### 4.2.16 Score per residue for model 16

- Molecule 1: Glutaredoxin



#### 4.2.17 Score per residue for model 17

- Molecule 1: Glutaredoxin







#### 4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Glutaredoxin

Chain A: 61% 27% 7% 6%



#### 4.2.19 Score per residue for model 19

- Molecule 1: Glutaredoxin

Chain A: 69% 20% 6% 6%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Glutaredoxin

Chain A: 65% 22% 7% 6%



## 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 least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	962
Number of shifts mapped to atoms	962
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

## 6 Model quality i

### 6.1 Standard geometry i

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 i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	675	670	670	11±3
All	All	13500	13400	13400	229

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ILE:HD11	1:A:62:VAL:HG23	0.84	1.50	12	2
1:A:18:ALA:O	1:A:22:LEU:HD22	0.64	1.92	11	3
1:A:25:LYS:HE3	1:A:81:LEU:HD11	0.62	1.70	1	5
1:A:22:LEU:HD23	1:A:29:TYR:HB3	0.61	1.70	17	4
1:A:9:ARG:HD2	1:A:34:ALA:HB2	0.61	1.73	14	1
1:A:36:THR:HG22	1:A:39:ARG:CZ	0.61	2.26	4	4
1:A:57:ILE:HD12	1:A:83:ASP:OD2	0.61	1.96	9	1
1:A:71:LEU:HD22	1:A:76:LYS:HG2	0.60	1.73	4	3
1:A:21:LEU:HD23	1:A:69:TYR:CE1	0.60	2.31	13	1
1:A:4:ILE:HB	1:A:84:VAL:HG12	0.60	1.72	20	8
1:A:77:LEU:HG	1:A:81:LEU:HD13	0.59	1.74	11	8
1:A:6:LEU:HD21	1:A:29:TYR:CD1	0.59	2.32	3	11
1:A:80:LEU:O	1:A:84:VAL:HG22	0.58	1.98	20	6
1:A:21:LEU:HD21	1:A:72:GLU:CD	0.58	2.19	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:ILE:CG1	1:A:57:ILE:HG22	0.58	2.29	10	10
1:A:21:LEU:HD11	1:A:72:GLU:OE1	0.57	1.99	14	7
1:A:25:LYS:CE	1:A:81:LEU:HD11	0.56	2.30	18	3
1:A:40:GLN:OE1	1:A:51:THR:HG23	0.56	2.00	8	1
1:A:57:ILE:CD1	1:A:62:VAL:HG23	0.55	2.32	2	2
1:A:21:LEU:HD11	1:A:72:GLU:HG3	0.55	1.79	2	3
1:A:22:LEU:HD23	1:A:29:TYR:CB	0.54	2.32	17	3
1:A:21:LEU:HD21	1:A:72:GLU:OE1	0.54	2.03	18	1
1:A:21:LEU:HD22	1:A:68:LEU:CD1	0.54	2.33	18	1
1:A:51:THR:HG23	1:A:52:PHE:CD2	0.53	2.39	3	1
1:A:4:ILE:HD12	1:A:22:LEU:HD21	0.53	1.80	8	2
1:A:72:GLU:O	1:A:77:LEU:HD23	0.53	2.03	20	1
1:A:4:ILE:HG12	1:A:57:ILE:HG22	0.52	1.81	5	12
1:A:21:LEU:HD13	1:A:68:LEU:CD1	0.52	2.33	14	3
1:A:22:LEU:CD1	1:A:84:VAL:HG11	0.52	2.35	14	1
1:A:47:ASN:ND2	1:A:49:ARG:H	0.51	2.03	14	5
1:A:22:LEU:HD13	1:A:29:TYR:HB3	0.51	1.81	13	2
1:A:55:ILE:HD12	1:A:64:GLY:O	0.51	2.06	8	3
1:A:4:ILE:HD13	1:A:5:ILE:N	0.50	2.21	8	10
1:A:55:ILE:HD13	1:A:64:GLY:O	0.50	2.06	18	6
1:A:25:LYS:HE2	1:A:81:LEU:HD21	0.50	1.82	4	1
1:A:4:ILE:HG21	1:A:22:LEU:HD22	0.50	1.83	4	1
1:A:80:LEU:O	1:A:84:VAL:HG13	0.49	2.07	2	2
1:A:71:LEU:HD22	1:A:76:LYS:CG	0.49	2.37	14	2
1:A:21:LEU:HD23	1:A:22:LEU:N	0.49	2.22	3	2
1:A:21:LEU:HD11	1:A:72:GLU:CD	0.49	2.27	9	2
1:A:21:LEU:HD21	1:A:72:GLU:OE2	0.49	2.08	15	2
1:A:25:LYS:HE3	1:A:81:LEU:HD21	0.49	1.84	8	1
1:A:21:LEU:HD13	1:A:69:TYR:CE1	0.48	2.42	18	3
1:A:57:ILE:HG22	1:A:83:ASP:HB3	0.48	1.85	17	1
1:A:77:LEU:HG	1:A:81:LEU:HD23	0.48	1.85	4	2
1:A:7:TYR:CE2	1:A:43:VAL:HG23	0.48	2.42	10	1
1:A:57:ILE:HD11	1:A:62:VAL:CG2	0.48	2.33	12	1
1:A:27:VAL:HG11	1:A:84:VAL:HG23	0.47	1.87	17	2
1:A:21:LEU:HD11	1:A:72:GLU:OE2	0.47	2.10	9	1
1:A:25:LYS:HE2	1:A:81:LEU:HD13	0.47	1.85	14	1
1:A:9:ARG:N	1:A:34:ALA:HB2	0.47	2.24	8	4
1:A:5:ILE:HG23	1:A:30:THR:HB	0.47	1.86	14	2
1:A:4:ILE:CB	1:A:84:VAL:HG12	0.47	2.40	14	1
1:A:7:TYR:CD1	1:A:32:ILE:HG21	0.46	2.45	13	4
1:A:37:SER:C	1:A:38:LEU:HD22	0.46	2.31	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ARG:O	1:A:43:VAL:HG12	0.46	2.10	13	7
1:A:7:TYR:CD2	1:A:32:ILE:HG21	0.46	2.45	8	2
1:A:32:ILE:HD12	1:A:42:MET:CE	0.46	2.40	3	1
1:A:55:ILE:HD13	1:A:64:GLY:C	0.46	2.31	3	5
1:A:71:LEU:HD22	1:A:76:LYS:HG3	0.45	1.87	17	1
1:A:36:THR:HG22	1:A:39:ARG:NH1	0.45	2.27	4	2
1:A:4:ILE:HG13	1:A:84:VAL:HG12	0.45	1.89	7	1
1:A:6:LEU:O	1:A:6:LEU:HD12	0.44	2.11	13	1
1:A:57:ILE:HG12	1:A:62:VAL:HG23	0.44	1.90	17	1
1:A:57:ILE:HD12	1:A:83:ASP:CG	0.44	2.32	10	1
1:A:32:ILE:HD12	1:A:42:MET:HE2	0.44	1.88	3	1
1:A:21:LEU:HD12	1:A:69:TYR:CE1	0.44	2.48	14	1
1:A:18:ALA:HA	1:A:68:LEU:HD21	0.44	1.89	13	1
1:A:6:LEU:HD21	1:A:29:TYR:HB2	0.43	1.90	2	1
1:A:57:ILE:CD1	1:A:80:LEU:HD13	0.43	2.43	15	1
1:A:72:GLU:HG2	1:A:77:LEU:HD12	0.43	1.88	16	1
1:A:7:TYR:CE1	1:A:32:ILE:HG21	0.43	2.49	15	3
1:A:22:LEU:O	1:A:27:VAL:HG22	0.43	2.14	5	1
1:A:7:TYR:O	1:A:8:THR:HG23	0.42	2.14	14	12
1:A:22:LEU:HD13	1:A:29:TYR:CB	0.42	2.44	13	1
1:A:22:LEU:HD12	1:A:84:VAL:HG11	0.42	1.90	14	1
1:A:43:VAL:HG22	1:A:47:ASN:HD21	0.42	1.74	11	1
1:A:43:VAL:HG21	1:A:50:ASN:HB3	0.42	1.92	17	1
1:A:6:LEU:HD21	1:A:29:TYR:HD1	0.42	1.75	1	1
1:A:71:LEU:HD23	1:A:74:LYS:NZ	0.41	2.29	12	1
1:A:27:VAL:HG21	1:A:84:VAL:HB	0.41	1.93	20	1
1:A:51:THR:HG23	1:A:52:PHE:CE2	0.41	2.50	3	1
1:A:68:LEU:HD12	1:A:68:LEU:C	0.41	2.35	20	1
1:A:39:ARG:HH22	1:A:52:PHE:N	0.41	2.13	19	1
1:A:25:LYS:CE	1:A:81:LEU:HD21	0.41	2.46	8	1
1:A:55:ILE:HD13	1:A:68:LEU:HD23	0.40	1.92	8	1
1:A:22:LEU:CD2	1:A:84:VAL:HG11	0.40	2.47	20	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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	83/89 (93%)	73±2 (88±2%)	9±2 (11±2%)	1±1 (1±1%)	17	64
All	All	1660/1780 (93%)	1457 (88%)	183 (11%)	20 (1%)	17	64

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	62	VAL	10
1	A	58	GLY	5
1	A	49	ARG	2
1	A	35	SER	1
1	A	50	ASN	1
1	A	51	THR	1

### 6.3.2 Protein sidechains [i](#)

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	74/77 (96%)	59±2 (80±3%)	15±2 (20±3%)	4	34
All	All	1480/1540 (96%)	1189 (80%)	291 (20%)	4	34

All 47 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	4	ILE	20
1	A	8	THR	19
1	A	56	PHE	19
1	A	69	TYR	15
1	A	6	LEU	14
1	A	54	GLN	13
1	A	47	ASN	13
1	A	27	VAL	12
1	A	74	LYS	12
1	A	77	LEU	11
1	A	22	LEU	10
1	A	28	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	42	MET	9
1	A	81	LEU	9
1	A	9	ARG	9
1	A	25	LYS	8
1	A	21	LEU	8
1	A	51	THR	7
1	A	2	LYS	6
1	A	67	ASP	6
1	A	68	LEU	5
1	A	19	ARG	5
1	A	3	GLU	4
1	A	57	ILE	4
1	A	39	ARG	4
1	A	76	LYS	4
1	A	17	ARG	3
1	A	72	GLU	3
1	A	45	ARG	3
1	A	78	ASP	3
1	A	65	CYS	3
1	A	38	LEU	2
1	A	14	TYR	2
1	A	24	LYS	2
1	A	40	GLN	2
1	A	44	GLN	1
1	A	83	ASP	1
1	A	66	ASP	1
1	A	11	ASN	1
1	A	16	LYS	1
1	A	59	ASP	1
1	A	41	GLU	1
1	A	15	CYS	1
1	A	23	ASP	1
1	A	37	SER	1
1	A	49	ARG	1
1	A	50	ASN	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 79% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping (i)

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	962
Number of shifts mapped to atoms	962
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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	88	$-0.42 \pm 0.09$	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	75	$0.16 \pm 0.13$	None needed (< 0.5 ppm)
$^{13}\text{C}'$	74	$0.37 \pm 0.09$	None needed (< 0.5 ppm)
$^{15}\text{N}$	82	$0.28 \pm 0.36$	None needed (< 0.5 ppm)

#### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 932 atoms were assigned a chemical shift out of a possible 1167. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	400/420 (95%)	167/171 (98%)	154/168 (92%)	79/81 (98%)
Sidechain	496/668 (74%)	376/429 (88%)	112/206 (54%)	8/33 (24%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	36/79 (46%)	32/38 (84%)	4/39 (10%)	0/2 (0%)
Overall	932/1167 (80%)	575/638 (90%)	270/413 (65%)	87/116 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 962 atoms were assigned a chemical shift out of a possible 1214. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	418/445 (94%)	174/182 (96%)	162/178 (91%)	82/85 (96%)
Sidechain	508/690 (74%)	385/444 (87%)	115/213 (54%)	8/33 (24%)
Aromatic	36/79 (46%)	32/38 (84%)	4/39 (10%)	0/2 (0%)
Overall	962/1214 (79%)	591/664 (89%)	281/430 (65%)	90/120 (75%)

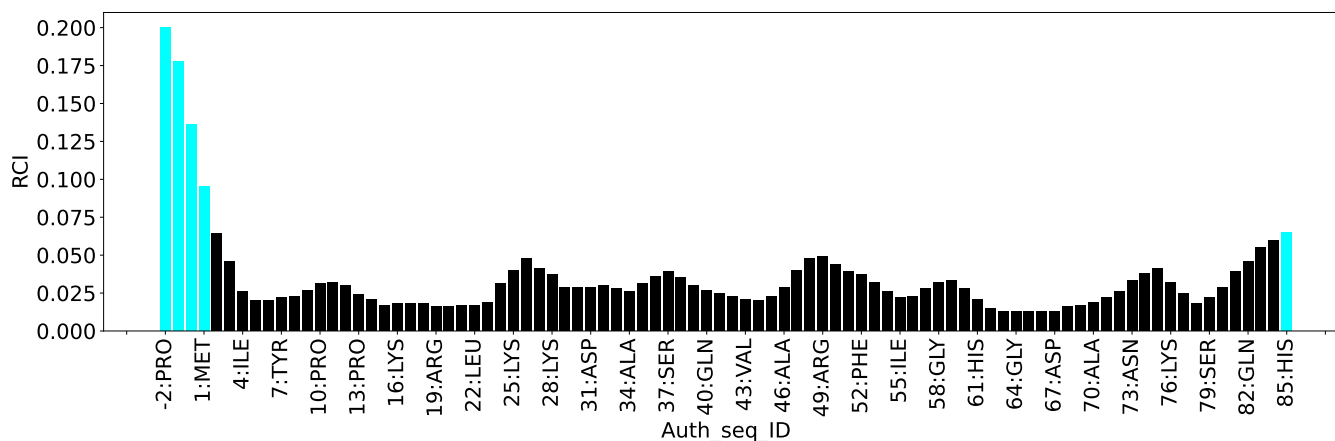
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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	1015
Intra-residue ( $ i-j =0$ )	268
Sequential ( $ i-j =1$ )	279
Medium range ( $ i-j >1$ and $ i-j <5$ )	202
Long range ( $ i-j \geq 5$ )	266
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.4
Number of long range restraints per residue <sup>1</sup>	3.0

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

### 8.2 Residual restraint violations

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

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

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.0	0.2
0.2-0.5 (Medium)	1.1	0.49
>0.5 (Large)	0.1	0.53

### 8.2.2 Average number of dihedral-angle violations per model

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

## 9 Distance violation analysis [i](#)

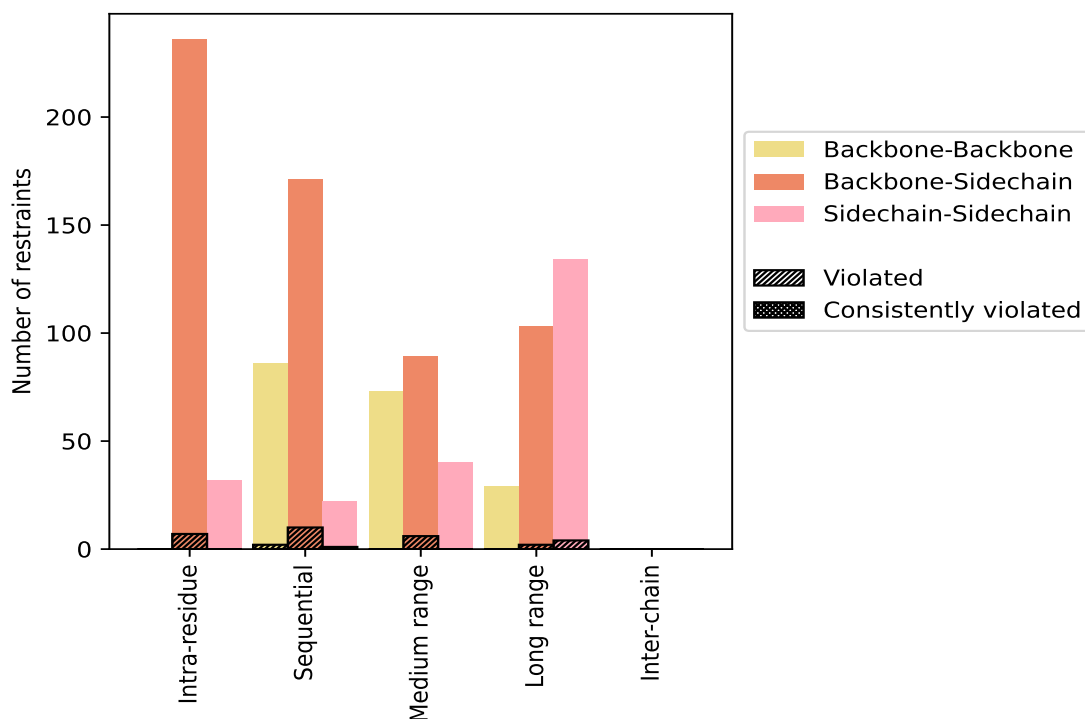
### 9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>268</b>	<b>26.4</b>	<b>7</b>	<b>2.6</b>	<b>0.7</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	236	23.3	7	3.0	0.7	0	0.0	0.0
Sidechain-Sidechain	32	3.2	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>279</b>	<b>27.5</b>	<b>13</b>	<b>4.7</b>	<b>1.3</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	86	8.5	2	2.3	0.2	0	0.0	0.0
Backbone-Sidechain	171	16.8	10	5.8	1.0	0	0.0	0.0
Sidechain-Sidechain	22	2.2	1	4.5	0.1	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>202</b>	<b>19.9</b>	<b>6</b>	<b>3.0</b>	<b>0.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	73	7.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	89	8.8	6	6.7	0.6	0	0.0	0.0
Sidechain-Sidechain	40	3.9	0	0.0	0.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>266</b>	<b>26.2</b>	<b>6</b>	<b>2.3</b>	<b>0.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	29	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	103	10.1	2	1.9	0.2	0	0.0	0.0
Sidechain-Sidechain	134	13.2	4	3.0	0.4	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1015</b>	<b>100.0</b>	<b>32</b>	<b>3.2</b>	<b>3.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	188	18.5	2	1.1	0.2	0	0.0	0.0
Backbone-Sidechain	599	59.0	25	4.2	2.5	0	0.0	0.0
Sidechain-Sidechain	228	22.5	5	2.2	0.5	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	1	0	0	0	1	0.12	0.12	0.0	0.12
2	0	3	0	1	0	4	0.16	0.24	0.04	0.15
3	1	2	0	1	0	4	0.12	0.13	0.01	0.12
4	0	4	1	0	0	5	0.13	0.14	0.01	0.13
5	0	3	0	1	0	4	0.15	0.19	0.03	0.15
6	1	4	1	0	0	6	0.14	0.2	0.03	0.12
7	1	2	0	1	0	4	0.19	0.23	0.04	0.21
8	0	4	1	1	0	6	0.15	0.21	0.04	0.14
9	1	3	0	0	0	4	0.18	0.23	0.05	0.18
10	0	4	1	1	0	6	0.17	0.27	0.06	0.17
11	3	2	0	0	0	5	0.17	0.21	0.03	0.18

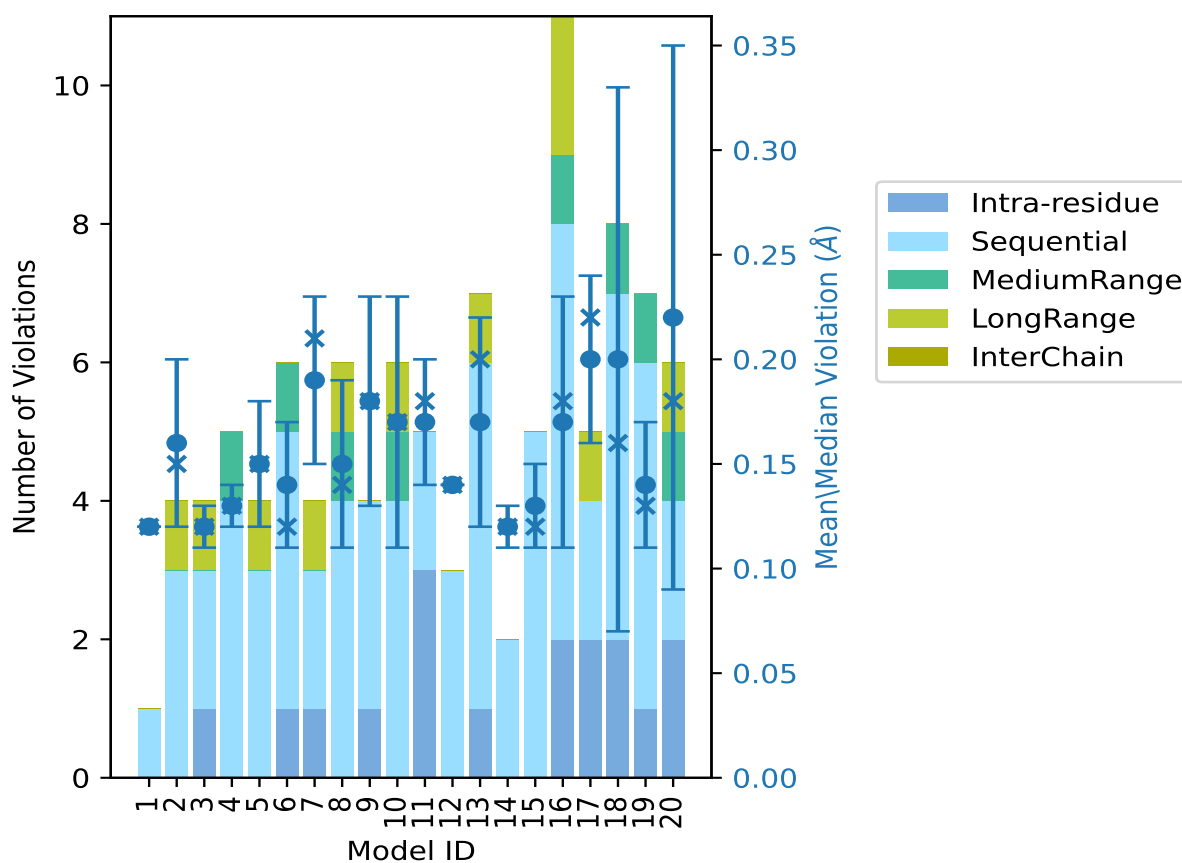
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>					
12	0	3	0	0	0	3	0.14	0.14	0.0	0.14
13	1	5	0	1	0	7	0.17	0.23	0.05	0.2
14	0	2	0	0	0	2	0.12	0.13	0.01	0.12
15	0	5	0	0	0	5	0.13	0.16	0.02	0.12
16	2	6	1	2	0	11	0.17	0.33	0.06	0.18
17	2	2	0	1	0	5	0.2	0.24	0.04	0.22
18	2	5	1	0	0	8	0.2	0.53	0.13	0.16
19	1	5	1	0	0	7	0.14	0.2	0.03	0.13
20	2	2	1	1	0	6	0.22	0.49	0.13	0.18

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [\(i\)](#)



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

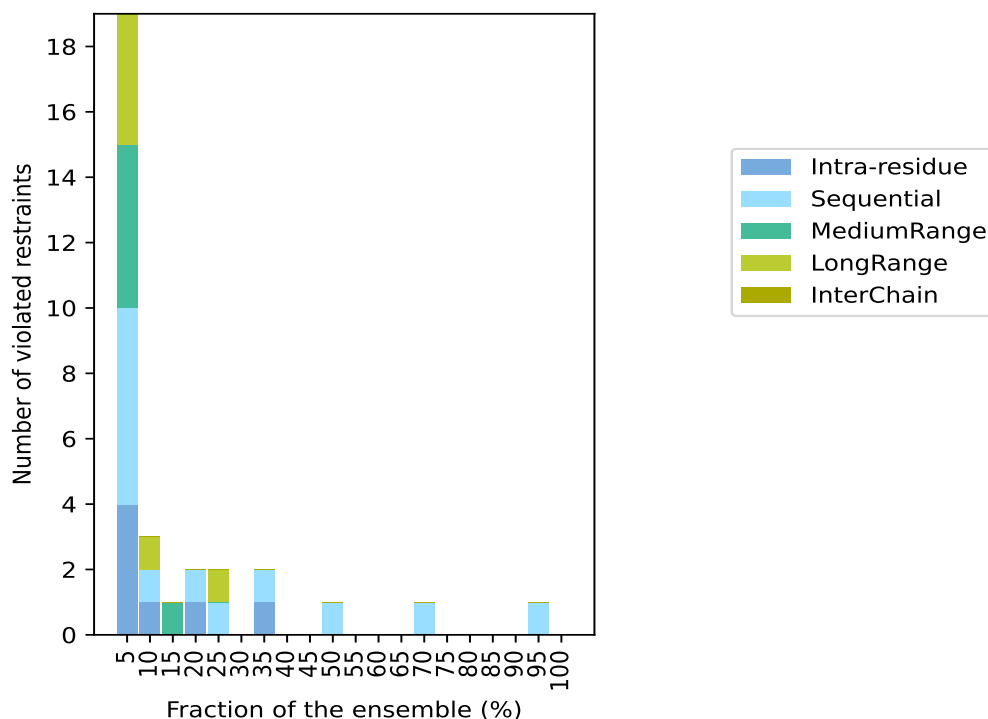
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 983(IR:261, SQ:266, MR:196, LR:260, IC:0) restraints are not violated in the ensemble.

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

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations



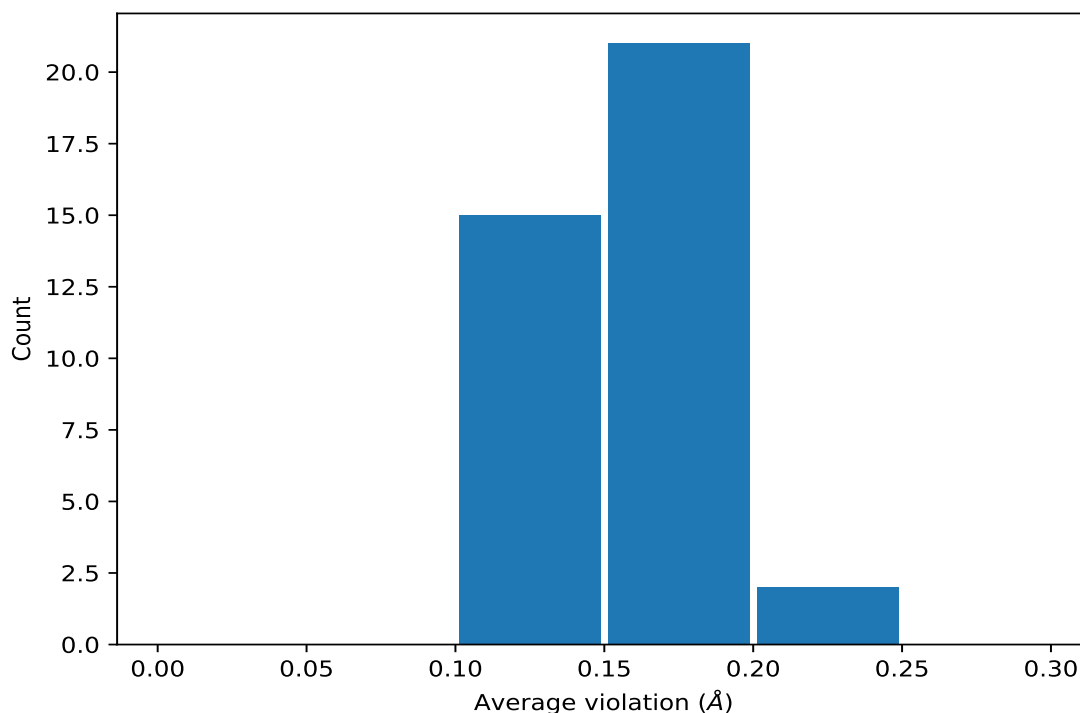
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	19	0.17	0.04	0.16
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	14	0.13	0.03	0.12
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	14	0.13	0.03	0.12
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	14	0.13	0.03	0.12
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	10	0.13	0.01	0.13
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG2	7	0.21	0.01	0.21
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG3	7	0.21	0.01	0.21
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD11	7	0.17	0.05	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD12	7	0.17	0.05	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD13	7	0.17	0.05	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD21	7	0.17	0.05	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD22	7	0.17	0.05	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD23	7	0.17	0.05	0.14
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD1	5	0.19	0.03	0.19
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD2	5	0.19	0.03	0.19
(1,198)	1:A:41:GLU:HG2	1:A:42:MET:H	5	0.11	0.0	0.11

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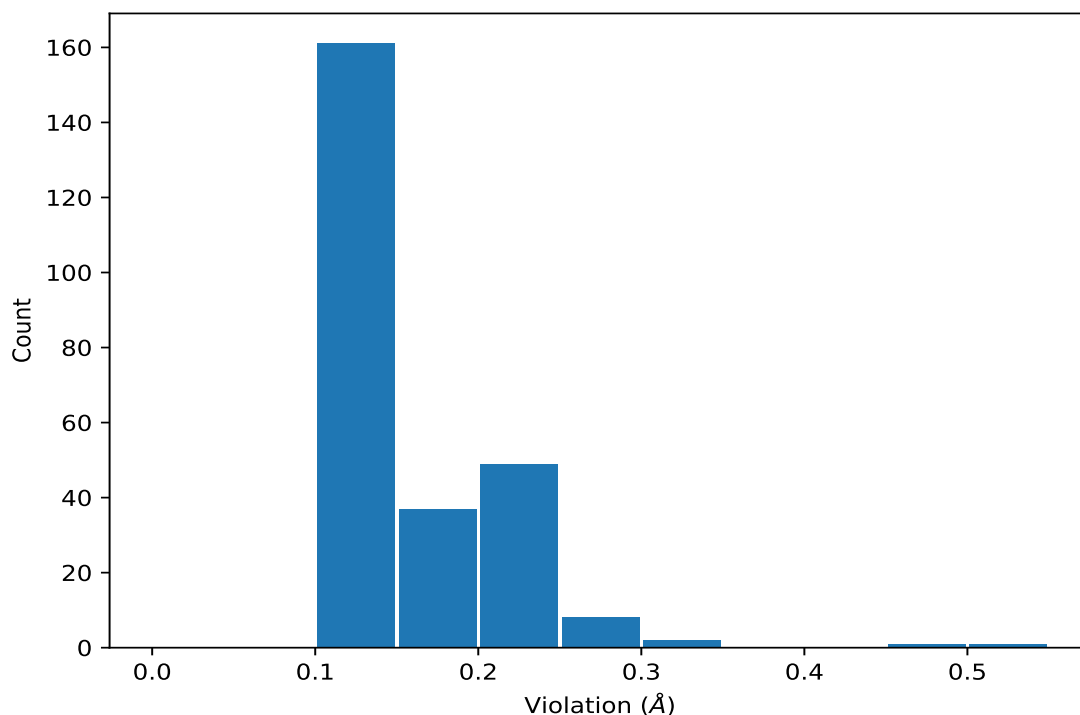
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,198)	1:A:41:GLU:HG3	1:A:42:MET:H	5	0.11	0.0	0.11
(1,811)	1:A:16:LYS:HB2	1:A:17:ARG:H	4	0.19	0.03	0.2
(1,811)	1:A:16:LYS:HB3	1:A:17:ARG:H	4	0.19	0.03	0.2
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG2	4	0.18	0.09	0.12
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG3	4	0.18	0.09	0.12
(1,855)	1:A:22:LEU:HD11	1:A:25:LYS:H	3	0.16	0.02	0.15
(1,855)	1:A:22:LEU:HD12	1:A:25:LYS:H	3	0.16	0.02	0.15
(1,855)	1:A:22:LEU:HD13	1:A:25:LYS:H	3	0.16	0.02	0.15
(1,855)	1:A:22:LEU:HD21	1:A:25:LYS:H	3	0.16	0.02	0.15
(1,855)	1:A:22:LEU:HD22	1:A:25:LYS:H	3	0.16	0.02	0.15
(1,855)	1:A:22:LEU:HD23	1:A:25:LYS:H	3	0.16	0.02	0.15
(1,351)	1:A:74:LYS:H	1:A:74:LYS:HD2	2	0.18	0.02	0.18
(1,351)	1:A:74:LYS:H	1:A:74:LYS:HD3	2	0.18	0.02	0.18
(1,170)	1:A:35:SER:H	1:A:36:THR:HG21	2	0.12	0.0	0.12
(1,170)	1:A:35:SER:H	1:A:36:THR:HG22	2	0.12	0.0	0.12
(1,170)	1:A:35:SER:H	1:A:36:THR:HG23	2	0.12	0.0	0.12
(1,947)	1:A:57:ILE:HG12	1:A:80:LEU:HD21	2	0.11	0.0	0.11
(1,947)	1:A:57:ILE:HG12	1:A:80:LEU:HD22	2	0.11	0.0	0.11
(1,947)	1:A:57:ILE:HG12	1:A:80:LEU:HD23	2	0.11	0.0	0.11
(1,947)	1:A:57:ILE:HG13	1:A:80:LEU:HD21	2	0.11	0.0	0.11
(1,947)	1:A:57:ILE:HG13	1:A:80:LEU:HD22	2	0.11	0.0	0.11
(1,947)	1:A:57:ILE:HG13	1:A:80:LEU:HD23	2	0.11	0.0	0.11

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:A:51:THR:HA	1:A:52:PHE:H	18	0.53
(1,376)	1:A:77:LEU:H	1:A:77:LEU:HB2	20	0.49
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG2	16	0.33
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG3	16	0.33
(1,807)	1:A:14:TYR:HB2	1:A:15:CYS:H	10	0.27
(1,807)	1:A:14:TYR:HB3	1:A:15:CYS:H	10	0.27
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD11	18	0.25
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD12	18	0.25
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD13	18	0.25
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD21	18	0.25
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD22	18	0.25
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD23	18	0.25
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD1	20	0.24
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD2	20	0.24
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	2	0.24
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG2	7	0.23
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG3	7	0.23
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD11	13	0.23
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD12	13	0.23
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD13	13	0.23
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD21	13	0.23
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD22	13	0.23
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD23	13	0.23
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	9	0.23
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	17	0.23
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	17	0.23
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	17	0.23
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG2	13	0.22
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG3	13	0.22
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG2	17	0.22
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG3	17	0.22
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	7	0.22
(1,539)	1:A:73:ASN:HB3	1:A:74:LYS:HG2	16	0.22
(1,539)	1:A:73:ASN:HB3	1:A:74:LYS:HG3	16	0.22
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG2	9	0.21
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG3	9	0.21
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG2	11	0.21
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG3	11	0.21
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG2	20	0.21
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG3	20	0.21
(1,895)	1:A:40:GLN:HA	1:A:43:VAL:HG11	10	0.21
(1,895)	1:A:40:GLN:HA	1:A:43:VAL:HG12	10	0.21
(1,895)	1:A:40:GLN:HA	1:A:43:VAL:HG13	10	0.21
(1,895)	1:A:40:GLN:HA	1:A:43:VAL:HG21	10	0.21
(1,895)	1:A:40:GLN:HA	1:A:43:VAL:HG22	10	0.21
(1,895)	1:A:40:GLN:HA	1:A:43:VAL:HG23	10	0.21
(1,811)	1:A:16:LYS:HB2	1:A:17:ARG:H	8	0.21
(1,811)	1:A:16:LYS:HB3	1:A:17:ARG:H	8	0.21
(1,811)	1:A:16:LYS:HB2	1:A:17:ARG:H	10	0.21
(1,811)	1:A:16:LYS:HB3	1:A:17:ARG:H	10	0.21
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD1	7	0.2
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD2	7	0.2
(1,811)	1:A:16:LYS:HB2	1:A:17:ARG:H	13	0.2
(1,811)	1:A:16:LYS:HB3	1:A:17:ARG:H	13	0.2
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	13	0.2
(1,570)	1:A:81:LEU:HA	1:A:81:LEU:HD11	19	0.2
(1,570)	1:A:81:LEU:HA	1:A:81:LEU:HD12	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:A:81:LEU:HA	1:A:81:LEU:HD13	19	0.2
(1,52)	1:A:14:TYR:H	1:A:16:LYS:HD2	6	0.2
(1,52)	1:A:14:TYR:H	1:A:16:LYS:HD3	6	0.2
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG2	18	0.19
(1,905)	1:A:44:GLN:H	1:A:44:GLN:HG3	18	0.19
(1,855)	1:A:22:LEU:HD11	1:A:25:LYS:H	16	0.19
(1,855)	1:A:22:LEU:HD12	1:A:25:LYS:H	16	0.19
(1,855)	1:A:22:LEU:HD13	1:A:25:LYS:H	16	0.19
(1,855)	1:A:22:LEU:HD21	1:A:25:LYS:H	16	0.19
(1,855)	1:A:22:LEU:HD22	1:A:25:LYS:H	16	0.19
(1,855)	1:A:22:LEU:HD23	1:A:25:LYS:H	16	0.19
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD1	16	0.19
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD2	16	0.19
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	5	0.19
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	8	0.19
(1,351)	1:A:74:LYS:H	1:A:74:LYS:HD2	16	0.19
(1,351)	1:A:74:LYS:H	1:A:74:LYS:HD3	16	0.19
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD1	17	0.18
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD2	17	0.18
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD11	16	0.18
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD12	16	0.18
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD13	16	0.18
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD21	16	0.18
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD22	16	0.18
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD23	16	0.18
(1,746)	1:A:81:LEU:HA	1:A:81:LEU:HD21	11	0.18
(1,746)	1:A:81:LEU:HA	1:A:81:LEU:HD22	11	0.18
(1,746)	1:A:81:LEU:HA	1:A:81:LEU:HD23	11	0.18
(1,223)	1:A:49:ARG:HA	1:A:50:ASN:H	11	0.18
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	11	0.17
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	19	0.17
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD1	2	0.16
(1,85)	1:A:21:LEU:H	1:A:69:TYR:HD2	2	0.16
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	15	0.16
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	18	0.16
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	5	0.16
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	5	0.16
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	5	0.16
(1,351)	1:A:74:LYS:H	1:A:74:LYS:HD2	6	0.16
(1,351)	1:A:74:LYS:H	1:A:74:LYS:HD3	6	0.16
(1,855)	1:A:22:LEU:HD11	1:A:25:LYS:H	18	0.15
(1,855)	1:A:22:LEU:HD12	1:A:25:LYS:H	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,855)	1:A:22:LEU:HD13	1:A:25:LYS:H	18	0.15
(1,855)	1:A:22:LEU:HD21	1:A:25:LYS:H	18	0.15
(1,855)	1:A:22:LEU:HD22	1:A:25:LYS:H	18	0.15
(1,855)	1:A:22:LEU:HD23	1:A:25:LYS:H	18	0.15
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	8	0.15
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	9	0.15
(1,984)	1:A:77:LEU:HA	1:A:81:LEU:HD11	19	0.14
(1,984)	1:A:77:LEU:HA	1:A:81:LEU:HD12	19	0.14
(1,984)	1:A:77:LEU:HA	1:A:81:LEU:HD13	19	0.14
(1,984)	1:A:77:LEU:HA	1:A:81:LEU:HD21	19	0.14
(1,984)	1:A:77:LEU:HA	1:A:81:LEU:HD22	19	0.14
(1,984)	1:A:77:LEU:HA	1:A:81:LEU:HD23	19	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD11	4	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD12	4	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD13	4	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD21	4	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD22	4	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD23	4	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD11	15	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD12	15	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD13	15	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD21	15	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD22	15	0.14
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD23	15	0.14
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	4	0.14
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	12	0.14
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	16	0.14
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	12	0.14
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	12	0.14
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	12	0.14
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	16	0.14
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	16	0.14
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	16	0.14
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	20	0.14
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	20	0.14
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	20	0.14
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	12	0.14
(1,855)	1:A:22:LEU:HD11	1:A:25:LYS:H	4	0.13
(1,855)	1:A:22:LEU:HD12	1:A:25:LYS:H	4	0.13
(1,855)	1:A:22:LEU:HD13	1:A:25:LYS:H	4	0.13
(1,855)	1:A:22:LEU:HD21	1:A:25:LYS:H	4	0.13
(1,855)	1:A:22:LEU:HD22	1:A:25:LYS:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,855)	1:A:22:LEU:HD23	1:A:25:LYS:H	4	0.13
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD11	2	0.13
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD12	2	0.13
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD13	2	0.13
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD21	2	0.13
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD22	2	0.13
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD23	2	0.13
(1,811)	1:A:16:LYS:HB2	1:A:17:ARG:H	2	0.13
(1,811)	1:A:16:LYS:HB3	1:A:17:ARG:H	2	0.13
(1,700)	1:A:7:TYR:HE1	1:A:43:VAL:HB	10	0.13
(1,700)	1:A:7:TYR:HE2	1:A:43:VAL:HB	10	0.13
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	14	0.13
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	20	0.13
(1,512)	1:A:56:PHE:HD1	1:A:57:ILE:HA	19	0.13
(1,512)	1:A:56:PHE:HD2	1:A:57:ILE:HA	19	0.13
(1,503)	1:A:55:ILE:HD11	1:A:56:PHE:H	13	0.13
(1,503)	1:A:55:ILE:HD12	1:A:56:PHE:H	13	0.13
(1,503)	1:A:55:ILE:HD13	1:A:56:PHE:H	13	0.13
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	4	0.13
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	5	0.13
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	19	0.13
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG2	3	0.13
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG3	3	0.13
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD11	7	0.12
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD12	7	0.12
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD13	7	0.12
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD21	7	0.12
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD22	7	0.12
(1,833)	1:A:21:LEU:H	1:A:22:LEU:HD23	7	0.12
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	1	0.12
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	6	0.12
(1,582)	1:A:4:ILE:HG21	1:A:22:LEU:HB2	8	0.12
(1,582)	1:A:4:ILE:HG22	1:A:22:LEU:HB2	8	0.12
(1,582)	1:A:4:ILE:HG23	1:A:22:LEU:HB2	8	0.12
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	3	0.12
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	3	0.12
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	3	0.12
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	4	0.12
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	4	0.12
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	4	0.12
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	6	0.12
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	6	0.12
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	10	0.12
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	10	0.12
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	10	0.12
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	13	0.12
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	15	0.12
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG2	17	0.12
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG3	17	0.12
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG2	18	0.12
(1,402)	1:A:74:LYS:H	1:A:74:LYS:HG3	18	0.12
(1,198)	1:A:41:GLU:HG2	1:A:42:MET:H	3	0.12
(1,198)	1:A:41:GLU:HG3	1:A:42:MET:H	3	0.12
(1,198)	1:A:41:GLU:HG2	1:A:42:MET:H	6	0.12
(1,198)	1:A:41:GLU:HG3	1:A:42:MET:H	6	0.12
(1,170)	1:A:35:SER:H	1:A:36:THR:HG21	15	0.12
(1,170)	1:A:35:SER:H	1:A:36:THR:HG22	15	0.12
(1,170)	1:A:35:SER:H	1:A:36:THR:HG23	15	0.12
(1,134)	1:A:28:LYS:H	1:A:28:LYS:HG2	11	0.12
(1,134)	1:A:28:LYS:H	1:A:28:LYS:HG3	11	0.12
(1,947)	1:A:57:ILE:HG12	1:A:80:LEU:HD21	3	0.11
(1,947)	1:A:57:ILE:HG12	1:A:80:LEU:HD22	3	0.11
(1,947)	1:A:57:ILE:HG12	1:A:80:LEU:HD23	3	0.11
(1,947)	1:A:57:ILE:HG13	1:A:80:LEU:HD21	3	0.11
(1,947)	1:A:57:ILE:HG13	1:A:80:LEU:HD22	3	0.11
(1,947)	1:A:57:ILE:HG13	1:A:80:LEU:HD23	3	0.11
(1,947)	1:A:57:ILE:HG12	1:A:80:LEU:HD21	5	0.11
(1,947)	1:A:57:ILE:HG12	1:A:80:LEU:HD22	5	0.11
(1,947)	1:A:57:ILE:HG12	1:A:80:LEU:HD23	5	0.11
(1,947)	1:A:57:ILE:HG13	1:A:80:LEU:HD21	5	0.11
(1,947)	1:A:57:ILE:HG13	1:A:80:LEU:HD22	5	0.11
(1,947)	1:A:57:ILE:HG13	1:A:80:LEU:HD23	5	0.11
(1,931)	1:A:54:GLN:HE21	1:A:57:ILE:H	8	0.11
(1,931)	1:A:54:GLN:HE22	1:A:57:ILE:H	8	0.11
(1,785)	1:A:6:LEU:HD11	1:A:19:ARG:HA	16	0.11
(1,785)	1:A:6:LEU:HD12	1:A:19:ARG:HA	16	0.11
(1,785)	1:A:6:LEU:HD13	1:A:19:ARG:HA	16	0.11
(1,785)	1:A:6:LEU:HD21	1:A:19:ARG:HA	16	0.11
(1,785)	1:A:6:LEU:HD22	1:A:19:ARG:HA	16	0.11
(1,785)	1:A:6:LEU:HD23	1:A:19:ARG:HA	16	0.11
(1,670)	1:A:66:ASP:HA	1:A:68:LEU:HD11	20	0.11
(1,670)	1:A:66:ASP:HA	1:A:68:LEU:HD12	20	0.11
(1,670)	1:A:66:ASP:HA	1:A:68:LEU:HD13	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:A:5:ILE:HD11	1:A:56:PHE:HD1	13	0.11
(1,667)	1:A:5:ILE:HD11	1:A:56:PHE:HD2	13	0.11
(1,667)	1:A:5:ILE:HD12	1:A:56:PHE:HD1	13	0.11
(1,667)	1:A:5:ILE:HD12	1:A:56:PHE:HD2	13	0.11
(1,667)	1:A:5:ILE:HD13	1:A:56:PHE:HD1	13	0.11
(1,667)	1:A:5:ILE:HD13	1:A:56:PHE:HD2	13	0.11
(1,613)	1:A:26:GLY:H	1:A:27:VAL:HB	10	0.11
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	8	0.11
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	8	0.11
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	8	0.11
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	9	0.11
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	9	0.11
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	9	0.11
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	15	0.11
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	15	0.11
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	15	0.11
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	18	0.11
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	18	0.11
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	18	0.11
(1,479)	1:A:27:VAL:HG11	1:A:28:LYS:HA	19	0.11
(1,479)	1:A:27:VAL:HG12	1:A:28:LYS:HA	19	0.11
(1,479)	1:A:27:VAL:HG13	1:A:28:LYS:HA	19	0.11
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	16	0.11
(1,473)	1:A:60:TYR:HA	1:A:61:HIS:HE1	18	0.11
(1,198)	1:A:41:GLU:HG2	1:A:42:MET:H	14	0.11
(1,198)	1:A:41:GLU:HG3	1:A:42:MET:H	14	0.11
(1,198)	1:A:41:GLU:HG2	1:A:42:MET:H	16	0.11
(1,198)	1:A:41:GLU:HG3	1:A:42:MET:H	16	0.11
(1,198)	1:A:41:GLU:HG2	1:A:42:MET:H	19	0.11
(1,198)	1:A:41:GLU:HG3	1:A:42:MET:H	19	0.11
(1,170)	1:A:35:SER:H	1:A:36:THR:HG21	6	0.11
(1,170)	1:A:35:SER:H	1:A:36:THR:HG22	6	0.11
(1,170)	1:A:35:SER:H	1:A:36:THR:HG23	6	0.11

## 10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value