



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:15 PM UTC

PDB ID : 6F9A / pdb_00006f9a
BMRB ID : 34219
Title : Solution structure of the MRH domain of Yos9 complexed with alpha3,alpha6-Man5
Authors : Kniss, A.; Kazemi, S.; Lohr, F.; Guntert, P.; Dotsch, V.
Deposited on : 2017-12-14

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

We welcome your comments at validation@mail.wwpdb.org

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<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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

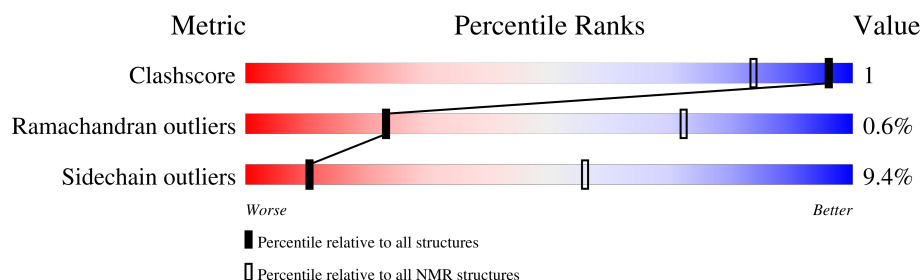
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	162	

2 Ensemble composition and analysis

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

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:95-A:142, A:148-A:149, A:156-A:245 (140)	0.40	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2534 atoms, of which 1248 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ER quality-control lectin.

Mol	Chain	Residues	Atoms						Trace
1	A	162	Total	C	H	N	O	S	0
			2534	814	1248	211	254	7	

There are 2 discrepancies between the modelled and reference sequences:

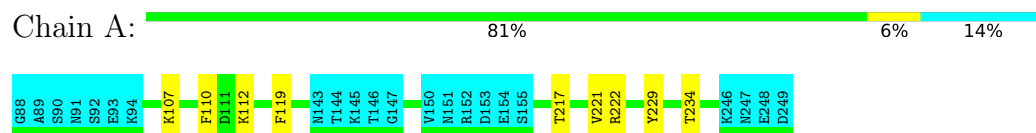
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLY	-	expression tag	UNP A0A250W9K2
A	89	ALA	-	expression tag	UNP A0A250W9K2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: ER quality-control lectin

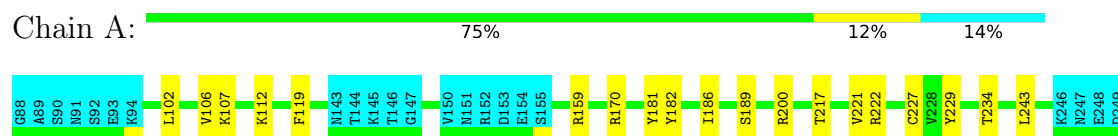


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

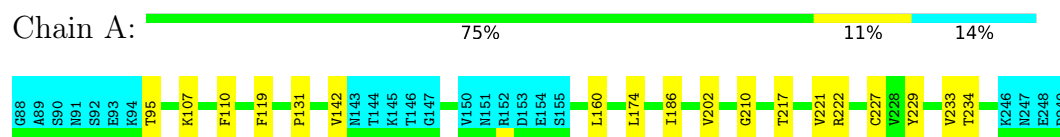
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: ER quality-control lectin



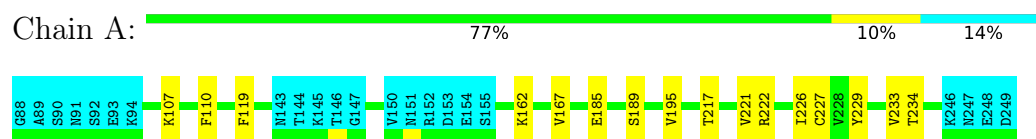
4.2.2 Score per residue for model 2

- Molecule 1: ER quality-control lectin



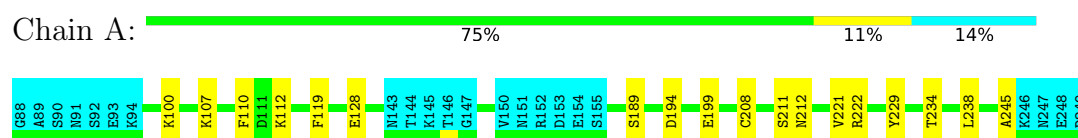
4.2.3 Score per residue for model 3

- Molecule 1: ER quality-control lectin



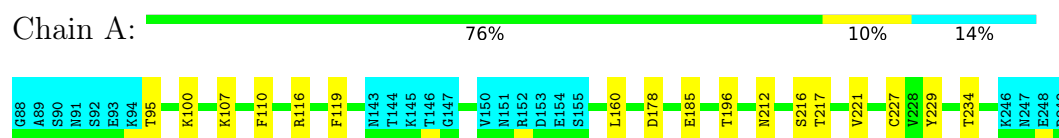
4.2.4 Score per residue for model 4

- Molecule 1: ER quality-control lectin



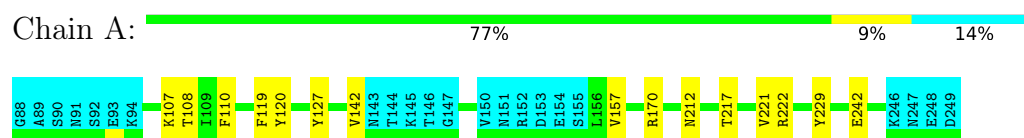
4.2.5 Score per residue for model 5

- Molecule 1: ER quality-control lectin



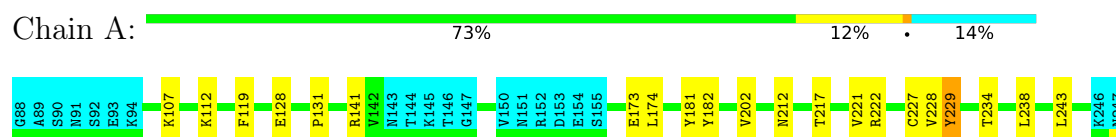
4.2.6 Score per residue for model 6

- Molecule 1: ER quality-control lectin



4.2.7 Score per residue for model 7

- Molecule 1: ER quality-control lectin



E248
D249

4.2.8 Score per residue for model 8

- Molecule 1: ER quality-control lectin

Chain A:  77% 9% 14%

G88 A89 S90 N91 S92 E93 K94 K107 F110 D111 K112 F119 E128 R141 Y142 N143 T144 K145 T146 G147 V150 N151 R152 D153 E154 S155 R170 M201 N212 T217 V221 R222 V228 Y229 T234 K246 N247 E248 D249

4.2.9 Score per residue for model 9

- Molecule 1: ER quality-control lectin

Chain A:  72% 14% 14%

G88 A89 S90 N91 S92 E93 K94 K100 K107 F110 D111 K112 F119 Y127 C130 P131 F135 R141 Y142 N143 T144 K145 T146 G147 V150 N151 R152 D153 E154 S155 Y181 E185 I186 S189 R200 T217 W220 V221 R222 C227 V228 Y229 T234 L243 L244 A245 K246 N247 E248 D249

4.2.10 Score per residue for model 10

- Molecule 1: ER quality-control lectin

Chain A:  74% 12% 14%

G88 A89 S90 N91 S92 E93 K94 L102 N103 V106 K107 F110 D111 K112 F119 R141 Y142 N143 T144 K145 T146 G147 I149 V150 N151 R152 D153 E154 S155 R159 Y181 R200 T217 V221 R222 C227 V228 Y229 T234 E237 L243 K246 N247 E248 D249

4.2.11 Score per residue for model 11

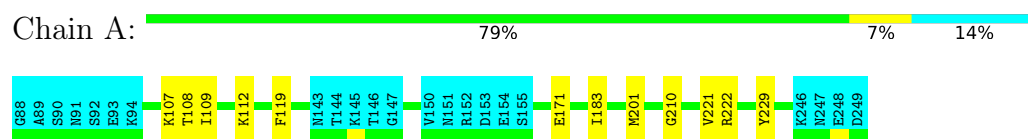
- Molecule 1: ER quality-control lectin

Chain A:  75% 11% 14%

G88 A89 S90 N91 S92 E93 K94 T101 F110 D111 K112 L113 M114 F119 N143 T144 K145 T146 G147 V150 N151 R152 D153 E154 S155 Y158 R170 E171 F172 D178 S184 E185 I186 N212 T217 V221 R222 Y229 T234 E242 K246 N247 E248 D249

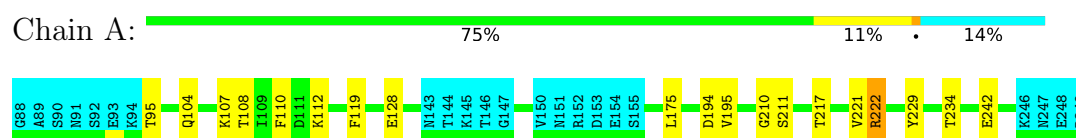
4.2.12 Score per residue for model 12

- Molecule 1: ER quality-control lectin



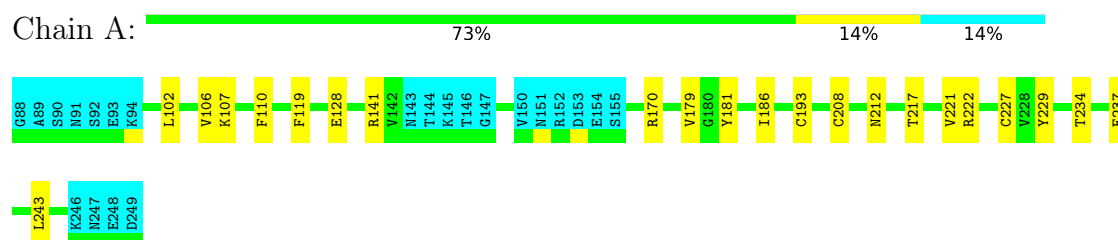
4.2.13 Score per residue for model 13

- Molecule 1: ER quality-control lectin



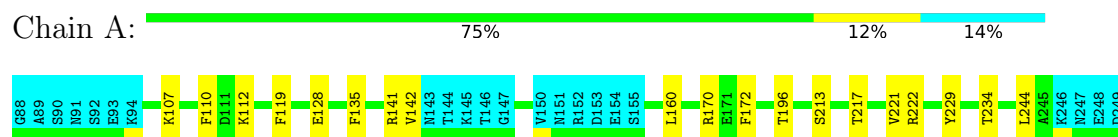
4.2.14 Score per residue for model 14

- Molecule 1: ER quality-control lectin



4.2.15 Score per residue for model 15

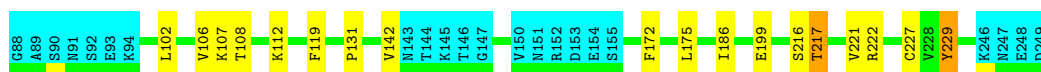
- Molecule 1: ER quality-control lectin



4.2.16 Score per residue for model 16

- Molecule 1: ER quality-control lectin





4.2.17 Score per residue for model 17

- Molecule 1: ER quality-control lectin

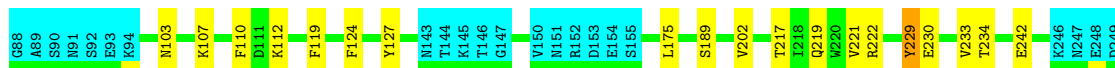
Chain A: 78% 7% 14%



4.2.18 Score per residue for model 18

- Molecule 1: ER quality-control lectin

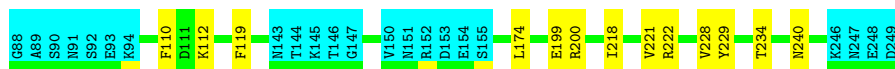
Chain A: 75% 11% 14%



4.2.19 Score per residue for model 19

- Molecule 1: ER quality-control lectin

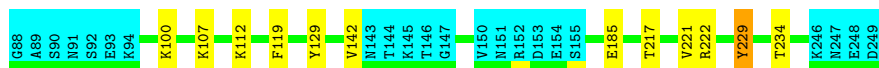
Chain A: 78% 8% 14%



4.2.20 Score per residue for model 20

- Molecule 1: ER quality-control lectin

Chain A: 79% 7% 14%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3.9
OPAL	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	1891
Number of shifts mapped to atoms	1891
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality i

6.1 Standard geometry i

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	0.60±0.01	0±0/1145 (0.0± 0.0%)	1.31±0.03	1±1/1554 (0.1± 0.1%)
All	All	0.60	0/22900 (0.0%)	1.31	26/31080 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.9
All	All	0	18

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	172	PHE	CA-CB-CG	6.68	120.48	113.80	15	2
1	A	211	SER	CA-C-N	6.40	133.77	121.54	4	1
1	A	211	SER	C-N-CA	6.40	133.77	121.54	4	1
1	A	179	VAL	N-CA-C	-6.20	105.10	110.74	14	1
1	A	135	PHE	CA-CB-CG	6.10	119.90	113.80	15	2
1	A	241	LEU	CA-C-N	5.80	128.85	120.38	17	1
1	A	241	LEU	C-N-CA	5.80	128.85	120.38	17	1
1	A	167	VAL	CA-C-N	5.70	129.72	120.60	3	1
1	A	167	VAL	C-N-CA	5.70	129.72	120.60	3	1
1	A	186	ILE	CB-CA-C	5.62	118.48	110.84	2	2
1	A	114	ASN	CA-C-N	5.39	127.77	120.44	11	1
1	A	114	ASN	C-N-CA	5.39	127.77	120.44	11	1
1	A	149	ILE	N-CA-C	-5.38	104.13	110.21	10	1
1	A	240	ASN	CA-C-N	5.26	128.81	121.24	19	1
1	A	240	ASN	C-N-CA	5.26	128.81	121.24	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	245	ALA	CA-C-N	5.24	131.38	121.69	9	2
1	A	245	ALA	C-N-CA	5.24	131.38	121.69	9	2
1	A	124	PHE	CA-CB-CG	5.16	118.96	113.80	18	1
1	A	196	THR	CA-CB-OG1	5.10	117.25	109.60	5	1
1	A	130	CYS	CA-C-N	5.06	126.16	119.84	9	1
1	A	130	CYS	C-N-CA	5.06	126.16	119.84	9	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	170	ARG	Sidechain	4
1	A	222	ARG	Sidechain	3
1	A	159	ARG	Sidechain	2
1	A	182	TYR	Sidechain	2
1	A	141	ARG	Sidechain	2
1	A	116	ARG	Sidechain	1
1	A	120	TYR	Sidechain	1
1	A	158	TYR	Sidechain	1
1	A	200	ARG	Sidechain	1
1	A	129	TYR	Sidechain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1121	1097	1097	2±1
All	All	22420	21940	21940	41

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:221:VAL:HG13	1:A:229:TYR:CE1	0.75	2.16	20	20
1:A:181:TYR:CE2	1:A:243:LEU:HD22	0.60	2.30	7	4
1:A:181:TYR:CE2	1:A:243:LEU:HD13	0.49	2.42	1	2
1:A:181:TYR:CZ	1:A:243:LEU:HD22	0.48	2.44	1	2
1:A:102:LEU:O	1:A:106:VAL:HG23	0.46	2.10	1	4
1:A:106:VAL:HG22	1:A:172:PHE:CD2	0.44	2.48	16	1
1:A:109:ILE:HD11	1:A:183:ILE:HD12	0.44	1.89	12	1
1:A:226:ILE:HD12	1:A:226:ILE:H	0.42	1.73	3	1
1:A:220:TRP:CE3	1:A:222:ARG:HD2	0.42	2.50	17	1
1:A:127:TYR:CD1	1:A:221:VAL:HG11	0.42	2.50	9	3
1:A:216:SER:O	1:A:217:THR:HG23	0.41	2.14	16	1
1:A:220:TRP:CE3	1:A:222:ARG:CD	0.40	3.04	9	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/162 (86%)	128±2 (91±1%)	11±2 (8±1%)	1±1 (1±1%)	23	72
All	All	2800/3240 (86%)	2558 (91%)	224 (8%)	18 (1%)	23	72

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	212	ASN	7
1	A	131	PRO	4
1	A	189	SER	3
1	A	210	GLY	3
1	A	200	ARG	1

6.3.2 Protein sidechains [i](#)

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	122/141 (87%)	111±3 (91±2%)	11±3 (9±2%)	10	56
All	All	2440/2820 (87%)	2211 (91%)	229 (9%)	10	56

All 51 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	119	PHE	20
1	A	107	LYS	18
1	A	222	ARG	18
1	A	234	THR	17
1	A	217	THR	16
1	A	110	PHE	15
1	A	112	LYS	14
1	A	227	CYS	9
1	A	128	GLU	6
1	A	142	VAL	5
1	A	186	ILE	4
1	A	185	GLU	4
1	A	100	LYS	4
1	A	108	THR	4
1	A	242	GLU	4
1	A	141	ARG	4
1	A	229	TYR	4
1	A	95	THR	3
1	A	160	LEU	3
1	A	174	LEU	3
1	A	202	VAL	3
1	A	233	VAL	3
1	A	199	GLU	3
1	A	208	CYS	3
1	A	228	VAL	3
1	A	175	LEU	3
1	A	200	ARG	2
1	A	189	SER	2
1	A	195	VAL	2
1	A	194	ASP	2
1	A	238	LEU	2
1	A	178	ASP	2
1	A	201	MET	2
1	A	103	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	237	GLU	2
1	A	170	ARG	2
1	A	230	GLU	2
1	A	162	LYS	1
1	A	216	SER	1
1	A	157	VAL	1
1	A	173	GLU	1
1	A	101	THR	1
1	A	184	SER	1
1	A	171	GLU	1
1	A	104	GLN	1
1	A	211	SER	1
1	A	193	CYS	1
1	A	196	THR	1
1	A	213	SER	1
1	A	219	GLN	1
1	A	218	ILE	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *minimized.str*

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	1891
Number of shifts mapped to atoms	1891
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	155	0.08 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	142	-0.12 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	146	0.28 ± 0.18	None needed (< 0.5 ppm)
^{15}N	146	0.10 ± 0.30	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1735 atoms were assigned a chemical shift out of a possible 1932. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	693/704 (98%)	285/288 (99%)	274/280 (98%)	134/136 (99%)
Sidechain	905/1056 (86%)	617/688 (90%)	288/333 (86%)	0/35 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	137/172 (80%)	76/82 (93%)	59/87 (68%)	2/3 (67%)
Overall	1735/1932 (90%)	978/1058 (92%)	621/700 (89%)	136/174 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1891 atoms were assigned a chemical shift out of a possible 2193. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	760/816 (93%)	313/334 (94%)	301/324 (93%)	146/158 (92%)
Sidechain	994/1205 (82%)	678/779 (87%)	316/381 (83%)	0/45 (0%)
Aromatic	137/172 (80%)	76/82 (93%)	59/87 (68%)	2/3 (67%)
Overall	1891/2193 (86%)	1067/1195 (89%)	676/792 (85%)	148/206 (72%)

7.1.4 Statistically unusual chemical shifts ⓘ

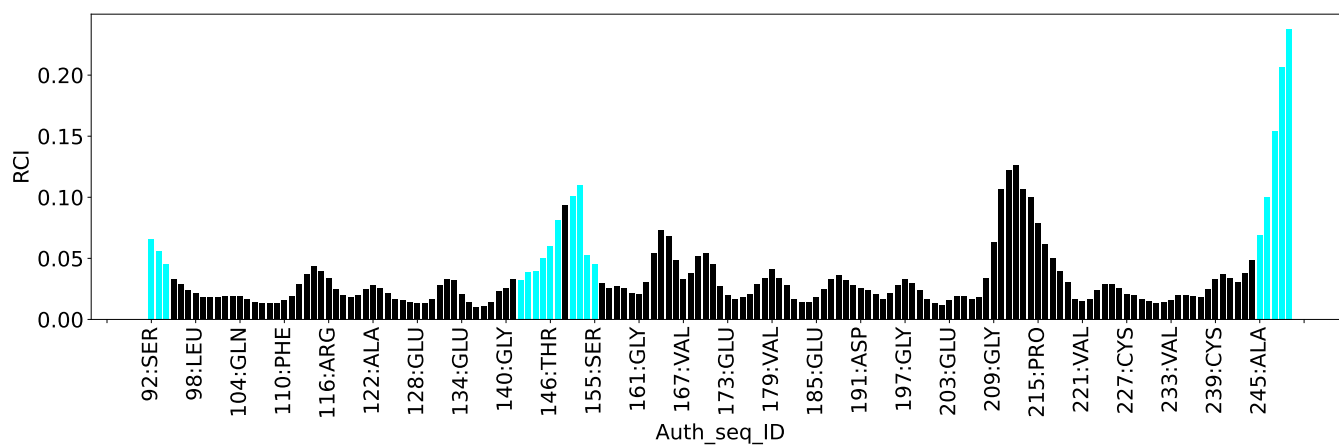
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	232	GLN	HB3	0.06	0.71 – 3.33	-7.5
1	A	232	GLN	HB2	0.25	0.80 – 3.29	-7.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3575
Intra-residue ($ i-j =0$)	666
Sequential ($ i-j =1$)	957
Medium range ($ i-j >1$ and $ i-j <5$)	521
Long range ($ i-j \geq 5$)	1431
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	509
Number of unmapped restraints	0
Number of restraints per residue	25.2
Number of long range restraints per residue ¹	8.8

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	1.9	0.12
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model [i](#)

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)	1.2	9.57
10.0-20.0 (Medium)	0.1	14.89
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

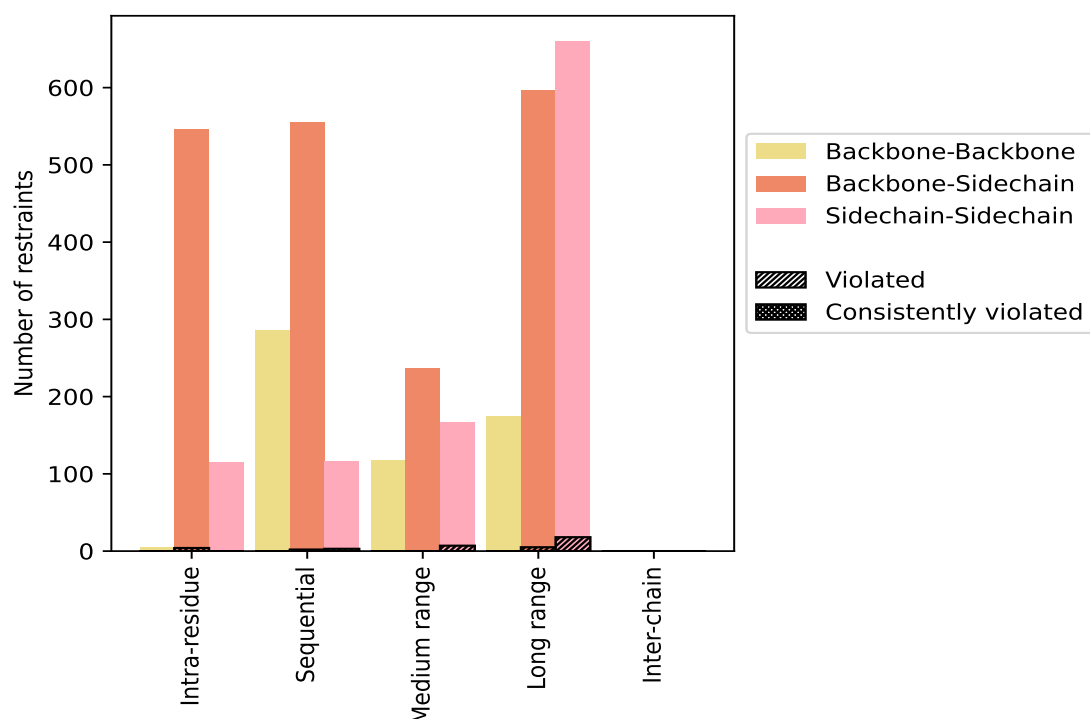
9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	666	18.6	4	0.6	0.1	0	0.0	0.0
Backbone-Backbone	5	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	546	15.3	4	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	115	3.2	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	957	26.8	5	0.5	0.1	0	0.0	0.0
Backbone-Backbone	286	8.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	555	15.5	2	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	116	3.2	3	2.6	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	521	14.6	7	1.3	0.2	0	0.0	0.0
Backbone-Backbone	117	3.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	237	6.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	167	4.7	7	4.2	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	1431	40.0	23	1.6	0.6	0	0.0	0.0
Backbone-Backbone	174	4.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	597	16.7	5	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	660	18.5	18	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	3575	100.0	39	1.1	1.1	0	0.0	0.0
Backbone-Backbone	582	16.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1935	54.1	11	0.6	0.3	0	0.0	0.0
Sidechain-Sidechain	1058	29.6	28	2.6	0.8	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	1	0	1	0.11	0.11	0.0	0.11
2	0	0	2	0	0	2	0.11	0.11	0.0	0.11
3	0	0	0	3	0	3	0.1	0.11	0.0	0.1
4	1	0	1	0	0	2	0.11	0.11	0.0	0.11
5	0	0	0	2	0	2	0.12	0.12	0.0	0.12
6	0	0	2	2	0	4	0.11	0.12	0.01	0.11
7	0	0	2	2	0	4	0.11	0.12	0.01	0.11
8	0	2	0	2	0	4	0.11	0.11	0.0	0.11
9	0	0	0	1	0	1	0.11	0.11	0.0	0.11
10	1	0	1	3	0	5	0.1	0.11	0.0	0.1

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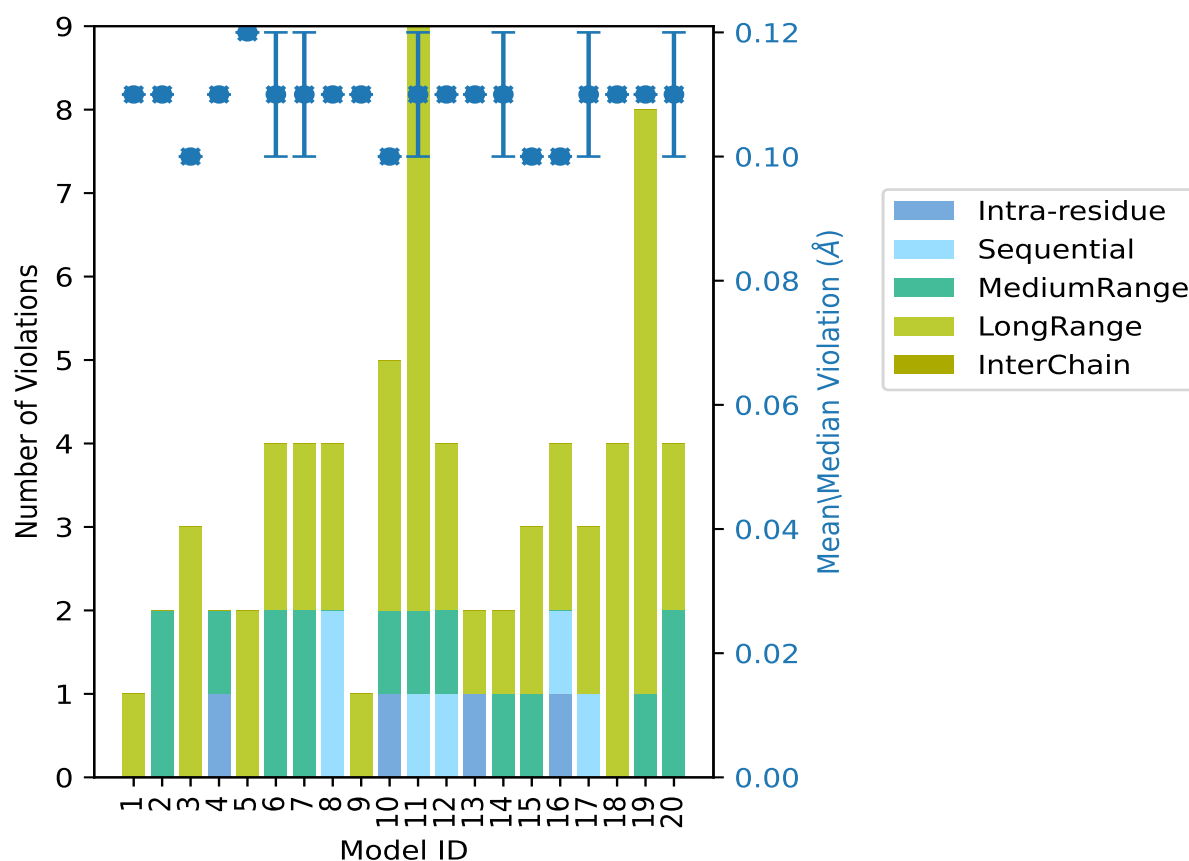
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	1	7	0	9	0.11	0.12	0.01	0.11
12	0	1	1	2	0	4	0.11	0.11	0.0	0.11
13	1	0	0	1	0	2	0.11	0.11	0.0	0.11
14	0	0	1	1	0	2	0.11	0.12	0.01	0.11
15	0	0	1	2	0	3	0.1	0.1	0.0	0.1
16	1	1	0	2	0	4	0.1	0.1	0.0	0.1
17	0	1	0	2	0	3	0.11	0.12	0.01	0.11
18	0	0	0	4	0	4	0.11	0.11	0.0	0.11
19	0	0	1	7	0	8	0.11	0.11	0.0	0.11
20	0	0	2	2	0	4	0.11	0.12	0.01	0.11

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

⁵Inter-chain restraints, ⁶Standard 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

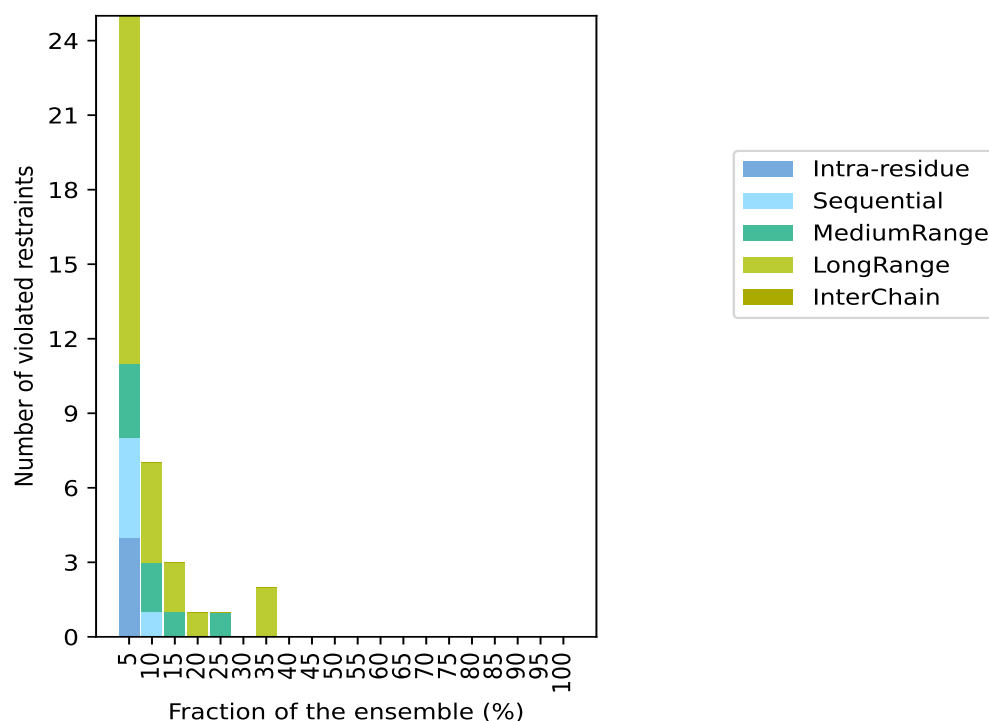
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3536(IR:662, SQ:952, MR:514, LR:1408, IC:0) restraints are 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	%
4	4	3	14	0	25	1	5.0
0	1	2	4	0	7	2	10.0
0	0	1	2	0	3	3	15.0
0	0	0	1	0	1	4	20.0
0	0	1	0	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	2	0	2	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

⁵Inter-chain restraints, ⁶ Number of models with violations

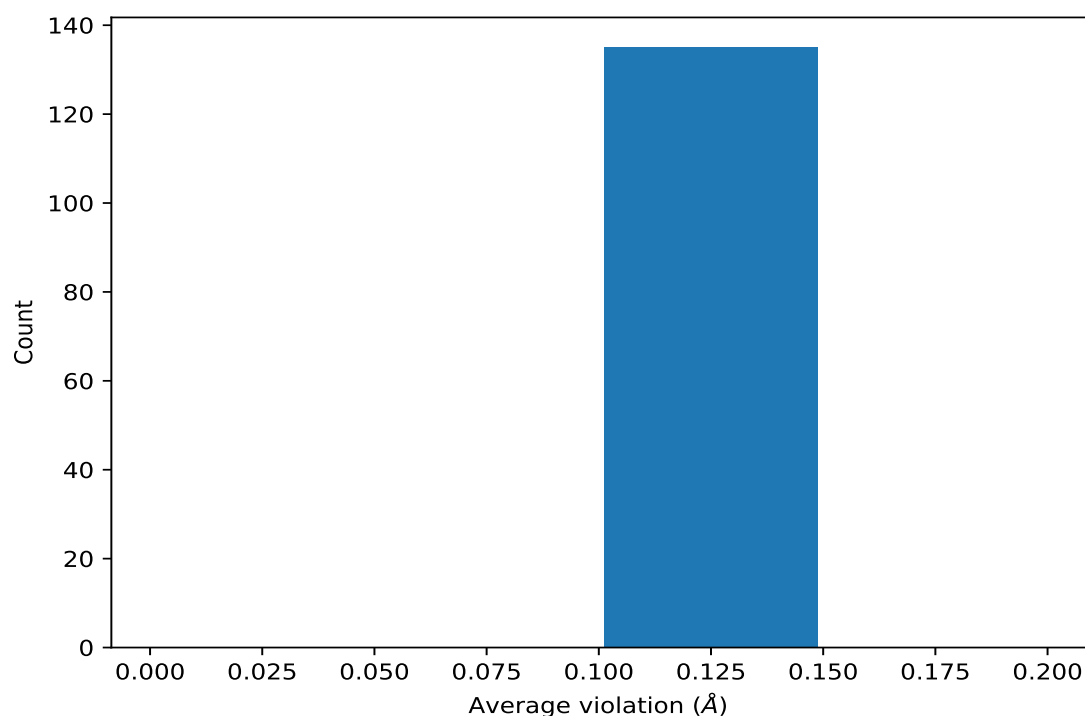
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD11	7	0.11	0.01	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD12	7	0.11	0.01	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD13	7	0.11	0.01	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD11	7	0.11	0.01	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD12	7	0.11	0.01	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD13	7	0.11	0.01	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD11	7	0.11	0.01	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD12	7	0.11	0.01	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD13	7	0.11	0.01	0.11
(1,3337)	1:175:A:LEU:HD11	1:183:A:ILE:HA	7	0.1	0.0	0.1
(1,3337)	1:175:A:LEU:HD12	1:183:A:ILE:HA	7	0.1	0.0	0.1
(1,3337)	1:175:A:LEU:HD13	1:183:A:ILE:HA	7	0.1	0.0	0.1
(1,3337)	1:175:A:LEU:HD21	1:183:A:ILE:HA	7	0.1	0.0	0.1
(1,3337)	1:175:A:LEU:HD22	1:183:A:ILE:HA	7	0.1	0.0	0.1
(1,3337)	1:175:A:LEU:HD23	1:183:A:ILE:HA	7	0.1	0.0	0.1
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD1	5	0.11	0.01	0.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD2	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD1	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD2	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD1	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD2	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD1	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD2	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD1	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD2	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD1	5	0.11	0.01	0.1
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD2	5	0.11	0.01	0.1
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB1	4	0.11	0.01	0.11
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB2	4	0.11	0.01	0.11
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB3	4	0.11	0.01	0.11
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB1	4	0.11	0.01	0.11
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB2	4	0.11	0.01	0.11
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB3	4	0.11	0.01	0.11
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB1	4	0.11	0.01	0.11
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB2	4	0.11	0.01	0.11
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB3	4	0.11	0.01	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG11	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG12	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG13	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG21	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG22	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG23	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG11	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG12	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG13	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG21	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG22	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG23	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG11	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG12	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG13	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG21	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG22	3	0.11	0.0	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG23	3	0.11	0.0	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG11	3	0.11	0.0	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG12	3	0.11	0.0	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG13	3	0.11	0.0	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG21	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG22	3	0.11	0.0	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG23	3	0.11	0.0	0.11
(1,1528)	1:109:A:ILE:HG21	1:112:A:LYS:HB2	3	0.1	0.0	0.1
(1,1528)	1:109:A:ILE:HG21	1:112:A:LYS:HB3	3	0.1	0.0	0.1
(1,1528)	1:109:A:ILE:HG22	1:112:A:LYS:HB2	3	0.1	0.0	0.1
(1,1528)	1:109:A:ILE:HG22	1:112:A:LYS:HB3	3	0.1	0.0	0.1
(1,1528)	1:109:A:ILE:HG23	1:112:A:LYS:HB2	3	0.1	0.0	0.1
(1,1528)	1:109:A:ILE:HG23	1:112:A:LYS:HB3	3	0.1	0.0	0.1
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD11	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD12	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD13	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD21	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD22	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD23	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD11	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD12	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD13	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD21	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD22	2	0.12	0.0	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD23	2	0.12	0.0	0.12
(1,1816)	1:109:A:ILE:HD11	1:241:A:LEU:HD11	2	0.11	0.0	0.11
(1,1816)	1:109:A:ILE:HD11	1:241:A:LEU:HD12	2	0.11	0.0	0.11
(1,1816)	1:109:A:ILE:HD11	1:241:A:LEU:HD13	2	0.11	0.0	0.11
(1,1816)	1:109:A:ILE:HD12	1:241:A:LEU:HD11	2	0.11	0.0	0.11
(1,1816)	1:109:A:ILE:HD12	1:241:A:LEU:HD12	2	0.11	0.0	0.11
(1,1816)	1:109:A:ILE:HD12	1:241:A:LEU:HD13	2	0.11	0.0	0.11
(1,1816)	1:109:A:ILE:HD13	1:241:A:LEU:HD11	2	0.11	0.0	0.11
(1,1816)	1:109:A:ILE:HD13	1:241:A:LEU:HD12	2	0.11	0.0	0.11
(1,1816)	1:109:A:ILE:HD13	1:241:A:LEU:HD13	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD11	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD12	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD13	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD21	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD22	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD23	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD11	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD12	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD13	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD21	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD22	2	0.11	0.0	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD23	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD11	1:202:A:VAL:HG11	2	0.11	0.0	0.11

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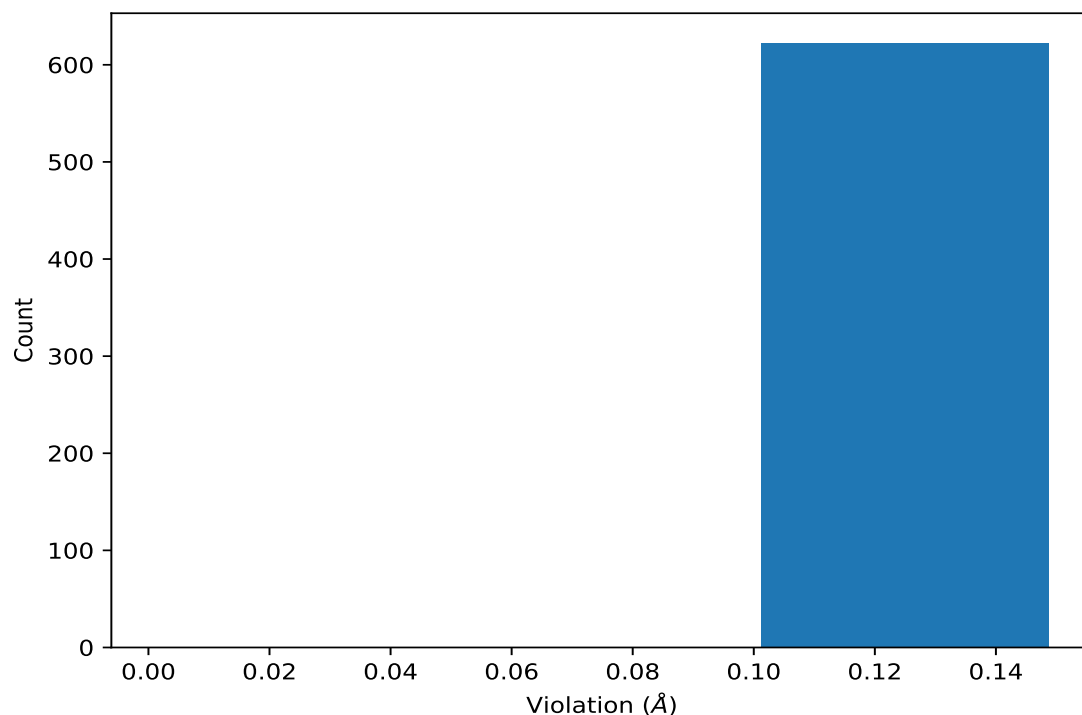
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3273)	1:160:A:LEU:HD11	1:202:A:VAL:HG12	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD11	1:202:A:VAL:HG13	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD12	1:202:A:VAL:HG11	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD12	1:202:A:VAL:HG12	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD12	1:202:A:VAL:HG13	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD13	1:202:A:VAL:HG11	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD13	1:202:A:VAL:HG12	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD13	1:202:A:VAL:HG13	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD21	1:202:A:VAL:HG11	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD21	1:202:A:VAL:HG12	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD21	1:202:A:VAL:HG13	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD22	1:202:A:VAL:HG11	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD22	1:202:A:VAL:HG12	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD22	1:202:A:VAL:HG13	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD23	1:202:A:VAL:HG11	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD23	1:202:A:VAL:HG12	2	0.11	0.0	0.11
(1,3273)	1:160:A:LEU:HD23	1:202:A:VAL:HG13	2	0.11	0.0	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD11	2	0.11	0.0	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD12	2	0.11	0.0	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD13	2	0.11	0.0	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD21	2	0.11	0.0	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD22	2	0.11	0.0	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD23	2	0.11	0.0	0.11
(1,3502)	1:226:A:ILE:HG21	1:227:A:CYS:HB2	2	0.11	0.0	0.11
(1,3502)	1:226:A:ILE:HG21	1:227:A:CYS:HB3	2	0.11	0.0	0.11
(1,3502)	1:226:A:ILE:HG22	1:227:A:CYS:HB2	2	0.11	0.0	0.11
(1,3502)	1:226:A:ILE:HG22	1:227:A:CYS:HB3	2	0.11	0.0	0.11
(1,3502)	1:226:A:ILE:HG23	1:227:A:CYS:HB2	2	0.11	0.0	0.11
(1,3502)	1:226:A:ILE:HG23	1:227:A:CYS:HB3	2	0.11	0.0	0.11
(1,1682)	1:135:A:PHE:HE1	1:218:A:ILE:HD11	2	0.1	0.0	0.1
(1,1682)	1:135:A:PHE:HE1	1:218:A:ILE:HD12	2	0.1	0.0	0.1
(1,1682)	1:135:A:PHE:HE1	1:218:A:ILE:HD13	2	0.1	0.0	0.1
(1,1682)	1:135:A:PHE:HE2	1:218:A:ILE:HD11	2	0.1	0.0	0.1
(1,1682)	1:135:A:PHE:HE2	1:218:A:ILE:HD12	2	0.1	0.0	0.1
(1,1682)	1:135:A:PHE:HE2	1:218:A:ILE:HD13	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD1	7	0.12
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD2	7	0.12
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD1	7	0.12
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD2	7	0.12
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD1	7	0.12
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD2	7	0.12
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD1	7	0.12
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD2	7	0.12
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD1	7	0.12
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD2	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD1	7	0.12
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD2	7	0.12
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD1	11	0.12
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD2	11	0.12
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD1	11	0.12
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD2	11	0.12
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD1	11	0.12
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD2	11	0.12
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD1	11	0.12
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD2	11	0.12
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD1	11	0.12
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD2	11	0.12
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD1	11	0.12
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD2	11	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD11	6	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD12	6	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD13	6	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD21	6	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD22	6	0.12
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD23	6	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD11	6	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD12	6	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD13	6	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD21	6	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD22	6	0.12
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD23	6	0.12
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB1	14	0.12
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB2	14	0.12
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB3	14	0.12
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB1	14	0.12
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB2	14	0.12
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB3	14	0.12
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB1	14	0.12
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB2	14	0.12
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB3	14	0.12
(1,1132)	1:108:A:THR:HG21	1:109:A:ILE:HD11	17	0.12
(1,1132)	1:108:A:THR:HG21	1:109:A:ILE:HD12	17	0.12
(1,1132)	1:108:A:THR:HG21	1:109:A:ILE:HD13	17	0.12
(1,1132)	1:108:A:THR:HG22	1:109:A:ILE:HD11	17	0.12
(1,1132)	1:108:A:THR:HG22	1:109:A:ILE:HD12	17	0.12
(1,1132)	1:108:A:THR:HG22	1:109:A:ILE:HD13	17	0.12
(1,1132)	1:108:A:THR:HG23	1:109:A:ILE:HD11	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	1:108:A:THR:HG23	1:109:A:ILE:HD12	17	0.12
(1,1132)	1:108:A:THR:HG23	1:109:A:ILE:HD13	17	0.12
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD11	5	0.12
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD12	5	0.12
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD13	5	0.12
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD11	5	0.12
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD12	5	0.12
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD13	5	0.12
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD11	5	0.12
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD12	5	0.12
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD13	5	0.12
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD11	20	0.12
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD12	20	0.12
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD13	20	0.12
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD11	20	0.12
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD12	20	0.12
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD13	20	0.12
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD11	20	0.12
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD12	20	0.12
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD13	20	0.12
(1,3502)	1:226:A:ILE:HG21	1:227:A:CYS:HB2	8	0.11
(1,3502)	1:226:A:ILE:HG21	1:227:A:CYS:HB3	8	0.11
(1,3502)	1:226:A:ILE:HG22	1:227:A:CYS:HB2	8	0.11
(1,3502)	1:226:A:ILE:HG22	1:227:A:CYS:HB3	8	0.11
(1,3502)	1:226:A:ILE:HG23	1:227:A:CYS:HB2	8	0.11
(1,3502)	1:226:A:ILE:HG23	1:227:A:CYS:HB3	8	0.11
(1,3498)	1:225:A:LYS:HE2	1:228:A:VAL:HG11	6	0.11
(1,3498)	1:225:A:LYS:HE2	1:228:A:VAL:HG12	6	0.11
(1,3498)	1:225:A:LYS:HE2	1:228:A:VAL:HG13	6	0.11
(1,3498)	1:225:A:LYS:HE2	1:228:A:VAL:HG21	6	0.11
(1,3498)	1:225:A:LYS:HE2	1:228:A:VAL:HG22	6	0.11
(1,3498)	1:225:A:LYS:HE2	1:228:A:VAL:HG23	6	0.11
(1,3498)	1:225:A:LYS:HE3	1:228:A:VAL:HG11	6	0.11
(1,3498)	1:225:A:LYS:HE3	1:228:A:VAL:HG12	6	0.11
(1,3498)	1:225:A:LYS:HE3	1:228:A:VAL:HG13	6	0.11
(1,3498)	1:225:A:LYS:HE3	1:228:A:VAL:HG21	6	0.11
(1,3498)	1:225:A:LYS:HE3	1:228:A:VAL:HG22	6	0.11
(1,3498)	1:225:A:LYS:HE3	1:228:A:VAL:HG23	6	0.11
(1,3462)	1:216:A:SER:HA	1:233:A:VAL:HG11	3	0.11
(1,3462)	1:216:A:SER:HA	1:233:A:VAL:HG12	3	0.11
(1,3462)	1:216:A:SER:HA	1:233:A:VAL:HG13	3	0.11
(1,3462)	1:216:A:SER:HA	1:233:A:VAL:HG21	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3462)	1:216:A:SER:HA	1:233:A:VAL:HG22	3	0.11
(1,3462)	1:216:A:SER:HA	1:233:A:VAL:HG23	3	0.11
(1,3373)	1:182:A:TYR:HD1	1:205:A:GLN:HG2	18	0.11
(1,3373)	1:182:A:TYR:HD1	1:205:A:GLN:HG3	18	0.11
(1,3373)	1:182:A:TYR:HD2	1:205:A:GLN:HG2	18	0.11
(1,3373)	1:182:A:TYR:HD2	1:205:A:GLN:HG3	18	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD11	17	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD12	17	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD13	17	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD21	17	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD22	17	0.11
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD23	17	0.11
(1,3337)	1:175:A:LEU:HD11	1:183:A:ILE:HA	5	0.11
(1,3337)	1:175:A:LEU:HD12	1:183:A:ILE:HA	5	0.11
(1,3337)	1:175:A:LEU:HD13	1:183:A:ILE:HA	5	0.11
(1,3337)	1:175:A:LEU:HD21	1:183:A:ILE:HA	5	0.11
(1,3337)	1:175:A:LEU:HD22	1:183:A:ILE:HA	5	0.11
(1,3337)	1:175:A:LEU:HD23	1:183:A:ILE:HA	5	0.11
(1,3337)	1:175:A:LEU:HD11	1:183:A:ILE:HA	8	0.11
(1,3337)	1:175:A:LEU:HD12	1:183:A:ILE:HA	8	0.11
(1,3337)	1:175:A:LEU:HD13	1:183:A:ILE:HA	8	0.11
(1,3337)	1:175:A:LEU:HD21	1:183:A:ILE:HA	8	0.11
(1,3337)	1:175:A:LEU:HD22	1:183:A:ILE:HA	8	0.11
(1,3337)	1:175:A:LEU:HD23	1:183:A:ILE:HA	8	0.11
(1,3337)	1:175:A:LEU:HD11	1:183:A:ILE:HA	11	0.11
(1,3337)	1:175:A:LEU:HD12	1:183:A:ILE:HA	11	0.11
(1,3337)	1:175:A:LEU:HD13	1:183:A:ILE:HA	11	0.11
(1,3337)	1:175:A:LEU:HD21	1:183:A:ILE:HA	11	0.11
(1,3337)	1:175:A:LEU:HD22	1:183:A:ILE:HA	11	0.11
(1,3337)	1:175:A:LEU:HD23	1:183:A:ILE:HA	11	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD11	4	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD12	4	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD13	4	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD21	4	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD22	4	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD23	4	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD11	4	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD12	4	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD13	4	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD21	4	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD22	4	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD23	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD11	12	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD12	12	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD13	12	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD21	12	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD22	12	0.11
(1,3315)	1:173:A:GLU:HG2	1:175:A:LEU:HD23	12	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD11	12	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD12	12	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD13	12	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD21	12	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD22	12	0.11
(1,3315)	1:173:A:GLU:HG3	1:175:A:LEU:HD23	12	0.11
(1,3273)	1:160:A:LEU:HD11	1:202:A:VAL:HG11	11	0.11
(1,3273)	1:160:A:LEU:HD11	1:202:A:VAL:HG12	11	0.11
(1,3273)	1:160:A:LEU:HD11	1:202:A:VAL:HG13	11	0.11
(1,3273)	1:160:A:LEU:HD12	1:202:A:VAL:HG11	11	0.11
(1,3273)	1:160:A:LEU:HD12	1:202:A:VAL:HG12	11	0.11
(1,3273)	1:160:A:LEU:HD12	1:202:A:VAL:HG13	11	0.11
(1,3273)	1:160:A:LEU:HD13	1:202:A:VAL:HG11	11	0.11
(1,3273)	1:160:A:LEU:HD13	1:202:A:VAL:HG12	11	0.11
(1,3273)	1:160:A:LEU:HD13	1:202:A:VAL:HG13	11	0.11
(1,3273)	1:160:A:LEU:HD21	1:202:A:VAL:HG11	11	0.11
(1,3273)	1:160:A:LEU:HD21	1:202:A:VAL:HG12	11	0.11
(1,3273)	1:160:A:LEU:HD21	1:202:A:VAL:HG13	11	0.11
(1,3273)	1:160:A:LEU:HD22	1:202:A:VAL:HG11	11	0.11
(1,3273)	1:160:A:LEU:HD22	1:202:A:VAL:HG12	11	0.11
(1,3273)	1:160:A:LEU:HD22	1:202:A:VAL:HG13	11	0.11
(1,3273)	1:160:A:LEU:HD23	1:202:A:VAL:HG11	11	0.11
(1,3273)	1:160:A:LEU:HD23	1:202:A:VAL:HG12	11	0.11
(1,3273)	1:160:A:LEU:HD23	1:202:A:VAL:HG13	11	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG11	9	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG12	9	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG13	9	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG21	9	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG22	9	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG23	9	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG11	10	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG12	10	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG13	10	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG21	10	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG22	10	0.11
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG23	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG11	11	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG12	11	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG13	11	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG21	11	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG22	11	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG23	11	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG11	11	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG12	11	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG13	11	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG21	11	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG22	11	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG23	11	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG11	11	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG12	11	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG13	11	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG21	11	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG22	11	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG23	11	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG11	12	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG12	12	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG13	12	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG21	12	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG22	12	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG23	12	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG11	12	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG12	12	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG13	12	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG21	12	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG22	12	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG23	12	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG11	12	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG12	12	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG13	12	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG21	12	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG22	12	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG23	12	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG11	19	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG12	19	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG13	19	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG21	19	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG22	19	0.11
(1,3175)	1:136:A:VAL:HG21	1:157:A:VAL:HG23	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG11	19	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG12	19	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG13	19	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG21	19	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG22	19	0.11
(1,3175)	1:136:A:VAL:HG22	1:157:A:VAL:HG23	19	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG11	19	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG12	19	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG13	19	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG21	19	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG22	19	0.11
(1,3175)	1:136:A:VAL:HG23	1:157:A:VAL:HG23	19	0.11
(1,3084)	1:110:A:PHE:HD1	1:113:A:LEU:HD11	7	0.11
(1,3084)	1:110:A:PHE:HD1	1:113:A:LEU:HD12	7	0.11
(1,3084)	1:110:A:PHE:HD1	1:113:A:LEU:HD13	7	0.11
(1,3084)	1:110:A:PHE:HD1	1:113:A:LEU:HD21	7	0.11
(1,3084)	1:110:A:PHE:HD1	1:113:A:LEU:HD22	7	0.11
(1,3084)	1:110:A:PHE:HD1	1:113:A:LEU:HD23	7	0.11
(1,3084)	1:110:A:PHE:HD2	1:113:A:LEU:HD11	7	0.11
(1,3084)	1:110:A:PHE:HD2	1:113:A:LEU:HD12	7	0.11
(1,3084)	1:110:A:PHE:HD2	1:113:A:LEU:HD13	7	0.11
(1,3084)	1:110:A:PHE:HD2	1:113:A:LEU:HD21	7	0.11
(1,3084)	1:110:A:PHE:HD2	1:113:A:LEU:HD22	7	0.11
(1,3084)	1:110:A:PHE:HD2	1:113:A:LEU:HD23	7	0.11
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD11	2	0.11
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD12	2	0.11
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD13	2	0.11
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD21	2	0.11
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD22	2	0.11
(1,2930)	1:94:A:LYS:HE2	1:98:A:LEU:HD23	2	0.11
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD11	2	0.11
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD12	2	0.11
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD13	2	0.11
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD21	2	0.11
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD22	2	0.11
(1,2930)	1:94:A:LYS:HE3	1:98:A:LEU:HD23	2	0.11
(1,1870)	1:182:A:TYR:HD1	1:207:A:VAL:HG11	18	0.11
(1,1870)	1:182:A:TYR:HD1	1:207:A:VAL:HG12	18	0.11
(1,1870)	1:182:A:TYR:HD1	1:207:A:VAL:HG13	18	0.11
(1,1870)	1:182:A:TYR:HD2	1:207:A:VAL:HG11	18	0.11
(1,1870)	1:182:A:TYR:HD2	1:207:A:VAL:HG12	18	0.11
(1,1870)	1:182:A:TYR:HD2	1:207:A:VAL:HG13	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1816)	1:109:A:ILE:HD11	1:241:A:LEU:HD11	11	0.11
(1,1816)	1:109:A:ILE:HD11	1:241:A:LEU:HD12	11	0.11
(1,1816)	1:109:A:ILE:HD11	1:241:A:LEU:HD13	11	0.11
(1,1816)	1:109:A:ILE:HD12	1:241:A:LEU:HD11	11	0.11
(1,1816)	1:109:A:ILE:HD12	1:241:A:LEU:HD12	11	0.11
(1,1816)	1:109:A:ILE:HD12	1:241:A:LEU:HD13	11	0.11
(1,1816)	1:109:A:ILE:HD13	1:241:A:LEU:HD11	11	0.11
(1,1816)	1:109:A:ILE:HD13	1:241:A:LEU:HD12	11	0.11
(1,1816)	1:109:A:ILE:HD13	1:241:A:LEU:HD13	11	0.11
(1,1816)	1:109:A:ILE:HD11	1:241:A:LEU:HD11	19	0.11
(1,1816)	1:109:A:ILE:HD11	1:241:A:LEU:HD12	19	0.11
(1,1816)	1:109:A:ILE:HD11	1:241:A:LEU:HD13	19	0.11
(1,1816)	1:109:A:ILE:HD12	1:241:A:LEU:HD11	19	0.11
(1,1816)	1:109:A:ILE:HD12	1:241:A:LEU:HD12	19	0.11
(1,1816)	1:109:A:ILE:HD12	1:241:A:LEU:HD13	19	0.11
(1,1816)	1:109:A:ILE:HD13	1:241:A:LEU:HD11	19	0.11
(1,1816)	1:109:A:ILE:HD13	1:241:A:LEU:HD12	19	0.11
(1,1816)	1:109:A:ILE:HD13	1:241:A:LEU:HD13	19	0.11
(1,1711)	1:183:A:ILE:H	1:183:A:ILE:HD11	10	0.11
(1,1711)	1:183:A:ILE:H	1:183:A:ILE:HD12	10	0.11
(1,1711)	1:183:A:ILE:H	1:183:A:ILE:HD13	10	0.11
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB1	19	0.11
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB2	19	0.11
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB3	19	0.11
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB1	19	0.11
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB2	19	0.11
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB3	19	0.11
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB1	19	0.11
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB2	19	0.11
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB3	19	0.11
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB1	20	0.11
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB2	20	0.11
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB3	20	0.11
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB1	20	0.11
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB2	20	0.11
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB3	20	0.11
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB1	20	0.11
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB2	20	0.11
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB3	20	0.11
(1,1089)	1:101:A:THR:HG21	1:244:A:LEU:HD21	1	0.11
(1,1089)	1:101:A:THR:HG21	1:244:A:LEU:HD22	1	0.11
(1,1089)	1:101:A:THR:HG21	1:244:A:LEU:HD23	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1089)	1:101:A:THR:HG22	1:244:A:LEU:HD21	1	0.11
(1,1089)	1:101:A:THR:HG22	1:244:A:LEU:HD22	1	0.11
(1,1089)	1:101:A:THR:HG22	1:244:A:LEU:HD23	1	0.11
(1,1089)	1:101:A:THR:HG23	1:244:A:LEU:HD21	1	0.11
(1,1089)	1:101:A:THR:HG23	1:244:A:LEU:HD22	1	0.11
(1,1089)	1:101:A:THR:HG23	1:244:A:LEU:HD23	1	0.11
(1,1069)	1:160:A:LEU:HD11	1:202:A:VAL:HG11	7	0.11
(1,1069)	1:160:A:LEU:HD11	1:202:A:VAL:HG12	7	0.11
(1,1069)	1:160:A:LEU:HD11	1:202:A:VAL:HG13	7	0.11
(1,1069)	1:160:A:LEU:HD12	1:202:A:VAL:HG11	7	0.11
(1,1069)	1:160:A:LEU:HD12	1:202:A:VAL:HG12	7	0.11
(1,1069)	1:160:A:LEU:HD12	1:202:A:VAL:HG13	7	0.11
(1,1069)	1:160:A:LEU:HD13	1:202:A:VAL:HG11	7	0.11
(1,1069)	1:160:A:LEU:HD13	1:202:A:VAL:HG12	7	0.11
(1,1069)	1:160:A:LEU:HD13	1:202:A:VAL:HG13	7	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD11	13	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD12	13	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD13	13	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD11	13	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD12	13	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD13	13	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD11	13	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD12	13	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD13	13	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD11	18	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD12	18	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD13	18	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD11	18	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD12	18	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD13	18	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD11	18	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD12	18	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD13	18	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD11	19	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD12	19	0.11
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD13	19	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD11	19	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD12	19	0.11
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD13	19	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD11	19	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD12	19	0.11
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD13	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:93:A:GLU:HA	1:93:A:GLU:HG2	13	0.11
(1,14)	1:93:A:GLU:HA	1:93:A:GLU:HG3	13	0.11
(1,3569)	1:246:A:LYS:HG2	1:247:A:ASN:HB2	8	0.1
(1,3569)	1:246:A:LYS:HG2	1:247:A:ASN:HB3	8	0.1
(1,3569)	1:246:A:LYS:HG3	1:247:A:ASN:HB2	8	0.1
(1,3569)	1:246:A:LYS:HG3	1:247:A:ASN:HB3	8	0.1
(1,3557)	1:244:A:LEU:HA	1:244:A:LEU:HD11	4	0.1
(1,3557)	1:244:A:LEU:HA	1:244:A:LEU:HD12	4	0.1
(1,3557)	1:244:A:LEU:HA	1:244:A:LEU:HD13	4	0.1
(1,3557)	1:244:A:LEU:HA	1:244:A:LEU:HD21	4	0.1
(1,3557)	1:244:A:LEU:HA	1:244:A:LEU:HD22	4	0.1
(1,3557)	1:244:A:LEU:HA	1:244:A:LEU:HD23	4	0.1
(1,3502)	1:226:A:ILE:HG21	1:227:A:CYS:HB2	12	0.1
(1,3502)	1:226:A:ILE:HG21	1:227:A:CYS:HB3	12	0.1
(1,3502)	1:226:A:ILE:HG22	1:227:A:CYS:HB2	12	0.1
(1,3502)	1:226:A:ILE:HG22	1:227:A:CYS:HB3	12	0.1
(1,3502)	1:226:A:ILE:HG23	1:227:A:CYS:HB2	12	0.1
(1,3502)	1:226:A:ILE:HG23	1:227:A:CYS:HB3	12	0.1
(1,3411)	1:201:A:MET:HE1	1:228:A:VAL:HG11	3	0.1
(1,3411)	1:201:A:MET:HE1	1:228:A:VAL:HG12	3	0.1
(1,3411)	1:201:A:MET:HE1	1:228:A:VAL:HG13	3	0.1
(1,3411)	1:201:A:MET:HE1	1:228:A:VAL:HG21	3	0.1
(1,3411)	1:201:A:MET:HE1	1:228:A:VAL:HG22	3	0.1
(1,3411)	1:201:A:MET:HE1	1:228:A:VAL:HG23	3	0.1
(1,3411)	1:201:A:MET:HE2	1:228:A:VAL:HG11	3	0.1
(1,3411)	1:201:A:MET:HE2	1:228:A:VAL:HG12	3	0.1
(1,3411)	1:201:A:MET:HE2	1:228:A:VAL:HG13	3	0.1
(1,3411)	1:201:A:MET:HE2	1:228:A:VAL:HG21	3	0.1
(1,3411)	1:201:A:MET:HE2	1:228:A:VAL:HG22	3	0.1
(1,3411)	1:201:A:MET:HE2	1:228:A:VAL:HG23	3	0.1
(1,3411)	1:201:A:MET:HE3	1:228:A:VAL:HG11	3	0.1
(1,3411)	1:201:A:MET:HE3	1:228:A:VAL:HG12	3	0.1
(1,3411)	1:201:A:MET:HE3	1:228:A:VAL:HG13	3	0.1
(1,3411)	1:201:A:MET:HE3	1:228:A:VAL:HG21	3	0.1
(1,3411)	1:201:A:MET:HE3	1:228:A:VAL:HG22	3	0.1
(1,3411)	1:201:A:MET:HE3	1:228:A:VAL:HG23	3	0.1
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD11	12	0.1
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD12	12	0.1
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD13	12	0.1
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD21	12	0.1
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD22	12	0.1
(1,3355)	1:181:A:TYR:HA	1:244:A:LEU:HD23	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3337)	1:175:A:LEU:HD11	1:183:A:ILE:HA	6	0.1
(1,3337)	1:175:A:LEU:HD12	1:183:A:ILE:HA	6	0.1
(1,3337)	1:175:A:LEU:HD13	1:183:A:ILE:HA	6	0.1
(1,3337)	1:175:A:LEU:HD21	1:183:A:ILE:HA	6	0.1
(1,3337)	1:175:A:LEU:HD22	1:183:A:ILE:HA	6	0.1
(1,3337)	1:175:A:LEU:HD23	1:183:A:ILE:HA	6	0.1
(1,3337)	1:175:A:LEU:HD11	1:183:A:ILE:HA	10	0.1
(1,3337)	1:175:A:LEU:HD12	1:183:A:ILE:HA	10	0.1
(1,3337)	1:175:A:LEU:HD13	1:183:A:ILE:HA	10	0.1
(1,3337)	1:175:A:LEU:HD21	1:183:A:ILE:HA	10	0.1
(1,3337)	1:175:A:LEU:HD22	1:183:A:ILE:HA	10	0.1
(1,3337)	1:175:A:LEU:HD23	1:183:A:ILE:HA	10	0.1
(1,3337)	1:175:A:LEU:HD11	1:183:A:ILE:HA	15	0.1
(1,3337)	1:175:A:LEU:HD12	1:183:A:ILE:HA	15	0.1
(1,3337)	1:175:A:LEU:HD13	1:183:A:ILE:HA	15	0.1
(1,3337)	1:175:A:LEU:HD21	1:183:A:ILE:HA	15	0.1
(1,3337)	1:175:A:LEU:HD22	1:183:A:ILE:HA	15	0.1
(1,3337)	1:175:A:LEU:HD23	1:183:A:ILE:HA	15	0.1
(1,3337)	1:175:A:LEU:HD11	1:183:A:ILE:HA	19	0.1
(1,3337)	1:175:A:LEU:HD12	1:183:A:ILE:HA	19	0.1
(1,3337)	1:175:A:LEU:HD13	1:183:A:ILE:HA	19	0.1
(1,3337)	1:175:A:LEU:HD21	1:183:A:ILE:HA	19	0.1
(1,3337)	1:175:A:LEU:HD22	1:183:A:ILE:HA	19	0.1
(1,3337)	1:175:A:LEU:HD23	1:183:A:ILE:HA	19	0.1
(1,3318)	1:174:A:LEU:H	1:175:A:LEU:HD11	16	0.1
(1,3318)	1:174:A:LEU:H	1:175:A:LEU:HD12	16	0.1
(1,3318)	1:174:A:LEU:H	1:175:A:LEU:HD13	16	0.1
(1,3318)	1:174:A:LEU:H	1:175:A:LEU:HD21	16	0.1
(1,3318)	1:174:A:LEU:H	1:175:A:LEU:HD22	16	0.1
(1,3318)	1:174:A:LEU:H	1:175:A:LEU:HD23	16	0.1
(1,3273)	1:160:A:LEU:HD11	1:202:A:VAL:HG11	6	0.1
(1,3273)	1:160:A:LEU:HD11	1:202:A:VAL:HG12	6	0.1
(1,3273)	1:160:A:LEU:HD11	1:202:A:VAL:HG13	6	0.1
(1,3273)	1:160:A:LEU:HD12	1:202:A:VAL:HG11	6	0.1
(1,3273)	1:160:A:LEU:HD12	1:202:A:VAL:HG12	6	0.1
(1,3273)	1:160:A:LEU:HD12	1:202:A:VAL:HG13	6	0.1
(1,3273)	1:160:A:LEU:HD13	1:202:A:VAL:HG11	6	0.1
(1,3273)	1:160:A:LEU:HD13	1:202:A:VAL:HG12	6	0.1
(1,3273)	1:160:A:LEU:HD13	1:202:A:VAL:HG13	6	0.1
(1,3273)	1:160:A:LEU:HD21	1:202:A:VAL:HG11	6	0.1
(1,3273)	1:160:A:LEU:HD21	1:202:A:VAL:HG12	6	0.1
(1,3273)	1:160:A:LEU:HD21	1:202:A:VAL:HG13	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3273)	1:160:A:LEU:HD22	1:202:A:VAL:HG11	6	0.1
(1,3273)	1:160:A:LEU:HD22	1:202:A:VAL:HG12	6	0.1
(1,3273)	1:160:A:LEU:HD22	1:202:A:VAL:HG13	6	0.1
(1,3273)	1:160:A:LEU:HD23	1:202:A:VAL:HG11	6	0.1
(1,3273)	1:160:A:LEU:HD23	1:202:A:VAL:HG12	6	0.1
(1,3273)	1:160:A:LEU:HD23	1:202:A:VAL:HG13	6	0.1
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD1	2	0.1
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD2	2	0.1
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD1	2	0.1
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD2	2	0.1
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD1	2	0.1
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD2	2	0.1
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD1	2	0.1
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD2	2	0.1
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD1	2	0.1
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD2	2	0.1
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD1	2	0.1
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD2	2	0.1
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD1	14	0.1
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD2	14	0.1
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD1	14	0.1
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD2	14	0.1
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD1	14	0.1
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD2	14	0.1
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD1	14	0.1
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD2	14	0.1
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD1	14	0.1
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD2	14	0.1
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD1	14	0.1
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD2	14	0.1
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD1	15	0.1
(1,3250)	1:156:A:LEU:HD11	1:158:A:TYR:HD2	15	0.1
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD1	15	0.1
(1,3250)	1:156:A:LEU:HD12	1:158:A:TYR:HD2	15	0.1
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD1	15	0.1
(1,3250)	1:156:A:LEU:HD13	1:158:A:TYR:HD2	15	0.1
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD1	15	0.1
(1,3250)	1:156:A:LEU:HD21	1:158:A:TYR:HD2	15	0.1
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD1	15	0.1
(1,3250)	1:156:A:LEU:HD22	1:158:A:TYR:HD2	15	0.1
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD1	15	0.1
(1,3250)	1:156:A:LEU:HD23	1:158:A:TYR:HD2	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG11	8	0.1
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG12	8	0.1
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG13	8	0.1
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG21	8	0.1
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG22	8	0.1
(1,3197)	1:141:A:ARG:HB2	1:150:A:VAL:HG23	8	0.1
(1,3159)	1:129:A:TYR:HE1	1:233:A:VAL:HG11	16	0.1
(1,3159)	1:129:A:TYR:HE1	1:233:A:VAL:HG12	16	0.1
(1,3159)	1:129:A:TYR:HE1	1:233:A:VAL:HG13	16	0.1
(1,3159)	1:129:A:TYR:HE1	1:233:A:VAL:HG21	16	0.1
(1,3159)	1:129:A:TYR:HE1	1:233:A:VAL:HG22	16	0.1
(1,3159)	1:129:A:TYR:HE1	1:233:A:VAL:HG23	16	0.1
(1,3159)	1:129:A:TYR:HE2	1:233:A:VAL:HG11	16	0.1
(1,3159)	1:129:A:TYR:HE2	1:233:A:VAL:HG12	16	0.1
(1,3159)	1:129:A:TYR:HE2	1:233:A:VAL:HG13	16	0.1
(1,3159)	1:129:A:TYR:HE2	1:233:A:VAL:HG21	16	0.1
(1,3159)	1:129:A:TYR:HE2	1:233:A:VAL:HG22	16	0.1
(1,3159)	1:129:A:TYR:HE2	1:233:A:VAL:HG23	16	0.1
(1,3070)	1:109:A:ILE:H	1:238:A:LEU:HD11	19	0.1
(1,3070)	1:109:A:ILE:H	1:238:A:LEU:HD12	19	0.1
(1,3070)	1:109:A:ILE:H	1:238:A:LEU:HD13	19	0.1
(1,3070)	1:109:A:ILE:H	1:238:A:LEU:HD21	19	0.1
(1,3070)	1:109:A:ILE:H	1:238:A:LEU:HD22	19	0.1
(1,3070)	1:109:A:ILE:H	1:238:A:LEU:HD23	19	0.1
(1,3039)	1:105:A:GLY:HA2	1:244:A:LEU:HD11	11	0.1
(1,3039)	1:105:A:GLY:HA2	1:244:A:LEU:HD12	11	0.1
(1,3039)	1:105:A:GLY:HA2	1:244:A:LEU:HD13	11	0.1
(1,3039)	1:105:A:GLY:HA2	1:244:A:LEU:HD21	11	0.1
(1,3039)	1:105:A:GLY:HA2	1:244:A:LEU:HD22	11	0.1
(1,3039)	1:105:A:GLY:HA2	1:244:A:LEU:HD23	11	0.1
(1,3039)	1:105:A:GLY:HA3	1:244:A:LEU:HD11	11	0.1
(1,3039)	1:105:A:GLY:HA3	1:244:A:LEU:HD12	11	0.1
(1,3039)	1:105:A:GLY:HA3	1:244:A:LEU:HD13	11	0.1
(1,3039)	1:105:A:GLY:HA3	1:244:A:LEU:HD21	11	0.1
(1,3039)	1:105:A:GLY:HA3	1:244:A:LEU:HD22	11	0.1
(1,3039)	1:105:A:GLY:HA3	1:244:A:LEU:HD23	11	0.1
(1,2964)	1:98:A:LEU:HD11	1:101:A:THR:HG21	20	0.1
(1,2964)	1:98:A:LEU:HD11	1:101:A:THR:HG22	20	0.1
(1,2964)	1:98:A:LEU:HD11	1:101:A:THR:HG23	20	0.1
(1,2964)	1:98:A:LEU:HD12	1:101:A:THR:HG21	20	0.1
(1,2964)	1:98:A:LEU:HD12	1:101:A:THR:HG22	20	0.1
(1,2964)	1:98:A:LEU:HD12	1:101:A:THR:HG23	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2964)	1:98:A:LEU:HD13	1:101:A:THR:HG21	20	0.1
(1,2964)	1:98:A:LEU:HD13	1:101:A:THR:HG22	20	0.1
(1,2964)	1:98:A:LEU:HD13	1:101:A:THR:HG23	20	0.1
(1,2964)	1:98:A:LEU:HD21	1:101:A:THR:HG21	20	0.1
(1,2964)	1:98:A:LEU:HD21	1:101:A:THR:HG22	20	0.1
(1,2964)	1:98:A:LEU:HD21	1:101:A:THR:HG23	20	0.1
(1,2964)	1:98:A:LEU:HD22	1:101:A:THR:HG21	20	0.1
(1,2964)	1:98:A:LEU:HD22	1:101:A:THR:HG22	20	0.1
(1,2964)	1:98:A:LEU:HD22	1:101:A:THR:HG23	20	0.1
(1,2964)	1:98:A:LEU:HD23	1:101:A:THR:HG21	20	0.1
(1,2964)	1:98:A:LEU:HD23	1:101:A:THR:HG22	20	0.1
(1,2964)	1:98:A:LEU:HD23	1:101:A:THR:HG23	20	0.1
(1,2879)	1:196:A:THR:HG21	1:197:A:GLY:H	11	0.1
(1,2879)	1:196:A:THR:HG22	1:197:A:GLY:H	11	0.1
(1,2879)	1:196:A:THR:HG23	1:197:A:GLY:H	11	0.1
(1,2033)	1:174:A:LEU:HD11	1:181:A:TYR:HE1	19	0.1
(1,2033)	1:174:A:LEU:HD11	1:181:A:TYR:HE2	19	0.1
(1,2033)	1:174:A:LEU:HD12	1:181:A:TYR:HE1	19	0.1
(1,2033)	1:174:A:LEU:HD12	1:181:A:TYR:HE2	19	0.1
(1,2033)	1:174:A:LEU:HD13	1:181:A:TYR:HE1	19	0.1
(1,2033)	1:174:A:LEU:HD13	1:181:A:TYR:HE2	19	0.1
(1,1729)	1:175:A:LEU:H	1:175:A:LEU:HD21	16	0.1
(1,1729)	1:175:A:LEU:H	1:175:A:LEU:HD22	16	0.1
(1,1729)	1:175:A:LEU:H	1:175:A:LEU:HD23	16	0.1
(1,1682)	1:135:A:PHE:HE1	1:218:A:ILE:HD11	7	0.1
(1,1682)	1:135:A:PHE:HE1	1:218:A:ILE:HD12	7	0.1
(1,1682)	1:135:A:PHE:HE1	1:218:A:ILE:HD13	7	0.1
(1,1682)	1:135:A:PHE:HE2	1:218:A:ILE:HD11	7	0.1
(1,1682)	1:135:A:PHE:HE2	1:218:A:ILE:HD12	7	0.1
(1,1682)	1:135:A:PHE:HE2	1:218:A:ILE:HD13	7	0.1
(1,1682)	1:135:A:PHE:HE1	1:218:A:ILE:HD11	18	0.1
(1,1682)	1:135:A:PHE:HE1	1:218:A:ILE:HD12	18	0.1
(1,1682)	1:135:A:PHE:HE1	1:218:A:ILE:HD13	18	0.1
(1,1682)	1:135:A:PHE:HE2	1:218:A:ILE:HD11	18	0.1
(1,1682)	1:135:A:PHE:HE2	1:218:A:ILE:HD12	18	0.1
(1,1682)	1:135:A:PHE:HE2	1:218:A:ILE:HD13	18	0.1
(1,1631)	1:100:A:LYS:HE2	1:241:A:LEU:HD21	11	0.1
(1,1631)	1:100:A:LYS:HE2	1:241:A:LEU:HD22	11	0.1
(1,1631)	1:100:A:LYS:HE2	1:241:A:LEU:HD23	11	0.1
(1,1631)	1:100:A:LYS:HE3	1:241:A:LEU:HD21	11	0.1
(1,1631)	1:100:A:LYS:HE3	1:241:A:LEU:HD22	11	0.1
(1,1631)	1:100:A:LYS:HE3	1:241:A:LEU:HD23	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1564)	1:109:A:ILE:HD11	1:185:A:GLU:HG2	11	0.1
(1,1564)	1:109:A:ILE:HD11	1:185:A:GLU:HG3	11	0.1
(1,1564)	1:109:A:ILE:HD12	1:185:A:GLU:HG2	11	0.1
(1,1564)	1:109:A:ILE:HD12	1:185:A:GLU:HG3	11	0.1
(1,1564)	1:109:A:ILE:HD13	1:185:A:GLU:HG2	11	0.1
(1,1564)	1:109:A:ILE:HD13	1:185:A:GLU:HG3	11	0.1
(1,1528)	1:109:A:ILE:HG21	1:112:A:LYS:HB2	10	0.1
(1,1528)	1:109:A:ILE:HG21	1:112:A:LYS:HB3	10	0.1
(1,1528)	1:109:A:ILE:HG22	1:112:A:LYS:HB2	10	0.1
(1,1528)	1:109:A:ILE:HG22	1:112:A:LYS:HB3	10	0.1
(1,1528)	1:109:A:ILE:HG23	1:112:A:LYS:HB2	10	0.1
(1,1528)	1:109:A:ILE:HG23	1:112:A:LYS:HB3	10	0.1
(1,1528)	1:109:A:ILE:HG21	1:112:A:LYS:HB2	19	0.1
(1,1528)	1:109:A:ILE:HG21	1:112:A:LYS:HB3	19	0.1
(1,1528)	1:109:A:ILE:HG22	1:112:A:LYS:HB2	19	0.1
(1,1528)	1:109:A:ILE:HG22	1:112:A:LYS:HB3	19	0.1
(1,1528)	1:109:A:ILE:HG23	1:112:A:LYS:HB2	19	0.1
(1,1528)	1:109:A:ILE:HG23	1:112:A:LYS:HB3	19	0.1
(1,1528)	1:109:A:ILE:HG21	1:112:A:LYS:HB2	20	0.1
(1,1528)	1:109:A:ILE:HG21	1:112:A:LYS:HB3	20	0.1
(1,1528)	1:109:A:ILE:HG22	1:112:A:LYS:HB2	20	0.1
(1,1528)	1:109:A:ILE:HG22	1:112:A:LYS:HB3	20	0.1
(1,1528)	1:109:A:ILE:HG23	1:112:A:LYS:HB2	20	0.1
(1,1528)	1:109:A:ILE:HG23	1:112:A:LYS:HB3	20	0.1
(1,1306)	1:192:A:ILE:HD11	1:198:A:ALA:HB1	3	0.1
(1,1306)	1:192:A:ILE:HD11	1:198:A:ALA:HB2	3	0.1
(1,1306)	1:192:A:ILE:HD11	1:198:A:ALA:HB3	3	0.1
(1,1306)	1:192:A:ILE:HD12	1:198:A:ALA:HB1	3	0.1
(1,1306)	1:192:A:ILE:HD12	1:198:A:ALA:HB2	3	0.1
(1,1306)	1:192:A:ILE:HD12	1:198:A:ALA:HB3	3	0.1
(1,1306)	1:192:A:ILE:HD13	1:198:A:ALA:HB1	3	0.1
(1,1306)	1:192:A:ILE:HD13	1:198:A:ALA:HB2	3	0.1
(1,1306)	1:192:A:ILE:HD13	1:198:A:ALA:HB3	3	0.1
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB1	17	0.1
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB2	17	0.1
(1,1291)	1:202:A:VAL:HG21	1:231:A:ALA:HB3	17	0.1
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB1	17	0.1
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB2	17	0.1
(1,1291)	1:202:A:VAL:HG22	1:231:A:ALA:HB3	17	0.1
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB1	17	0.1
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB2	17	0.1
(1,1291)	1:202:A:VAL:HG23	1:231:A:ALA:HB3	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1243)	1:138:A:PHE:HB2	1:157:A:VAL:HG11	15	0.1
(1,1243)	1:138:A:PHE:HB2	1:157:A:VAL:HG12	15	0.1
(1,1243)	1:138:A:PHE:HB2	1:157:A:VAL:HG13	15	0.1
(1,1243)	1:138:A:PHE:HB3	1:157:A:VAL:HG11	15	0.1
(1,1243)	1:138:A:PHE:HB3	1:157:A:VAL:HG12	15	0.1
(1,1243)	1:138:A:PHE:HB3	1:157:A:VAL:HG13	15	0.1
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD11	10	0.1
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD12	10	0.1
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD13	10	0.1
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD11	10	0.1
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD12	10	0.1
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD13	10	0.1
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD11	10	0.1
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD12	10	0.1
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD13	10	0.1
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD11	16	0.1
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD12	16	0.1
(1,971)	1:101:A:THR:HG21	1:244:A:LEU:HD13	16	0.1
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD11	16	0.1
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD12	16	0.1
(1,971)	1:101:A:THR:HG22	1:244:A:LEU:HD13	16	0.1
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD11	16	0.1
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD12	16	0.1
(1,971)	1:101:A:THR:HG23	1:244:A:LEU:HD13	16	0.1

10 Dihedral-angle violation analysis [i](#)

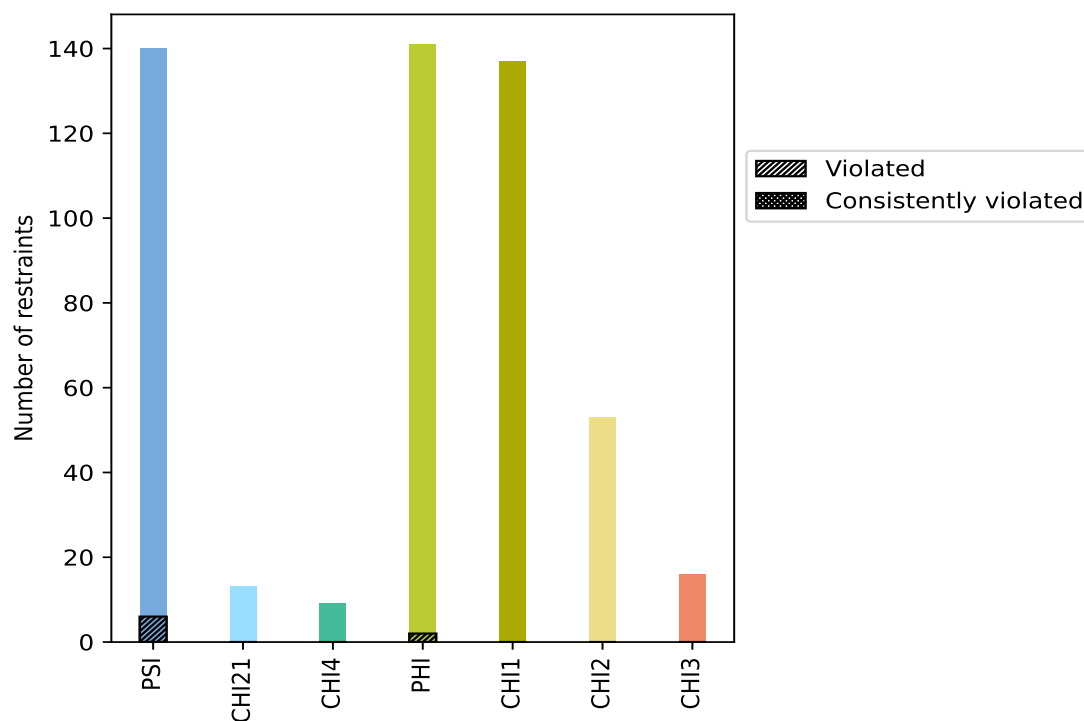
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	140	27.5	6	4.3	1.2	0	0.0	0.0
CHI21	13	2.6	0	0.0	0.0	0	0.0	0.0
CHI4	9	1.8	0	0.0	0.0	0	0.0	0.0
PHI	141	27.7	2	1.4	0.4	0	0.0	0.0
CHI1	137	26.9	0	0.0	0.0	0	0.0	0.0
CHI2	53	10.4	0	0.0	0.0	0	0.0	0.0
CHI3	16	3.1	0	0.0	0.0	0	0.0	0.0
Total	509	100.0	8	1.6	1.6	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 [i](#)



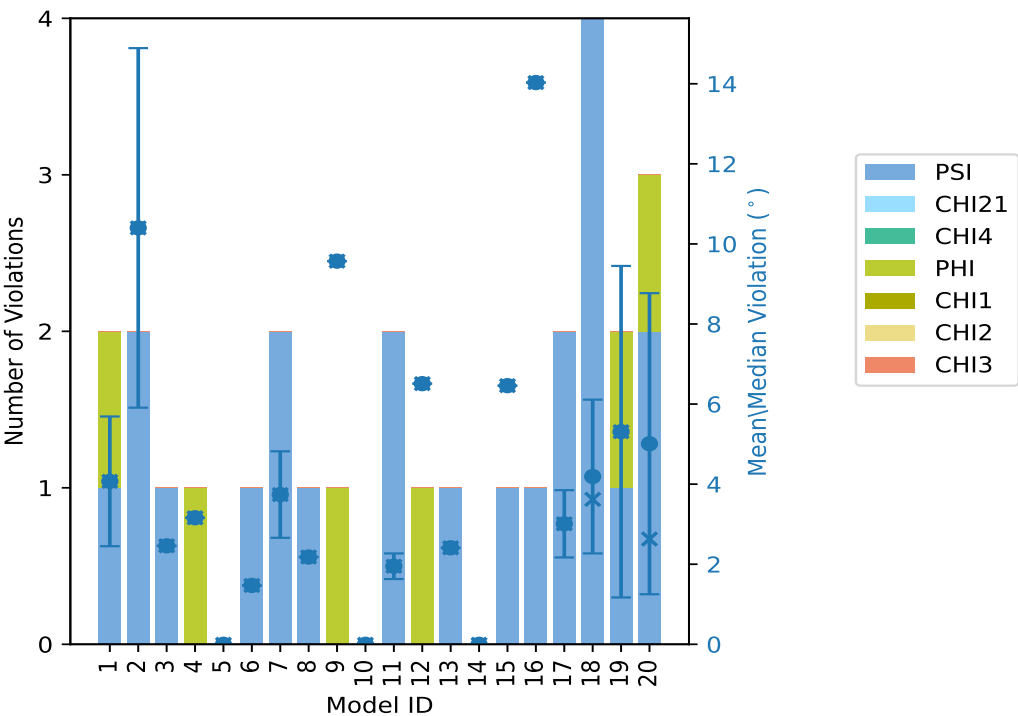
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations								Total	Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	CHI21	CHI4	PHI	CHI1	CHI2	CHI3						
1	1	0	0	1	0	0	0	2	4.07	5.69	1.62	4.07	
2	2	0	0	0	0	0	0	2	10.4	14.89	4.49	10.4	
3	1	0	0	0	0	0	0	1	2.46	2.46	0.0	2.46	
4	0	0	0	1	0	0	0	1	3.16	3.16	0.0	3.16	
5	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0	
6	1	0	0	0	0	0	0	1	1.47	1.47	0.0	1.47	
7	2	0	0	0	0	0	0	2	3.74	4.82	1.08	3.74	
8	1	0	0	0	0	0	0	1	2.18	2.18	0.0	2.18	
9	0	0	0	1	0	0	0	1	9.57	9.57	0.0	9.57	
10	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0	
11	2	0	0	0	0	0	0	2	1.95	2.28	0.32	1.95	
12	0	0	0	1	0	0	0	1	6.51	6.51	0.0	6.51	
13	1	0	0	0	0	0	0	1	2.41	2.41	0.0	2.41	
14	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0	
15	1	0	0	0	0	0	0	1	6.46	6.46	0.0	6.46	
16	1	0	0	0	0	0	0	1	14.03	14.03	0.0	14.03	
17	2	0	0	0	0	0	0	2	3.01	3.85	0.84	3.01	
18	4	0	0	0	0	0	0	4	4.19	7.35	1.92	3.62	
19	1	0	0	1	0	0	0	2	5.31	9.45	4.14	5.31	
20	2	0	0	1	0	0	0	3	5.01	10.32	3.76	2.63	

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

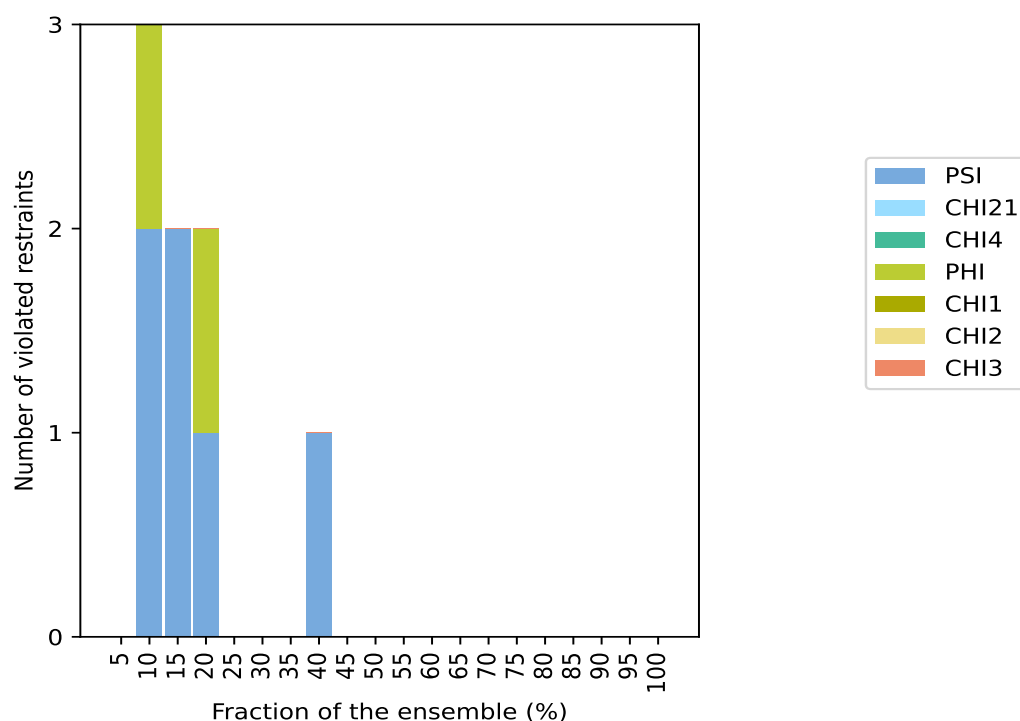
10.3 Dihedral-angle violation statistics for the ensemble

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.

PSI	Number of violated restraints							Fraction of the ensemble	
	CHI21	CHI4	PHI	CHI1	CHI2	CHI3	Total	Count ¹	%
0	0	0	0	0	0	0	0	1	5.0
2	0	0	1	0	0	0	3	2	10.0
2	0	0	0	0	0	0	2	3	15.0
1	0	0	1	0	0	0	2	4	20.0
0	0	0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	0	0	7	35.0
1	0	0	0	0	0	0	1	8	40.0
0	0	0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	0	0	20	100.0

¹ Number of models with violations

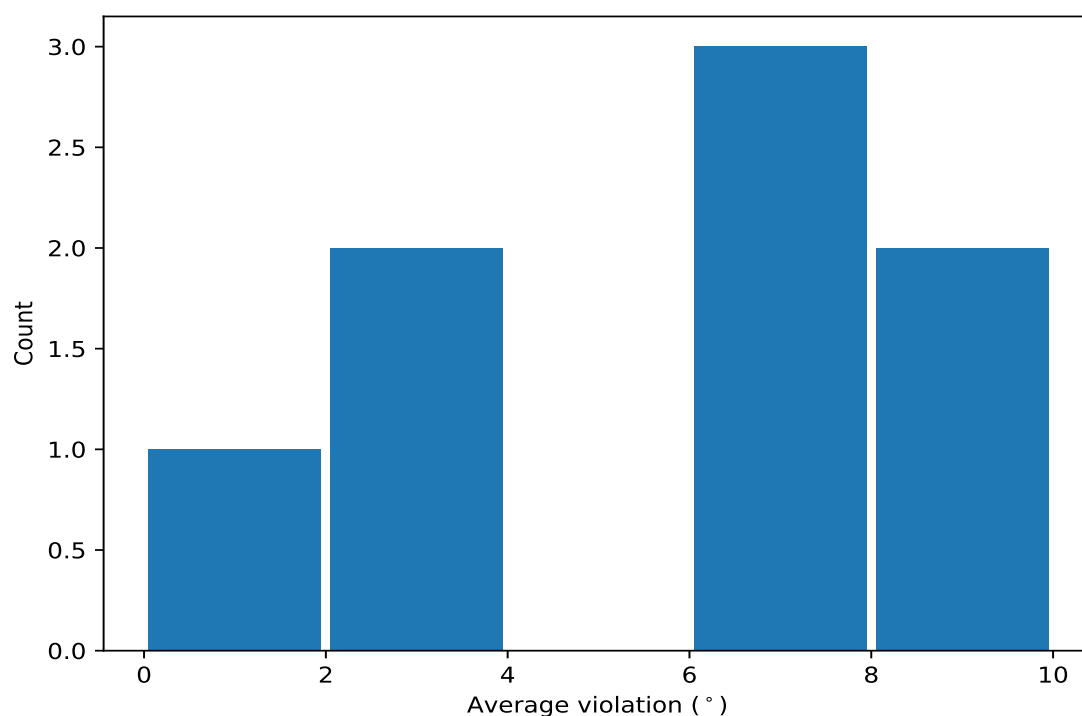
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

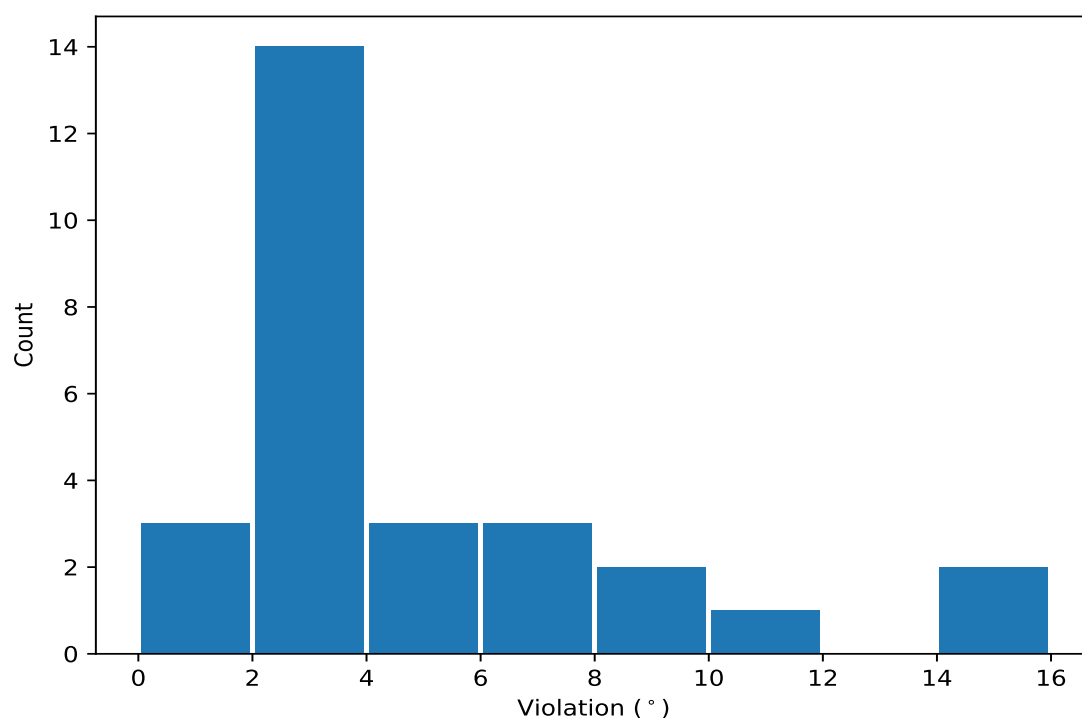
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,238)	1:225:A:LYS:N	1:225:A:LYS:CA	1:225:A:LYS:C	1:226:A:ILE:N	8	2.22	0.42	2.34
(1,177)	1:188:A:GLY:C	1:189:A:SER:N	1:189:A:SER:CA	1:189:A:SER:C	4	6.97	2.7	7.57
(1,130)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:GLY:N	4	6.56	4.34	4.34
(1,2)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:SER:N	3	3.9	1.57	3.7
(1,158)	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	1:178:A:ASP:N	3	1.76	0.3	1.63
(1,4)	1:90:A:SER:N	1:90:A:SER:CA	1:90:A:SER:C	1:91:A:ASN:N	2	8.78	6.12	8.78
(1,277)	1:246:A:LYS:C	1:247:A:ASN:N	1:247:A:ASN:CA	1:247:A:ASN:C	2	8.41	1.91	8.41
(1,110)	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	1:151:A:ASN:N	2	6.9	0.44	6.9

¹ Number of violated models, ²Standard 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 (°)
(1,4)	1:90:A:SER:N	1:90:A:SER:CA	1:90:A:SER:C	1:91:A:ASN:N	2	14.89
(1,130)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:GLY:N	16	14.03
(1,277)	1:246:A:LYS:C	1:247:A:ASN:N	1:247:A:ASN:CA	1:247:A:ASN:C	20	10.32
(1,177)	1:188:A:GLY:C	1:189:A:SER:N	1:189:A:SER:CA	1:189:A:SER:C	9	9.57
(1,177)	1:188:A:GLY:C	1:189:A:SER:N	1:189:A:SER:CA	1:189:A:SER:C	19	9.45
(1,110)	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	1:151:A:ASN:N	18	7.35
(1,277)	1:246:A:LYS:C	1:247:A:ASN:N	1:247:A:ASN:CA	1:247:A:ASN:C	12	6.51
(1,110)	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	1:151:A:ASN:N	15	6.46
(1,2)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:SER:N	2	5.91
(1,177)	1:188:A:GLY:C	1:189:A:SER:N	1:189:A:SER:CA	1:189:A:SER:C	1	5.69
(1,130)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:GLY:N	7	4.82
(1,130)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:GLY:N	17	3.85
(1,2)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:SER:N	18	3.7
(1,130)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:GLY:N	18	3.53
(1,177)	1:188:A:GLY:C	1:189:A:SER:N	1:189:A:SER:CA	1:189:A:SER:C	4	3.16
(1,4)	1:90:A:SER:N	1:90:A:SER:CA	1:90:A:SER:C	1:91:A:ASN:N	7	2.66
(1,238)	1:225:A:LYS:N	1:225:A:LYS:CA	1:225:A:LYS:C	1:226:A:ILE:N	20	2.63
(1,238)	1:225:A:LYS:N	1:225:A:LYS:CA	1:225:A:LYS:C	1:226:A:ILE:N	3	2.46
(1,238)	1:225:A:LYS:N	1:225:A:LYS:CA	1:225:A:LYS:C	1:226:A:ILE:N	1	2.45
(1,238)	1:225:A:LYS:N	1:225:A:LYS:CA	1:225:A:LYS:C	1:226:A:ILE:N	13	2.41
(1,238)	1:225:A:LYS:N	1:225:A:LYS:CA	1:225:A:LYS:C	1:226:A:ILE:N	11	2.28

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,238)	1:225:A:LYS:N	1:225:A:LYS:CA	1:225:A:LYS:C	1:226:A:ILE:N	8	2.18
(1,238)	1:225:A:LYS:N	1:225:A:LYS:CA	1:225:A:LYS:C	1:226:A:ILE:N	18	2.17
(1,158)	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	1:178:A:ASP:N	17	2.17
(1,2)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:SER:N	20	2.09
(1,158)	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	1:178:A:ASP:N	11	1.63
(1,158)	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	1:178:A:ASP:N	6	1.47
(1,238)	1:225:A:LYS:N	1:225:A:LYS:CA	1:225:A:LYS:C	1:226:A:ILE:N	19	1.17