W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 08:32 pm BST

PDB ID	:	6ZV0
BMRB ID	:	34537
Title	:	TFIIS N-terminal domain (TND) from human LEDGF/p75
Authors	:	Veverka, V.
Deposited on	:	2020-07-23

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

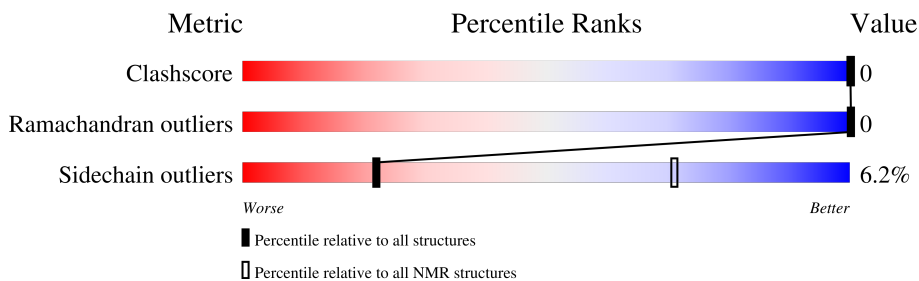|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance ⓘ

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

The overall completeness of chemical shifts assignment is 92%.

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
Sidechain outliers		6.2%

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	92	86% • 12%

2 Ensemble composition and analysis ⓘ

This entry contains 50 models. Model 39 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:348-A:428 (81)	0.33	39

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 8 clusters and 2 single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 1511 atoms, of which 771 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	92	1511	459	771	132	142	7	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	SER	-	expression tag	UNP O75475
A	341	ASN	-	expression tag	UNP O75475
A	342	ALA	-	expression tag	UNP O75475
A	343	ALA	-	expression tag	UNP O75475
A	344	SER	-	expression tag	UNP O75475

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

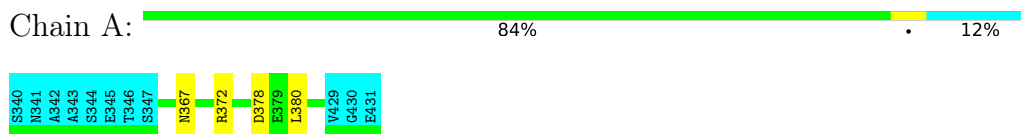• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
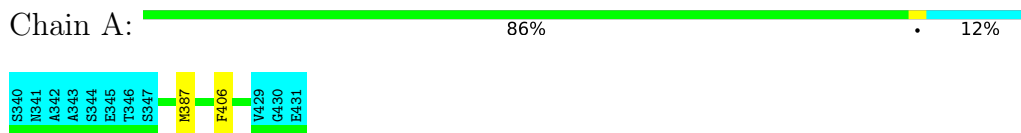
4.2 Scores per residue for each member of the ensemble
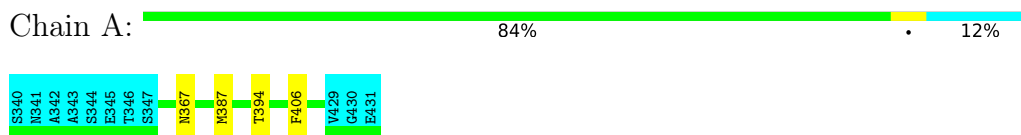
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.3　Score per residue for model 3

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.4　Score per residue for model 4

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.5　Score per residue for model 5

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.6　Score per residue for model 6

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.7　Score per residue for model 7

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: PC4 and SFRS1-interacting protein
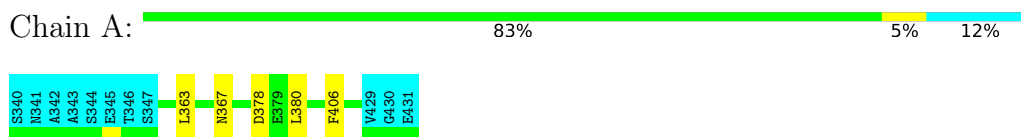
Chain A:

4.2.9 Score per residue for model 9

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.11 Score per residue for model 11

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.12 Score per residue for model 12
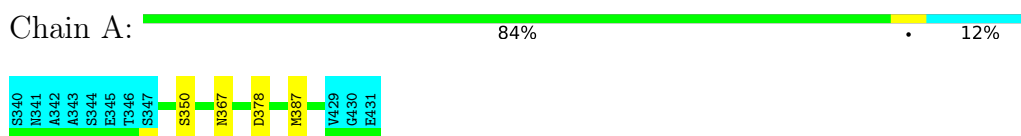
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.13 Score per residue for model 13

• Molecule 1: PC4 and SFRS1-interacting protein
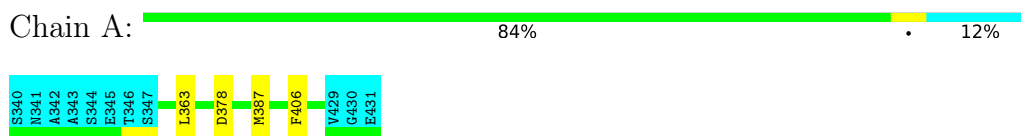
Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.17 Score per residue for model 17

• Molecule 1: PC4 and SFRS1-interacting protein
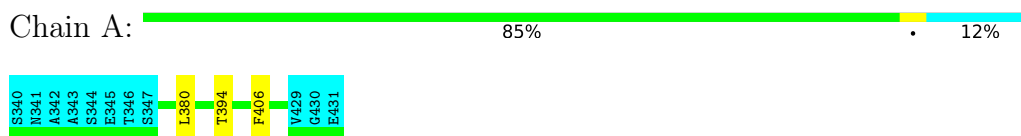
Chain A:

4.2.18 Score per residue for model 18

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.19 Score per residue for model 19

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.20 Score per residue for model 20
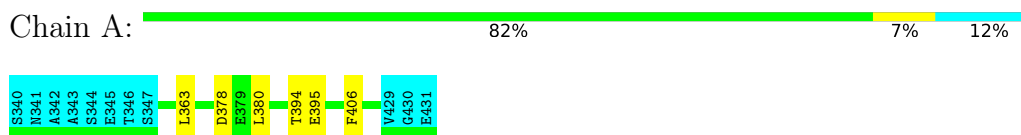
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.21 Score per residue for model 21

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.22 Score per residue for model 22
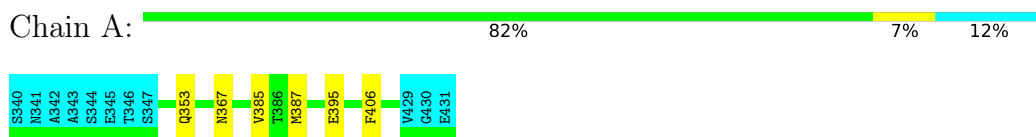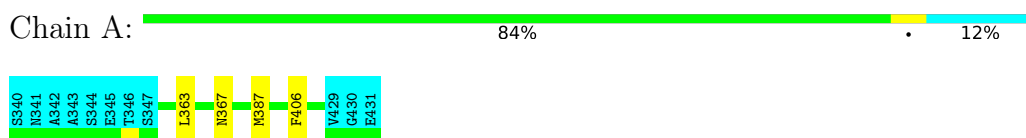
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

4.2.23　Score per residue for model 23

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:　　　　　　　　　　　　　　84%　　　　　　　　　　　　　•　　12%

S340 N341 A342 A343 S344 E345 T346 S347 R354 M387 F406 N425 V429 G430 E431

4.2.24　Score per residue for model 24

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:　　　　　　　　　　　　　　82%　　　　　　　　　　　　7%　　12%

S340 N341 A342 A343 S344 E345 T346 S347 R351 D378 E379 M387 T394 F406 V429 G430 E431
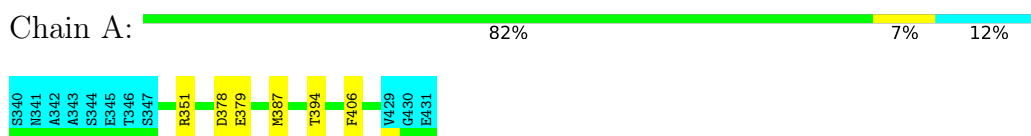
4.2.25　Score per residue for model 25

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:　　　　　　　　　　　　　　83%　　　　　　　　　　　　5%　　12%

S340 N341 A342 A343 S344 E345 T346 S347 N367 M387 Q388 Q389 T394 F406 V429 G430 E431
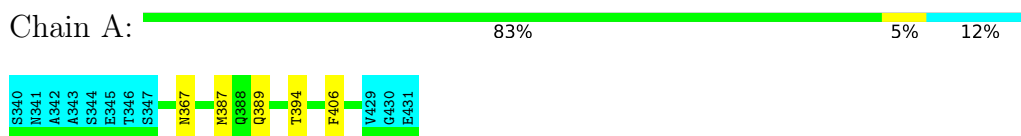
4.2.26　Score per residue for model 26

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:　　　　　　　　　　　　　　78%　　　　　　　　　　10%　　12%

S340 N341 A342 A343 S344 E345 T346 S347 M348 D349 N367 D378 E379 L380 V385 T386 M387 Q388 Q389 T394 F406 V429 G430 E431
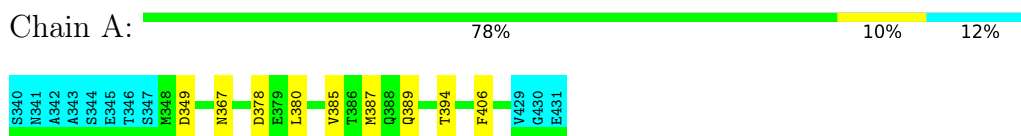
4.2.27　Score per residue for model 27

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:　　　　　　　　　　　　　　84%　　　　　　　　　　　　•　　12%

S340 N341 A342 A343 S344 E345 T346 S347 N367 L380 E395 F406 V429 G430 E431
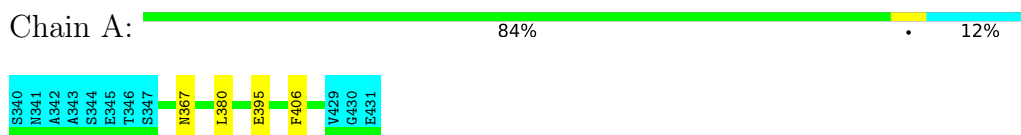
4.2.28 Score per residue for model 28

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
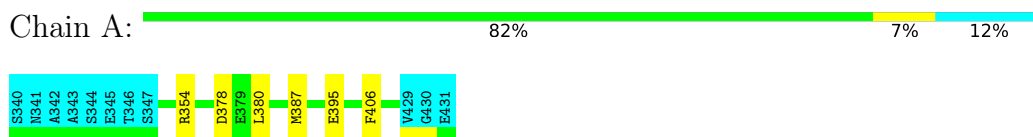
4.2.29 Score per residue for model 29
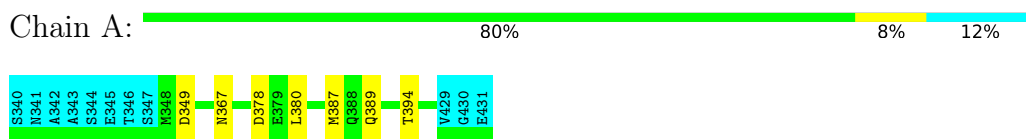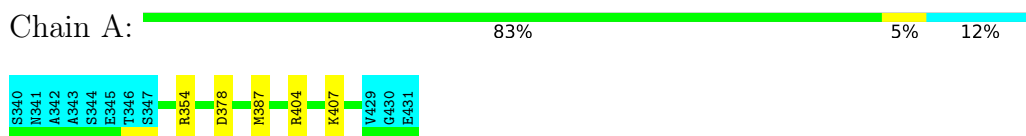
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
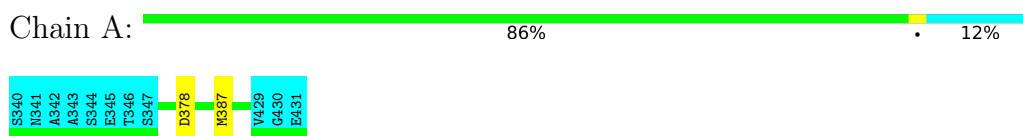
4.2.30 Score per residue for model 30

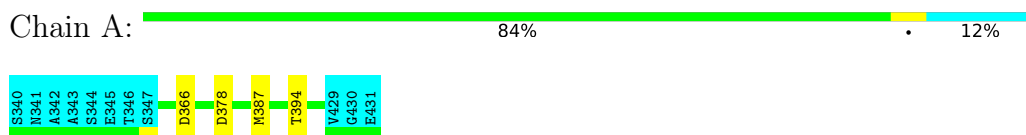• Molecule 1: PC4 and SFRS1-interacting protein
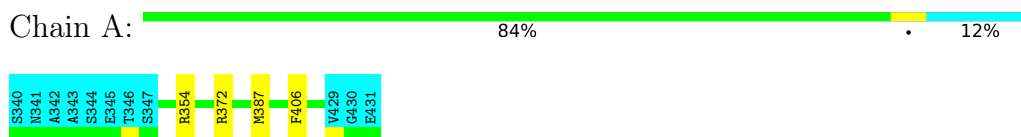
Chain A:
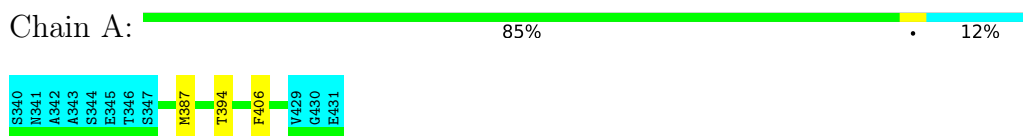
4.2.31 Score per residue for model 31

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
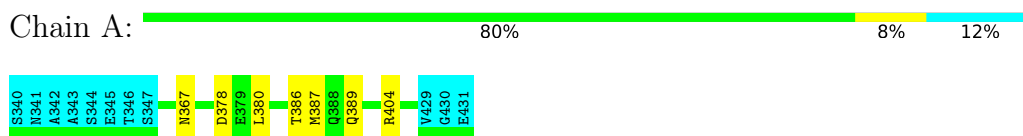
4.2.32 Score per residue for model 32

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
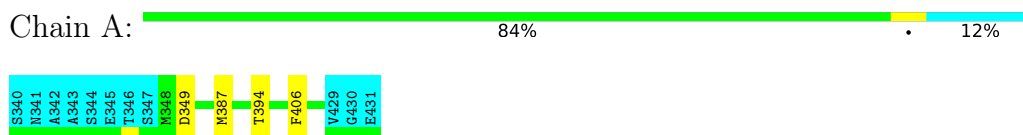
4.2.33 Score per residue for model 33

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
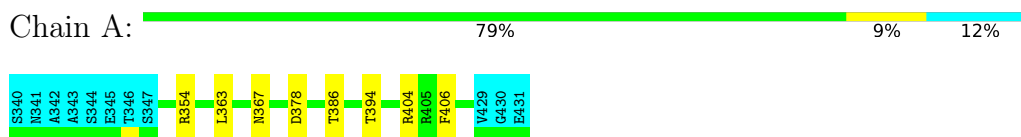
4.2.34 Score per residue for model 34

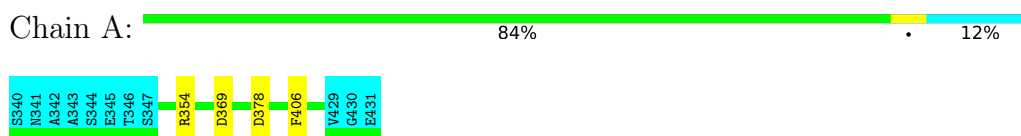• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
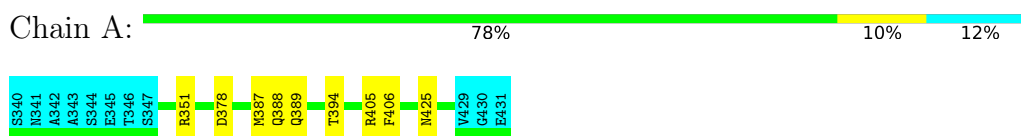
4.2.35 Score per residue for model 35

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
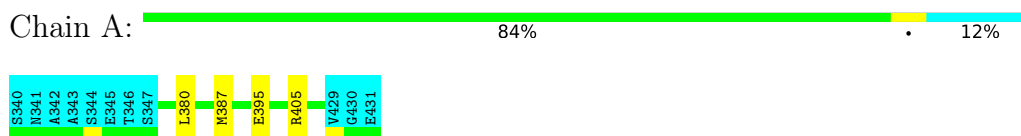
4.2.36 Score per residue for model 36

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
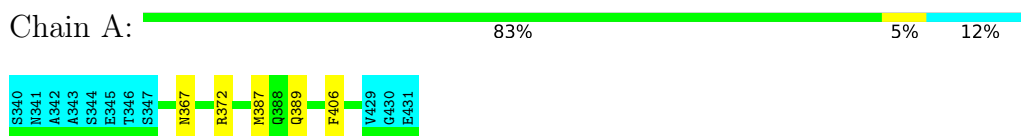
4.2.37 Score per residue for model 37

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
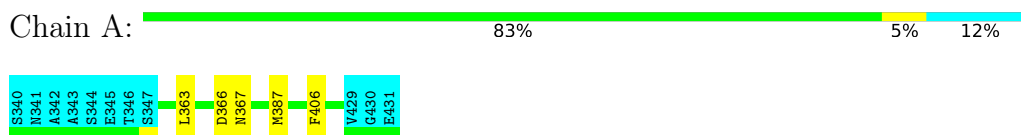
4.2.38　Score per residue for model 38
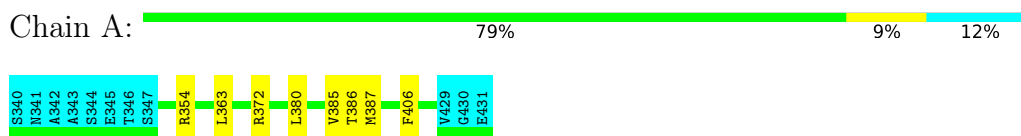
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
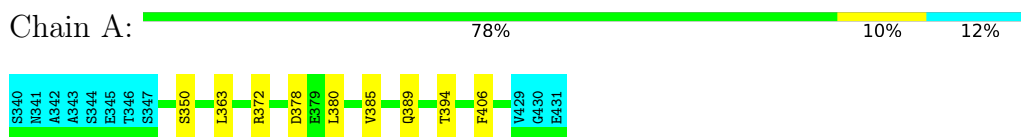
4.2.39　Score per residue for model 39 (medoid)

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
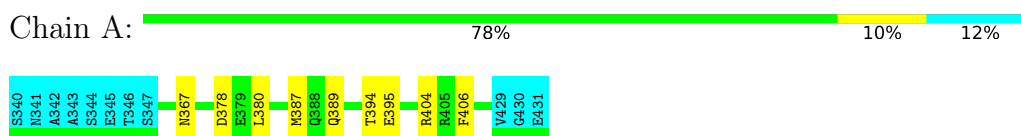
4.2.40　Score per residue for model 40
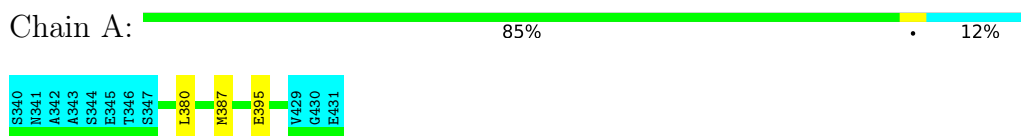
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
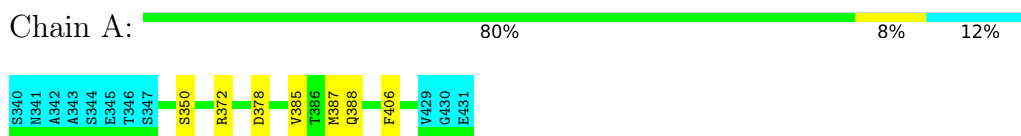
4.2.41　Score per residue for model 41

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
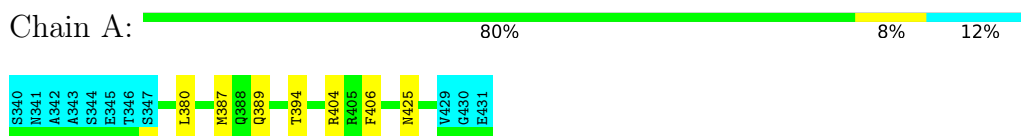
4.2.42　Score per residue for model 42

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
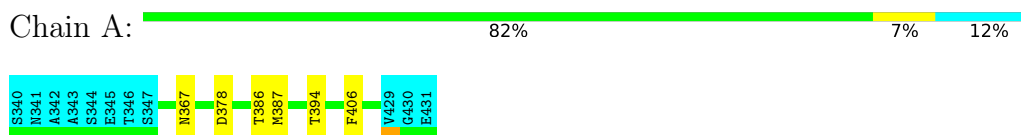
4.2.43 Score per residue for model 43
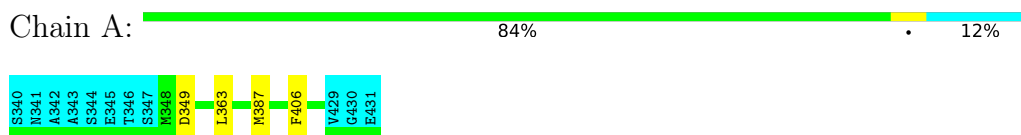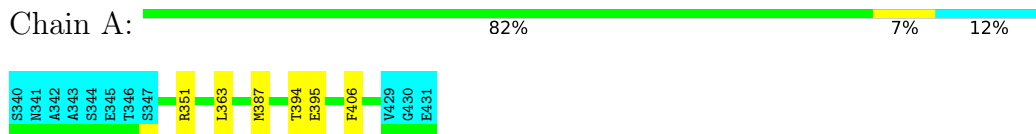
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 82% 7% 12%
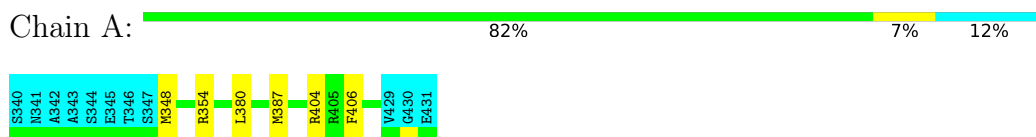
4.2.44 Score per residue for model 44

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 83% 5% 12%
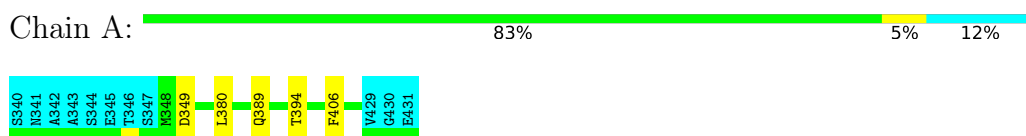
4.2.45 Score per residue for model 45

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 82% 7% 12%
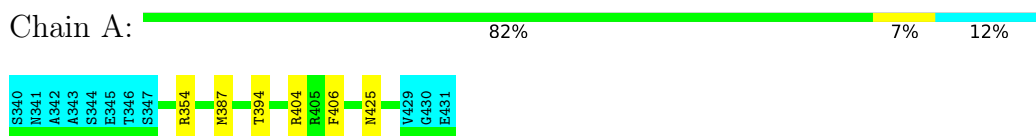
4.2.46 Score per residue for model 46

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 83% 5% 12%
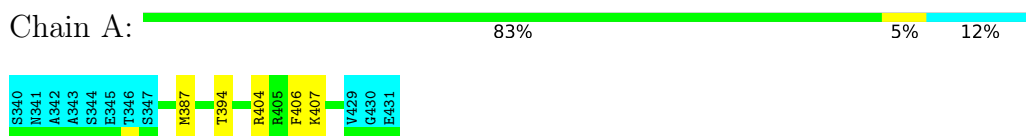
4.2.47 Score per residue for model 47

• Molecule 1: PC4 and SFRS1-interacting protein

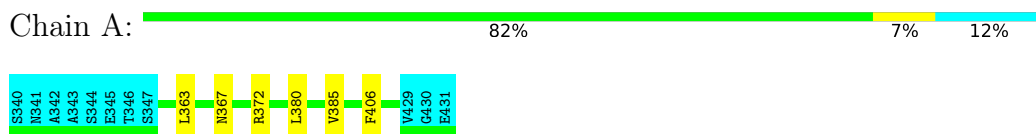Chain A: 83% 5% 12%
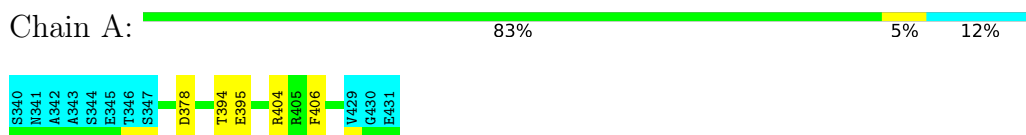
4.2.48 Score per residue for model 48

• Molecule 1: PC4 and SFRS1-interacting protein
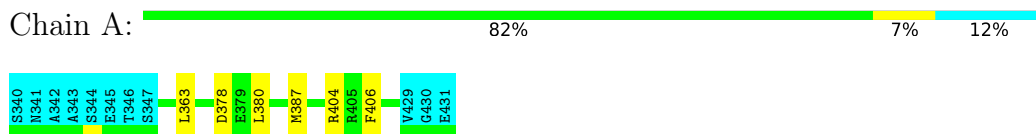
Chain A:
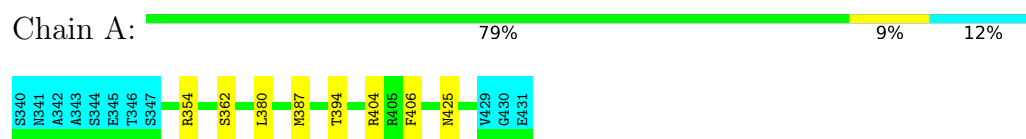
4.2.49 Score per residue for model 49
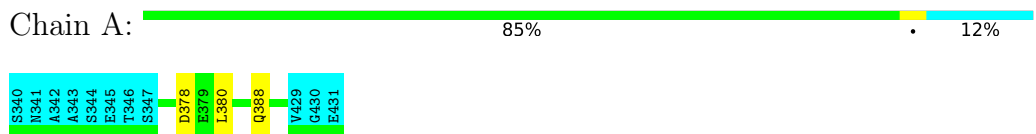
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
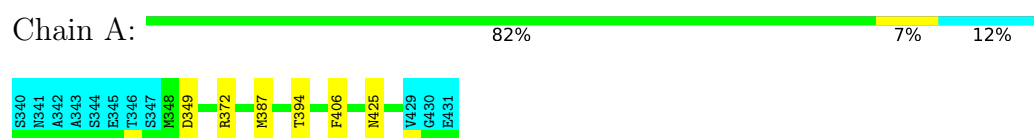
4.2.50 Score per residue for model 50
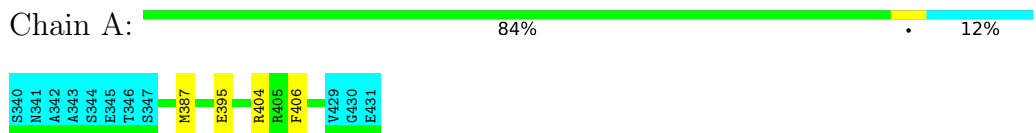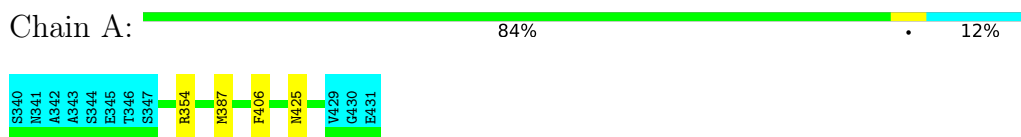
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
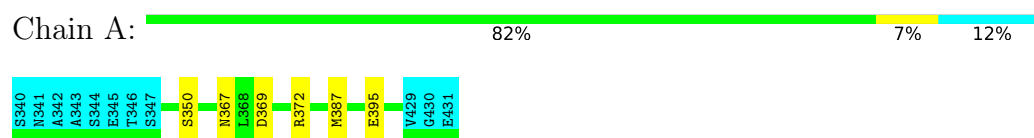
5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 50 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	1189
Number of shifts mapped to atoms	1189
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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	0.59±0.01	0±0/673 (0.0± 0.0%)	0.69±0.02	1±1/898 (0.1± 0.1%)
All	All	0.59	0/33650 (0.0%)	0.69	33/44900 (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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	351	ARG	NE-CZ-NH1	6.22	123.41	120.30	18	3
1	A	404	ARG	NE-CZ-NH1	6.19	123.39	120.30	48	12
1	A	372	ARG	NE-CZ-NH1	6.18	123.39	120.30	1	9
1	A	354	ARG	NE-CZ-NH1	5.73	123.16	120.30	48	9

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	33350	35350	35350	-

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is -.

There are no clashes.

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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	81/92 (88%)	79±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
All	All	4050/4600 (88%)	3964 (98%)	86 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	77/85 (91%)	72±2 (94±2%)	5±2 (6±2%)	22	71
All	All	3850/4250 (91%)	3613 (94%)	237 (6%)	22	71

All 24 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	406	PHE	39
1	A	387	MET	38
1	A	378	ASP	23
1	A	394	THR	23
1	A	380	LEU	21
1	A	367	ASN	18
1	A	363	LEU	12
1	A	395	GLU	11
1	A	389	GLN	10
1	A	385	VAL	6
1	A	349	ASP	6
1	A	425	ASN	6
1	A	350	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	386	THR	4
1	A	388	GLN	3
1	A	407	LYS	2
1	A	366	ASP	2
1	A	369	ASP	2
1	A	405	ARG	2
1	A	353	GLN	1
1	A	379	GLU	1
1	A	348	MET	1
1	A	354	ARG	1
1	A	362	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 92% for the well-defined parts and 90% 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	1189
Number of shifts mapped to atoms	1189
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	90	-0.67 ± 0.15	Should be checked
$^{13}C_\beta$	89	0.16 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	85	-0.39 ± 0.12	None needed (< 0.5 ppm)
^{15}N	87	0.12 ± 0.36	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 92%, i.e. 1100 atoms were assigned a chemical shift out of a possible 1201. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	398/405 (98%)	160/162 (99%)	159/162 (98%)	79/81 (98%)
Sidechain	664/743 (89%)	452/481 (94%)	202/227 (89%)	10/35 (29%)

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	Total	**^{1}H**	**^{13}C**	**^{15}N**
Aromatic	38/53 (72%)	23/27 (85%)	15/24 (62%)	0/2 (0%)
Overall	1100/1201 (92%)	635/670 (95%)	376/413 (91%)	89/118 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1184 atoms were assigned a chemical shift out of a possible 1311. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	440/461 (95%)	178/185 (96%)	175/184 (95%)	87/92 (95%)
Sidechain	706/797 (89%)	481/516 (93%)	215/245 (88%)	10/36 (28%)
Aromatic	38/53 (72%)	23/27 (85%)	15/24 (62%)	0/2 (0%)
Overall	1184/1311 (90%)	682/728 (94%)	405/453 (89%)	97/130 (75%)

7.1.4   Statistically unusual chemical shifts (i)

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	417	THR	HG1	5.62	0.08 − 2.19	21.2
1	A	386	THR	HG1	5.57	0.08 − 2.19	21.0
1	A	399	THR	HG1	3.87	0.08 − 2.19	12.9

7.1.5   Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:
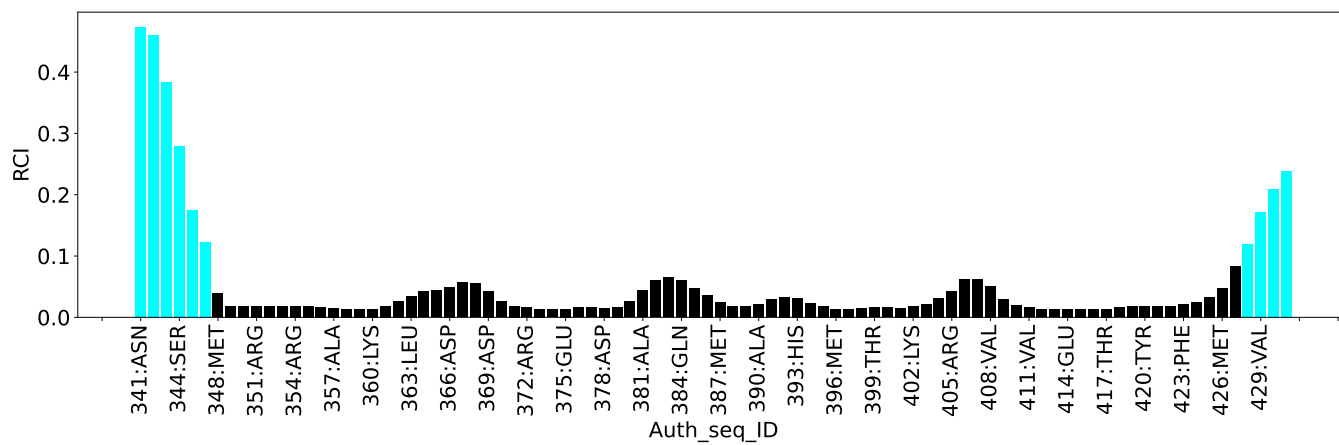
8 NMR restraints analysis ⓘ

8.1 Conformationally restricting restraints ⓘ

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1959
Intra-residue ($|i-j|=0$)	602
Sequential ($|i-j|=1$)	392
Medium range ($|i-j|>1$ and $|i-j|<5$)	484
Long range ($|i-j|\geq 5$)	481
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	154
Number of unmapped restraints	0
Number of restraints per residue	23.0
Number of long range restraints per residue[1]	5.2

[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)	1.5	0.2
0.2-0.5 (Medium)	0.5	0.49
>0.5 (Large)	0.8	1.02

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)	1.7	5.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

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)	602	30.7	1	0.2	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	478	24.4	1	0.2	0.1	0	0.0	0.0
Sidechain-Sidechain	124	6.3	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	392	20.0	3	0.8	0.2	0	0.0	0.0
Backbone-Backbone	80	4.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	265	13.5	3	1.1	0.2	0	0.0	0.0
Sidechain-Sidechain	47	2.4	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	484	24.7	6	1.2	0.3	0	0.0	0.0
Backbone-Backbone	81	4.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	225	11.5	1	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	178	9.1	5	2.8	0.3	0	0.0	0.0
Long range (|i-j|≥5)	481	24.6	14	2.9	0.7	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	144	7.4	5	3.5	0.3	0	0.0	0.0
Sidechain-Sidechain	336	17.2	9	2.7	0.5	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	1959	100.0	24	1.2	1.2	0	0.0	0.0
Backbone-Backbone	162	8.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1112	56.8	10	0.9	0.5	0	0.0	0.0
Sidechain-Sidechain	685	35.0	14	2.0	0.7	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 ⓘ
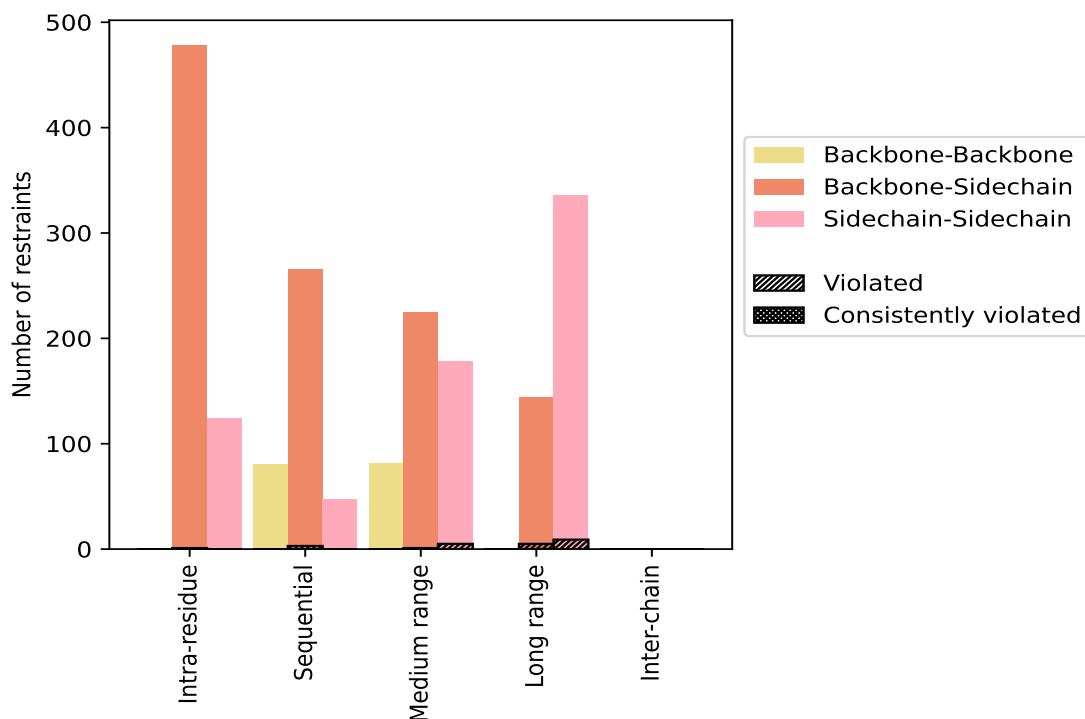
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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	0	1	0	1	0	2	0.12	0.13	0.01	0.12
2	1	0	0	0	0	1	0.91	0.91	0.0	0.91
3	1	0	0	4	0	5	0.33	0.95	0.32	0.16
4	1	0	1	1	0	3	0.48	0.94	0.33	0.26
5	1	1	0	1	0	3	0.43	0.95	0.37	0.18
6	1	0	0	0	0	1	0.93	0.93	0.0	0.93
7	0	1	0	2	0	3	0.14	0.16	0.02	0.14
8	1	0	1	2	0	4	0.32	0.93	0.35	0.12
9	1	0	1	4	0	6	0.25	0.92	0.3	0.12
10	1	0	1	1	0	3	0.48	0.95	0.33	0.31
11	1	1	1	4	0	7	0.28	0.91	0.26	0.17

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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	1	1	2	1	0	5	0.17	0.23	0.04	0.16
13	1	0	1	1	0	3	0.4	0.96	0.4	0.12
14	1	1	0	1	0	3	0.42	0.92	0.36	0.2
15	1	1	1	2	0	5	0.31	1.0	0.34	0.14
16	1	1	1	2	0	5	0.32	0.9	0.29	0.18
17	1	2	0	2	0	5	0.32	1.02	0.35	0.16
18	1	0	1	0	0	2	0.53	0.93	0.4	0.53
19	1	1	0	1	0	3	0.16	0.17	0.0	0.16
20	1	1	0	2	0	4	0.38	0.99	0.35	0.22
21	1	0	0	1	0	2	0.54	0.92	0.38	0.54
22	1	0	0	1	0	2	0.54	0.94	0.39	0.54
23	1	0	1	1	0	3	0.44	0.97	0.38	0.2
24	1	0	1	1	0	3	0.41	0.9	0.35	0.22
25	1	0	1	1	0	3	0.14	0.21	0.05	0.11
26	1	0	0	1	0	2	0.52	0.89	0.36	0.52
27	1	0	0	0	0	1	0.88	0.88	0.0	0.88
28	1	0	1	1	0	3	0.39	0.94	0.39	0.11
29	1	1	0	0	0	2	0.55	0.91	0.36	0.55
30	1	0	0	0	0	1	0.94	0.94	0.0	0.94
31	1	0	1	2	0	4	0.39	0.93	0.32	0.24
32	1	1	0	0	0	2	0.2	0.22	0.02	0.2
33	1	1	0	2	0	4	0.33	0.89	0.32	0.16
34	1	0	0	0	0	1	0.74	0.74	0.0	0.74
35	1	0	0	1	0	2	0.17	0.23	0.06	0.17
36	1	0	0	1	0	2	0.2	0.28	0.08	0.2
37	1	0	0	0	0	1	0.89	0.89	0.0	0.89
38	1	0	0	3	0	4	0.37	0.91	0.32	0.22
39	1	0	0	1	0	2	0.54	0.94	0.4	0.54
40	1	0	0	0	0	1	0.9	0.9	0.0	0.9
41	1	1	0	1	0	3	0.42	0.88	0.33	0.25
42	1	0	0	0	0	1	0.39	0.39	0.0	0.39
43	1	1	0	0	0	2	0.57	0.94	0.37	0.57
44	1	0	0	1	0	2	0.58	0.89	0.3	0.58
45	1	0	0	0	0	1	0.86	0.86	0.0	0.86
46	1	0	0	1	0	2	0.51	0.89	0.38	0.51
47	1	1	0	0	0	2	0.15	0.18	0.03	0.15
48	1	0	0	1	0	2	0.53	0.94	0.41	0.53
49	1	0	0	0	0	1	0.79	0.79	0.0	0.79
50	1	0	0	1	0	2	0.38	0.49	0.11	0.38

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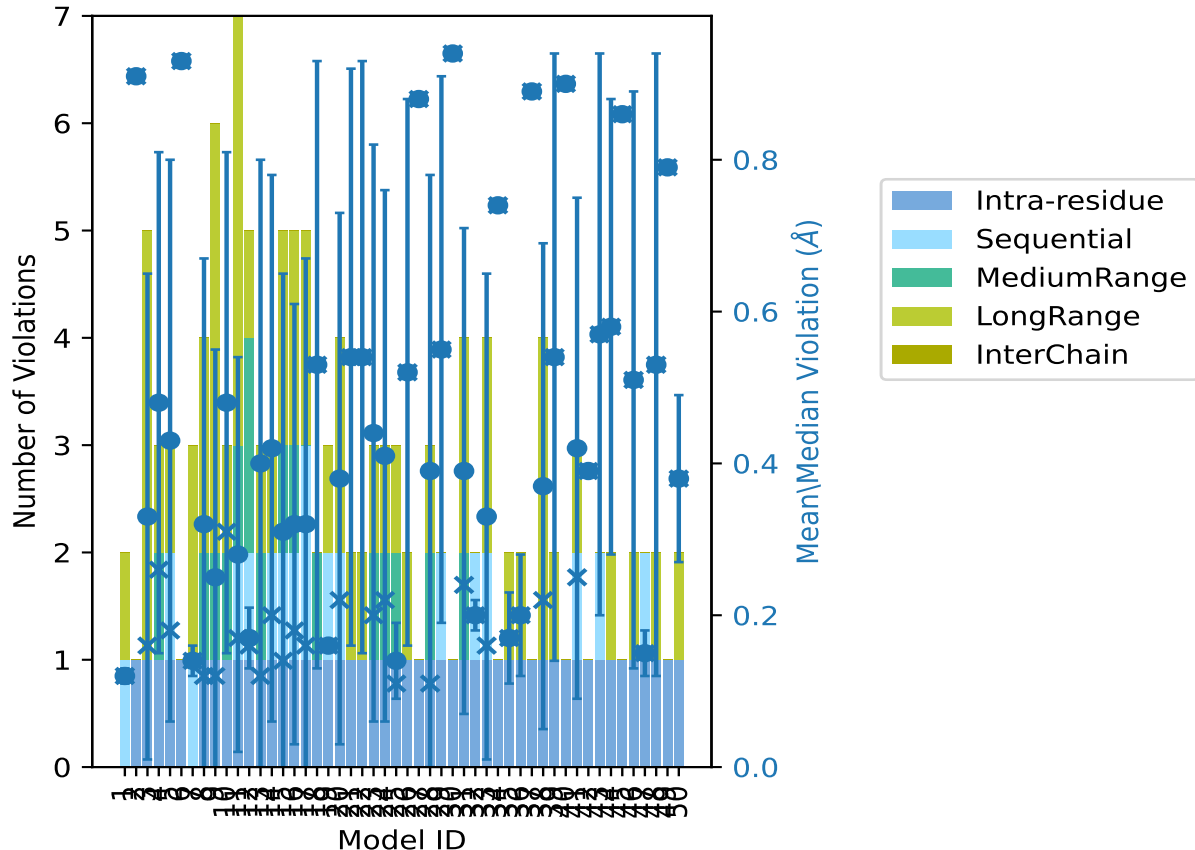
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

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, 1935(IR:601, SQ:389, MR:478, LR:467, 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	4	0	5	1	2.0
0	1	2	4	0	7	2	4.0
0	1	2	1	0	4	3	6.0
0	0	0	0	0	0	4	8.0
0	0	1	0	0	1	5	10.0
0	0	0	1	0	1	6	12.0

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Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	2	0	2	7	14.0
0	0	0	0	0	0	8	16.0
0	0	0	1	0	1	9	18.0
0	0	0	1	0	1	10	20.0
0	0	0	0	0	0	11	22.0
0	0	0	0	0	0	12	24.0
0	1	0	0	0	1	13	26.0
0	0	0	0	0	0	14	28.0
0	0	0	0	0	0	15	30.0
0	0	0	0	0	0	16	32.0
0	0	0	0	0	0	17	34.0
0	0	0	0	0	0	18	36.0
0	0	0	0	0	0	19	38.0
0	0	0	0	0	0	20	40.0
0	0	0	0	0	0	21	42.0
0	0	0	0	0	0	22	44.0
0	0	0	0	0	0	23	46.0
0	0	0	0	0	0	24	48.0
0	0	0	0	0	0	25	50.0
0	0	0	0	0	0	26	52.0
0	0	0	0	0	0	27	54.0
0	0	0	0	0	0	28	56.0
0	0	0	0	0	0	29	58.0
0	0	0	0	0	0	30	60.0
0	0	0	0	0	0	31	62.0
0	0	0	0	0	0	32	64.0
0	0	0	0	0	0	33	66.0
0	0	0	0	0	0	34	68.0
0	0	0	0	0	0	35	70.0
0	0	0	0	0	0	36	72.0
0	0	0	0	0	0	37	74.0
0	0	0	0	0	0	38	76.0
0	0	0	0	0	0	39	78.0
0	0	0	0	0	0	40	80.0
0	0	0	0	0	0	41	82.0
0	0	0	0	0	0	42	84.0
0	0	0	0	0	0	43	86.0
0	0	0	0	0	0	44	88.0
0	0	0	0	0	0	45	90.0
0	0	0	0	0	0	46	92.0
0	0	0	0	0	0	47	94.0

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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]	%
1	0	0	0	0	1	48	96.0
0	0	0	0	0	0	49	98.0
0	0	0	0	0	0	50	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ
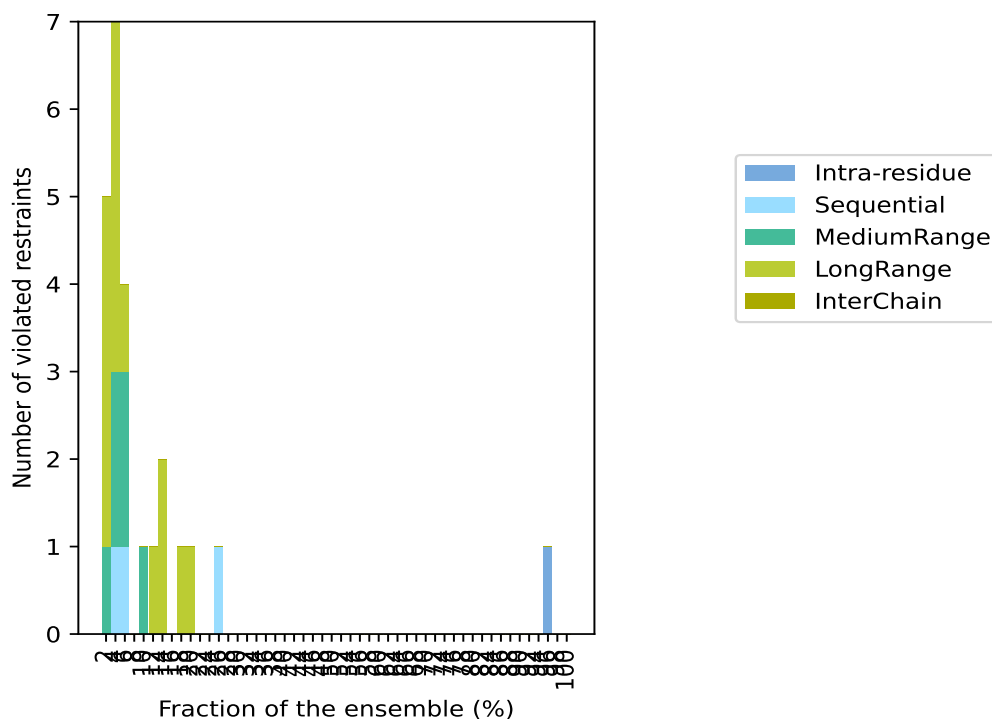
9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble
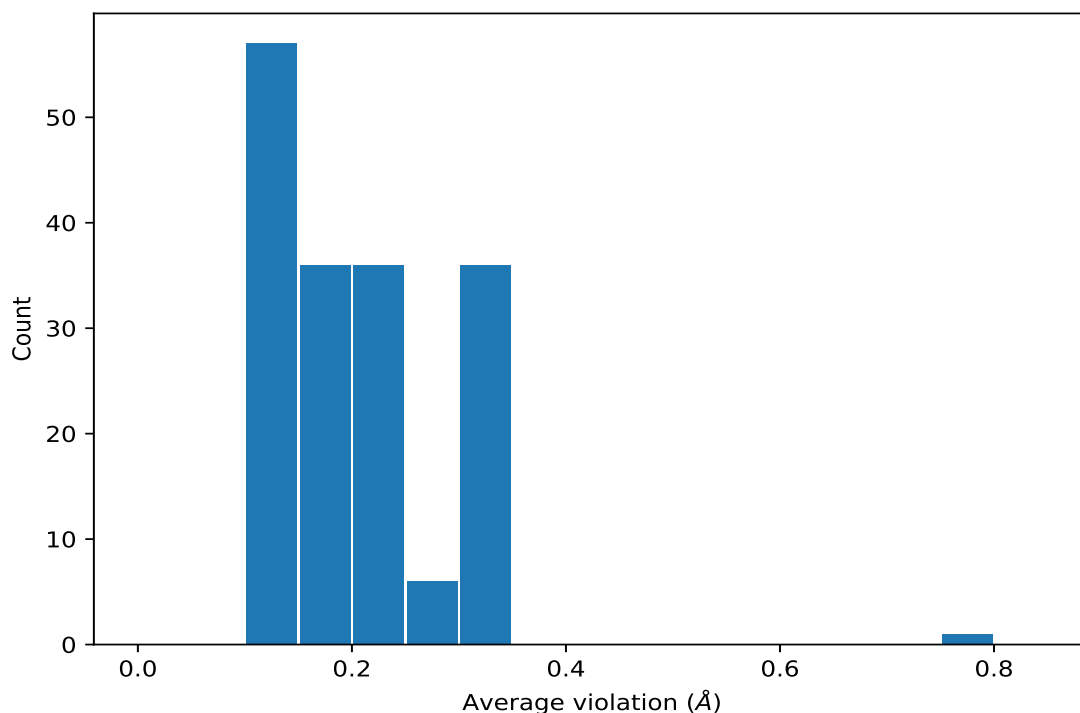
9.4.2　Table: Most violated distance restraints ⓘ

The following table provides the mean and the standard deviation of 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)
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	48	0.79	0.28	0.91
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	13	0.15	0.03	0.16
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	13	0.15	0.03	0.16
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	13	0.15	0.03	0.16
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	10	0.14	0.02	0.14
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	10	0.14	0.02	0.14
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	10	0.14	0.02	0.14
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	10	0.14	0.02	0.14
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	10	0.14	0.02	0.14
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	10	0.14	0.02	0.14
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	9	0.25	0.04	0.26
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	9	0.25	0.04	0.26
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	9	0.25	0.04	0.26
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	9	0.25	0.04	0.26
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	9	0.25	0.04	0.26
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	9	0.25	0.04	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD11	7	0.14	0.02	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD12	7	0.14	0.02	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD13	7	0.14	0.02	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD21	7	0.14	0.02	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD22	7	0.14	0.02	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD23	7	0.14	0.02	0.14
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD21	7	0.13	0.02	0.12
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD22	7	0.13	0.02	0.12
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD23	7	0.13	0.02	0.12
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD21	7	0.13	0.02	0.12
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD22	7	0.13	0.02	0.12
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD23	7	0.13	0.02	0.12
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD21	7	0.13	0.02	0.12
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD22	7	0.13	0.02	0.12
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD23	7	0.13	0.02	0.12
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG11	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG12	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG13	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG21	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG22	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG23	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG11	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG12	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG13	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG21	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG22	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG23	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG11	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG12	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG13	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG21	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG22	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG23	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG11	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG12	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG13	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG21	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG22	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG23	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG11	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG12	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG13	6	0.3	0.1	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG21	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG22	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG23	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG11	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG12	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG13	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG21	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG22	6	0.3	0.1	0.29
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG23	6	0.3	0.1	0.29
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG11	5	0.17	0.04	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG12	5	0.17	0.04	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG13	5	0.17	0.04	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG21	5	0.17	0.04	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG22	5	0.17	0.04	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG23	5	0.17	0.04	0.17
(1,1713)	1:A:386:THR:HG21	1:A:389:GLN:HE21	3	0.17	0.03	0.16
(1,1713)	1:A:386:THR:HG21	1:A:389:GLN:HE22	3	0.17	0.03	0.16
(1,1713)	1:A:386:THR:HG22	1:A:389:GLN:HE21	3	0.17	0.03	0.16
(1,1713)	1:A:386:THR:HG22	1:A:389:GLN:HE22	3	0.17	0.03	0.16
(1,1713)	1:A:386:THR:HG23	1:A:389:GLN:HE21	3	0.17	0.03	0.16
(1,1713)	1:A:386:THR:HG23	1:A:389:GLN:HE22	3	0.17	0.03	0.16
(1,1955)	1:A:428:LEU:HD11	1:A:429:VAL:HA	3	0.13	0.03	0.12
(1,1955)	1:A:428:LEU:HD12	1:A:429:VAL:HA	3	0.13	0.03	0.12
(1,1955)	1:A:428:LEU:HD13	1:A:429:VAL:HA	3	0.13	0.03	0.12
(1,1955)	1:A:428:LEU:HD21	1:A:429:VAL:HA	3	0.13	0.03	0.12
(1,1955)	1:A:428:LEU:HD22	1:A:429:VAL:HA	3	0.13	0.03	0.12
(1,1955)	1:A:428:LEU:HD23	1:A:429:VAL:HA	3	0.13	0.03	0.12
(1,28)	1:A:348:MET:HE1	1:A:384:GLN:H	3	0.13	0.02	0.12
(1,28)	1:A:348:MET:HE2	1:A:384:GLN:H	3	0.13	0.02	0.12
(1,28)	1:A:348:MET:HE3	1:A:384:GLN:H	3	0.13	0.02	0.12
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD21	3	0.12	0.01	0.11
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD22	3	0.12	0.01	0.11
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD23	3	0.12	0.01	0.11
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG11	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG12	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG13	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG21	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG22	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG23	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG11	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG12	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG13	2	0.22	0.01	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG21	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG22	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG23	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG11	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG12	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG13	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG21	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG22	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG23	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG11	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG12	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG13	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG21	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG22	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG23	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG11	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG12	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG13	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG21	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG22	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG23	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG11	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG12	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG13	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG21	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG22	2	0.22	0.01	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG23	2	0.22	0.01	0.22
(1,1954)	1:A:428:LEU:HD11	1:A:429:VAL:H	2	0.18	0.02	0.18
(1,1954)	1:A:428:LEU:HD12	1:A:429:VAL:H	2	0.18	0.02	0.18
(1,1954)	1:A:428:LEU:HD13	1:A:429:VAL:H	2	0.18	0.02	0.18
(1,1954)	1:A:428:LEU:HD21	1:A:429:VAL:H	2	0.18	0.02	0.18
(1,1954)	1:A:428:LEU:HD22	1:A:429:VAL:H	2	0.18	0.02	0.18
(1,1954)	1:A:428:LEU:HD23	1:A:429:VAL:H	2	0.18	0.02	0.18
(1,1536)	1:A:363:LEU:HD11	1:A:368:LEU:HB2	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD11	1:A:368:LEU:HB3	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD12	1:A:368:LEU:HB2	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD12	1:A:368:LEU:HB3	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD13	1:A:368:LEU:HB2	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD13	1:A:368:LEU:HB3	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD21	1:A:368:LEU:HB2	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD21	1:A:368:LEU:HB3	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD22	1:A:368:LEU:HB2	2	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1536)	1:A:363:LEU:HD22	1:A:368:LEU:HB3	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD23	1:A:368:LEU:HB2	2	0.16	0.02	0.16
(1,1536)	1:A:363:LEU:HD23	1:A:368:LEU:HB3	2	0.16	0.02	0.16
(1,188)	1:A:359:ILE:HG21	1:A:363:LEU:HG	2	0.16	0.0	0.16
(1,188)	1:A:359:ILE:HG22	1:A:363:LEU:HG	2	0.16	0.0	0.16
(1,188)	1:A:359:ILE:HG23	1:A:363:LEU:HG	2	0.16	0.0	0.16
(1,1632)	1:A:377:LEU:HD11	1:A:412:ILE:H	2	0.14	0.01	0.14
(1,1632)	1:A:377:LEU:HD12	1:A:412:ILE:H	2	0.14	0.01	0.14
(1,1632)	1:A:377:LEU:HD13	1:A:412:ILE:H	2	0.14	0.01	0.14
(1,1632)	1:A:377:LEU:HD21	1:A:412:ILE:H	2	0.14	0.01	0.14
(1,1632)	1:A:377:LEU:HD22	1:A:412:ILE:H	2	0.14	0.01	0.14
(1,1632)	1:A:377:LEU:HD23	1:A:412:ILE:H	2	0.14	0.01	0.14
(1,1452)	1:A:348:MET:HE1	1:A:389:GLN:HE21	2	0.12	0.01	0.12
(1,1452)	1:A:348:MET:HE1	1:A:389:GLN:HE22	2	0.12	0.01	0.12
(1,1452)	1:A:348:MET:HE2	1:A:389:GLN:HE21	2	0.12	0.01	0.12
(1,1452)	1:A:348:MET:HE2	1:A:389:GLN:HE22	2	0.12	0.01	0.12
(1,1452)	1:A:348:MET:HE3	1:A:389:GLN:HE21	2	0.12	0.01	0.12
(1,1452)	1:A:348:MET:HE3	1:A:389:GLN:HE22	2	0.12	0.01	0.12
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG11	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG12	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG13	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG21	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG22	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG23	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG11	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG12	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG13	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG21	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG22	2	0.11	0.0	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG23	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.
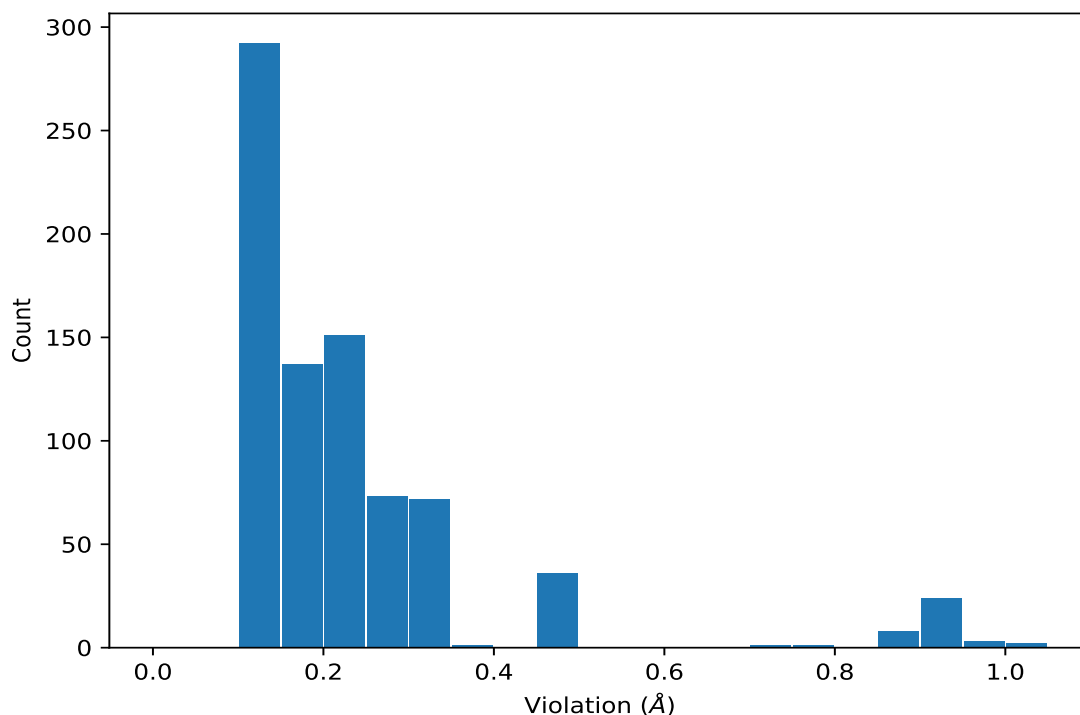
9.5.2 Table : All distance violations ⓘ

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)
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	17	1.02
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	15	1.0
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	20	0.99
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	23	0.97
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	13	0.96
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	3	0.95
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	5	0.95
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	10	0.95
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	4	0.94
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	22	0.94
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	28	0.94
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	30	0.94
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	39	0.94
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	43	0.94
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	48	0.94
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	6	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	8	0.93
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	18	0.93
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	31	0.93
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	9	0.92
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	14	0.92
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	21	0.92
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	2	0.91
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	11	0.91
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	29	0.91
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	38	0.91
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	16	0.9
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	24	0.9
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	40	0.9
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	26	0.89
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	33	0.89
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	37	0.89
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	44	0.89
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	46	0.89
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	27	0.88
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	41	0.88
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	45	0.86
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	49	0.79
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	34	0.74
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG11	50	0.49
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG12	50	0.49
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG13	50	0.49
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG21	50	0.49
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG22	50	0.49
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG23	50	0.49
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG11	50	0.49
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG12	50	0.49
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG13	50	0.49
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG21	50	0.49
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG22	50	0.49
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG23	50	0.49
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG11	50	0.49
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG12	50	0.49
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG13	50	0.49
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG21	50	0.49
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG22	50	0.49
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG23	50	0.49
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG11	50	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG12	50	0.49
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG13	50	0.49
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG21	50	0.49
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG22	50	0.49
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG23	50	0.49
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG11	50	0.49
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG12	50	0.49
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG13	50	0.49
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG21	50	0.49
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG22	50	0.49
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG23	50	0.49
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG11	50	0.49
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG12	50	0.49
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG13	50	0.49
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG21	50	0.49
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG22	50	0.49
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG23	50	0.49
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	42	0.39
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG11	31	0.32
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG12	31	0.32
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG13	31	0.32
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG21	31	0.32
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG22	31	0.32
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG23	31	0.32
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG11	31	0.32
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG12	31	0.32
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG13	31	0.32
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG21	31	0.32
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG22	31	0.32
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG23	31	0.32
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG11	31	0.32
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG12	31	0.32
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG13	31	0.32
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG21	31	0.32
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG22	31	0.32
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG23	31	0.32
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG11	31	0.32
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG12	31	0.32
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG13	31	0.32
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG21	31	0.32
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG22	31	0.32
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG23	31	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG11	31	0.32
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG12	31	0.32
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG13	31	0.32
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG21	31	0.32
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG22	31	0.32
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG23	31	0.32
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG11	31	0.32
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG12	31	0.32
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG13	31	0.32
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG21	31	0.32
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG22	31	0.32
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG23	31	0.32
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG11	10	0.31
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG12	10	0.31
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG13	10	0.31
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG21	10	0.31
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG22	10	0.31
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG23	10	0.31
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG11	10	0.31
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG12	10	0.31
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG13	10	0.31
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG21	10	0.31
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG22	10	0.31
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG23	10	0.31
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG11	10	0.31
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG12	10	0.31
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG13	10	0.31
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG21	10	0.31
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG22	10	0.31
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG23	10	0.31
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG11	10	0.31
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG12	10	0.31
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG13	10	0.31
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG21	10	0.31
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG22	10	0.31
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG23	10	0.31
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG11	10	0.31
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG12	10	0.31
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG13	10	0.31
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG21	10	0.31
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG22	10	0.31
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG23	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG11	10	0.31
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG12	10	0.31
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG13	10	0.31
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG21	10	0.31
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG22	10	0.31
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG23	10	0.31
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	36	0.28
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	36	0.28
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	36	0.28
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	36	0.28
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	36	0.28
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	36	0.28
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	44	0.28
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	44	0.28
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	44	0.28
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	44	0.28
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	44	0.28
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	44	0.28
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	3	0.27
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	3	0.27
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	3	0.27
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	3	0.27
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	3	0.27
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	3	0.27
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	20	0.27
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	20	0.27
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	20	0.27
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	20	0.27
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	20	0.27
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	20	0.27
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	50	0.27
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	38	0.26
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	38	0.26
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	38	0.26
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	38	0.26
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	38	0.26
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	38	0.26
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG11	4	0.26
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG12	4	0.26
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG13	4	0.26
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG21	4	0.26
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG22	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG23	4	0.26
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG11	4	0.26
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG12	4	0.26
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG13	4	0.26
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG21	4	0.26
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG22	4	0.26
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG23	4	0.26
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG11	4	0.26
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG12	4	0.26
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG13	4	0.26
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG21	4	0.26
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG22	4	0.26
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG23	4	0.26
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG11	4	0.26
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG12	4	0.26
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG13	4	0.26
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG21	4	0.26
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG22	4	0.26
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG23	4	0.26
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG11	4	0.26
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG12	4	0.26
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG13	4	0.26
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG21	4	0.26
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG22	4	0.26
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG23	4	0.26
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG11	4	0.26
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG12	4	0.26
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG13	4	0.26
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG21	4	0.26
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG22	4	0.26
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG23	4	0.26
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	41	0.25
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	41	0.25
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	41	0.25
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	41	0.25
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	41	0.25
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	41	0.25
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG11	4	0.23
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG12	4	0.23
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG13	4	0.23
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG21	4	0.23
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG22	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG23	4	0.23
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	11	0.23
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	11	0.23
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	11	0.23
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	11	0.23
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	11	0.23
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	11	0.23
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG11	12	0.23
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG12	12	0.23
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG13	12	0.23
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG21	12	0.23
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG22	12	0.23
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG23	12	0.23
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG11	12	0.23
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG12	12	0.23
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG13	12	0.23
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG21	12	0.23
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG22	12	0.23
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG23	12	0.23
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG11	12	0.23
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG12	12	0.23
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG13	12	0.23
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG21	12	0.23
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG22	12	0.23
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG23	12	0.23
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG11	12	0.23
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG12	12	0.23
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG13	12	0.23
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG21	12	0.23
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG22	12	0.23
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG23	12	0.23
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG11	12	0.23
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG12	12	0.23
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG13	12	0.23
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG21	12	0.23
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG22	12	0.23
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG23	12	0.23
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG11	12	0.23
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG12	12	0.23
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG13	12	0.23
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG21	12	0.23
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG22	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG23	12	0.23
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	35	0.23
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	24	0.22
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	24	0.22
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	24	0.22
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	24	0.22
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	24	0.22
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	24	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG11	11	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG12	11	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG13	11	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG21	11	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG22	11	0.22
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG23	11	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG11	11	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG12	11	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG13	11	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG21	11	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG22	11	0.22
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG23	11	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG11	11	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG12	11	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG13	11	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG21	11	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG22	11	0.22
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG23	11	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG11	11	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG12	11	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG13	11	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG21	11	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG22	11	0.22
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG23	11	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG11	11	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG12	11	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG13	11	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG21	11	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG22	11	0.22
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG23	11	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG11	11	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG12	11	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG13	11	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG21	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG22	11	0.22
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG23	11	0.22
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	32	0.22
(1,1713)	1:A:386:THR:HG21	1:A:389:GLN:HE21	15	0.21
(1,1713)	1:A:386:THR:HG21	1:A:389:GLN:HE22	15	0.21
(1,1713)	1:A:386:THR:HG22	1:A:389:GLN:HE21	15	0.21
(1,1713)	1:A:386:THR:HG22	1:A:389:GLN:HE22	15	0.21
(1,1713)	1:A:386:THR:HG23	1:A:389:GLN:HE21	15	0.21
(1,1713)	1:A:386:THR:HG23	1:A:389:GLN:HE22	15	0.21
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG11	16	0.21
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG12	16	0.21
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG13	16	0.21
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG21	16	0.21
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG22	16	0.21
(1,1541)	1:A:363:LEU:HD11	1:A:370:VAL:HG23	16	0.21
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG11	16	0.21
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG12	16	0.21
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG13	16	0.21
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG21	16	0.21
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG22	16	0.21
(1,1541)	1:A:363:LEU:HD12	1:A:370:VAL:HG23	16	0.21
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG11	16	0.21
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG12	16	0.21
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG13	16	0.21
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG21	16	0.21
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG22	16	0.21
(1,1541)	1:A:363:LEU:HD13	1:A:370:VAL:HG23	16	0.21
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG11	16	0.21
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG12	16	0.21
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG13	16	0.21
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG21	16	0.21
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG22	16	0.21
(1,1541)	1:A:363:LEU:HD21	1:A:370:VAL:HG23	16	0.21
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG11	16	0.21
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG12	16	0.21
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG13	16	0.21
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG21	16	0.21
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG22	16	0.21
(1,1541)	1:A:363:LEU:HD22	1:A:370:VAL:HG23	16	0.21
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG11	16	0.21
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG12	16	0.21
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG13	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG21	16	0.21
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG22	16	0.21
(1,1541)	1:A:363:LEU:HD23	1:A:370:VAL:HG23	16	0.21
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	12	0.21
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	25	0.21
(1,575)	1:A:398:THR:HG21	1:A:402:LYS:HD2	23	0.2
(1,575)	1:A:398:THR:HG21	1:A:402:LYS:HD3	23	0.2
(1,575)	1:A:398:THR:HG22	1:A:402:LYS:HD2	23	0.2
(1,575)	1:A:398:THR:HG22	1:A:402:LYS:HD3	23	0.2
(1,575)	1:A:398:THR:HG23	1:A:402:LYS:HD2	23	0.2
(1,575)	1:A:398:THR:HG23	1:A:402:LYS:HD3	23	0.2
(1,1954)	1:A:428:LEU:HD11	1:A:429:VAL:H	43	0.2
(1,1954)	1:A:428:LEU:HD12	1:A:429:VAL:H	43	0.2
(1,1954)	1:A:428:LEU:HD13	1:A:429:VAL:H	43	0.2
(1,1954)	1:A:428:LEU:HD21	1:A:429:VAL:H	43	0.2
(1,1954)	1:A:428:LEU:HD22	1:A:429:VAL:H	43	0.2
(1,1954)	1:A:428:LEU:HD23	1:A:429:VAL:H	43	0.2
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	14	0.2
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	14	0.2
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	14	0.2
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG11	10	0.19
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG12	10	0.19
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG13	10	0.19
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG21	10	0.19
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG22	10	0.19
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG23	10	0.19
(1,1536)	1:A:363:LEU:HD11	1:A:368:LEU:HB2	16	0.18
(1,1536)	1:A:363:LEU:HD11	1:A:368:LEU:HB3	16	0.18
(1,1536)	1:A:363:LEU:HD12	1:A:368:LEU:HB2	16	0.18
(1,1536)	1:A:363:LEU:HD12	1:A:368:LEU:HB3	16	0.18
(1,1536)	1:A:363:LEU:HD13	1:A:368:LEU:HB2	16	0.18
(1,1536)	1:A:363:LEU:HD13	1:A:368:LEU:HB3	16	0.18
(1,1536)	1:A:363:LEU:HD21	1:A:368:LEU:HB2	16	0.18
(1,1536)	1:A:363:LEU:HD21	1:A:368:LEU:HB3	16	0.18
(1,1536)	1:A:363:LEU:HD22	1:A:368:LEU:HB2	16	0.18
(1,1536)	1:A:363:LEU:HD22	1:A:368:LEU:HB3	16	0.18
(1,1536)	1:A:363:LEU:HD23	1:A:368:LEU:HB2	16	0.18
(1,1536)	1:A:363:LEU:HD23	1:A:368:LEU:HB3	16	0.18
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	47	0.18
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	5	0.18
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	5	0.18
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	29	0.18
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	29	0.18
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	29	0.18
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	33	0.18
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	33	0.18
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	33	0.18
(1,1955)	1:A:428:LEU:HD11	1:A:429:VAL:HA	17	0.17
(1,1955)	1:A:428:LEU:HD12	1:A:429:VAL:HA	17	0.17
(1,1955)	1:A:428:LEU:HD13	1:A:429:VAL:HA	17	0.17
(1,1955)	1:A:428:LEU:HD21	1:A:429:VAL:HA	17	0.17
(1,1955)	1:A:428:LEU:HD22	1:A:429:VAL:HA	17	0.17
(1,1955)	1:A:428:LEU:HD23	1:A:429:VAL:HA	17	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG11	31	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG12	31	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG13	31	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG21	31	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG22	31	0.17
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG23	31	0.17
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD11	38	0.17
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD12	38	0.17
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD13	38	0.17
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD21	38	0.17
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD22	38	0.17
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD23	38	0.17
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG11	11	0.17
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG12	11	0.17
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG13	11	0.17
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG21	11	0.17
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG22	11	0.17
(1,1556)	1:A:363:LEU:HD11	1:A:408:VAL:HG23	11	0.17
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG11	11	0.17
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG12	11	0.17
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG13	11	0.17
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG21	11	0.17
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG22	11	0.17
(1,1556)	1:A:363:LEU:HD12	1:A:408:VAL:HG23	11	0.17
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG11	11	0.17
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG12	11	0.17
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG13	11	0.17
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG21	11	0.17
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG22	11	0.17
(1,1556)	1:A:363:LEU:HD13	1:A:408:VAL:HG23	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG11	11	0.17
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG12	11	0.17
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG13	11	0.17
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG21	11	0.17
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG22	11	0.17
(1,1556)	1:A:363:LEU:HD21	1:A:408:VAL:HG23	11	0.17
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG11	11	0.17
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG12	11	0.17
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG13	11	0.17
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG21	11	0.17
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG22	11	0.17
(1,1556)	1:A:363:LEU:HD22	1:A:408:VAL:HG23	11	0.17
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG11	11	0.17
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG12	11	0.17
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG13	11	0.17
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG21	11	0.17
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG22	11	0.17
(1,1556)	1:A:363:LEU:HD23	1:A:408:VAL:HG23	11	0.17
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	19	0.17
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	19	0.17
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	19	0.17
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	32	0.17
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	32	0.17
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	32	0.17
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD21	20	0.16
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD22	20	0.16
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD23	20	0.16
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD21	20	0.16
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD22	20	0.16
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD23	20	0.16
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD21	20	0.16
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD22	20	0.16
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD23	20	0.16
(1,1954)	1:A:428:LEU:HD11	1:A:429:VAL:H	17	0.16
(1,1954)	1:A:428:LEU:HD12	1:A:429:VAL:H	17	0.16
(1,1954)	1:A:428:LEU:HD13	1:A:429:VAL:H	17	0.16
(1,1954)	1:A:428:LEU:HD21	1:A:429:VAL:H	17	0.16
(1,1954)	1:A:428:LEU:HD22	1:A:429:VAL:H	17	0.16
(1,1954)	1:A:428:LEU:HD23	1:A:429:VAL:H	17	0.16
(1,188)	1:A:359:ILE:HG21	1:A:363:LEU:HG	11	0.16
(1,188)	1:A:359:ILE:HG22	1:A:363:LEU:HG	11	0.16
(1,188)	1:A:359:ILE:HG23	1:A:363:LEU:HG	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:A:359:ILE:HG21	1:A:363:LEU:HG	16	0.16
(1,188)	1:A:359:ILE:HG22	1:A:363:LEU:HG	16	0.16
(1,188)	1:A:359:ILE:HG23	1:A:363:LEU:HG	16	0.16
(1,1713)	1:A:386:THR:HG21	1:A:389:GLN:HE21	12	0.16
(1,1713)	1:A:386:THR:HG21	1:A:389:GLN:HE22	12	0.16
(1,1713)	1:A:386:THR:HG22	1:A:389:GLN:HE21	12	0.16
(1,1713)	1:A:386:THR:HG22	1:A:389:GLN:HE22	12	0.16
(1,1713)	1:A:386:THR:HG23	1:A:389:GLN:HE21	12	0.16
(1,1713)	1:A:386:THR:HG23	1:A:389:GLN:HE22	12	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD11	3	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD12	3	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD13	3	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD21	3	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD22	3	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD23	3	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD11	26	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD12	26	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD13	26	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD21	26	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD22	26	0.16
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD23	26	0.16
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	19	0.16
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	19	0.16
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	19	0.16
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	19	0.16
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	19	0.16
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	19	0.16
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	19	0.16
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	7	0.16
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	7	0.16
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	7	0.16
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD21	21	0.15
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD22	21	0.15
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD23	21	0.15
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD21	21	0.15
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD22	21	0.15
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD23	21	0.15
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD21	21	0.15
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD22	21	0.15
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD23	21	0.15
(1,28)	1:A:348:MET:HE1	1:A:384:GLN:H	3	0.15
(1,28)	1:A:348:MET:HE2	1:A:384:GLN:H	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:A:348:MET:HE3	1:A:384:GLN:H	3	0.15
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG11	12	0.15
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG12	12	0.15
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG13	12	0.15
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG21	12	0.15
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG22	12	0.15
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG23	12	0.15
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB2	22	0.15
(1,1767)	1:A:397:ILE:HD11	1:A:426:MET:HB3	22	0.15
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB2	22	0.15
(1,1767)	1:A:397:ILE:HD12	1:A:426:MET:HB3	22	0.15
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB2	22	0.15
(1,1767)	1:A:397:ILE:HD13	1:A:426:MET:HB3	22	0.15
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	5	0.15
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	5	0.15
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	5	0.15
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	5	0.15
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	5	0.15
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	5	0.15
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	17	0.15
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	17	0.15
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	17	0.15
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	17	0.15
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	17	0.15
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	17	0.15
(1,1536)	1:A:363:LEU:HD11	1:A:368:LEU:HB2	11	0.15
(1,1536)	1:A:363:LEU:HD11	1:A:368:LEU:HB3	11	0.15
(1,1536)	1:A:363:LEU:HD12	1:A:368:LEU:HB2	11	0.15
(1,1536)	1:A:363:LEU:HD12	1:A:368:LEU:HB3	11	0.15
(1,1536)	1:A:363:LEU:HD13	1:A:368:LEU:HB2	11	0.15
(1,1536)	1:A:363:LEU:HD13	1:A:368:LEU:HB3	11	0.15
(1,1536)	1:A:363:LEU:HD21	1:A:368:LEU:HB2	11	0.15
(1,1536)	1:A:363:LEU:HD21	1:A:368:LEU:HB3	11	0.15
(1,1536)	1:A:363:LEU:HD22	1:A:368:LEU:HB2	11	0.15
(1,1536)	1:A:363:LEU:HD22	1:A:368:LEU:HB3	11	0.15
(1,1536)	1:A:363:LEU:HD23	1:A:368:LEU:HB2	11	0.15
(1,1536)	1:A:363:LEU:HD23	1:A:368:LEU:HB3	11	0.15
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	16	0.15
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	16	0.15
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	16	0.15
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD21	31	0.14
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD22	31	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD23	31	0.14
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD21	31	0.14
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD22	31	0.14
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD23	31	0.14
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD21	31	0.14
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD22	31	0.14
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD23	31	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD11	7	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD12	7	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD13	7	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD21	7	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD22	7	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD23	7	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD11	39	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD12	39	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD13	39	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD21	39	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD22	39	0.14
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD23	39	0.14
(1,1632)	1:A:377:LEU:HD11	1:A:412:ILE:H	33	0.14
(1,1632)	1:A:377:LEU:HD12	1:A:412:ILE:H	33	0.14
(1,1632)	1:A:377:LEU:HD13	1:A:412:ILE:H	33	0.14
(1,1632)	1:A:377:LEU:HD21	1:A:412:ILE:H	33	0.14
(1,1632)	1:A:377:LEU:HD22	1:A:412:ILE:H	33	0.14
(1,1632)	1:A:377:LEU:HD23	1:A:412:ILE:H	33	0.14
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	15	0.14
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	15	0.14
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	15	0.14
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	15	0.14
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	15	0.14
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	15	0.14
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	23	0.14
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	23	0.14
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	23	0.14
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	23	0.14
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	23	0.14
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	23	0.14
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	41	0.14
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	41	0.14
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	41	0.14
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD21	8	0.13
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD22	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD23	8	0.13
(1,1713)	1:A:386:THR:HG21	1:A:389:GLN:HE21	18	0.13
(1,1713)	1:A:386:THR:HG21	1:A:389:GLN:HE22	18	0.13
(1,1713)	1:A:386:THR:HG22	1:A:389:GLN:HE21	18	0.13
(1,1713)	1:A:386:THR:HG22	1:A:389:GLN:HE22	18	0.13
(1,1713)	1:A:386:THR:HG23	1:A:389:GLN:HE21	18	0.13
(1,1713)	1:A:386:THR:HG23	1:A:389:GLN:HE22	18	0.13
(1,1632)	1:A:377:LEU:HD11	1:A:412:ILE:H	14	0.13
(1,1632)	1:A:377:LEU:HD12	1:A:412:ILE:H	14	0.13
(1,1632)	1:A:377:LEU:HD13	1:A:412:ILE:H	14	0.13
(1,1632)	1:A:377:LEU:HD21	1:A:412:ILE:H	14	0.13
(1,1632)	1:A:377:LEU:HD22	1:A:412:ILE:H	14	0.13
(1,1632)	1:A:377:LEU:HD23	1:A:412:ILE:H	14	0.13
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	9	0.13
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	9	0.13
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	9	0.13
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	9	0.13
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	9	0.13
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	9	0.13
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	38	0.13
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	38	0.13
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	38	0.13
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	38	0.13
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	38	0.13
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	38	0.13
(1,1452)	1:A:348:MET:HE1	1:A:389:GLN:HE21	46	0.13
(1,1452)	1:A:348:MET:HE1	1:A:389:GLN:HE22	46	0.13
(1,1452)	1:A:348:MET:HE2	1:A:389:GLN:HE21	46	0.13
(1,1452)	1:A:348:MET:HE2	1:A:389:GLN:HE22	46	0.13
(1,1452)	1:A:348:MET:HE3	1:A:389:GLN:HE21	46	0.13
(1,1452)	1:A:348:MET:HE3	1:A:389:GLN:HE22	46	0.13
(1,1061)	1:A:425:ASN:H	1:A:425:ASN:HD21	36	0.13
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	1	0.13
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	1	0.13
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	1	0.13
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD21	9	0.12
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD22	9	0.12
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD23	9	0.12
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD21	9	0.12
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD22	9	0.12
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD23	9	0.12
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD21	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD22	9	0.12
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD23	9	0.12
(1,28)	1:A:348:MET:HE1	1:A:384:GLN:H	13	0.12
(1,28)	1:A:348:MET:HE2	1:A:384:GLN:H	13	0.12
(1,28)	1:A:348:MET:HE3	1:A:384:GLN:H	13	0.12
(1,1955)	1:A:428:LEU:HD11	1:A:429:VAL:HA	20	0.12
(1,1955)	1:A:428:LEU:HD12	1:A:429:VAL:HA	20	0.12
(1,1955)	1:A:428:LEU:HD13	1:A:429:VAL:HA	20	0.12
(1,1955)	1:A:428:LEU:HD21	1:A:429:VAL:HA	20	0.12
(1,1955)	1:A:428:LEU:HD22	1:A:429:VAL:HA	20	0.12
(1,1955)	1:A:428:LEU:HD23	1:A:429:VAL:HA	20	0.12
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD11	48	0.12
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD12	48	0.12
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD13	48	0.12
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD21	48	0.12
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD22	48	0.12
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD23	48	0.12
(1,1549)	1:A:363:LEU:HD11	1:A:403:ILE:HA	9	0.12
(1,1549)	1:A:363:LEU:HD12	1:A:403:ILE:HA	9	0.12
(1,1549)	1:A:363:LEU:HD13	1:A:403:ILE:HA	9	0.12
(1,1549)	1:A:363:LEU:HD21	1:A:403:ILE:HA	9	0.12
(1,1549)	1:A:363:LEU:HD22	1:A:403:ILE:HA	9	0.12
(1,1549)	1:A:363:LEU:HD23	1:A:403:ILE:HA	9	0.12
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	7	0.12
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	7	0.12
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	7	0.12
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	7	0.12
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	7	0.12
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	7	0.12
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	33	0.12
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	33	0.12
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	33	0.12
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	33	0.12
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	33	0.12
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	33	0.12
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	11	0.12
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	11	0.12
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	11	0.12
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	47	0.12
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	47	0.12
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	47	0.12
(1,832)	1:A:363:LEU:HD11	1:A:412:ILE:HG21	25	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,832)	1:A:363:LEU:HD11	1:A:412:ILE:HG22	25	0.11
(1,832)	1:A:363:LEU:HD11	1:A:412:ILE:HG23	25	0.11
(1,832)	1:A:363:LEU:HD12	1:A:412:ILE:HG21	25	0.11
(1,832)	1:A:363:LEU:HD12	1:A:412:ILE:HG22	25	0.11
(1,832)	1:A:363:LEU:HD12	1:A:412:ILE:HG23	25	0.11
(1,832)	1:A:363:LEU:HD13	1:A:412:ILE:HG21	25	0.11
(1,832)	1:A:363:LEU:HD13	1:A:412:ILE:HG22	25	0.11
(1,832)	1:A:363:LEU:HD13	1:A:412:ILE:HG23	25	0.11
(1,812)	1:A:406:PHE:HE1	1:A:412:ILE:HD11	28	0.11
(1,812)	1:A:406:PHE:HE1	1:A:412:ILE:HD12	28	0.11
(1,812)	1:A:406:PHE:HE1	1:A:412:ILE:HD13	28	0.11
(1,812)	1:A:406:PHE:HE2	1:A:412:ILE:HD11	28	0.11
(1,812)	1:A:406:PHE:HE2	1:A:412:ILE:HD12	28	0.11
(1,812)	1:A:406:PHE:HE2	1:A:412:ILE:HD13	28	0.11
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD21	1	0.11
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD22	1	0.11
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD23	1	0.11
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD21	1	0.11
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD22	1	0.11
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD23	1	0.11
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD21	1	0.11
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD22	1	0.11
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD23	1	0.11
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD21	8	0.11
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD22	8	0.11
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD23	8	0.11
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD21	8	0.11
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD22	8	0.11
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD23	8	0.11
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD21	8	0.11
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD22	8	0.11
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD23	8	0.11
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD21	15	0.11
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD22	15	0.11
(1,473)	1:A:352:LEU:HD21	1:A:383:LEU:HD23	15	0.11
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD21	15	0.11
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD22	15	0.11
(1,473)	1:A:352:LEU:HD22	1:A:383:LEU:HD23	15	0.11
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD21	15	0.11
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD22	15	0.11
(1,473)	1:A:352:LEU:HD23	1:A:383:LEU:HD23	15	0.11
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD21	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD22	9	0.11
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD23	9	0.11
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD21	28	0.11
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD22	28	0.11
(1,286)	1:A:364:LYS:H	1:A:368:LEU:HD23	28	0.11
(1,28)	1:A:348:MET:HE1	1:A:384:GLN:H	9	0.11
(1,28)	1:A:348:MET:HE2	1:A:384:GLN:H	9	0.11
(1,28)	1:A:348:MET:HE3	1:A:384:GLN:H	9	0.11
(1,1955)	1:A:428:LEU:HD11	1:A:429:VAL:HA	15	0.11
(1,1955)	1:A:428:LEU:HD12	1:A:429:VAL:HA	15	0.11
(1,1955)	1:A:428:LEU:HD13	1:A:429:VAL:HA	15	0.11
(1,1955)	1:A:428:LEU:HD21	1:A:429:VAL:HA	15	0.11
(1,1955)	1:A:428:LEU:HD22	1:A:429:VAL:HA	15	0.11
(1,1955)	1:A:428:LEU:HD23	1:A:429:VAL:HA	15	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG11	24	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG12	24	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG13	24	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG21	24	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG22	24	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG23	24	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG11	24	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG12	24	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG13	24	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG21	24	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG22	24	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG23	24	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG11	25	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG12	25	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG13	25	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG21	25	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG22	25	0.11
(1,1947)	1:A:427:PHE:HB2	1:A:429:VAL:HG23	25	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG11	25	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG12	25	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG13	25	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG21	25	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG22	25	0.11
(1,1947)	1:A:427:PHE:HB3	1:A:429:VAL:HG23	25	0.11
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG11	13	0.11
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG12	13	0.11
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG13	13	0.11
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG21	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG22	13	0.11
(1,1835)	1:A:406:PHE:HB2	1:A:408:VAL:HG23	13	0.11
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD11	35	0.11
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD12	35	0.11
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD13	35	0.11
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD21	35	0.11
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD22	35	0.11
(1,1660)	1:A:380:LEU:HG	1:A:419:LEU:HD23	35	0.11
(1,1548)	1:A:363:LEU:HD11	1:A:403:ILE:H	3	0.11
(1,1548)	1:A:363:LEU:HD12	1:A:403:ILE:H	3	0.11
(1,1548)	1:A:363:LEU:HD13	1:A:403:ILE:H	3	0.11
(1,1548)	1:A:363:LEU:HD21	1:A:403:ILE:H	3	0.11
(1,1548)	1:A:363:LEU:HD22	1:A:403:ILE:H	3	0.11
(1,1548)	1:A:363:LEU:HD23	1:A:403:ILE:H	3	0.11
(1,1531)	1:A:363:LEU:HA	1:A:370:VAL:HG11	8	0.11
(1,1531)	1:A:363:LEU:HA	1:A:370:VAL:HG12	8	0.11
(1,1531)	1:A:363:LEU:HA	1:A:370:VAL:HG13	8	0.11
(1,1531)	1:A:363:LEU:HA	1:A:370:VAL:HG21	8	0.11
(1,1531)	1:A:363:LEU:HA	1:A:370:VAL:HG22	8	0.11
(1,1531)	1:A:363:LEU:HA	1:A:370:VAL:HG23	8	0.11
(1,1452)	1:A:348:MET:HE1	1:A:389:GLN:HE21	17	0.11
(1,1452)	1:A:348:MET:HE1	1:A:389:GLN:HE22	17	0.11
(1,1452)	1:A:348:MET:HE2	1:A:389:GLN:HE21	17	0.11
(1,1452)	1:A:348:MET:HE2	1:A:389:GLN:HE22	17	0.11
(1,1452)	1:A:348:MET:HE3	1:A:389:GLN:HE21	17	0.11
(1,1452)	1:A:348:MET:HE3	1:A:389:GLN:HE22	17	0.11
(1,1026)	1:A:428:LEU:HD11	1:A:429:VAL:H	12	0.11
(1,1026)	1:A:428:LEU:HD12	1:A:429:VAL:H	12	0.11
(1,1026)	1:A:428:LEU:HD13	1:A:429:VAL:H	12	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	77	50.0	5	6.5	3.2	0	0.0	0.0
PSI	77	50.0	4	5.2	2.6	0	0.0	0.0
Total	154	100.0	9	5.8	5.8	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 ⓘ
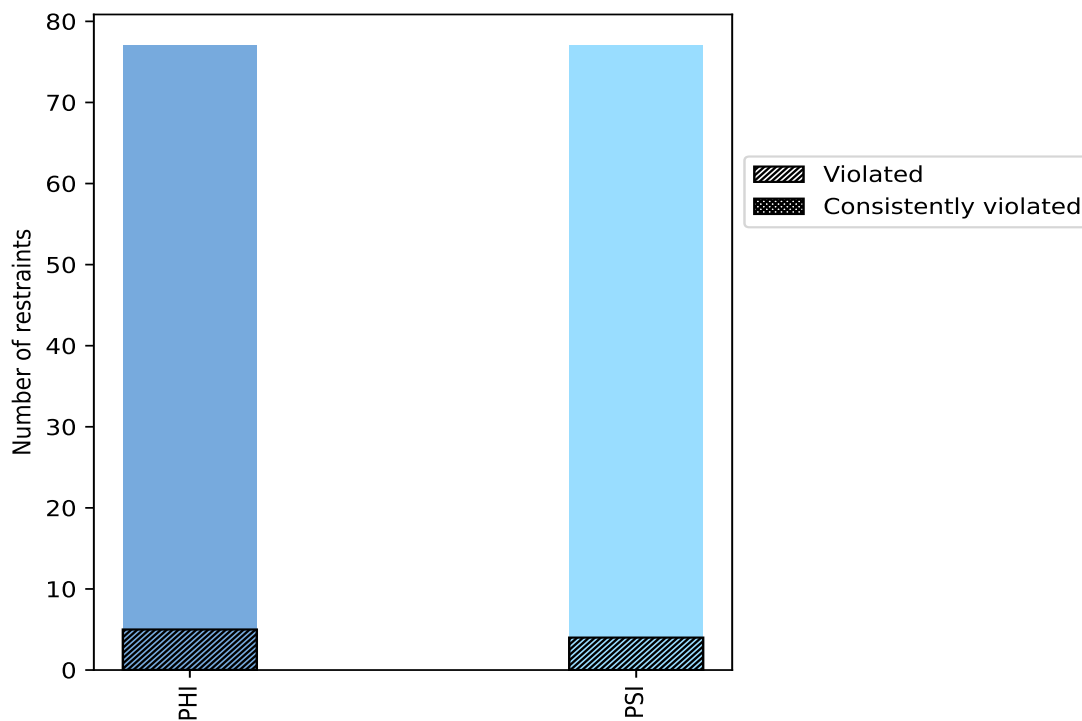
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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	2	0	2	3.4	3.4	0.0	3.4
2	0	1	1	4.5	4.5	0.0	4.5
3	1	0	1	4.0	4.0	0.0	4.0
4	2	0	2	3.55	4.3	0.75	3.55
5	2	2	4	3.32	4.0	0.5	3.35
6	2	0	2	3.1	4.9	1.8	3.1
7	1	0	1	4.5	4.5	0.0	4.5
8	2	1	3	2.67	4.9	1.59	1.8
9	1	2	3	2.73	3.4	0.87	3.3
10	2	0	2	3.7	4.6	0.9	3.7
11	2	0	2	3.75	4.2	0.45	3.75
12	1	0	1	4.9	4.9	0.0	4.9
13	0	1	1	4.9	4.9	0.0	4.9
14	1	1	2	2.2	2.7	0.5	2.2
15	1	1	2	4.3	4.6	0.3	4.3
16	2	0	2	2.95	4.5	1.55	2.95
17	2	2	4	3.45	4.8	1.32	3.6
18	1	0	1	4.8	4.8	0.0	4.8
19	2	1	3	2.67	4.6	1.45	2.3
20	0	1	1	4.7	4.7	0.0	4.7
21	1	0	1	4.2	4.2	0.0	4.2
22	2	0	2	3.15	4.8	1.65	3.15
23	2	0	2	3.35	4.3	0.95	3.35
24	1	0	1	4.1	4.1	0.0	4.1
25	1	0	1	3.9	3.9	0.0	3.9
26	1	1	2	3.4	4.8	1.4	3.4
27	1	0	1	5.0	5.0	0.0	5.0
28	5	1	6	3.48	5.0	1.3	3.65
29	2	0	2	4.45	4.6	0.15	4.45
30	1	0	1	4.2	4.2	0.0	4.2
31	2	0	2	2.8	3.1	0.3	2.8
32	2	0	2	2.7	3.4	0.7	2.7
33	2	1	3	3.1	4.2	1.42	4.0
34	1	0	1	4.9	4.9	0.0	4.9
35	1	0	1	4.8	4.8	0.0	4.8
36	1	2	3	3.03	3.8	0.88	3.5
37	1	0	1	4.8	4.8	0.0	4.8
38	1	0	1	4.2	4.2	0.0	4.2

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	0	1	1	3.9	3.9	0.0	3.9
40	2	1	3	2.37	2.9	0.75	2.9
41	1	0	1	4.5	4.5	0.0	4.5
42	1	0	1	4.8	4.8	0.0	4.8
43	1	0	1	5.0	5.0	0.0	5.0
44	1	0	1	4.6	4.6	0.0	4.6
45	1	0	1	4.8	4.8	0.0	4.8
46	1	0	1	4.9	4.9	0.0	4.9
47	1	1	2	3.15	4.9	1.75	3.15
48	1	0	1	4.8	4.8	0.0	4.8
49	1	0	1	4.9	4.9	0.0	4.9
50	0	0	0	0.0	0.0	0.0	0.0

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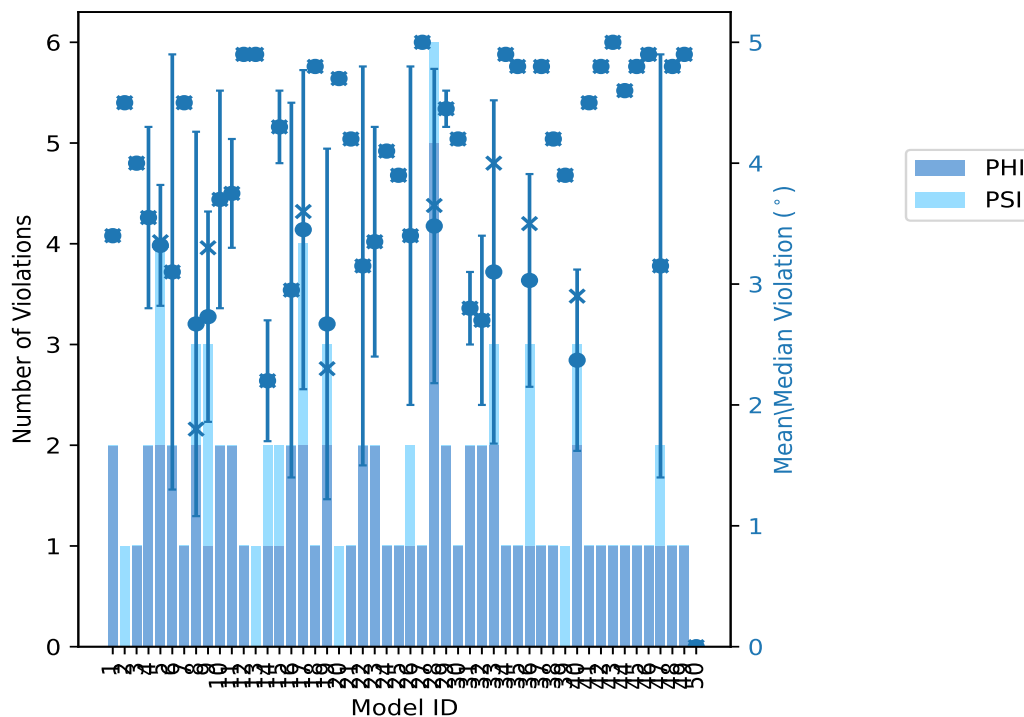
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

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]	%
1	2	3	1	2.0
1	0	1	2	4.0
0	0	0	3	6.0
1	0	1	4	8.0
0	0	0	5	10.0
0	1	1	6	12.0
0	0	0	7	14.0
0	0	0	8	16.0
0	0	0	9	18.0
0	0	0	10	20.0
0	0	0	11	22.0
0	0	0	12	24.0
0	1	1	13	26.0
0	0	0	14	28.0
0	0	0	15	30.0
0	0	0	16	32.0
0	0	0	17	34.0
0	0	0	18	36.0
0	0	0	19	38.0
0	0	0	20	40.0
0	0	0	21	42.0
0	0	0	22	44.0
0	0	0	23	46.0
0	0	0	24	48.0
0	0	0	25	50.0
0	0	0	26	52.0
0	0	0	27	54.0
1	0	1	28	56.0
0	0	0	29	58.0
0	0	0	30	60.0
1	0	1	31	62.0
0	0	0	32	64.0
0	0	0	33	66.0
0	0	0	34	68.0
0	0	0	35	70.0
0	0	0	36	72.0
0	0	0	37	74.0

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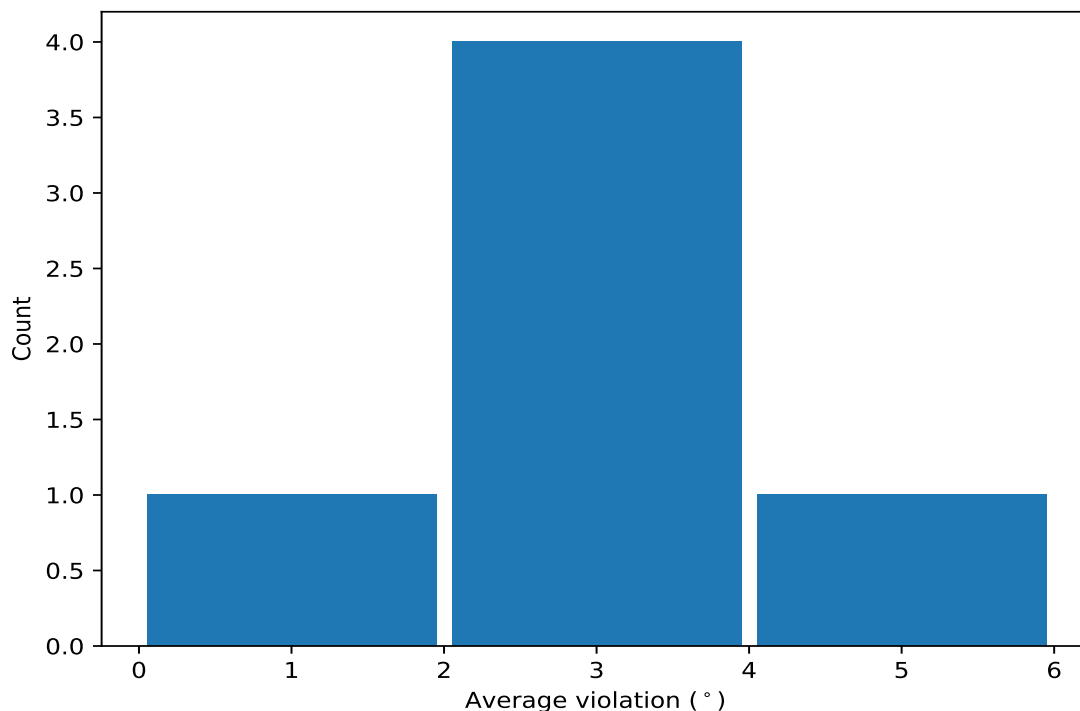| Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	38	76.0
0	0	0	39	78.0
0	0	0	40	80.0
0	0	0	41	82.0
0	0	0	42	84.0
0	0	0	43	86.0
0	0	0	44	88.0
0	0	0	45	90.0
0	0	0	46	92.0
0	0	0	47	94.0
0	0	0	48	96.0
0	0	0	49	98.0
0	0	0	50	100.0

[1] Number of models with violations

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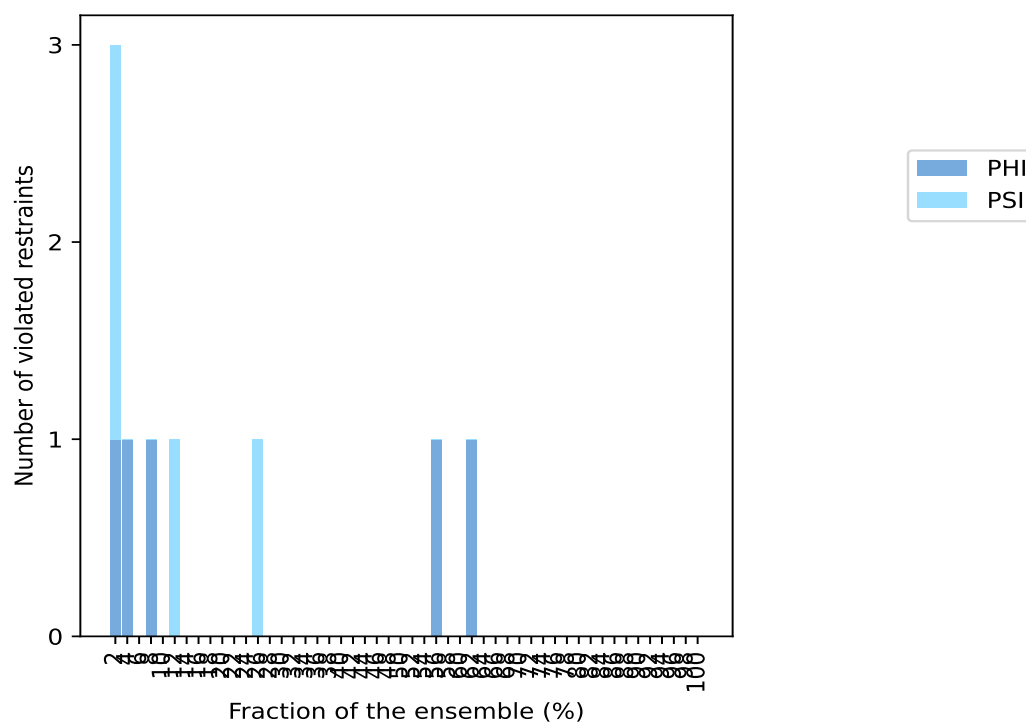
10.4   Most violated dihedral-angle restraints in the ensemble   ⓘ

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
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	31	3.67	1.23	4.1
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	28	4.04	0.83	4.2
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	13	3.21	1.24	3.5
(1,34)	1:A:363:LEU:N	1:A:363:LEU:CA	1:A:363:LEU:C	1:A:364:LYS:N	6	3.4	1.57	4.0
(1,3)	1:A:347:SER:C	1:A:348:MET:N	1:A:348:MET:CA	1:A:348:MET:C	4	3.05	1.24	3.05
(1,29)	1:A:360:LYS:C	1:A:361:ASN:N	1:A:361:ASN:CA	1:A:361:ASN:C	2	1.5	0.3	1.5

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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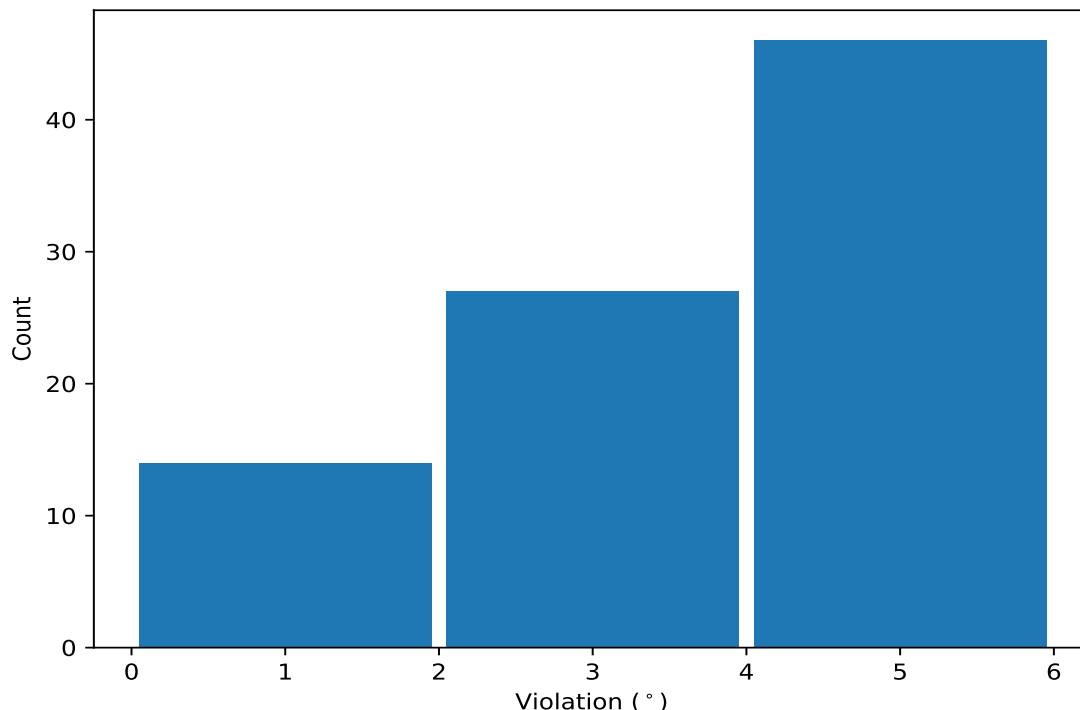
10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	27	5.0
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	43	5.0
(1,34)	1:A:363:LEU:N	1:A:363:LEU:CA	1:A:363:LEU:C	1:A:364:LYS:N	28	5.0
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	12	4.9
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	34	4.9
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	46	4.9
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	49	4.9
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	13	4.9
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	6	4.9
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	8	4.9
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	47	4.9
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	18	4.8
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	35	4.8
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	37	4.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	42	4.8
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	45	4.8
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	48	4.8
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	26	4.8
(1,34)	1:A:363:LEU:N	1:A:363:LEU:CA	1:A:363:LEU:C	1:A:364:LYS:N	17	4.8
(1,3)	1:A:347:SER:C	1:A:348:MET:N	1:A:348:MET:CA	1:A:348:MET:C	22	4.8
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	20	4.7
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	17	4.7
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	28	4.7
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	15	4.6
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	44	4.6
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	10	4.6
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	29	4.6
(1,34)	1:A:363:LEU:N	1:A:363:LEU:CA	1:A:363:LEU:C	1:A:364:LYS:N	19	4.6
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	2	4.5
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	7	4.5
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	16	4.5
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	41	4.5
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	29	4.3
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	4	4.3
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	23	4.3
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	11	4.2
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	21	4.2
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	30	4.2
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	33	4.2
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	38	4.2
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	28	4.1
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	24	4.1
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	33	4.0
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	5	4.0
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	15	4.0
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	3	4.0
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	39	3.9
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	25	3.9
(1,44)	1:A:368:LEU:N	1:A:368:LEU:CA	1:A:368:LEU:C	1:A:369:ASP:N	36	3.8
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	36	3.5
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	1	3.4
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	9	3.4
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1	3.4
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	32	3.4
(1,34)	1:A:363:LEU:N	1:A:363:LEU:CA	1:A:363:LEU:C	1:A:364:LYS:N	5	3.4
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	9	3.3
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	11	3.3
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	5	3.3
(1,3)	1:A:347:SER:C	1:A:348:MET:N	1:A:348:MET:CA	1:A:348:MET:C	28	3.2
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	31	3.1
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	40	2.9
(1,3)	1:A:347:SER:C	1:A:348:MET:N	1:A:348:MET:CA	1:A:348:MET:C	40	2.9
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	4	2.8
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	10	2.8
(1,73)	1:A:384:GLN:C	1:A:385:VAL:N	1:A:385:VAL:CA	1:A:385:VAL:C	28	2.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	14	2.7
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	5	2.6
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	31	2.5
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	17	2.5
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	23	2.4
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	19	2.3
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	32	2.0
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	26	2.0
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	8	1.8
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	36	1.8
(1,29)	1:A:360:LYS:C	1:A:361:ASN:N	1:A:361:ASN:CA	1:A:361:ASN:C	17	1.8
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	14	1.7
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	22	1.5
(1,34)	1:A:363:LEU:N	1:A:363:LEU:CA	1:A:363:LEU:C	1:A:364:LYS:N	9	1.5
(1,81)	1:A:388:GLN:C	1:A:389:GLN:N	1:A:389:GLN:CA	1:A:389:GLN:C	16	1.4
(1,10)	1:A:351:ARG:N	1:A:351:ARG:CA	1:A:351:ARG:C	1:A:352:LEU:N	47	1.4
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	8	1.3
(1,42)	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	1:A:368:LEU:N	40	1.3
(1,3)	1:A:347:SER:C	1:A:348:MET:N	1:A:348:MET:CA	1:A:348:MET:C	6	1.3
(1,29)	1:A:360:LYS:C	1:A:361:ASN:N	1:A:361:ASN:CA	1:A:361:ASN:C	28	1.2
(1,41)	1:A:366:ASP:C	1:A:367:ASN:N	1:A:367:ASN:CA	1:A:367:ASN:C	19	1.1
(1,34)	1:A:363:LEU:N	1:A:363:LEU:CA	1:A:363:LEU:C	1:A:364:LYS:N	33	1.1