WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 01:44 pm BST

|		
PDB ID	:	5LKN
BMRB ID	:	34026
Title	:	NMR solution structure of human FNIII domain 2 of NCAM
Authors	:	Slapsak, U.; Salzano, G.; Amin, L.; Abskharon, R.N.N.; Ilc, G.; Zupancic, B.; Biljan, I.; Plavec, J.; Giachin, G.; Legname, G.
Deposited on	:	2016-07-22

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 82%.

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	Percentile Ranks	Value
Clashscore		0
Ramachandran outliers		0.5%
Sidechain outliers		15.9%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures
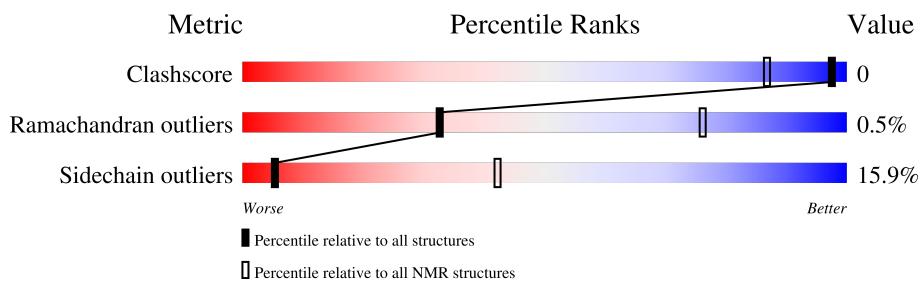
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	103	81% 12% 8%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:598-A:692 (95)	0.50	1

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. No single-model clusters were found.

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

3 Entity composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 1641 atoms, of which 805 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Neural cell adhesion molecule 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	103	1641	523	805	157	153	3	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	595	MET	-	expression tag	UNP P13591
A	596	GLN	-	expression tag	UNP P13591
A	597	PRO	-	expression tag	UNP P13591
A	598	VAL	-	expression tag	UNP P13591
A	599	ARG	-	expression tag	UNP P13591
A	692	HIS	-	expression tag	UNP P13591
A	693	HIS	-	expression tag	UNP P13591
A	694	HIS	-	expression tag	UNP P13591
A	695	HIS	-	expression tag	UNP P13591
A	696	HIS	-	expression tag	UNP P13591
A	697	HIS	-	expression tag	UNP P13591

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: Neural cell adhesion molecule 1

Chain A:
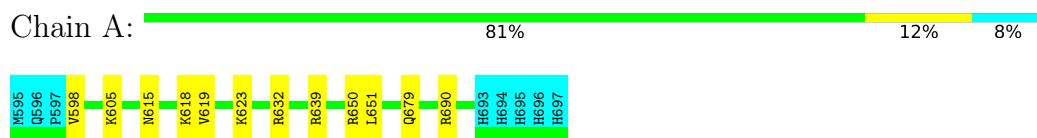
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
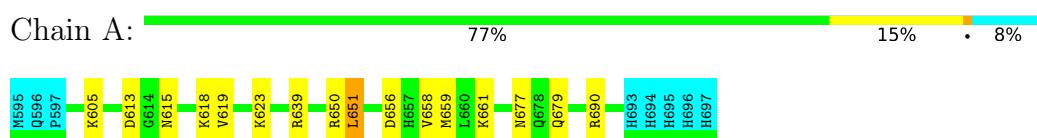
4.2.2 Score per residue for model 2

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
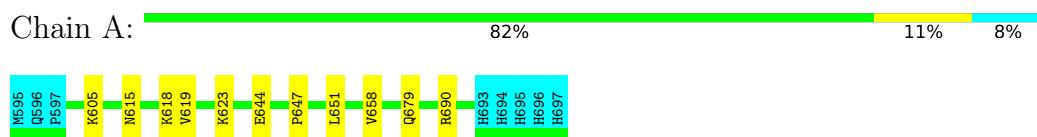
4.2.3 Score per residue for model 3

• Molecule 1: Neural cell adhesion molecule 1

Chain A:

83% 8% ⠈⠈ 8%

M595 Q596 P597 E612 N615 V619 K623 R632 R639 R650 L651 E676 R690 H693 H694 H695 H696 H697
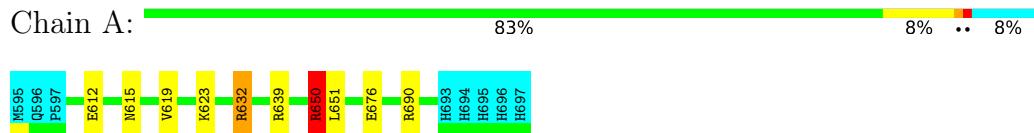
4.2.4 Score per residue for model 4

• Molecule 1: Neural cell adhesion molecule 1

Chain A:

82% 11% 8%

M595 Q596 P597 K605 N615 K618 V619 K623 R632 K646 L651 V658 M659 R690 H693 H694 H695 H696 H697
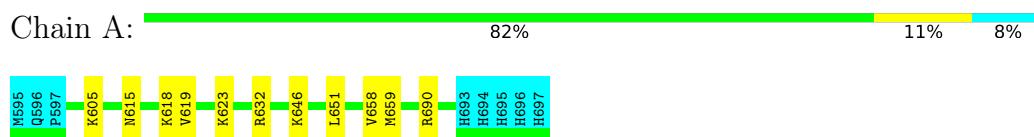
4.2.5 Score per residue for model 5

• Molecule 1: Neural cell adhesion molecule 1

Chain A:

83% 10% 8%

M595 Q596 P597 N615 V619 K623 R639 A640 L641 K646 L651 M659 E668 R690 H693 H694 H695 H696 H697
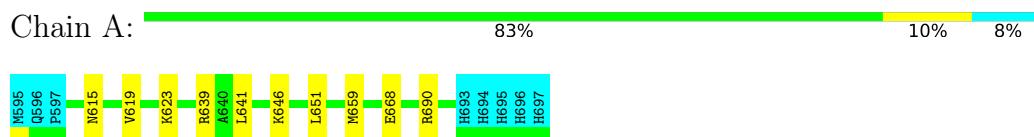
4.2.6 Score per residue for model 6

• Molecule 1: Neural cell adhesion molecule 1

Chain A:

77% 14% • 8%

M595 Q596 P597 V598 R599 K605 E612 N615 K618 V619 K623 Q624 R639 P647 L651 P652 S653 V658 Q679 R690 H693 H694 H695 H696 H697
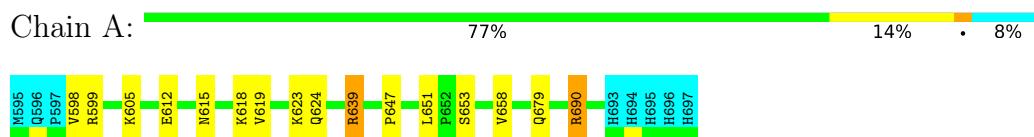
4.2.7 Score per residue for model 7

• Molecule 1: Neural cell adhesion molecule 1

Chain A:

75% 17% • 8%

M595 Q596 P597 V598 K605 N615 K618 V619 N620 K623 I631 R632 H633 Y634 R637 Y638 R639 P647 R650 L651 M659 E676 R690 H693 H694 H695 H696 H697
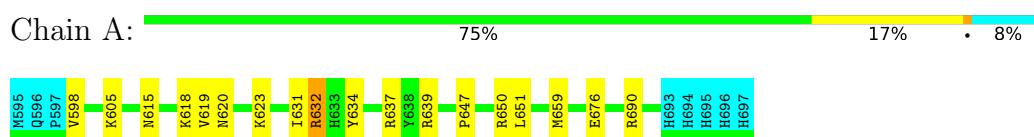
4.2.8 Score per residue for model 8

• Molecule 1: Neural cell adhesion molecule 1

Chain A: 76% 15% 8%

M595 Q596 P597 V598 K605 D613 G614 N615 V619 N620 K623 G627 I631 R632 H633 Y634 R639 E648 I649 R650 L651 V658 R690 H693 H694 H695 H696 H697
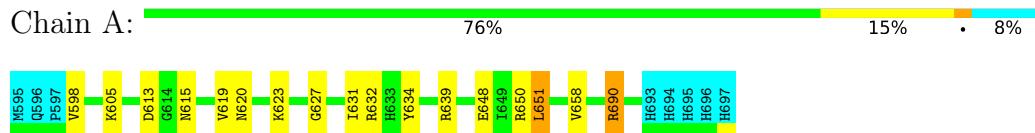
4.2.9 Score per residue for model 9

• Molecule 1: Neural cell adhesion molecule 1

Chain A: 76% 16% 8%

M595 Q596 P597 K605 L606 E607 G608 Q609 N615 K618 V619 N620 I631 R632 H633 Y634 R639 A640 L641 E648 L651 M659 Q679 R690 H693 H694 H695 H696 H697
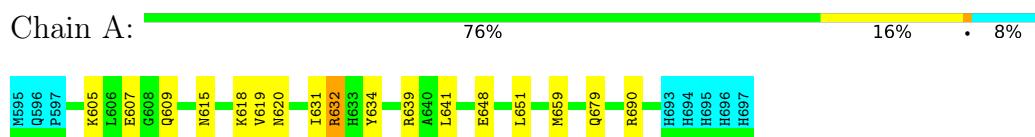
4.2.10 Score per residue for model 10

• Molecule 1: Neural cell adhesion molecule 1

Chain A: 72% 20% 8%

M595 Q596 P597 V598 R599 K605 E612 N615 K618 V619 N620 K623 D626 G627 I631 Y634 R639 L651 V658 M659 E668 E676 Q679 R690 H693 H694 H695 H696 H697
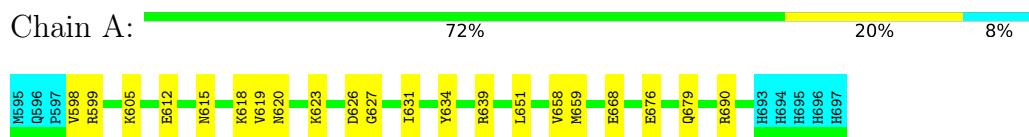
4.2.11 Score per residue for model 11

• Molecule 1: Neural cell adhesion molecule 1

Chain A: 78% 14% 8%

M595 Q596 P597 V598 K605 M610 D613 G614 N615 V619 N620 K623 R639 L651 E668 N677 Q678 Q679 R690 H693 H694 H695 H696 H697
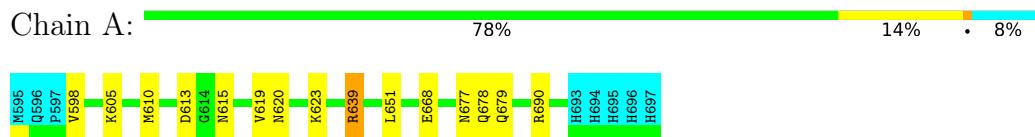
4.2.12 Score per residue for model 12

• Molecule 1: Neural cell adhesion molecule 1

Chain A: 78% 14% 8%

M595 Q596 P597 V598 K605 D613 G614 N615 K618 V619 N620 K623 R639 E644 R650 L651 V658 K661 Q679 H693 H694 H695 H696 H697
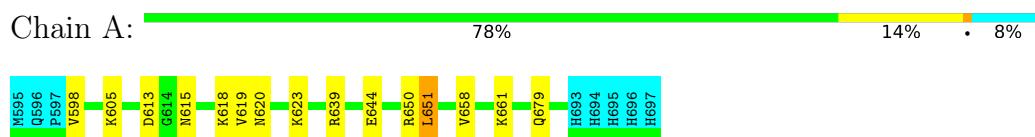
4.2.13   Score per residue for model 13

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
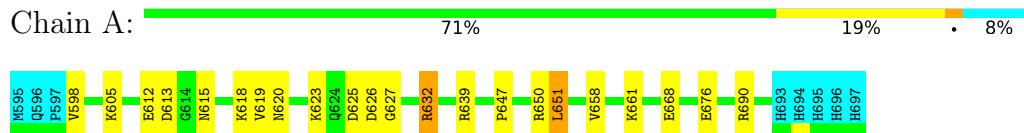
4.2.14   Score per residue for model 14

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
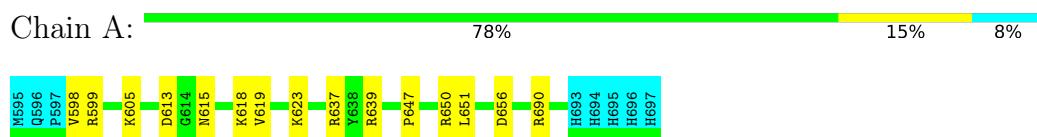
4.2.15   Score per residue for model 15

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
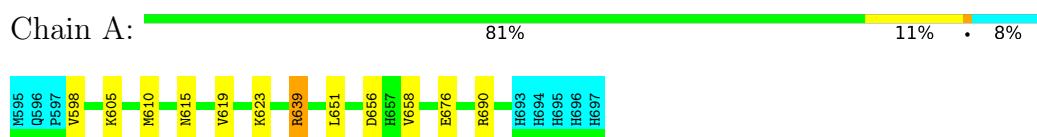
4.2.16   Score per residue for model 16

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
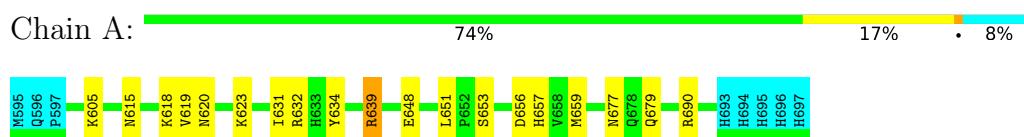
4.2.17   Score per residue for model 17

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
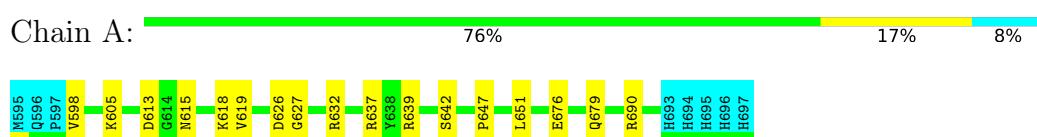
4.2.18 Score per residue for model 18

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
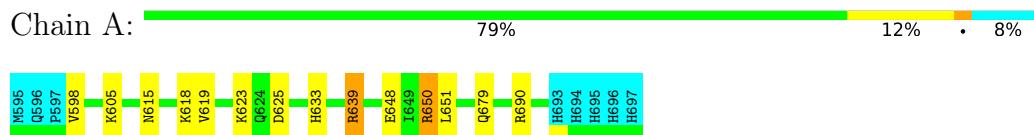
#### 4.2.19 Score per residue for model 19

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
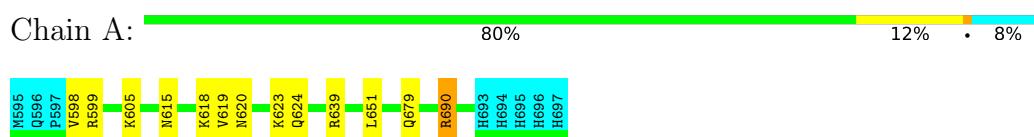
4.2.20 Score per residue for model 20

• Molecule 1: Neural cell adhesion molecule 1

Chain A:
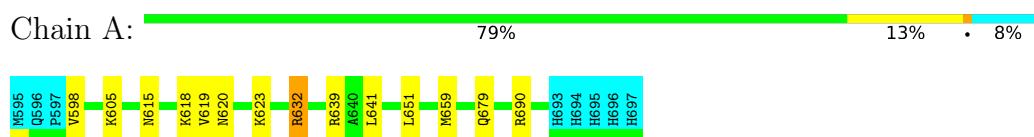
5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	structure calculation	
YASARA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1106
Number of shifts mapped to atoms	1106
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6   Model quality ⓘ

6.1   Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.67±0.01	0±0/780 (0.0± 0.0%)	0.84±0.02	1±1/1054 (0.1± 0.1%)
All	All	0.67	0/15600 (0.0%)	0.84	25/21080 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	690	ARG	NE-CZ-NH1	6.39	123.49	120.30	8	3
1	A	637	ARG	NE-CZ-NH1	6.13	123.36	120.30	17	3
1	A	599	ARG	NE-CZ-NH1	5.97	123.29	120.30	10	4
1	A	632	ARG	NE-CZ-NH1	5.86	123.23	120.30	13	9
1	A	639	ARG	NE-CZ-NH1	5.42	123.01	120.30	16	5
1	A	650	ARG	NE-CZ-NH1	5.17	122.89	120.30	3	1

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
1	A	761	744	744	1±1
All	All	15220	14880	14880	14

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:650:ARG:C	1:A:651:LEU:HD22	0.53	2.24	3	4
1:A:631:ILE:HG21	1:A:634:TYR:CE2	0.49	2.41	8	4
1:A:631:ILE:HG21	1:A:634:TYR:CZ	0.47	2.44	7	1
1:A:650:ARG:O	1:A:651:LEU:HD22	0.43	2.13	1	4
1:A:607:GLU:HG2	1:A:620:ASN:HD22	0.41	1.75	9	1

6.3　Torsion angles　ⓘ

6.3.1　Protein backbone　ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/103 (92%)	92±1 (96±1%)	3±2 (3±2%)	0±1 (1±1%)	32	76
All	All	1900/2060 (92%)	1831 (96%)	59 (3%)	10 (1%)	32	76

All 2 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	647	PRO	6
1	A	627	GLY	4

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	82/90 (91%)	69±3 (84±3%)	13±3 (16±3%)	5	42
All	All	1640/1800 (91%)	1380 (84%)	260 (16%)	5	42

All 36 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	615	ASN	20
1	A	619	VAL	20
1	A	690	ARG	19
1	A	605	LYS	18
1	A	623	LYS	18
1	A	639	ARG	18
1	A	651	LEU	16
1	A	618	LYS	15
1	A	598	VAL	13
1	A	679	GLN	12
1	A	658	VAL	9
1	A	620	ASN	9
1	A	659	MET	8
1	A	613	ASP	7
1	A	676	GLU	6
1	A	632	ARG	5
1	A	656	ASP	4
1	A	612	GLU	4
1	A	668	GLU	4
1	A	648	GLU	4
1	A	661	LYS	3
1	A	677	ASN	3
1	A	641	LEU	3
1	A	626	ASP	3
1	A	644	GLU	2
1	A	650	ARG	2
1	A	646	LYS	2
1	A	624	GLN	2
1	A	653	SER	2
1	A	610	MET	2
1	A	625	ASP	2
1	A	609	GLN	1
1	A	678	GLN	1
1	A	657	HIS	1
1	A	642	SER	1
1	A	633	HIS	1

6.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *shift_set_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	1106
Number of shifts mapped to atoms	1106
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, *ppm*	Suggested action
$^{13}C_\alpha$	95	0.36 ± 0.21	None needed (< 0.5 ppm)
$^{13}C_\beta$	91	-0.25 ± 0.24	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	90	0.18 ± 0.51	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1068 atoms were assigned a chemical shift out of a possible 1304. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	369/472 (78%)	188/192 (98%)	93/190 (49%)	88/90 (98%)
Sidechain	621/724 (86%)	423/467 (91%)	190/224 (85%)	8/33 (24%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	78/108 (72%)	39/54 (72%)	37/48 (77%)	2/6 (33%)
Overall	1068/1304 (82%)	650/713 (91%)	320/462 (69%)	98/129 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1106 atoms were assigned a chemical shift out of a possible 1421. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	377/510 (74%)	192/207 (93%)	95/206 (46%)	90/97 (93%)
Sidechain	649/768 (85%)	442/496 (89%)	198/238 (83%)	9/34 (26%)
Aromatic	80/143 (56%)	40/74 (54%)	38/58 (66%)	2/11 (18%)
Overall	1106/1421 (78%)	674/777 (87%)	331/502 (66%)	101/142 (71%)

7.1.4 Statistically unusual chemical shifts ⓘ

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

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	639	ARG	HD2	0.46	1.97 − 4.26	-11.6
1	A	615	ASN	HB2	0.61	1.27 − 4.34	-7.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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:
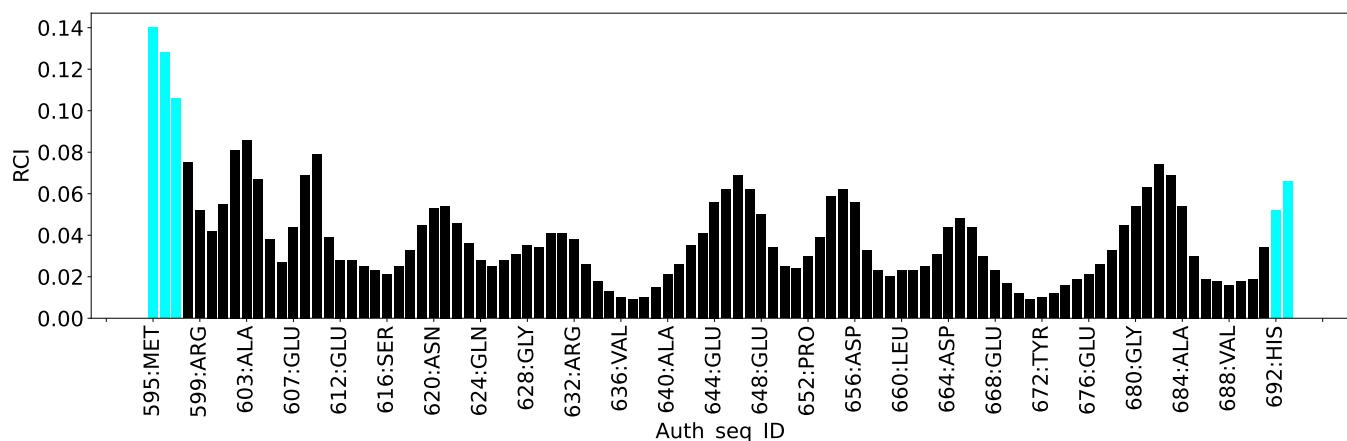
8 NMR restraints analysis ⓘ

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	1658
Intra-residue ($|i\text{-}j|$=0)	337
Sequential ($|i\text{-}j|$=1)	441
Medium range ($|i\text{-}j|$>1 and $|i\text{-}j|$<5)	108
Long range ($|i\text{-}j|$≥5)	772
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	136
Number of unmapped restraints	0
Number of restraints per residue	17.4
Number of long range restraints per residue[1]	7.5

[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)	1.9	0.2
0.2-0.5 (Medium)	5.0	0.5
>0.5 (Large)	8.4	1.65

8.2.2 Average number of dihedral-angle violations per model ⓘ

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	None	None
10.0-20.0 (Medium)	None	None
>20.0 (Large)	0.3	27.9

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)	337	20.3	3	0.9	0.2	1	0.3	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	279	16.8	2	0.7	0.1	1	0.4	0.1
Sidechain-Sidechain	58	3.5	1	1.7	0.1	0	0.0	0.0
Sequential (|i-j|=1)	441	26.6	4	0.9	0.2	2	0.5	0.1
Backbone-Backbone	143	8.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	250	15.1	2	0.8	0.1	1	0.4	0.1
Sidechain-Sidechain	48	2.9	2	4.2	0.1	1	2.1	0.1
Medium range (|i-j|>1 & |i-j|<5)	108	6.5	1	0.9	0.1	0	0.0	0.0
Backbone-Backbone	24	1.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	46	2.8	1	2.2	0.1	0	0.0	0.0
Sidechain-Sidechain	38	2.3	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	772	46.6	21	2.7	1.3	6	0.8	0.4
Backbone-Backbone	133	8.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	323	19.5	10	3.1	0.6	4	1.2	0.2
Sidechain-Sidechain	316	19.1	11	3.5	0.7	2	0.6	0.1
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	1658	100.0	29	1.7	1.7	9	0.5	0.5
Backbone-Backbone	300	18.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	898	54.2	15	1.7	0.9	6	0.7	0.4
Sidechain-Sidechain	460	27.7	14	3.0	0.8	3	0.7	0.2

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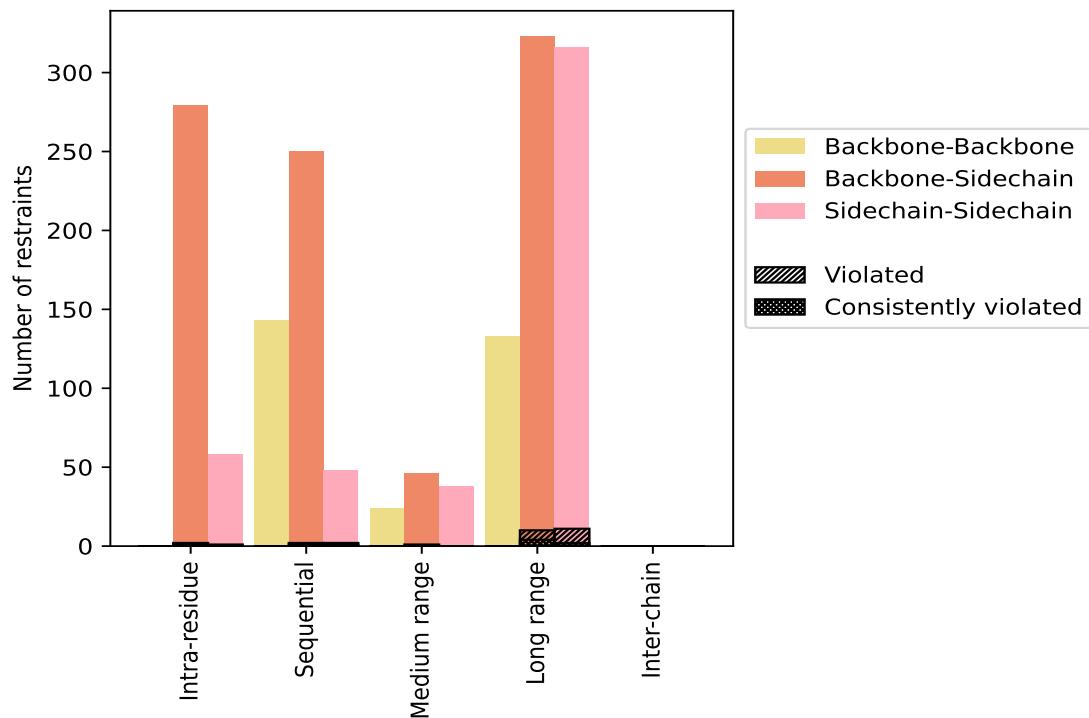
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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	1	3	0	10	0	14	0.7	1.53	0.37	0.66
2	1	3	0	9	0	13	0.61	1.4	0.38	0.5
3	1	3	0	12	0	16	0.74	1.33	0.35	0.84
4	1	3	0	11	0	15	0.8	1.63	0.38	0.77
5	3	4	0	13	0	20	0.56	1.55	0.41	0.4
6	1	3	0	8	0	12	0.61	1.42	0.39	0.53
7	2	3	0	12	0	17	0.66	1.38	0.42	0.47
8	2	3	0	10	0	15	0.74	1.57	0.38	0.76
9	1	4	0	8	0	13	0.63	1.02	0.25	0.62
10	2	4	0	8	0	14	0.68	1.58	0.43	0.63
11	2	3	0	12	0	17	0.63	1.48	0.35	0.53

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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				
12	2	4	0	12	0	18	0.63	1.5	0.4	0.55
13	2	3	0	9	0	14	0.7	1.47	0.38	0.6
14	1	3	0	10	0	14	0.54	1.45	0.35	0.46
15	2	3	0	10	0	15	0.77	1.43	0.35	0.75
16	2	4	0	11	0	17	0.78	1.54	0.34	0.77
17	2	3	1	8	0	14	0.71	1.65	0.42	0.62
18	1	2	0	9	0	12	0.57	1.16	0.27	0.54
19	2	4	0	11	0	17	0.53	1.38	0.32	0.48
20	2	3	0	13	0	18	0.46	1.45	0.4	0.28

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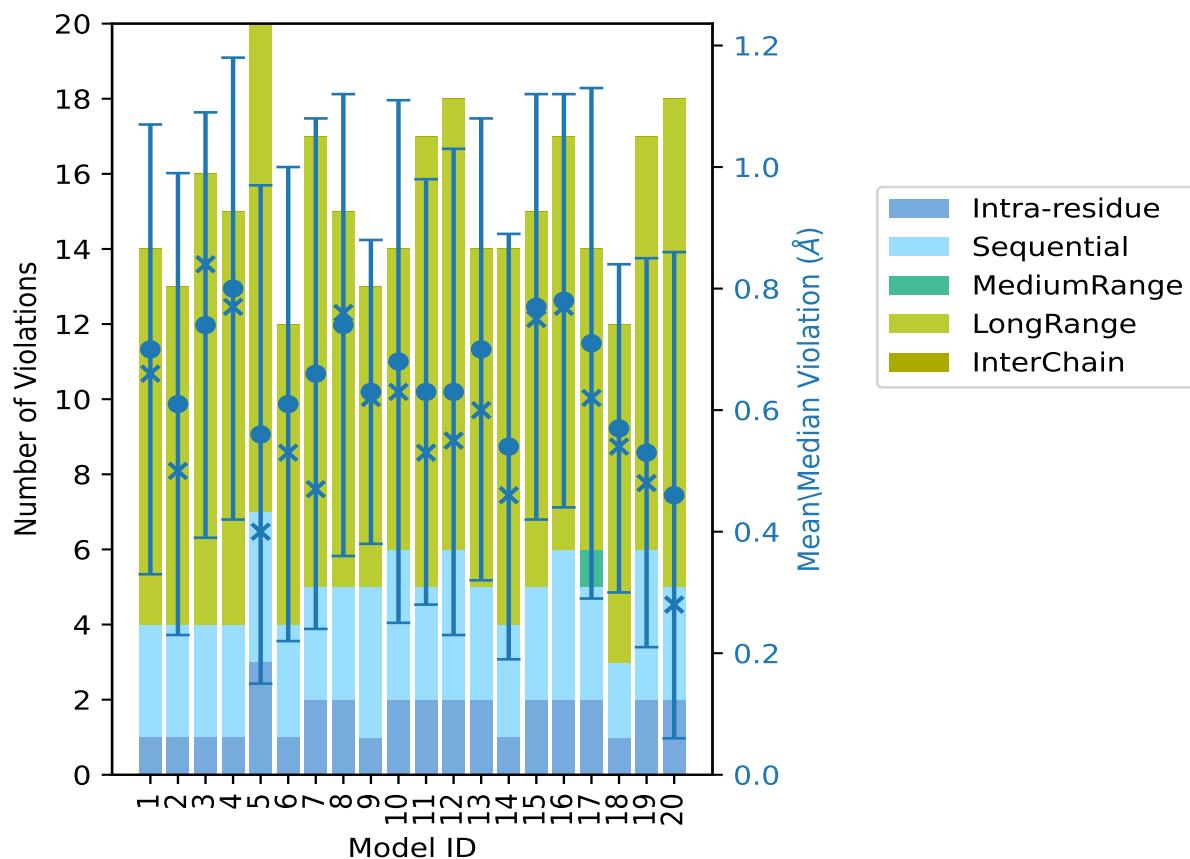
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

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, 1629(IR:334, SQ:437, MR:107, LR:751, 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]	%
0	0	1	2	0	3	1	5.0
0	0	0	2	0	2	2	10.0
1	0	0	1	0	2	3	15.0
0	0	0	2	0	2	4	20.0
0	0	0	2	0	2	5	25.0
0	0	0	1	0	1	6	30.0
0	0	0	1	0	1	7	35.0
0	0	0	1	0	1	8	40.0
0	0	0	1	0	1	9	45.0
1	1	0	0	0	2	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	1	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	1	0	0	0	1	15	75.0
0	0	0	1	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
1	2	0	6	0	9	20	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 ⓘ
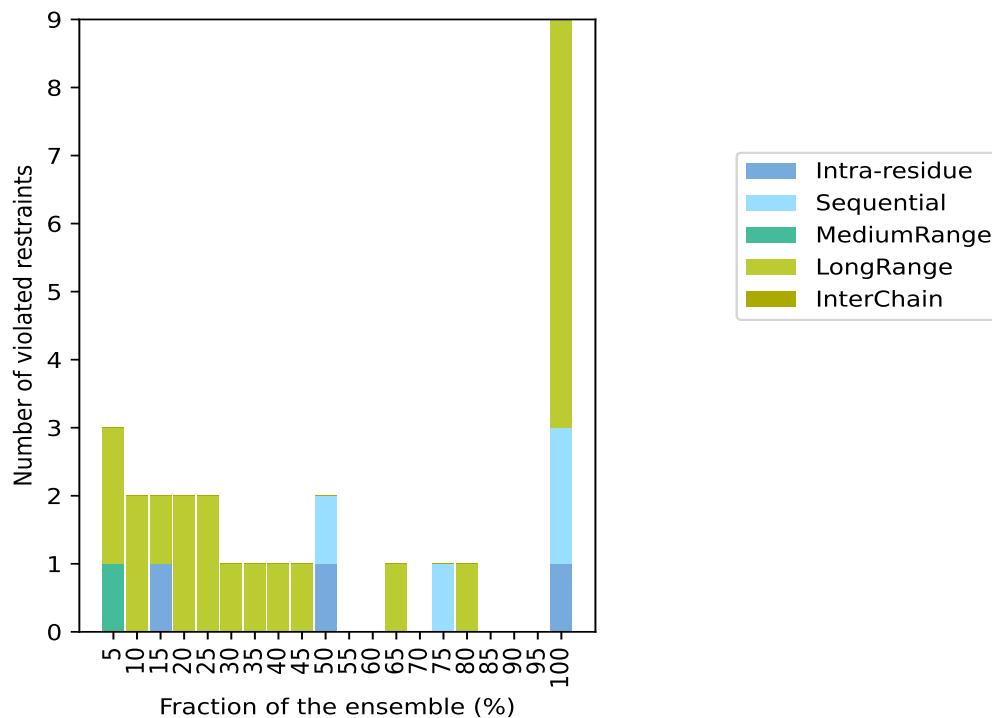
9.4 Most violated distance restraints in the ensemble ⓘ

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
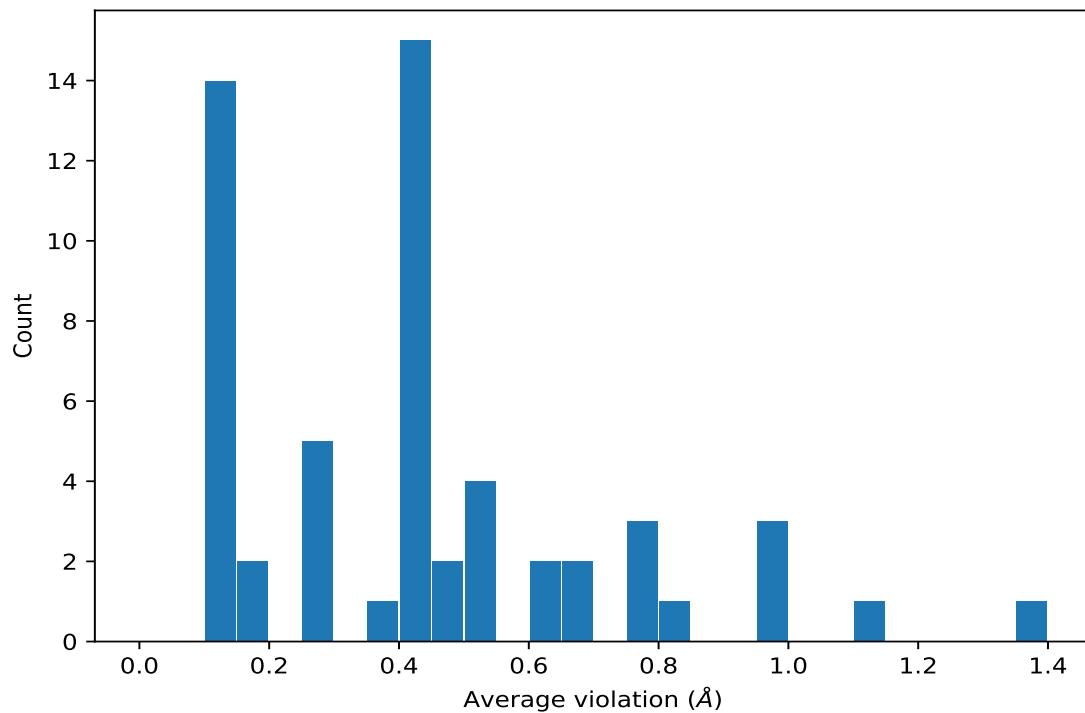
9.4.2 Table: Most violated distance restraints ⓘ

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	20	1.35	0.14	1.39
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	20	1.11	0.45	1.23
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	20	0.96	0.04	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	20	0.96	0.04	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	20	0.96	0.04	0.98
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	20	0.77	0.33	0.88
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	20	0.77	0.09	0.8
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	20	0.75	0.37	0.84
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	20	0.51	0.08	0.52
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	20	0.49	0.27	0.51
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	20	0.49	0.27	0.51
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	20	0.4	0.05	0.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	20	0.4	0.05	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	20	0.4	0.05	0.38
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	16	0.6	0.28	0.64
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	16	0.6	0.28	0.64
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	15	0.67	0.2	0.64
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	15	0.67	0.2	0.64
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	13	0.52	0.28	0.45
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	10	0.42	0.22	0.34
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	10	0.28	0.1	0.32
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	9	0.54	0.24	0.49
(1,533)	1:A:609:GLN:H	1:A:620:ASN:HD21	8	0.52	0.25	0.47
(1,404)	1:A:601:PRO:HD2	1:A:677:ASN:HD22	7	0.25	0.11	0.22
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG2	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG3	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG2	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG3	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG2	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG3	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG2	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG3	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG2	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG3	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG2	6	0.13	0.03	0.12
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG3	6	0.13	0.03	0.12
(1,411)	1:A:605:LYS:HE3	1:A:624:GLN:HE22	5	0.83	0.27	0.81
(1,320)	1:A:605:LYS:HE2	1:A:624:GLN:HE22	5	0.19	0.04	0.19
(1,1425)	1:A:605:LYS:HD2	1:A:624:GLN:HE22	4	0.44	0.21	0.4
(1,1425)	1:A:605:LYS:HD3	1:A:624:GLN:HE22	4	0.44	0.21	0.4
(1,716)	1:A:629:SER:H	1:A:677:ASN:HD21	4	0.39	0.12	0.36
(1,624)	1:A:679:GLN:HB2	1:A:679:GLN:HE21	3	0.28	0.02	0.28
(1,1476)	1:A:629:SER:HB2	1:A:679:GLN:HE21	3	0.14	0.01	0.15
(1,1476)	1:A:629:SER:HB3	1:A:679:GLN:HE21	3	0.14	0.01	0.15
(1,1427)	1:A:605:LYS:HE2	1:A:624:GLN:HE22	2	0.26	0.1	0.26
(1,1427)	1:A:605:LYS:HE3	1:A:624:GLN:HE22	2	0.26	0.1	0.26
(1,385)	1:A:607:GLU:H	1:A:620:ASN:HD21	2	0.15	0.02	0.15

[1]Number of violated models, [2]Standard deviation

9.5   All violated distance restraints ⓘ

9.5.1   Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
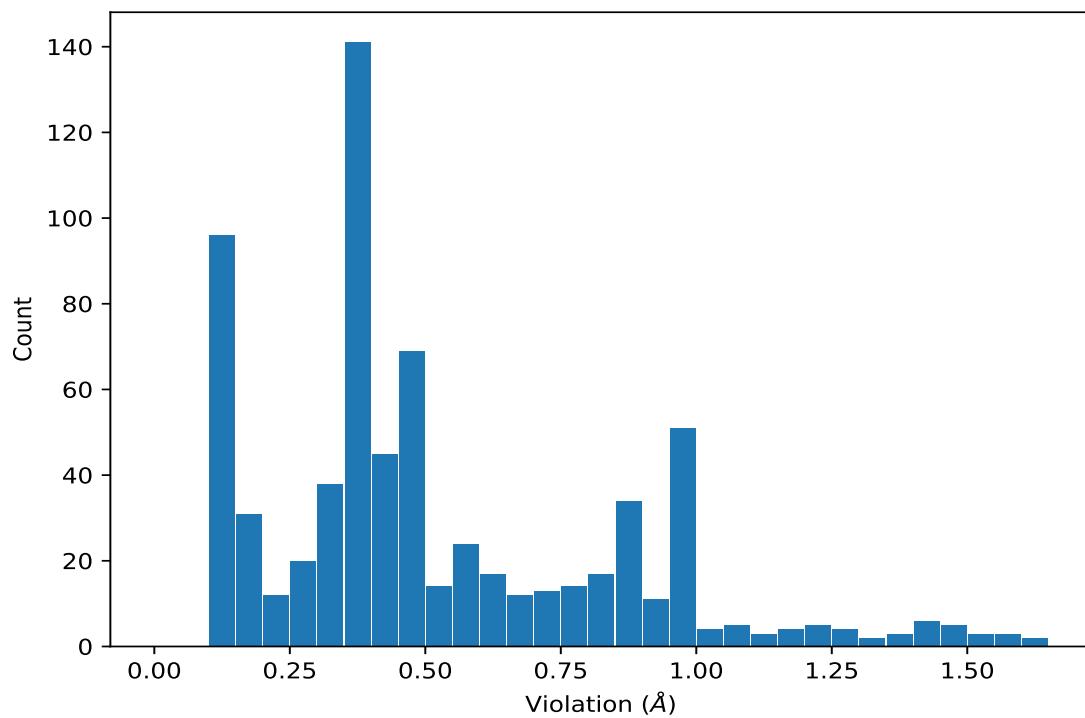
9.5.2   Table : All distance violations ⓘ

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	17	1.65
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	4	1.63
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	10	1.58
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	8	1.57
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	5	1.55
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	16	1.54
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	1	1.53
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	12	1.5
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	11	1.48
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	13	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	13	1.47
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	14	1.45
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	20	1.45
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	15	1.43
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	6	1.42
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	16	1.42
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	10	1.41
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	2	1.4
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	17	1.4
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	19	1.38
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	7	1.38
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	7	1.36
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	3	1.33
(1,411)	1:A:605:LYS:HE3	1:A:624:GLN:HE22	7	1.3
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	15	1.29
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	5	1.27
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	8	1.26
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	1	1.25
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	6	1.24
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	4	1.23
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	15	1.23
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	4	1.23
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	12	1.22
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	2	1.16
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	18	1.16
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	11	1.16
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	20	1.15
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	3	1.12
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	5	1.12
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	3	1.1
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	7	1.08
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	8	1.08
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	16	1.07
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	4	1.06
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	4	1.05
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	12	1.04
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	12	1.04
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	8	1.03
(1,788)	1:A:608:GLY:H	1:A:620:ASN:HD21	9	1.02
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	19	0.99
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	19	0.99
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	19	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	5	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	5	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	5	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	6	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	6	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	6	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	7	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	7	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	7	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	8	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	8	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	8	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	10	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	10	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	10	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	11	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	11	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	11	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	12	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	12	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	12	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	13	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	13	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	13	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	15	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	15	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	15	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	16	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	16	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	16	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	20	0.98
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	20	0.98
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	20	0.98
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	1	0.98
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	3	0.97
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	3	0.97
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	3	0.97
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	9	0.97
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	9	0.97
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	9	0.97
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	14	0.97
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	14	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	14	0.97
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	17	0.97
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	17	0.97
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	17	0.97
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	12	0.96
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	16	0.95
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	2	0.94
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	2	0.94
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	2	0.94
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	16	0.94
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	16	0.94
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	11	0.93
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	9	0.93
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	9	0.92
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	7	0.92
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	7	0.92
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	15	0.91
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	17	0.89
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	7	0.89
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	18	0.89
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	18	0.89
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	18	0.89
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	3	0.89
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	10	0.89
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	10	0.89
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	1	0.88
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	4	0.88
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	4	0.88
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	4	0.88
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	3	0.88
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	3	0.88
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	5	0.88
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	5	0.88
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	11	0.88
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	11	0.88
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	14	0.88
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	14	0.88
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	17	0.88
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	17	0.88
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	15	0.88
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	15	0.88
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	3	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	19	0.87
(1,411)	1:A:605:LYS:HE3	1:A:624:GLN:HE22	16	0.87
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	19	0.87
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	3	0.87
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	3	0.87
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	11	0.86
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	11	0.86
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	8	0.85
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	13	0.85
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	4	0.84
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	12	0.84
(1,533)	1:A:609:GLN:H	1:A:620:ASN:HD21	12	0.84
(1,271)	1:A:606:LEU:HD21	1:A:620:ASN:HD21	1	0.84
(1,271)	1:A:606:LEU:HD22	1:A:620:ASN:HD21	1	0.84
(1,271)	1:A:606:LEU:HD23	1:A:620:ASN:HD21	1	0.84
(1,533)	1:A:609:GLN:H	1:A:620:ASN:HD21	10	0.83
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	16	0.82
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	17	0.82
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	20	0.82
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	13	0.82
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	10	0.82
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	1	0.81
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	15	0.81
(1,411)	1:A:605:LYS:HE3	1:A:624:GLN:HE22	12	0.81
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	3	0.8
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	10	0.8
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	2	0.79
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	2	0.79
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	5	0.79
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	5	0.79
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	5	0.78
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	4	0.77
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	4	0.77
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	16	0.77
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	16	0.77
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	8	0.76
(1,533)	1:A:609:GLN:H	1:A:620:ASN:HD21	13	0.76
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	8	0.76
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	8	0.76
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	15	0.75
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	2	0.74
(1,411)	1:A:605:LYS:HE3	1:A:624:GLN:HE22	20	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	2	0.73
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	15	0.73
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	13	0.72
(1,1425)	1:A:605:LYS:HD2	1:A:624:GLN:HE22	3	0.72
(1,1425)	1:A:605:LYS:HD3	1:A:624:GLN:HE22	3	0.72
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	18	0.71
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	9	0.71
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	4	0.71
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	4	0.71
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	18	0.7
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	18	0.7
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	18	0.69
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	1	0.69
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	1	0.69
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	14	0.67
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	3	0.67
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	3	0.67
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	11	0.66
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	18	0.66
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	8	0.66
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	8	0.66
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	3	0.66
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	17	0.65
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	9	0.64
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	9	0.64
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	15	0.64
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	15	0.64
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	16	0.63
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	16	0.63
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	1	0.63
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	1	0.63
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	6	0.63
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	6	0.63
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	16	0.62
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	12	0.62
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	9	0.62
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	9	0.62
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	1	0.61
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	1	0.61
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	15	0.6
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	6	0.59
(1,555)	1:A:624:GLN:HA	1:A:624:GLN:HE21	19	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	5	0.59
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	11	0.59
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	17	0.59
(1,716)	1:A:629:SER:H	1:A:677:ASN:HD21	4	0.57
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	6	0.57
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	19	0.57
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	20	0.57
(1,533)	1:A:609:GLN:H	1:A:620:ASN:HD21	16	0.56
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	1	0.56
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	14	0.55
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	3	0.55
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	3	0.55
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	3	0.55
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	3	0.55
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	3	0.55
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	3	0.55
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	3	0.55
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	3	0.55
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	3	0.55
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	3	0.55
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	3	0.55
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	3	0.55
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	19	0.54
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	19	0.54
(1,1425)	1:A:605:LYS:HD2	1:A:624:GLN:HE22	4	0.54
(1,1425)	1:A:605:LYS:HD3	1:A:624:GLN:HE22	4	0.54
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	11	0.53
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	19	0.53
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	19	0.53
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	11	0.52
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	9	0.52
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	14	0.52
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	8	0.51
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	2	0.5
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	7	0.5
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	16	0.5
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	6	0.49
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	12	0.49
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	8	0.49
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	8	0.49
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	8	0.49
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	8	0.49
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	8	0.49
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	8	0.49
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	8	0.49
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	8	0.49
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	8	0.49
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	8	0.49
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	8	0.49
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	4	0.49
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	4	0.49
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	17	0.49
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	17	0.49
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	19	0.48
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	13	0.48
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	20	0.47
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	7	0.47
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	5	0.47
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	11	0.47
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	11	0.47
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	11	0.47
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	11	0.47
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	11	0.47
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	11	0.47
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	11	0.47
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	11	0.47
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	11	0.47
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	11	0.47
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	11	0.47
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	11	0.47
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	2	0.47
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	2	0.47
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	13	0.47
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	13	0.47
(1,411)	1:A:605:LYS:HE3	1:A:624:GLN:HE22	14	0.46
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	17	0.46
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	10	0.46
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	14	0.46
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	4	0.46
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	7	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	14	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	14	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	14	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	14	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	14	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	14	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	14	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	14	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	14	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	14	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	14	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	16	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	16	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	16	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	16	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	16	0.45
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	16	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	16	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	16	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	16	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	16	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	16	0.45
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	16	0.45
(1,716)	1:A:629:SER:H	1:A:677:ASN:HD21	2	0.44
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	9	0.43
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	9	0.43
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	9	0.43
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	9	0.43
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	9	0.43
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	9	0.43
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	9	0.43
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	9	0.43
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	9	0.43
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	9	0.43
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	9	0.43
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	9	0.43
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	13	0.43
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	18	0.42
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	18	0.42
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	5	0.42
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	5	0.42
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	5	0.42
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	5	0.42
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	5	0.42
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	5	0.42
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	5	0.42
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	5	0.42
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	5	0.42
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	5	0.42
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	5	0.42
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	7	0.41
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	7	0.41
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	7	0.41
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	7	0.41
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	7	0.41
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	7	0.41
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	7	0.41
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	7	0.41
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	7	0.41
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	7	0.41
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	7	0.41
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	7	0.41
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	13	0.4
(1,404)	1:A:601:PRO:HD2	1:A:677:ASN:HD22	16	0.4
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	6	0.4
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	6	0.4
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	9	0.4
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	1	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	1	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	1	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	1	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	1	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	1	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	1	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	1	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	1	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	1	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	1	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	1	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	18	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	18	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	18	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	18	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	18	0.39
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	18	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	18	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	18	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	18	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	18	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	18	0.39
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	18	0.39
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	12	0.39
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	18	0.39
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	5	0.38
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	9	0.38
(1,533)	1:A:609:GLN:H	1:A:620:ASN:HD21	7	0.38
(1,404)	1:A:601:PRO:HD2	1:A:677:ASN:HD22	11	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	12	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	12	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	12	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	12	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	12	0.38
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	12	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	12	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	12	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	12	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	12	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	12	0.38
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	12	0.38
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	5	0.37
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	10	0.37
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	12	0.37
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	13	0.37
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	16	0.37
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	6	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	2	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	2	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	2	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	2	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	2	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	2	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	2	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	2	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	2	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	2	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	2	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	13	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	13	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	13	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	13	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	13	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	13	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	13	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	13	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	13	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	13	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	13	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	13	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	19	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	19	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	19	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	19	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	19	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	19	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	19	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	19	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	19	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	19	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	19	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	19	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	20	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	20	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	20	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	20	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	20	0.37
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	20	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	20	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	20	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	20	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	20	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	20	0.37
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	20	0.37
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	9	0.36
(1,533)	1:A:609:GLN:H	1:A:620:ASN:HD21	5	0.36
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	11	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	4	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	4	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	4	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	4	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	4	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	4	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	4	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	4	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	4	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	4	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	4	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	15	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	15	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	15	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	15	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	15	0.36
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	15	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	15	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	15	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	15	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	15	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	15	0.36
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	15	0.36
(1,1427)	1:A:605:LYS:HE2	1:A:624:GLN:HE22	20	0.36
(1,1427)	1:A:605:LYS:HE3	1:A:624:GLN:HE22	20	0.36
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	15	0.36
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	15	0.36
(1,1041)	1:A:607:GLU:HA	1:A:620:ASN:HD21	10	0.36
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	16	0.35
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	17	0.35
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	17	0.35
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	17	0.35
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	17	0.35
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	17	0.35
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	17	0.35
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	17	0.35
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	17	0.35
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	17	0.35
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	17	0.35
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	17	0.35
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	17	0.35
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	19	0.34
(1,171)	1:A:626:ASP:HB2	1:A:628:GLY:H	17	0.34
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	6	0.34
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	6	0.34
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	6	0.34
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	6	0.34
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	6	0.34
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	6	0.34
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	6	0.34
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	6	0.34
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	6	0.34
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	6	0.34
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	6	0.34
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	19	0.34
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	19	0.34
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	8	0.33
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD11	10	0.33
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD12	10	0.33
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD13	10	0.33
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD21	10	0.33
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD22	10	0.33
(1,1530)	1:A:650:ARG:HG2	1:A:651:LEU:HD23	10	0.33
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD11	10	0.33
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD12	10	0.33
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD13	10	0.33
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD21	10	0.33
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD22	10	0.33
(1,1530)	1:A:650:ARG:HG3	1:A:651:LEU:HD23	10	0.33
(1,241)	1:A:624:GLN:HE21	1:A:625:ASP:HA	19	0.32
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	17	0.31
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	17	0.31
(1,624)	1:A:679:GLN:HB2	1:A:679:GLN:HE21	8	0.3
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	9	0.3
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	14	0.3
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	14	0.3
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	18	0.3
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	18	0.3
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	14	0.29
(1,404)	1:A:601:PRO:HD2	1:A:677:ASN:HD22	15	0.29
(1,1466)	1:A:623:LYS:HD2	1:A:624:GLN:HE22	12	0.29
(1,1466)	1:A:623:LYS:HD3	1:A:624:GLN:HE22	12	0.29
(1,716)	1:A:629:SER:H	1:A:677:ASN:HD21	7	0.28
(1,624)	1:A:679:GLN:HB2	1:A:679:GLN:HE21	5	0.28
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	11	0.28
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	10	0.28
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	10	0.28
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	13	0.27
(1,716)	1:A:629:SER:H	1:A:677:ASN:HD21	14	0.27
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	7	0.27
(1,533)	1:A:609:GLN:H	1:A:620:ASN:HD21	11	0.27
(1,1425)	1:A:605:LYS:HD2	1:A:624:GLN:HE22	8	0.26
(1,1425)	1:A:605:LYS:HD3	1:A:624:GLN:HE22	8	0.26
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	1	0.25
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	5	0.25
(1,624)	1:A:679:GLN:HB2	1:A:679:GLN:HE21	15	0.25
(1,320)	1:A:605:LYS:HE2	1:A:624:GLN:HE22	19	0.25
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	7	0.24
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	11	0.23
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	19	0.22
(1,404)	1:A:601:PRO:HD2	1:A:677:ASN:HD22	5	0.22
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	8	0.22
(1,1425)	1:A:605:LYS:HD2	1:A:624:GLN:HE22	1	0.22
(1,1425)	1:A:605:LYS:HD3	1:A:624:GLN:HE22	1	0.22
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	7	0.22
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	7	0.22
(1,404)	1:A:601:PRO:HD2	1:A:677:ASN:HD22	1	0.2
(1,320)	1:A:605:LYS:HE2	1:A:624:GLN:HE22	10	0.2
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	12	0.2
(1,320)	1:A:605:LYS:HE2	1:A:624:GLN:HE22	11	0.19
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG2	20	0.19
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG3	20	0.19
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG2	20	0.19
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG3	20	0.19
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG2	20	0.19
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG3	20	0.19
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG2	20	0.19
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG3	20	0.19
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG2	20	0.19
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG3	20	0.19
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG2	20	0.19
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG3	20	0.19
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	5	0.19
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	5	0.19
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	2	0.18
(2,38)	1:A:599:ARG:H	1:A:677:ASN:HD22	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:A:607:GLU:H	1:A:620:ASN:HD21	5	0.17
(1,191)	1:A:600:GLU:H	1:A:677:ASN:HD22	20	0.17
(1,320)	1:A:605:LYS:HE2	1:A:624:GLN:HE22	4	0.16
(1,1424)	1:A:605:LYS:HG2	1:A:624:GLN:HE22	20	0.16
(1,1424)	1:A:605:LYS:HG3	1:A:624:GLN:HE22	20	0.16
(2,30)	1:A:605:LYS:H	1:A:624:GLN:HE22	10	0.15
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	20	0.15
(1,533)	1:A:609:GLN:H	1:A:620:ASN:HD21	20	0.15
(1,1476)	1:A:629:SER:HB2	1:A:679:GLN:HE21	3	0.15
(1,1476)	1:A:629:SER:HB3	1:A:679:GLN:HE21	3	0.15
(1,1476)	1:A:629:SER:HB2	1:A:679:GLN:HE21	19	0.15
(1,1476)	1:A:629:SER:HB3	1:A:679:GLN:HE21	19	0.15
(1,1427)	1:A:605:LYS:HE2	1:A:624:GLN:HE22	7	0.15
(1,1427)	1:A:605:LYS:HE3	1:A:624:GLN:HE22	7	0.15
(1,495)	1:A:595:MET:HA	1:A:679:GLN:HE22	19	0.14
(1,404)	1:A:601:PRO:HD2	1:A:677:ASN:HD22	3	0.13
(1,385)	1:A:607:GLU:H	1:A:620:ASN:HD21	12	0.13
(1,320)	1:A:605:LYS:HE2	1:A:624:GLN:HE22	20	0.13
(1,174)	1:A:619:VAL:HA	1:A:620:ASN:HD21	20	0.13
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG2	2	0.13
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG3	2	0.13
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG2	2	0.13
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG3	2	0.13
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG2	2	0.13
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG3	2	0.13
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG2	2	0.13
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG3	2	0.13
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG2	2	0.13
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG3	2	0.13
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG2	2	0.13
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG3	2	0.13
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG2	12	0.13
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG3	12	0.13
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG2	12	0.13
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG3	12	0.13
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG2	12	0.13
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG3	12	0.13
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG2	12	0.13
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG3	12	0.13
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG2	12	0.13
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG3	12	0.13
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG2	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG3	12	0.13
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	2	0.13
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	2	0.13
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	6	0.13
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	6	0.13
(1,240)	1:A:627:GLY:H	1:A:677:ASN:HD21	5	0.12
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG2	14	0.12
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG3	14	0.12
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG2	14	0.12
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG3	14	0.12
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG2	14	0.12
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG3	14	0.12
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG2	14	0.12
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG3	14	0.12
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG2	14	0.12
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG3	14	0.12
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG2	14	0.12
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG3	14	0.12
(1,1476)	1:A:629:SER:HB2	1:A:679:GLN:HE21	6	0.12
(1,1476)	1:A:629:SER:HB3	1:A:679:GLN:HE21	6	0.12
(1,1454)	1:A:621:LEU:HD11	1:A:651:LEU:HD11	3	0.12
(1,1454)	1:A:621:LEU:HD11	1:A:651:LEU:HD12	3	0.12
(1,1454)	1:A:621:LEU:HD11	1:A:651:LEU:HD13	3	0.12
(1,1454)	1:A:621:LEU:HD11	1:A:651:LEU:HD21	3	0.12
(1,1454)	1:A:621:LEU:HD11	1:A:651:LEU:HD22	3	0.12
(1,1454)	1:A:621:LEU:HD11	1:A:651:LEU:HD23	3	0.12
(1,1454)	1:A:621:LEU:HD12	1:A:651:LEU:HD11	3	0.12
(1,1454)	1:A:621:LEU:HD12	1:A:651:LEU:HD12	3	0.12
(1,1454)	1:A:621:LEU:HD12	1:A:651:LEU:HD13	3	0.12
(1,1454)	1:A:621:LEU:HD12	1:A:651:LEU:HD21	3	0.12
(1,1454)	1:A:621:LEU:HD12	1:A:651:LEU:HD22	3	0.12
(1,1454)	1:A:621:LEU:HD12	1:A:651:LEU:HD23	3	0.12
(1,1454)	1:A:621:LEU:HD13	1:A:651:LEU:HD11	3	0.12
(1,1454)	1:A:621:LEU:HD13	1:A:651:LEU:HD12	3	0.12
(1,1454)	1:A:621:LEU:HD13	1:A:651:LEU:HD13	3	0.12
(1,1454)	1:A:621:LEU:HD13	1:A:651:LEU:HD21	3	0.12
(1,1454)	1:A:621:LEU:HD13	1:A:651:LEU:HD22	3	0.12
(1,1454)	1:A:621:LEU:HD13	1:A:651:LEU:HD23	3	0.12
(1,604)	1:A:620:ASN:H	1:A:620:ASN:HD21	17	0.11
(1,404)	1:A:601:PRO:HD2	1:A:677:ASN:HD22	20	0.11
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG2	5	0.11
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG2	5	0.11
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG3	5	0.11
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG2	5	0.11
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG3	5	0.11
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG2	5	0.11
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG3	5	0.11
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG2	5	0.11
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG3	5	0.11
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG2	5	0.11
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG3	5	0.11
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG2	18	0.11
(1,1501)	1:A:635:LEU:HD11	1:A:676:GLU:HG3	18	0.11
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG2	18	0.11
(1,1501)	1:A:635:LEU:HD12	1:A:676:GLU:HG3	18	0.11
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG2	18	0.11
(1,1501)	1:A:635:LEU:HD13	1:A:676:GLU:HG3	18	0.11
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG2	18	0.11
(1,1501)	1:A:635:LEU:HD21	1:A:676:GLU:HG3	18	0.11
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG2	18	0.11
(1,1501)	1:A:635:LEU:HD22	1:A:676:GLU:HG3	18	0.11
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG2	18	0.11
(1,1501)	1:A:635:LEU:HD23	1:A:676:GLU:HG3	18	0.11
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	12	0.11
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	12	0.11
(1,1411)	1:A:600:GLU:HB2	1:A:677:ASN:HD22	20	0.11
(1,1411)	1:A:600:GLU:HB3	1:A:677:ASN:HD22	20	0.11

10 Dihedral-angle violation analysis ⓘ

## 10.1 Summary of dihedral-angle violations ⓘ

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	$\%^1$	Violated[3]			Consistently Violated[4]		
			Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
PHI	68	50.0	0	0.0	0.0	0	0.0	0.0
PSI	68	50.0	1	1.5	0.7	0	0.0	0.0
Total	136	100.0	1	0.7	0.7	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations ⓘ
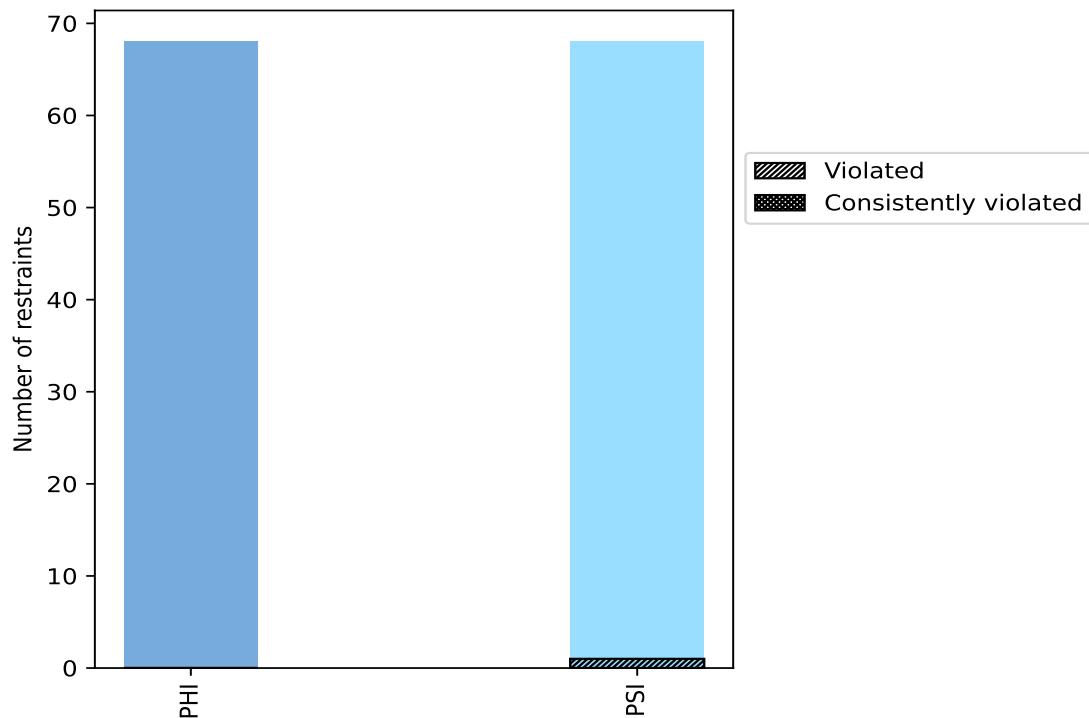

Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2   Dihedral-angle violation statistics for each model ⓘ

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	1	1	27.7	27.7	0.0	27.7
6	0	1	1	27.9	27.9	0.0	27.9
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	1	1	27.8	27.8	0.0	27.8
10	0	1	1	27.5	27.5	0.0	27.5
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	1	1	27.9	27.9	0.0	27.9
14	0	1	1	27.9	27.9	0.0	27.9
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	0	1	1	27.9	27.9	0.0	27.9
20	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ
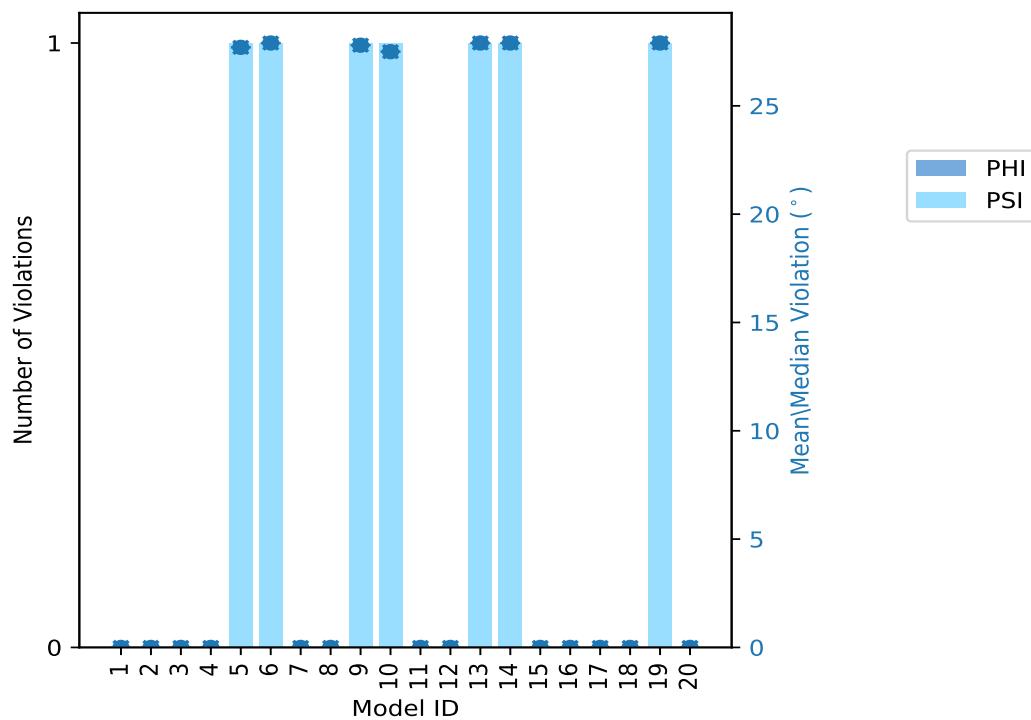
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
0	1	1	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ
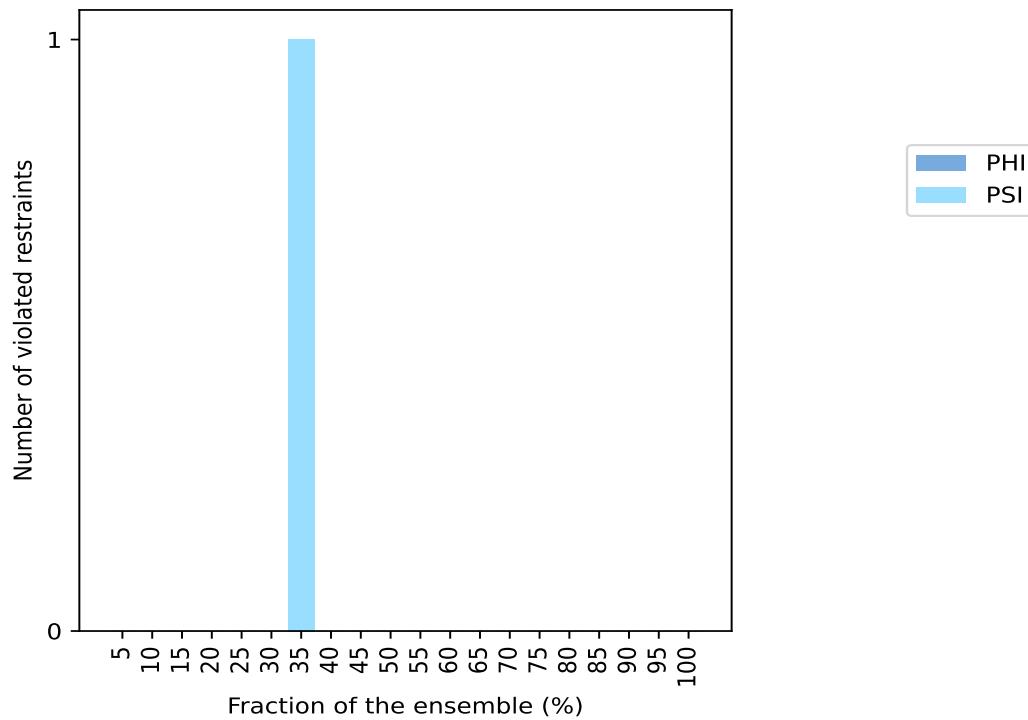
## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle 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
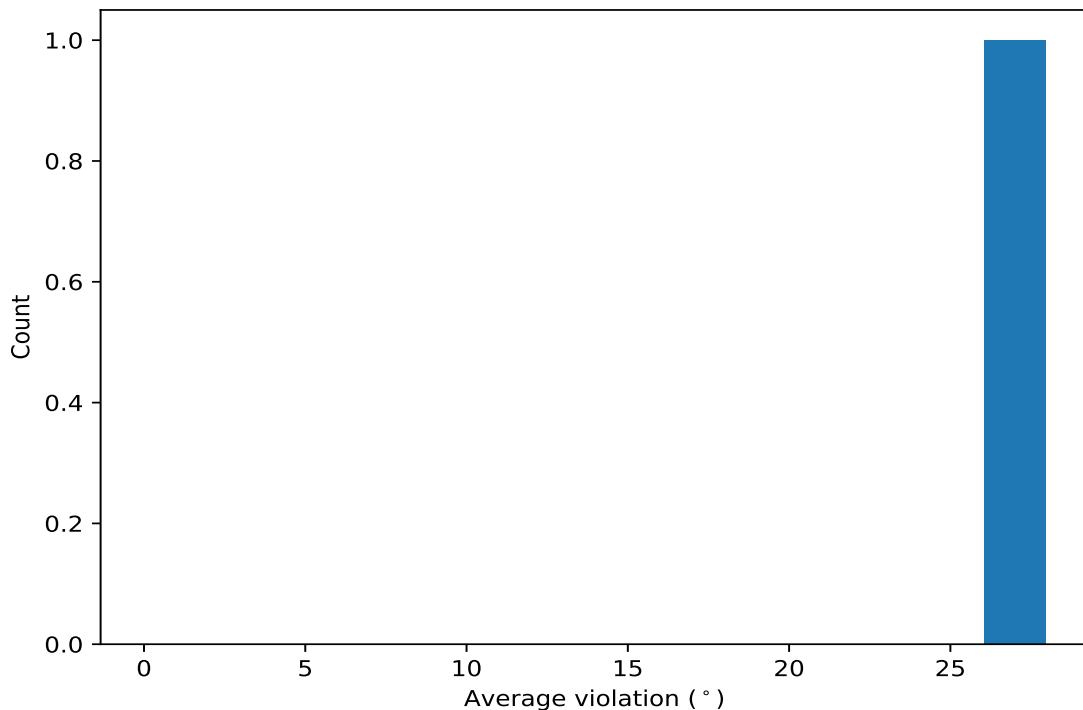
10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,34)	1:A:621:LEU:N	1:A:621:LEU:CA	1:A:621:LEU:C	1:A:622:ILE:N	7	27.8	0.14	27.9

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
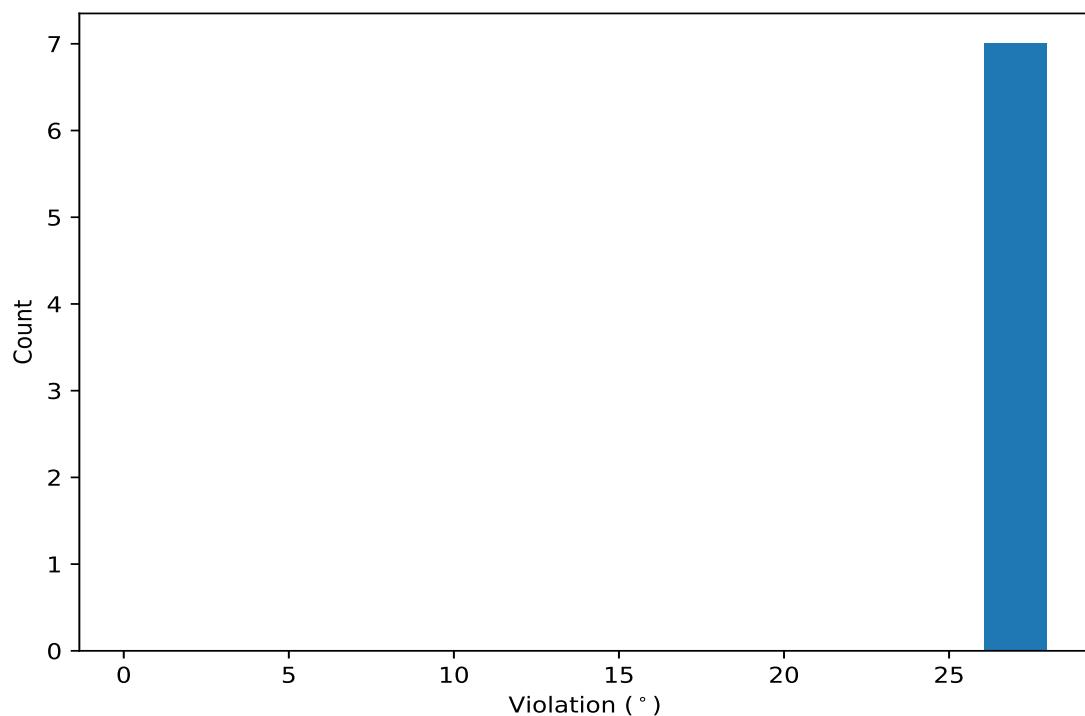
10.5.2 Table: All violated dihedral-angle restraints ⓘ

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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:A:621:LEU:N	1:A:621:LEU:CA	1:A:621:LEU:C	1:A:622:ILE:N	6	27.9
(1,34)	1:A:621:LEU:N	1:A:621:LEU:CA	1:A:621:LEU:C	1:A:622:ILE:N	13	27.9
(1,34)	1:A:621:LEU:N	1:A:621:LEU:CA	1:A:621:LEU:C	1:A:622:ILE:N	14	27.9
(1,34)	1:A:621:LEU:N	1:A:621:LEU:CA	1:A:621:LEU:C	1:A:622:ILE:N	19	27.9
(1,34)	1:A:621:LEU:N	1:A:621:LEU:CA	1:A:621:LEU:C	1:A:622:ILE:N	9	27.8
(1,34)	1:A:621:LEU:N	1:A:621:LEU:CA	1:A:621:LEU:C	1:A:622:ILE:N	5	27.7
(1,34)	1:A:621:LEU:N	1:A:621:LEU:CA	1:A:621:LEU:C	1:A:622:ILE:N	10	27.5