WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 07:57 pm BST

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PDB ID	:	6QVW
BMRB ID	:	34364
Title	:	Solution structure of the free FOXO1 DNA binding domain
Authors	:	Psenakova, K.; Obsil, T.; Veverka, V.; Obsilova, V.; Kohoutova, K.
Deposited on	:	2019-03-05

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 90%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
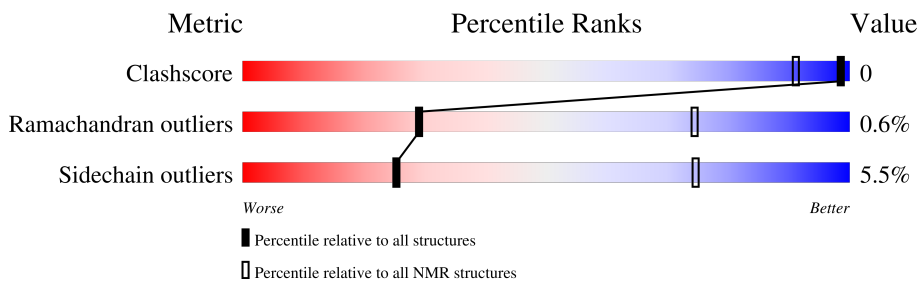
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	119	58% • 39%

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. Model 12 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:160-A:224, A:232-A:238 (72)	0.47	12

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 5, 6, 12, 13, 14, 16, 17, 19, 22, 23, 27, 29, 30
2	11, 18, 21, 24, 25, 26
3	2, 4, 7, 10
4	15, 20, 28
Single-model clusters	8; 9

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1857 atoms, of which 927 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Forkhead box protein O1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	119	1857	579	927	175	173	3	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	GLY	-	expression tag	UNP Q12778
A	152	PRO	-	expression tag	UNP Q12778
A	153	LEU	-	expression tag	UNP Q12778
A	154	GLY	-	expression tag	UNP Q12778
A	155	SER	-	expression tag	UNP Q12778
A	265	GLY	SER	conflict	UNP Q12778

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: Forkhead box protein O1
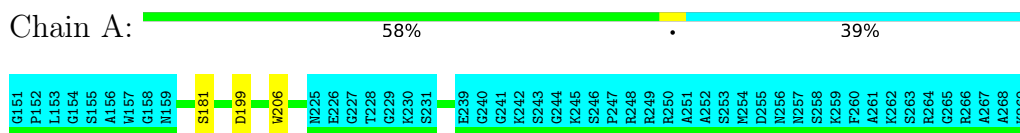
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Forkhead box protein O1
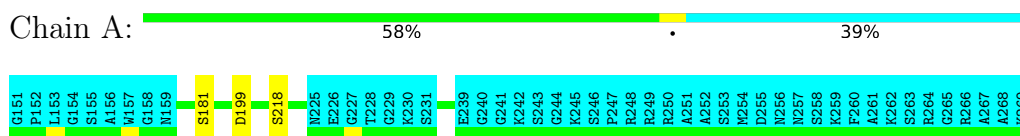
4.2.2 Score per residue for model 2

• Molecule 1: Forkhead box protein O1

4.2.3 Score per residue for model 3

• Molecule 1: Forkhead box protein O1

4.2.4 Score per residue for model 4

• Molecule 1: Forkhead box protein O1

4.2.5 Score per residue for model 5

• Molecule 1: Forkhead box protein O1

4.2.6 Score per residue for model 6

• Molecule 1: Forkhead box protein O1

4.2.7 Score per residue for model 7

• Molecule 1: Forkhead box protein O1

4.2.8 Score per residue for model 8

• Molecule 1: Forkhead box protein O1

Chain A:

4.2.9 Score per residue for model 9

• Molecule 1: Forkhead box protein O1

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: Forkhead box protein O1

Chain A:

4.2.11 Score per residue for model 11

• Molecule 1: Forkhead box protein O1

Chain A:

4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: Forkhead box protein O1

Chain A:

4.2.13　Score per residue for model 13

• Molecule 1: Forkhead box protein O1

Chain A:

4.2.14　Score per residue for model 14

• Molecule 1: Forkhead box protein O1

Chain A:

4.2.15　Score per residue for model 15

• Molecule 1: Forkhead box protein O1

Chain A:
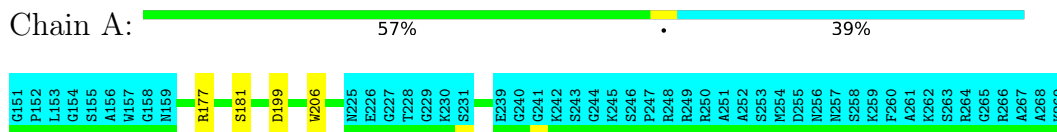
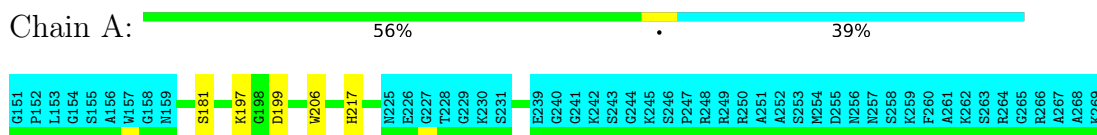
4.2.16　Score per residue for model 16

• Molecule 1: Forkhead box protein O1

Chain A:
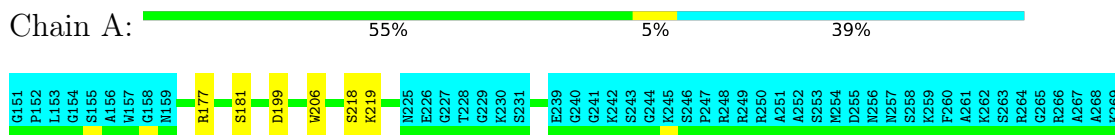
4.2.17　Score per residue for model 17

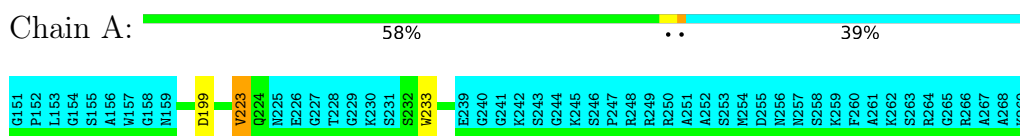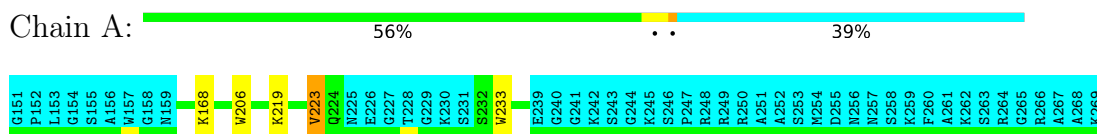• Molecule 1: Forkhead box protein O1

Chain A:

G151 P152 L153 G154 S155 A156 W157 G158 N159 K168 W206 H217 V223 Q224 N225 E226 G227 T228 G229 K230 S231 S232 W233 E239 G240 G241 K242 S243 G244 K245 S246 P247 R248 R249 R250 A251 A252 S253 M254 D255 N256 N257 S258 K259 F260 A261 K262 S263 R264 G265 R266 A267 A268 K269
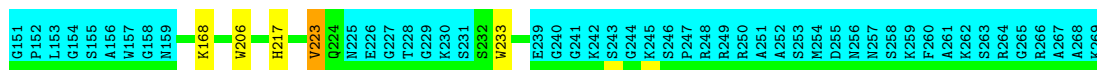
4.2.18 Score per residue for model 18

• Molecule 1: Forkhead box protein O1

Chain A: 57%   ·   39%

G151 P152 L153 G154 S155 A156 W157 G158 N159 S181 K189 K197 G198 D199 N225 E226 G227 T228 G229 K230 S231 E239 G240 G241 K242 S243 G244 K245 S246 P247 R248 R249 R250 A251 A252 S253 M254 D255 N256 N257 S258 K259 F260 A261 K262 S263 R264 G265 R266 A267 A268 K269
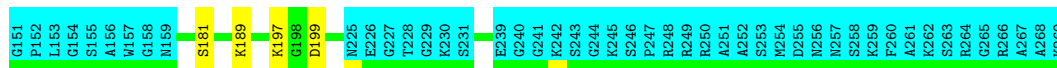
4.2.19 Score per residue for model 19

• Molecule 1: Forkhead box protein O1

Chain A: 55%   5%   39%

G151 P152 L153 G154 S155 A156 W157 G158 N159 D164 S181 D199 W206 H217 S218 K219 N225 E226 G227 T228 G229 K230 S231 E239 G240 G241 K242 S243 G244 K245 S246 P247 R248 R249 R250 A251 A252 S253 M254 D255 N256 N257 S258 K259 F260 A261 K262 S263 R264 G265 R266 A267 A268

K269
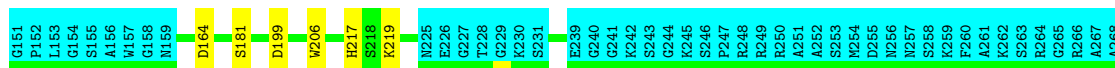
4.2.20 Score per residue for model 20

• Molecule 1: Forkhead box protein O1

Chain A: 57%   ·   39%

G151 P152 L153 G154 S155 A156 W157 G158 N159 S181 D199 H217 S218 K219 N225 E226 G227 G229 K230 S231 E239 G240 G241 K242 S243 G244 K245 S246 P247 R248 R249 R250 A251 A252 S253 M254 D255 N256 N257 S258 K259 F260 A261 K262 S263 R264 G265 R266 A267 A268 K269
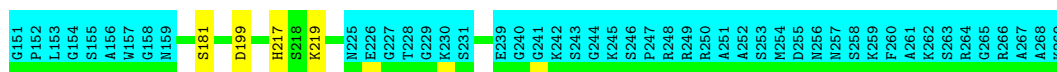
4.2.21 Score per residue for model 21

• Molecule 1: Forkhead box protein O1

Chain A: 58%   ·   39%

G151 P152 L153 G154 S155 A156 W157 G158 N159 R177 D199 S218 N225 E226 G227 T228 G229 K230 S231 E239 G240 G241 K242 S243 G244 K245 S246 P247 R248 R249 R250 A251 A252 S253 M254 D255 N256 N257 S258 K259 F260 A261 K262 S263 R264 G265 R266 A267 A268 K269
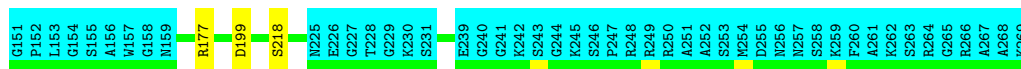
4.2.22 Score per residue for model 22

• Molecule 1: Forkhead box protein O1

Chain A:
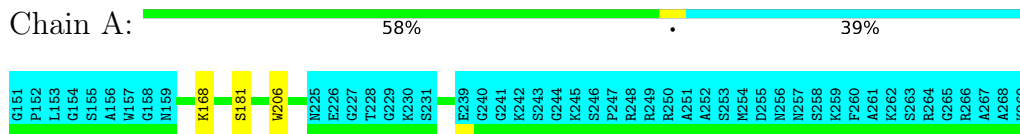
4.2.23 Score per residue for model 23

• Molecule 1: Forkhead box protein O1

Chain A:
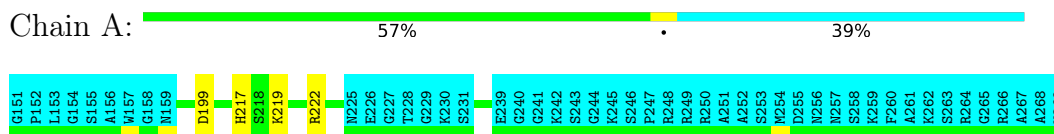
4.2.24 Score per residue for model 24
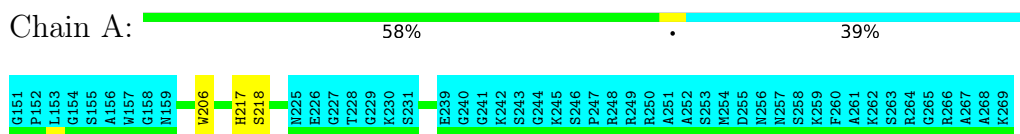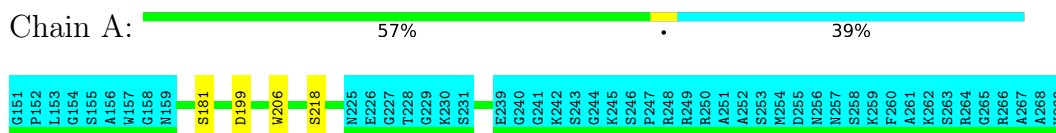
• Molecule 1: Forkhead box protein O1

Chain A:
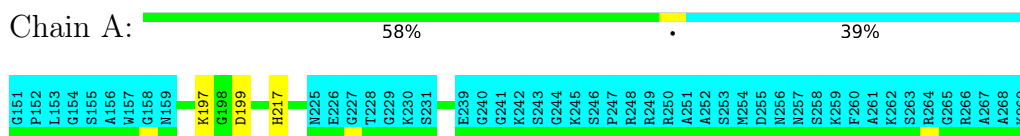
4.2.25 Score per residue for model 25

• Molecule 1: Forkhead box protein O1

Chain A:
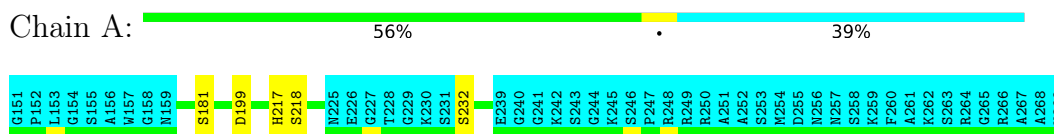
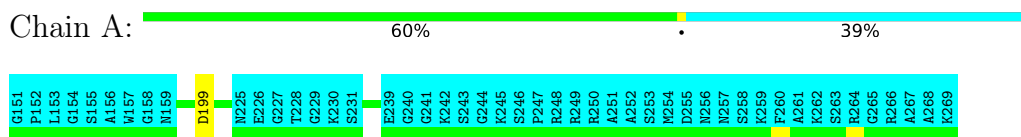**4.2.26 Score per residue for model 26**

• Molecule 1: Forkhead box protein O1

Chain A:
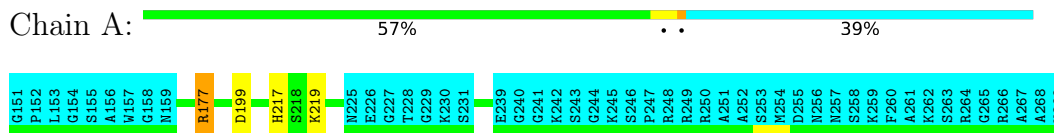
4.2.27 Score per residue for model 27

• Molecule 1: Forkhead box protein O1
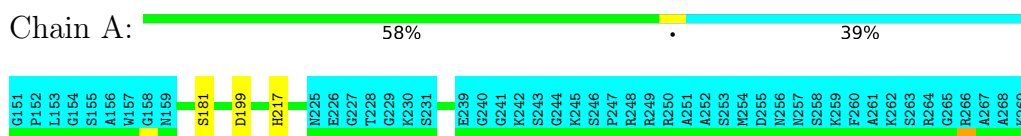
Chain A:
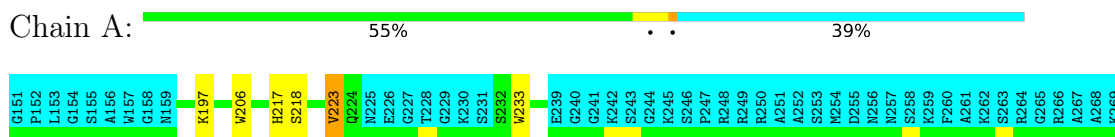
4.2.28 Score per residue for model 28

• Molecule 1: Forkhead box protein O1
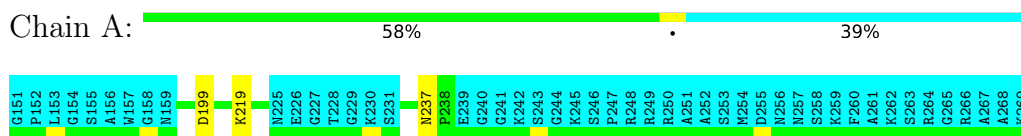
Chain A:
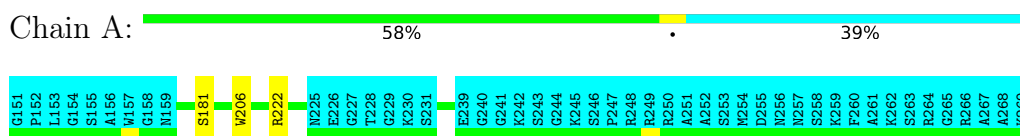
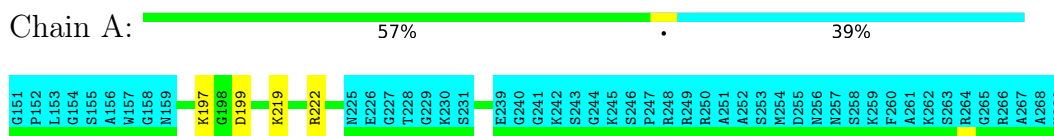#### 4.2.29 Score per residue for model 29

• Molecule 1: Forkhead box protein O1

Chain A:

4.2.30 Score per residue for model 30
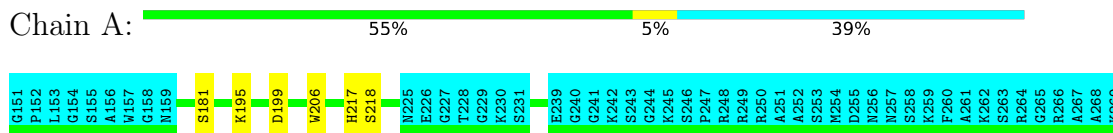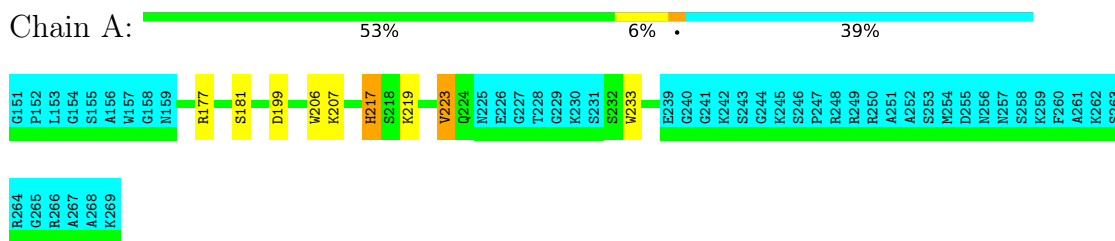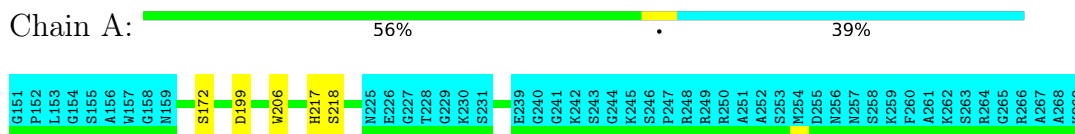
• Molecule 1: Forkhead box protein O1

Chain A:
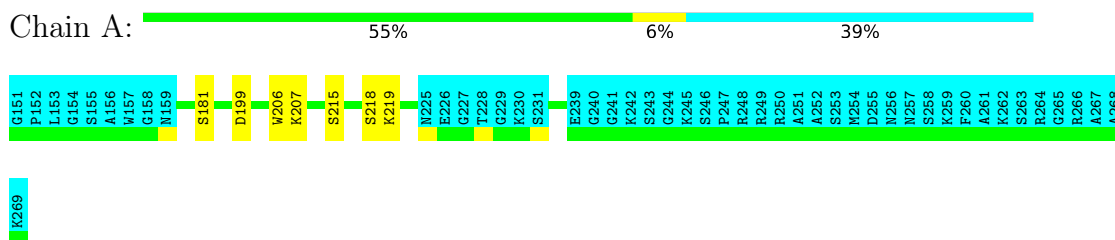
5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 30 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 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	1361
Number of shifts mapped to atoms	1361
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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	0.66±0.01	0±0/609 (0.0± 0.0%)	0.68±0.02	0±0/824 (0.0± 0.1%)
All	All	0.66	0/18270 (0.0%)	0.68	8/24720 (0.0%)

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	177	ARG	NE-CZ-NH1	5.70	123.15	120.30	15	5
1	A	222	ARG	NE-CZ-NH1	5.37	122.98	120.30	11	3

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	592	590	590	0±0
All	All	17760	17700	17700	5

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:223:VAL:HG13	1:A:233:TRP:CB	0.44	2.42	4	5

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	72/119 (61%)	71±1 (98±1%)	1±1 (1±1%)	0±1 (1±1%)	29	74
All	All	2160/3570 (61%)	2118 (98%)	29 (1%)	13 (1%)	29	74

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	217	HIS	12
1	A	232	SER	1

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	66/98 (67%)	62±1 (95±2%)	4±1 (5±2%)	25	74
All	All	1980/2940 (67%)	1872 (95%)	108 (5%)	25	74

All 18 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	199	ASP	23
1	A	206	TRP	17
1	A	181	SER	16

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Mol	Chain	Res	Type	Models (Total)
1	A	218	SER	12
1	A	219	LYS	12
1	A	223	VAL	6
1	A	197	LYS	5
1	A	168	LYS	4
1	A	217	HIS	3
1	A	207	LYS	2
1	A	237	ASN	1
1	A	195	LYS	1
1	A	172	SER	1
1	A	189	LYS	1
1	A	164	ASP	1
1	A	177	ARG	1
1	A	224	GLN	1
1	A	215	SER	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

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 90% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	1361
Number of shifts mapped to atoms	1361
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	117	-0.31 ± 0.07	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	107	0.12 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	114	-0.63 ± 0.09	Should be applied
^{15}N	110	0.17 ± 0.26	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 90%, i.e. 911 atoms were assigned a chemical shift out of a possible 1014. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	343/358 (96%)	138/144 (96%)	139/144 (97%)	66/70 (94%)
Sidechain	485/547 (89%)	328/356 (92%)	151/169 (89%)	6/22 (27%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	83/109 (76%)	47/54 (87%)	33/49 (67%)	3/6 (50%)
Overall	911/1014 (90%)	513/554 (93%)	323/362 (89%)	75/98 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1359 atoms were assigned a chemical shift out of a possible 1588. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	576/598 (96%)	235/245 (96%)	231/238 (97%)	110/115 (96%)
Sidechain	685/859 (80%)	459/553 (83%)	217/259 (84%)	9/47 (19%)
Aromatic	98/131 (75%)	55/65 (85%)	39/59 (66%)	4/7 (57%)
Overall	1359/1588 (86%)	749/863 (87%)	487/556 (88%)	123/169 (73%)

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	167	THR	HG1	5.09	0.08 – 2.19	18.7
1	A	190	SER	HB2	2.12	2.61 – 5.13	-7.0
1	A	177	ARG	HD2	1.69	1.97 – 4.26	-6.2
1	A	169	ALA	HA	1.85	2.13 – 6.34	-5.7

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:
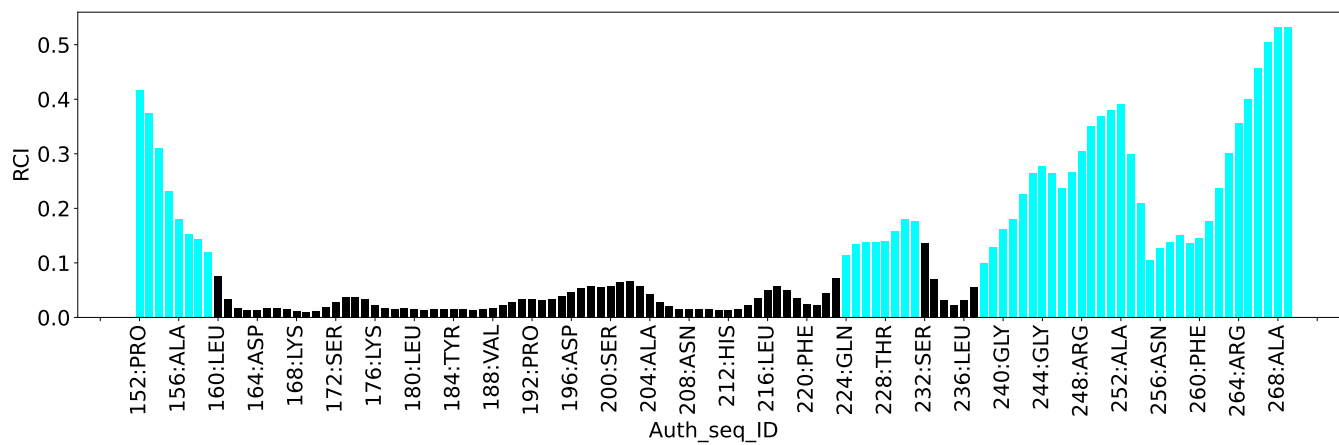
8   NMR restraints analysis ⓘ

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	1577
Intra-residue ($\vert$i-j$\vert$=0)	413
Sequential ($\vert$i-j$\vert$=1)	375
Medium range ($\vert$i-j$\vert$>1 and $\vert$i-j$\vert$<5)	298
Long range ($\vert$i-j$\vert$≥5)	491
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	13.3
Number of long range restraints per residue[1]	4.1

[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)	3.9	0.2
0.2-0.5 (Medium)	0.8	0.35
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model ⓘ

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

9 Distance violation analysis ⓘ

9.1 Summary of distance violations ⓘ

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	413	26.2	3	0.7	0.2	0	0.0	0.0
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	322	20.4	3	0.9	0.2	0	0.0	0.0
Sidechain-Sidechain	88	5.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	375	23.8	11	2.9	0.7	0	0.0	0.0
Backbone-Backbone	96	6.1	2	2.1	0.1	0	0.0	0.0
Backbone-Sidechain	222	14.1	3	1.4	0.2	0	0.0	0.0
Sidechain-Sidechain	57	3.6	6	10.5	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	298	18.9	7	2.3	0.4	0	0.0	0.0
Backbone-Backbone	45	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	140	8.9	2	1.4	0.1	0	0.0	0.0
Sidechain-Sidechain	113	7.2	5	4.4	0.3	0	0.0	0.0
Long range (|i-j|≥5)	491	31.1	12	2.4	0.8	0	0.0	0.0
Backbone-Backbone	13	0.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	161	10.2	2	1.2	0.1	0	0.0	0.0
Sidechain-Sidechain	317	20.1	10	3.2	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1577	100.0	33	2.1	2.1	0	0.0	0.0
Backbone-Backbone	157	10.0	2	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	845	53.6	10	1.2	0.6	0	0.0	0.0
Sidechain-Sidechain	575	36.5	21	3.7	1.3	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations (i)
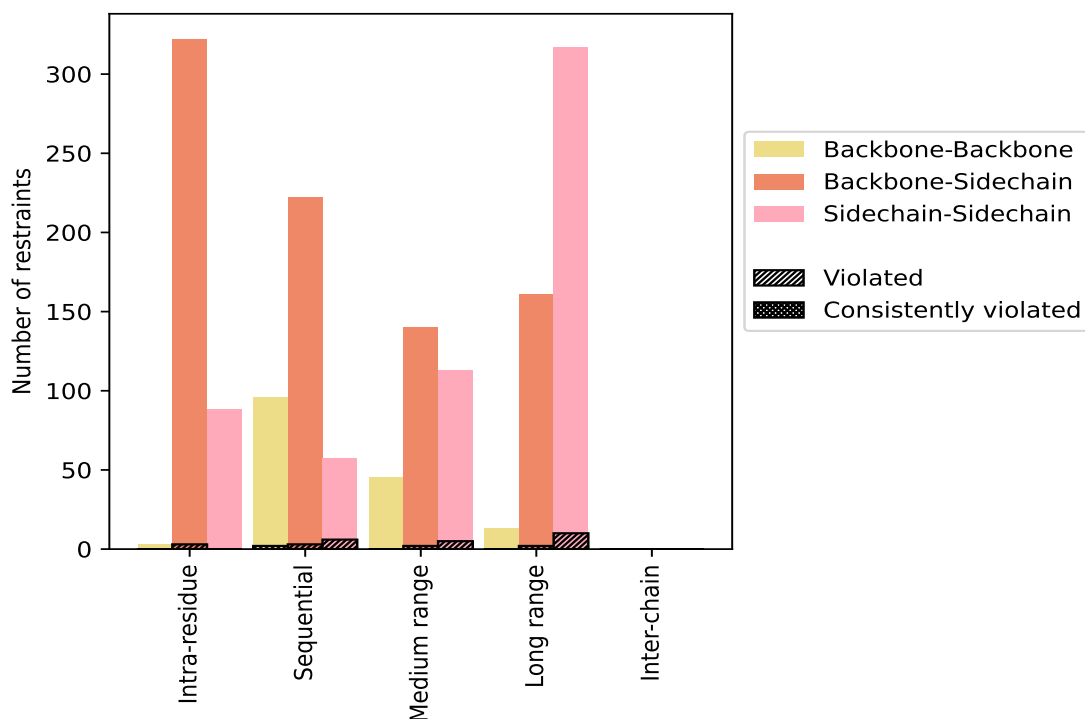
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	1	1	3	0	5	0.15	0.17	0.02	0.15
2	0	0	2	3	0	5	0.16	0.2	0.03	0.17
3	0	2	2	3	0	7	0.15	0.21	0.03	0.16
4	0	0	1	3	0	4	0.15	0.16	0.01	0.15
5	0	1	0	4	0	5	0.13	0.15	0.01	0.13
6	0	1	2	2	0	5	0.16	0.22	0.05	0.13
7	0	0	0	2	0	2	0.13	0.14	0.01	0.13
8	0	0	0	2	0	2	0.15	0.16	0.02	0.15
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	4	1	2	0	7	0.17	0.26	0.05	0.18
11	0	1	2	1	0	4	0.18	0.29	0.07	0.16

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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	0	1	2	3	0	6	0.16	0.2	0.03	0.16
13	0	1	1	3	0	5	0.15	0.21	0.04	0.13
14	0	1	2	3	0	6	0.18	0.27	0.06	0.16
15	0	0	0	1	0	1	0.17	0.17	0.0	0.17
16	0	0	0	1	0	1	0.12	0.12	0.0	0.12
17	0	3	1	3	0	7	0.15	0.23	0.04	0.13
18	0	1	1	2	0	4	0.16	0.22	0.04	0.15
19	1	1	1	2	0	5	0.16	0.24	0.05	0.14
20	0	0	1	1	0	2	0.12	0.12	0.0	0.12
21	0	0	0	0	0	0	0.0	0.0	0.0	0.0
22	0	0	0	2	0	2	0.14	0.16	0.02	0.14
23	0	1	3	4	0	8	0.16	0.22	0.04	0.16
24	0	2	1	3	0	6	0.14	0.2	0.03	0.12
25	0	1	2	2	0	5	0.16	0.2	0.02	0.15
26	0	0	0	0	0	0	0.0	0.0	0.0	0.0
27	0	1	2	2	0	5	0.19	0.35	0.09	0.14
28	0	4	3	6	0	13	0.17	0.3	0.06	0.14
29	2	4	4	7	0	17	0.16	0.26	0.05	0.14
30	0	0	0	2	0	2	0.18	0.2	0.03	0.18

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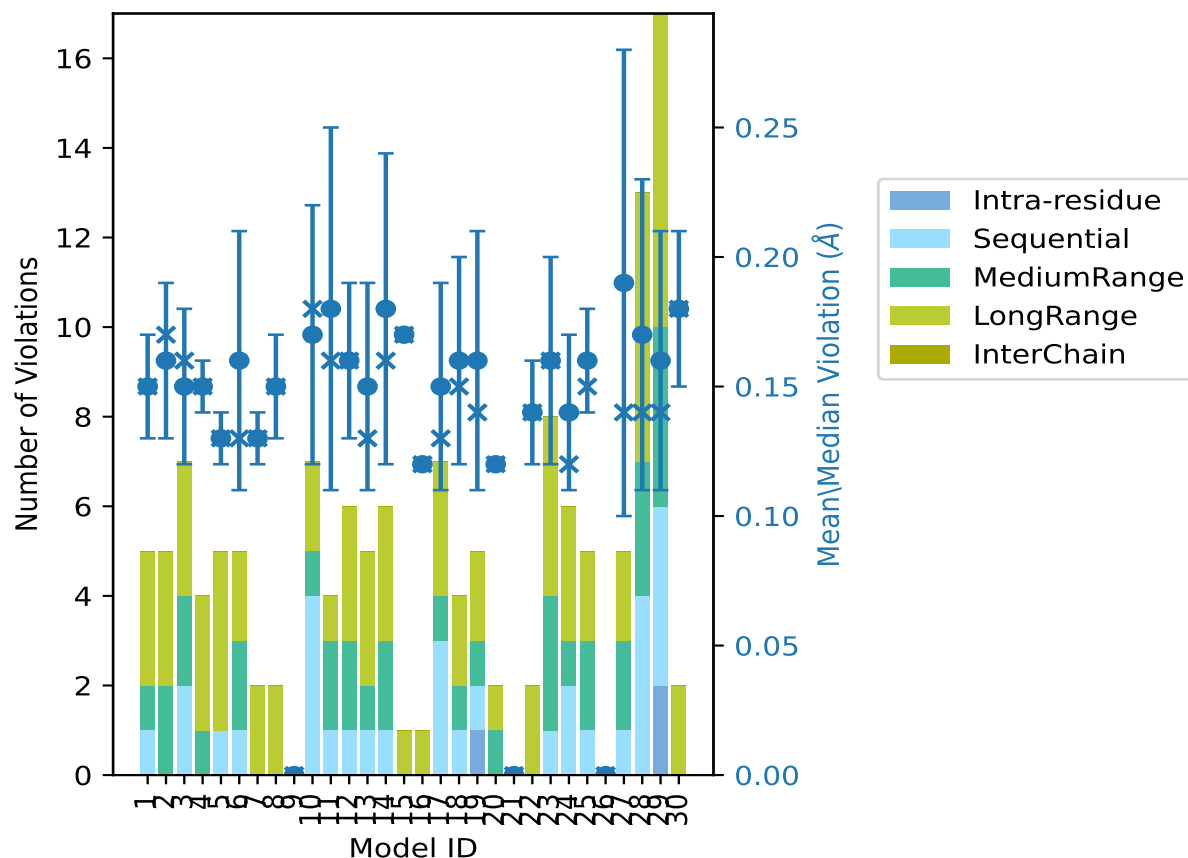
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

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, 1544(IR:410, SQ:364, MR:291, LR:479, 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]	%
3	6	4	3	0	16	1	3.3
0	0	0	6	0	6	2	6.7
0	2	0	0	0	2	3	10.0
0	1	0	0	0	1	4	13.3
0	0	0	0	0	0	5	16.7
0	0	1	0	0	1	6	20.0

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Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	1	0	0	0	1	7	23.3
0	1	0	0	0	1	8	26.7
0	0	1	0	0	1	9	30.0
0	0	0	0	0	0	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	15	50.0
0	0	1	0	0	1	16	53.3
0	0	0	2	0	2	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	1	0	1	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
0	0	0	0	0	0	30	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 ⓘ
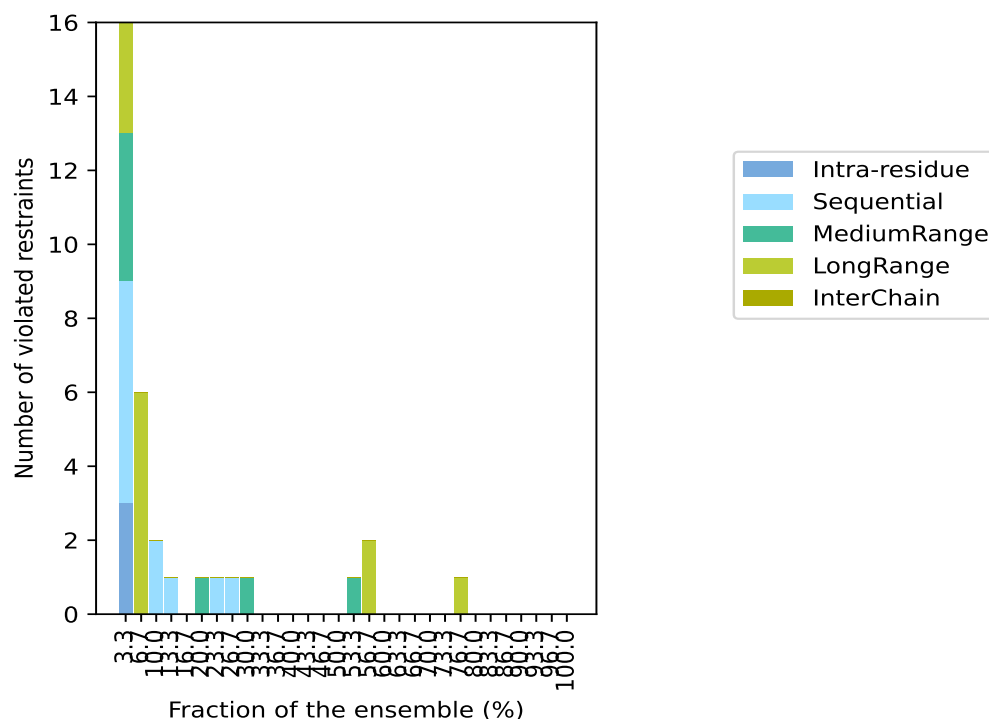
9.4 Most violated distance restraints in the ensemble ⓘ

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
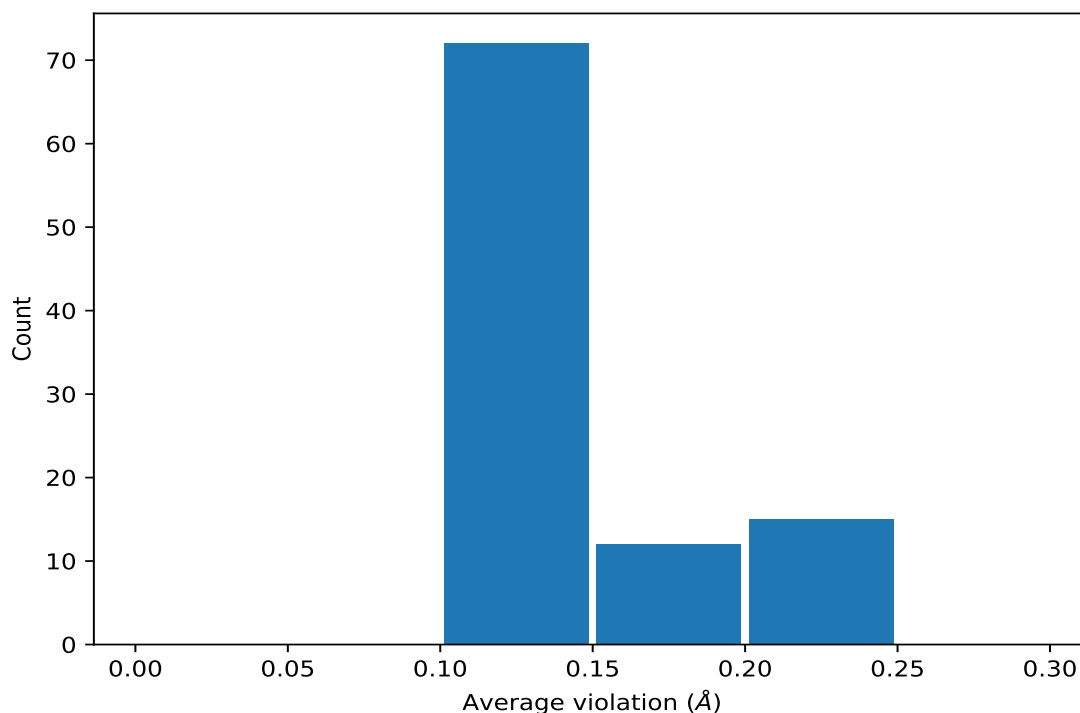
9.4.2 Table: Most violated distance restraints ⓘ

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)
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	23	0.2	0.04	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	23	0.2	0.04	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	23	0.2	0.04	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	23	0.2	0.04	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	23	0.2	0.04	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	23	0.2	0.04	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	23	0.2	0.04	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	23	0.2	0.04	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	23	0.2	0.04	0.2
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	17	0.15	0.03	0.14
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	17	0.15	0.03	0.14
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	17	0.15	0.03	0.14
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	17	0.14	0.02	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	17	0.14	0.02	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	17	0.14	0.02	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	17	0.14	0.02	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	17	0.14	0.02	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	17	0.14	0.02	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	17	0.14	0.02	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	17	0.14	0.02	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	17	0.14	0.02	0.15
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	16	0.18	0.04	0.18
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	16	0.18	0.04	0.18
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	16	0.18	0.04	0.18
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	16	0.18	0.04	0.18
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	16	0.18	0.04	0.18
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	16	0.18	0.04	0.18
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	9	0.12	0.01	0.12
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	9	0.12	0.01	0.12
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	9	0.12	0.01	0.12
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	9	0.12	0.01	0.12
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	9	0.12	0.01	0.12
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	9	0.12	0.01	0.12
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	9	0.12	0.01	0.12
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	9	0.12	0.01	0.12
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	9	0.12	0.01	0.12
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD11	8	0.14	0.03	0.13
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD12	8	0.14	0.03	0.13
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD13	8	0.14	0.03	0.13
(1,995)	1:A:228:THR:HG21	1:A:229:GLY:H	7	0.17	0.03	0.17
(1,995)	1:A:228:THR:HG22	1:A:229:GLY:H	7	0.17	0.03	0.17
(1,995)	1:A:228:THR:HG23	1:A:229:GLY:H	7	0.17	0.03	0.17
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG21	6	0.22	0.08	0.21
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG22	6	0.22	0.08	0.21
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG23	6	0.22	0.08	0.21
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG21	6	0.22	0.08	0.21
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG22	6	0.22	0.08	0.21
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG23	6	0.22	0.08	0.21
(1,735)	1:A:223:VAL:HG11	1:A:224:GLN:H	4	0.12	0.01	0.13
(1,735)	1:A:223:VAL:HG12	1:A:224:GLN:H	4	0.12	0.01	0.13
(1,735)	1:A:223:VAL:HG13	1:A:224:GLN:H	4	0.12	0.01	0.13
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG21	3	0.13	0.01	0.12
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG22	3	0.13	0.01	0.12
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG23	3	0.13	0.01	0.12
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG21	3	0.13	0.01	0.12
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG22	3	0.13	0.01	0.12
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG23	3	0.13	0.01	0.12
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG21	3	0.13	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG22	3	0.13	0.01	0.12
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG23	3	0.13	0.01	0.12
(1,135)	1:A:166:ILE:HG21	1:A:167:THR:HB	3	0.12	0.01	0.12
(1,135)	1:A:166:ILE:HG22	1:A:167:THR:HB	3	0.12	0.01	0.12
(1,135)	1:A:166:ILE:HG23	1:A:167:THR:HB	3	0.12	0.01	0.12
(1,5)	1:A:160:LEU:HD11	1:A:165:LEU:H	2	0.12	0.01	0.12
(1,5)	1:A:160:LEU:HD12	1:A:165:LEU:H	2	0.12	0.01	0.12
(1,5)	1:A:160:LEU:HD13	1:A:165:LEU:H	2	0.12	0.01	0.12
(1,444)	1:A:223:VAL:HG11	1:A:233:TRP:HB3	2	0.12	0.01	0.12
(1,444)	1:A:223:VAL:HG12	1:A:233:TRP:HB3	2	0.12	0.01	0.12
(1,444)	1:A:223:VAL:HG13	1:A:233:TRP:HB3	2	0.12	0.01	0.12
(1,688)	1:A:167:THR:HB	1:A:236:LEU:HD11	2	0.12	0.02	0.12
(1,688)	1:A:167:THR:HB	1:A:236:LEU:HD12	2	0.12	0.02	0.12
(1,688)	1:A:167:THR:HB	1:A:236:LEU:HD13	2	0.12	0.02	0.12
(1,1229)	1:A:160:LEU:HD11	1:A:168:LYS:HB2	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD11	1:A:168:LYS:HB3	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD12	1:A:168:LYS:HB2	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD12	1:A:168:LYS:HB3	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD13	1:A:168:LYS:HB2	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD13	1:A:168:LYS:HB3	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD21	1:A:168:LYS:HB2	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD21	1:A:168:LYS:HB3	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD22	1:A:168:LYS:HB2	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD22	1:A:168:LYS:HB3	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD23	1:A:168:LYS:HB2	2	0.12	0.01	0.12
(1,1229)	1:A:160:LEU:HD23	1:A:168:LYS:HB3	2	0.12	0.01	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG11	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG12	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG13	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG21	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG22	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG23	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG11	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG12	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG13	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG21	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG22	2	0.12	0.0	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG23	2	0.12	0.0	0.12
(1,334)	1:A:180:LEU:HD11	1:A:207:LYS:HA	2	0.11	0.0	0.11
(1,334)	1:A:180:LEU:HD12	1:A:207:LYS:HA	2	0.11	0.0	0.11
(1,334)	1:A:180:LEU:HD13	1:A:207:LYS:HA	2	0.11	0.0	0.11

[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.
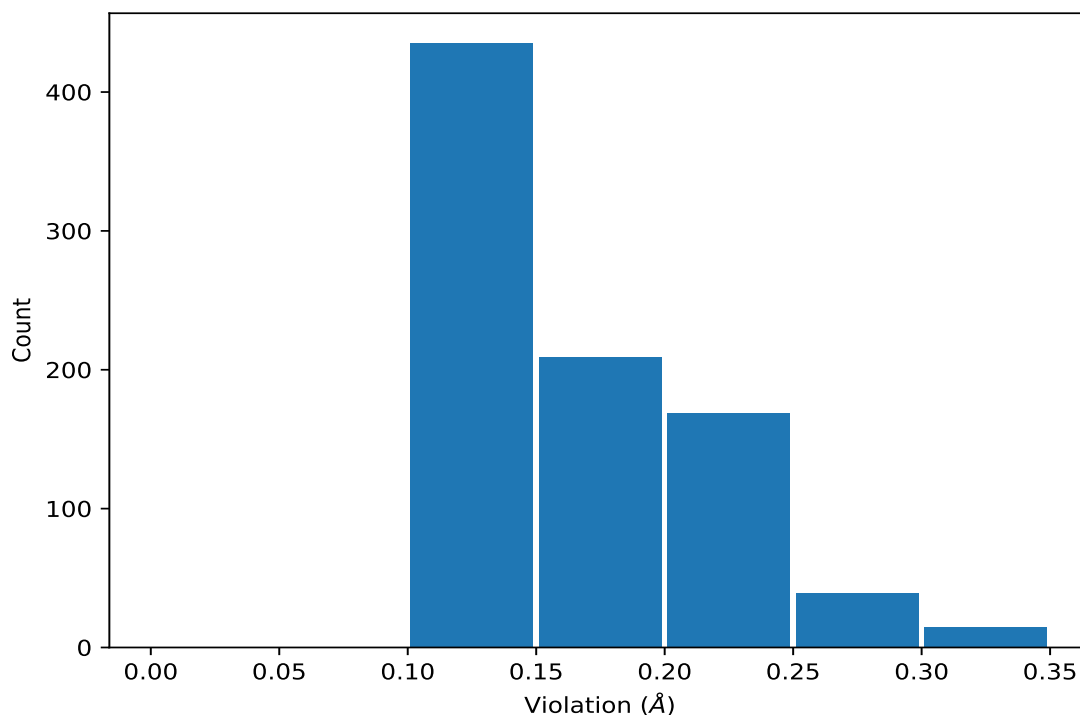
9.5.2   Table : All distance violations ⓘ

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)
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG21	27	0.35
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG22	27	0.35
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG23	27	0.35
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG21	27	0.35
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG22	27	0.35
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG23	27	0.35
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	28	0.3
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	28	0.3
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	28	0.3
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	28	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	28	0.3
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	28	0.3
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	28	0.3
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	28	0.3
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	28	0.3
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG21	11	0.29
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG22	11	0.29
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG23	11	0.29
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG21	11	0.29
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG22	11	0.29
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG23	11	0.29
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	14	0.27
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	14	0.27
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	14	0.27
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	14	0.27
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	14	0.27
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	14	0.27
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	14	0.27
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	14	0.27
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	14	0.27
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	10	0.26
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	10	0.26
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	10	0.26
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	10	0.26
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	10	0.26
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	10	0.26
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	10	0.26
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	10	0.26
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	10	0.26
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	29	0.26
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	29	0.26
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	29	0.26
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	29	0.26
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	29	0.26
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	29	0.26
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	29	0.26
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	29	0.26
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	29	0.26
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG21	28	0.26
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG22	28	0.26
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG23	28	0.26
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG21	28	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG22	28	0.26
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG23	28	0.26
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	29	0.24
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	29	0.24
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	29	0.24
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	19	0.24
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	19	0.24
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	19	0.24
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	19	0.24
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	19	0.24
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	19	0.24
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	19	0.24
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	19	0.24
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	19	0.24
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	14	0.24
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	14	0.24
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	14	0.24
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	14	0.24
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	14	0.24
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	14	0.24
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	17	0.23
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	17	0.23
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	17	0.23
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	17	0.23
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	17	0.23
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	17	0.23
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	17	0.23
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	17	0.23
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	17	0.23
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	18	0.22
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	18	0.22
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	18	0.22
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	18	0.22
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	18	0.22
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	18	0.22
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	18	0.22
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	18	0.22
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	18	0.22
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	6	0.22
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	6	0.22
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	6	0.22
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	6	0.22
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	6	0.22
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	23	0.22
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	23	0.22
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	23	0.22
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	23	0.22
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	23	0.22
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	23	0.22
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	28	0.22
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	28	0.22
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	28	0.22
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	28	0.22
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	28	0.22
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	28	0.22
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	29	0.22
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	29	0.22
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	29	0.22
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	29	0.22
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	29	0.22
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	29	0.22
(1,995)	1:A:228:THR:HG21	1:A:229:GLY:H	17	0.21
(1,995)	1:A:228:THR:HG22	1:A:229:GLY:H	17	0.21
(1,995)	1:A:228:THR:HG23	1:A:229:GLY:H	17	0.21
(1,995)	1:A:228:THR:HG21	1:A:229:GLY:H	29	0.21
(1,995)	1:A:228:THR:HG22	1:A:229:GLY:H	29	0.21
(1,995)	1:A:228:THR:HG23	1:A:229:GLY:H	29	0.21
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	10	0.21
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	10	0.21
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	10	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	3	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	3	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	3	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	3	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	3	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	3	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	3	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	3	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	3	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	6	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	6	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	6	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	6	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	6	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	6	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	6	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	6	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	13	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	13	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	13	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	13	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	13	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	13	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	13	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	13	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	13	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	23	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	23	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	23	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	23	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	23	0.21
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	23	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	23	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	23	0.21
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	23	0.21
(1,1055)	1:A:228:THR:H	1:A:228:THR:HB	29	0.21
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	2	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	2	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	2	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	2	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	2	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	2	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	2	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	2	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	2	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	12	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	12	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	12	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	12	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	12	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	12	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	12	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	12	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	24	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	24	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	24	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	24	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	24	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	24	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	24	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	24	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	24	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	25	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	25	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	25	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	25	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	25	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	25	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	25	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	25	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	25	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	27	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	27	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	27	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	27	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	27	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	27	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	27	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	27	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	27	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	30	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	30	0.2
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	30	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	30	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	30	0.2
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	30	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	30	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	30	0.2
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	30	0.2
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD11	29	0.2
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD12	29	0.2
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD13	29	0.2
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	12	0.2
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	12	0.2
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	12	0.2
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	12	0.2
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	12	0.2
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	28	0.19
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	28	0.19
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	28	0.19
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	29	0.19
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	29	0.19
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	29	0.19
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	29	0.19
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	29	0.19
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	29	0.19
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	29	0.19
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	29	0.19
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	29	0.19
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	10	0.19
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	10	0.19
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	10	0.19
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	10	0.19
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	10	0.19
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	10	0.19
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	19	0.19
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	19	0.19
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	19	0.19
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	19	0.19
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	19	0.19
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	19	0.19
(1,995)	1:A:228:THR:HG21	1:A:229:GLY:H	10	0.18
(1,995)	1:A:228:THR:HG22	1:A:229:GLY:H	10	0.18
(1,995)	1:A:228:THR:HG23	1:A:229:GLY:H	10	0.18
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	2	0.18
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	2	0.18
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	2	0.18
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	2	0.18
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	2	0.18
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	2	0.18
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	3	0.18
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	3	0.18
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	3	0.18
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	3	0.18
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	3	0.18
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	11	0.18
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	11	0.18
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	11	0.18
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	11	0.18
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	11	0.18
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	11	0.18
(1,995)	1:A:228:THR:HG21	1:A:229:GLY:H	25	0.17
(1,995)	1:A:228:THR:HG22	1:A:229:GLY:H	25	0.17
(1,995)	1:A:228:THR:HG23	1:A:229:GLY:H	25	0.17
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	15	0.17
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	15	0.17
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	15	0.17
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	15	0.17
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	15	0.17
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	15	0.17
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	15	0.17
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	15	0.17
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	15	0.17
(1,610)	1:A:206:TRP:HH2	1:A:210:ILE:HD11	23	0.17
(1,610)	1:A:206:TRP:HH2	1:A:210:ILE:HD12	23	0.17
(1,610)	1:A:206:TRP:HH2	1:A:210:ILE:HD13	23	0.17
(1,1548)	1:A:230:LYS:HB2	1:A:231:SER:H	14	0.17
(1,1548)	1:A:230:LYS:HB3	1:A:231:SER:H	14	0.17
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	1	0.17
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	1	0.17
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	1	0.17
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	1	0.17
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	1	0.17
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	1	0.17
(1,1264)	1:A:165:LEU:HD11	1:A:168:LYS:HD2	2	0.17
(1,1264)	1:A:165:LEU:HD11	1:A:168:LYS:HD3	2	0.17
(1,1264)	1:A:165:LEU:HD12	1:A:168:LYS:HD2	2	0.17
(1,1264)	1:A:165:LEU:HD12	1:A:168:LYS:HD3	2	0.17
(1,1264)	1:A:165:LEU:HD13	1:A:168:LYS:HD2	2	0.17
(1,1264)	1:A:165:LEU:HD13	1:A:168:LYS:HD3	2	0.17
(1,1264)	1:A:165:LEU:HD21	1:A:168:LYS:HD2	2	0.17
(1,1264)	1:A:165:LEU:HD21	1:A:168:LYS:HD3	2	0.17
(1,1264)	1:A:165:LEU:HD22	1:A:168:LYS:HD2	2	0.17
(1,1264)	1:A:165:LEU:HD22	1:A:168:LYS:HD3	2	0.17
(1,1264)	1:A:165:LEU:HD23	1:A:168:LYS:HD2	2	0.17
(1,1264)	1:A:165:LEU:HD23	1:A:168:LYS:HD3	2	0.17
(1,995)	1:A:228:THR:HG21	1:A:229:GLY:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:A:228:THR:HG22	1:A:229:GLY:H	18	0.16
(1,995)	1:A:228:THR:HG23	1:A:229:GLY:H	18	0.16
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	3	0.16
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	3	0.16
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	3	0.16
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	12	0.16
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	12	0.16
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	12	0.16
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	13	0.16
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	13	0.16
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	13	0.16
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	8	0.16
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	8	0.16
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	8	0.16
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	8	0.16
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	8	0.16
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	8	0.16
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	8	0.16
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	8	0.16
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	8	0.16
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD11	23	0.16
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD12	23	0.16
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD13	23	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	1	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	1	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	1	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	1	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	1	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	1	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	1	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	1	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	1	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	3	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	3	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	3	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	3	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	3	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	3	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	3	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	3	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	3	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	22	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	22	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	22	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	22	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	22	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	22	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	22	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	22	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	22	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	28	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	28	0.16
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	28	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	28	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	28	0.16
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	28	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	28	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	28	0.16
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	28	0.16
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG21	4	0.16
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG22	4	0.16
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG23	4	0.16
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG21	4	0.16
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG22	4	0.16
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG23	4	0.16
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	30	0.15
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	30	0.15
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	30	0.15
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	1	0.15
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	1	0.15
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	1	0.15
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	1	0.15
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	1	0.15
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	1	0.15
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	1	0.15
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	1	0.15
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	1	0.15
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	4	0.15
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	4	0.15
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	4	0.15
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	4	0.15
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	4	0.15
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	4	0.15
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	4	0.15
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	4	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	5	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	5	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	5	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	5	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	5	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	5	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	5	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	5	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	5	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	12	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	12	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	12	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	12	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	12	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	12	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	12	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	12	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	12	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	23	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	23	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	23	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	23	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	23	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	23	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	23	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	23	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	23	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	25	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	25	0.15
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	25	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	25	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	25	0.15
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	25	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	25	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	25	0.15
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	25	0.15
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG21	17	0.15
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG22	17	0.15
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG23	17	0.15
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG21	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG22	17	0.15
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG23	17	0.15
(1,998)	1:A:229:GLY:H	1:A:230:LYS:H	29	0.14
(1,995)	1:A:228:THR:HG21	1:A:229:GLY:H	11	0.14
(1,995)	1:A:228:THR:HG22	1:A:229:GLY:H	11	0.14
(1,995)	1:A:228:THR:HG23	1:A:229:GLY:H	11	0.14
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	14	0.14
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	14	0.14
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	14	0.14
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	19	0.14
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	19	0.14
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	19	0.14
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	27	0.14
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	27	0.14
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	27	0.14
(1,688)	1:A:167:THR:HB	1:A:236:LEU:HD11	29	0.14
(1,688)	1:A:167:THR:HB	1:A:236:LEU:HD12	29	0.14
(1,688)	1:A:167:THR:HB	1:A:236:LEU:HD13	29	0.14
(1,532)	1:A:211:ARG:HA	1:A:211:ARG:HD2	29	0.14
(1,532)	1:A:211:ARG:HA	1:A:211:ARG:HD3	29	0.14
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD11	12	0.14
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD12	12	0.14
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD13	12	0.14
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	28	0.14
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	28	0.14
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	28	0.14
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	28	0.14
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	28	0.14
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	28	0.14
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	28	0.14
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	28	0.14
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	28	0.14
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	4	0.14
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	4	0.14
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	4	0.14
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	4	0.14
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	4	0.14
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	4	0.14
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	4	0.14
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	4	0.14
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	4	0.14
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	7	0.14
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	7	0.14
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	7	0.14
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	7	0.14
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	7	0.14
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	7	0.14
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	7	0.14
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	7	0.14
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	24	0.14
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	24	0.14
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	24	0.14
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	24	0.14
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	24	0.14
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	24	0.14
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	25	0.14
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	25	0.14
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	25	0.14
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	25	0.14
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	25	0.14
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	25	0.14
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG21	28	0.14
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG22	28	0.14
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG23	28	0.14
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG21	28	0.14
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG22	28	0.14
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG23	28	0.14
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG21	28	0.14
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG22	28	0.14
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG23	28	0.14
(1,988)	1:A:227:GLY:H	1:A:228:THR:H	28	0.13
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	1	0.13
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	1	0.13
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	1	0.13
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	2	0.13
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	2	0.13
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	2	0.13
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	4	0.13
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	4	0.13
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	4	0.13
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	5	0.13
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	5	0.13
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	6	0.13
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	6	0.13
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	6	0.13
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	17	0.13
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	17	0.13
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	17	0.13
(1,89)	1:A:166:ILE:HG21	1:A:210:ILE:HB	23	0.13
(1,89)	1:A:166:ILE:HG22	1:A:210:ILE:HB	23	0.13
(1,89)	1:A:166:ILE:HG23	1:A:210:ILE:HB	23	0.13
(1,735)	1:A:223:VAL:HG11	1:A:224:GLN:H	13	0.13
(1,735)	1:A:223:VAL:HG12	1:A:224:GLN:H	13	0.13
(1,735)	1:A:223:VAL:HG13	1:A:224:GLN:H	13	0.13
(1,735)	1:A:223:VAL:HG11	1:A:224:GLN:H	17	0.13
(1,735)	1:A:223:VAL:HG12	1:A:224:GLN:H	17	0.13
(1,735)	1:A:223:VAL:HG13	1:A:224:GLN:H	17	0.13
(1,735)	1:A:223:VAL:HG11	1:A:224:GLN:H	27	0.13
(1,735)	1:A:223:VAL:HG12	1:A:224:GLN:H	27	0.13
(1,735)	1:A:223:VAL:HG13	1:A:224:GLN:H	27	0.13
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	5	0.13
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	5	0.13
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	5	0.13
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	5	0.13
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	5	0.13
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	5	0.13
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	5	0.13
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	5	0.13
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	5	0.13
(1,5)	1:A:160:LEU:HD11	1:A:165:LEU:H	28	0.13
(1,5)	1:A:160:LEU:HD12	1:A:165:LEU:H	28	0.13
(1,5)	1:A:160:LEU:HD13	1:A:165:LEU:H	28	0.13
(1,444)	1:A:223:VAL:HG11	1:A:233:TRP:HB3	29	0.13
(1,444)	1:A:223:VAL:HG12	1:A:233:TRP:HB3	29	0.13
(1,444)	1:A:223:VAL:HG13	1:A:233:TRP:HB3	29	0.13
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD11	10	0.13
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD12	10	0.13
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD13	10	0.13
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD11	28	0.13
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD12	28	0.13
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD13	28	0.13
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	3	0.13
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	3	0.13
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	3	0.13
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	3	0.13
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	3	0.13
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	3	0.13
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	3	0.13
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	3	0.13
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	29	0.13
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	29	0.13
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	29	0.13
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	29	0.13
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	29	0.13
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	29	0.13
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	29	0.13
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	29	0.13
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	29	0.13
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	18	0.13
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	18	0.13
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	18	0.13
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	18	0.13
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	18	0.13
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	18	0.13
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG21	25	0.13
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG22	25	0.13
(1,1490)	1:A:219:LYS:HE2	1:A:221:ILE:HG23	25	0.13
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG21	25	0.13
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG22	25	0.13
(1,1490)	1:A:219:LYS:HE3	1:A:221:ILE:HG23	25	0.13
(1,1483)	1:A:215:SER:HB2	1:A:216:LEU:HD11	24	0.13
(1,1483)	1:A:215:SER:HB2	1:A:216:LEU:HD12	24	0.13
(1,1483)	1:A:215:SER:HB2	1:A:216:LEU:HD13	24	0.13
(1,1483)	1:A:215:SER:HB2	1:A:216:LEU:HD21	24	0.13
(1,1483)	1:A:215:SER:HB2	1:A:216:LEU:HD22	24	0.13
(1,1483)	1:A:215:SER:HB2	1:A:216:LEU:HD23	24	0.13
(1,1483)	1:A:215:SER:HB3	1:A:216:LEU:HD11	24	0.13
(1,1483)	1:A:215:SER:HB3	1:A:216:LEU:HD12	24	0.13
(1,1483)	1:A:215:SER:HB3	1:A:216:LEU:HD13	24	0.13
(1,1483)	1:A:215:SER:HB3	1:A:216:LEU:HD21	24	0.13
(1,1483)	1:A:215:SER:HB3	1:A:216:LEU:HD22	24	0.13
(1,1483)	1:A:215:SER:HB3	1:A:216:LEU:HD23	24	0.13
(1,135)	1:A:166:ILE:HG21	1:A:167:THR:HB	29	0.13
(1,135)	1:A:166:ILE:HG22	1:A:167:THR:HB	29	0.13
(1,135)	1:A:166:ILE:HG23	1:A:167:THR:HB	29	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1283)	1:A:166:ILE:HD11	1:A:213:ASN:HD21	23	0.13
(1,1283)	1:A:166:ILE:HD11	1:A:213:ASN:HD22	23	0.13
(1,1283)	1:A:166:ILE:HD12	1:A:213:ASN:HD21	23	0.13
(1,1283)	1:A:166:ILE:HD12	1:A:213:ASN:HD22	23	0.13
(1,1283)	1:A:166:ILE:HD13	1:A:213:ASN:HD21	23	0.13
(1,1283)	1:A:166:ILE:HD13	1:A:213:ASN:HD22	23	0.13
(1,1229)	1:A:160:LEU:HD11	1:A:168:LYS:HB2	8	0.13
(1,1229)	1:A:160:LEU:HD11	1:A:168:LYS:HB3	8	0.13
(1,1229)	1:A:160:LEU:HD12	1:A:168:LYS:HB2	8	0.13
(1,1229)	1:A:160:LEU:HD12	1:A:168:LYS:HB3	8	0.13
(1,1229)	1:A:160:LEU:HD13	1:A:168:LYS:HB2	8	0.13
(1,1229)	1:A:160:LEU:HD13	1:A:168:LYS:HB3	8	0.13
(1,1229)	1:A:160:LEU:HD21	1:A:168:LYS:HB2	8	0.13
(1,1229)	1:A:160:LEU:HD21	1:A:168:LYS:HB3	8	0.13
(1,1229)	1:A:160:LEU:HD22	1:A:168:LYS:HB2	8	0.13
(1,1229)	1:A:160:LEU:HD22	1:A:168:LYS:HB3	8	0.13
(1,1229)	1:A:160:LEU:HD23	1:A:168:LYS:HB2	8	0.13
(1,1229)	1:A:160:LEU:HD23	1:A:168:LYS:HB3	8	0.13
(1,995)	1:A:228:THR:HG21	1:A:229:GLY:H	1	0.12
(1,995)	1:A:228:THR:HG22	1:A:229:GLY:H	1	0.12
(1,995)	1:A:228:THR:HG23	1:A:229:GLY:H	1	0.12
(1,509)	1:A:201:ASN:HB2	1:A:204:ALA:HB1	29	0.12
(1,509)	1:A:201:ASN:HB2	1:A:204:ALA:HB2	29	0.12
(1,509)	1:A:201:ASN:HB2	1:A:204:ALA:HB3	29	0.12
(1,509)	1:A:201:ASN:HB3	1:A:204:ALA:HB1	29	0.12
(1,509)	1:A:201:ASN:HB3	1:A:204:ALA:HB2	29	0.12
(1,509)	1:A:201:ASN:HB3	1:A:204:ALA:HB3	29	0.12
(1,5)	1:A:160:LEU:HD11	1:A:165:LEU:H	29	0.12
(1,5)	1:A:160:LEU:HD12	1:A:165:LEU:H	29	0.12
(1,5)	1:A:160:LEU:HD13	1:A:165:LEU:H	29	0.12
(1,444)	1:A:223:VAL:HG11	1:A:233:TRP:HB3	28	0.12
(1,444)	1:A:223:VAL:HG12	1:A:233:TRP:HB3	28	0.12
(1,444)	1:A:223:VAL:HG13	1:A:233:TRP:HB3	28	0.12
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD11	19	0.12
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD12	19	0.12
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD13	19	0.12
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	12	0.12
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	12	0.12
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	12	0.12
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	12	0.12
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	12	0.12
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	12	0.12
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	12	0.12
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	12	0.12
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	27	0.12
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	27	0.12
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	27	0.12
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	27	0.12
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	27	0.12
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	27	0.12
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	27	0.12
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	27	0.12
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	27	0.12
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	13	0.12
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	13	0.12
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	13	0.12
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	13	0.12
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	13	0.12
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	13	0.12
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	13	0.12
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	13	0.12
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	13	0.12
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	14	0.12
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	14	0.12
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	14	0.12
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	14	0.12
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	14	0.12
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	14	0.12
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	14	0.12
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	14	0.12
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	14	0.12
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	16	0.12
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	16	0.12
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	16	0.12
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	16	0.12
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	16	0.12
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	16	0.12
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	16	0.12
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	16	0.12
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	16	0.12
(1,1534)	1:A:225:ASN:H	1:A:225:ASN:HD21	19	0.12
(1,1534)	1:A:225:ASN:H	1:A:225:ASN:HD22	19	0.12
(1,1518)	1:A:223:VAL:HG11	1:A:225:ASN:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:A:223:VAL:HG12	1:A:225:ASN:H	20	0.12
(1,1518)	1:A:223:VAL:HG13	1:A:225:ASN:H	20	0.12
(1,1518)	1:A:223:VAL:HG21	1:A:225:ASN:H	20	0.12
(1,1518)	1:A:223:VAL:HG22	1:A:225:ASN:H	20	0.12
(1,1518)	1:A:223:VAL:HG23	1:A:225:ASN:H	20	0.12
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG21	3	0.12
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG22	3	0.12
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG23	3	0.12
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG21	3	0.12
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG22	3	0.12
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG23	3	0.12
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG21	3	0.12
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG22	3	0.12
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG23	3	0.12
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG21	10	0.12
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG22	10	0.12
(1,148)	1:A:166:ILE:HG21	1:A:167:THR:HG23	10	0.12
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG21	10	0.12
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG22	10	0.12
(1,148)	1:A:166:ILE:HG22	1:A:167:THR:HG23	10	0.12
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG21	10	0.12
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG22	10	0.12
(1,148)	1:A:166:ILE:HG23	1:A:167:THR:HG23	10	0.12
(1,135)	1:A:166:ILE:HG21	1:A:167:THR:HB	28	0.12
(1,135)	1:A:166:ILE:HG22	1:A:167:THR:HB	28	0.12
(1,135)	1:A:166:ILE:HG23	1:A:167:THR:HB	28	0.12
(1,1346)	1:A:180:LEU:HD11	1:A:211:ARG:HD2	7	0.12
(1,1346)	1:A:180:LEU:HD11	1:A:211:ARG:HD3	7	0.12
(1,1346)	1:A:180:LEU:HD12	1:A:211:ARG:HD2	7	0.12
(1,1346)	1:A:180:LEU:HD12	1:A:211:ARG:HD3	7	0.12
(1,1346)	1:A:180:LEU:HD13	1:A:211:ARG:HD2	7	0.12
(1,1346)	1:A:180:LEU:HD13	1:A:211:ARG:HD3	7	0.12
(1,1346)	1:A:180:LEU:HD21	1:A:211:ARG:HD2	7	0.12
(1,1346)	1:A:180:LEU:HD21	1:A:211:ARG:HD3	7	0.12
(1,1346)	1:A:180:LEU:HD22	1:A:211:ARG:HD2	7	0.12
(1,1346)	1:A:180:LEU:HD22	1:A:211:ARG:HD3	7	0.12
(1,1346)	1:A:180:LEU:HD23	1:A:211:ARG:HD2	7	0.12
(1,1346)	1:A:180:LEU:HD23	1:A:211:ARG:HD3	7	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG11	5	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG12	5	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG13	5	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG21	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG22	5	0.12
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG23	5	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG11	5	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG12	5	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG13	5	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG21	5	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG22	5	0.12
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG23	5	0.12
(1,1229)	1:A:160:LEU:HD11	1:A:168:LYS:HB2	24	0.12
(1,1229)	1:A:160:LEU:HD11	1:A:168:LYS:HB3	24	0.12
(1,1229)	1:A:160:LEU:HD12	1:A:168:LYS:HB2	24	0.12
(1,1229)	1:A:160:LEU:HD12	1:A:168:LYS:HB3	24	0.12
(1,1229)	1:A:160:LEU:HD13	1:A:168:LYS:HB2	24	0.12
(1,1229)	1:A:160:LEU:HD13	1:A:168:LYS:HB3	24	0.12
(1,1229)	1:A:160:LEU:HD21	1:A:168:LYS:HB2	24	0.12
(1,1229)	1:A:160:LEU:HD21	1:A:168:LYS:HB3	24	0.12
(1,1229)	1:A:160:LEU:HD22	1:A:168:LYS:HB2	24	0.12
(1,1229)	1:A:160:LEU:HD22	1:A:168:LYS:HB3	24	0.12
(1,1229)	1:A:160:LEU:HD23	1:A:168:LYS:HB2	24	0.12
(1,1229)	1:A:160:LEU:HD23	1:A:168:LYS:HB3	24	0.12
(1,735)	1:A:223:VAL:HG11	1:A:224:GLN:H	5	0.11
(1,735)	1:A:223:VAL:HG12	1:A:224:GLN:H	5	0.11
(1,735)	1:A:223:VAL:HG13	1:A:224:GLN:H	5	0.11
(1,708)	1:A:171:GLU:HG2	1:A:236:LEU:HD21	29	0.11
(1,708)	1:A:171:GLU:HG2	1:A:236:LEU:HD22	29	0.11
(1,708)	1:A:171:GLU:HG2	1:A:236:LEU:HD23	29	0.11
(1,688)	1:A:167:THR:HB	1:A:236:LEU:HD11	28	0.11
(1,688)	1:A:167:THR:HB	1:A:236:LEU:HD12	28	0.11
(1,688)	1:A:167:THR:HB	1:A:236:LEU:HD13	28	0.11
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE1	22	0.11
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE2	22	0.11
(1,653)	1:A:221:ILE:HG21	1:A:235:MET:HE3	22	0.11
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE1	22	0.11
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE2	22	0.11
(1,653)	1:A:221:ILE:HG22	1:A:235:MET:HE3	22	0.11
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE1	22	0.11
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE2	22	0.11
(1,653)	1:A:221:ILE:HG23	1:A:235:MET:HE3	22	0.11
(1,615)	1:A:210:ILE:HG21	1:A:211:ARG:HD2	3	0.11
(1,615)	1:A:210:ILE:HG21	1:A:211:ARG:HD3	3	0.11
(1,615)	1:A:210:ILE:HG22	1:A:211:ARG:HD2	3	0.11
(1,615)	1:A:210:ILE:HG22	1:A:211:ARG:HD3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:A:210:ILE:HG23	1:A:211:ARG:HD2	3	0.11
(1,615)	1:A:210:ILE:HG23	1:A:211:ARG:HD3	3	0.11
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD11	6	0.11
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD12	6	0.11
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD13	6	0.11
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD11	24	0.11
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD12	24	0.11
(1,401)	1:A:182:GLN:HB3	1:A:183:ILE:HD13	24	0.11
(1,334)	1:A:180:LEU:HD11	1:A:207:LYS:HA	11	0.11
(1,334)	1:A:180:LEU:HD12	1:A:207:LYS:HA	11	0.11
(1,334)	1:A:180:LEU:HD13	1:A:207:LYS:HA	11	0.11
(1,334)	1:A:180:LEU:HD11	1:A:207:LYS:HA	18	0.11
(1,334)	1:A:180:LEU:HD12	1:A:207:LYS:HA	18	0.11
(1,334)	1:A:180:LEU:HD13	1:A:207:LYS:HA	18	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	6	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	6	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	6	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	6	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	6	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	6	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	6	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	6	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	6	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	13	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	13	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	13	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	13	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	13	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	13	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	13	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	13	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	13	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	14	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	14	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	14	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	14	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	14	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	14	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	14	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	14	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	14	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG21	23	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG22	23	0.11
(1,249)	1:A:167:THR:HG21	1:A:170:ILE:HG23	23	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG21	23	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG22	23	0.11
(1,249)	1:A:167:THR:HG22	1:A:170:ILE:HG23	23	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG21	23	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG22	23	0.11
(1,249)	1:A:167:THR:HG23	1:A:170:ILE:HG23	23	0.11
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	17	0.11
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	17	0.11
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	17	0.11
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	17	0.11
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	17	0.11
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	17	0.11
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	17	0.11
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	17	0.11
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	17	0.11
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	20	0.11
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	20	0.11
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	20	0.11
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	20	0.11
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	20	0.11
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	20	0.11
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	20	0.11
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	20	0.11
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	20	0.11
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD21	24	0.11
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD22	24	0.11
(1,200)	1:A:169:ALA:HB1	1:A:236:LEU:HD23	24	0.11
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD21	24	0.11
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD22	24	0.11
(1,200)	1:A:169:ALA:HB2	1:A:236:LEU:HD23	24	0.11
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD21	24	0.11
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD22	24	0.11
(1,200)	1:A:169:ALA:HB3	1:A:236:LEU:HD23	24	0.11
(1,135)	1:A:166:ILE:HG21	1:A:167:THR:HB	10	0.11
(1,135)	1:A:166:ILE:HG22	1:A:167:THR:HB	10	0.11
(1,135)	1:A:166:ILE:HG23	1:A:167:THR:HB	10	0.11
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG11	2	0.11
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG12	2	0.11
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG13	2	0.11
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG21	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG22	2	0.11
(1,1292)	1:A:168:LYS:HD2	1:A:191:VAL:HG23	2	0.11
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG11	2	0.11
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG12	2	0.11
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG13	2	0.11
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG21	2	0.11
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG22	2	0.11
(1,1292)	1:A:168:LYS:HD3	1:A:191:VAL:HG23	2	0.11
(1,1206)	1:A:155:SER:HB2	1:A:156:ALA:HB1	17	0.11
(1,1206)	1:A:155:SER:HB2	1:A:156:ALA:HB2	17	0.11
(1,1206)	1:A:155:SER:HB2	1:A:156:ALA:HB3	17	0.11
(1,1206)	1:A:155:SER:HB3	1:A:156:ALA:HB1	17	0.11
(1,1206)	1:A:155:SER:HB3	1:A:156:ALA:HB2	17	0.11
(1,1206)	1:A:155:SER:HB3	1:A:156:ALA:HB3	17	0.11
(1,1168)	1:A:169:ALA:HB1	1:A:173:SER:H	29	0.11
(1,1168)	1:A:169:ALA:HB2	1:A:173:SER:H	29	0.11
(1,1168)	1:A:169:ALA:HB3	1:A:173:SER:H	29	0.11

10 Dihedral-angle violation analysis ⓘ

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