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Full wwPDB NMR Structure Validation Report ⓘ

Jun 4, 2023 – 05:48 AM EDT

PDB ID	:	2LML
BMRB ID	:	16860
Title	:	Solution NMR structure of holo acyl carrier protein from geobacter Metallireducens refined with nh rdcs, Northeast Structural Genomics consortium target gmr141
Authors	:	Ramelot, T.A.; Smola, M.J.; Lee, H.; Zhao, L.; Ciccosanti, C.; Foote, E.L.; Hamilton, K.; Nair, R.; Rost, B.; Swapna, G.; Acton, T.B.; Xiao, R.; Everett, J.K.; Prestegard, J.H.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2011-12-05

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:

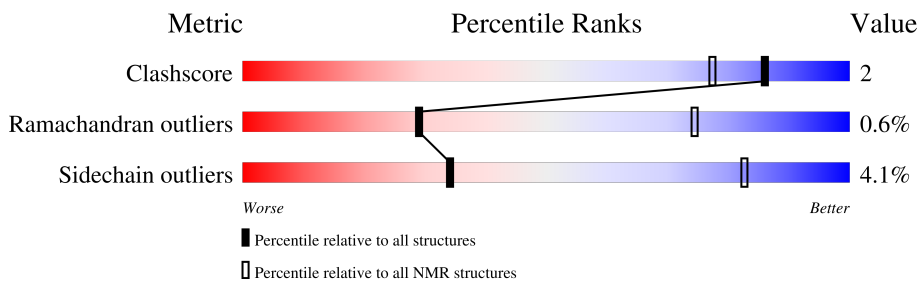|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2

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 94%.

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		2
Ramachandran outliers		0.6%
Sidechain outliers		4.1%

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	87	86% · 10%

Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

W O R L D W I D E

wwPDB

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2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:79 (78)	0.68	12

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

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

The models can be grouped into 3 clusters and 14 single-model clusters were found.

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

3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 1459 atoms, of which 732 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative acyl carrier protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	87	1417	448	711	125	131	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	LEU	-	expression tag	UNP Q39T60
A	81	GLU	-	expression tag	UNP Q39T60
A	82	HIS	-	expression tag	UNP Q39T60
A	83	HIS	-	expression tag	UNP Q39T60
A	84	HIS	-	expression tag	UNP Q39T60
A	85	HIS	-	expression tag	UNP Q39T60
A	86	HIS	-	expression tag	UNP Q39T60
A	87	HIS	-	expression tag	UNP Q39T60

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).
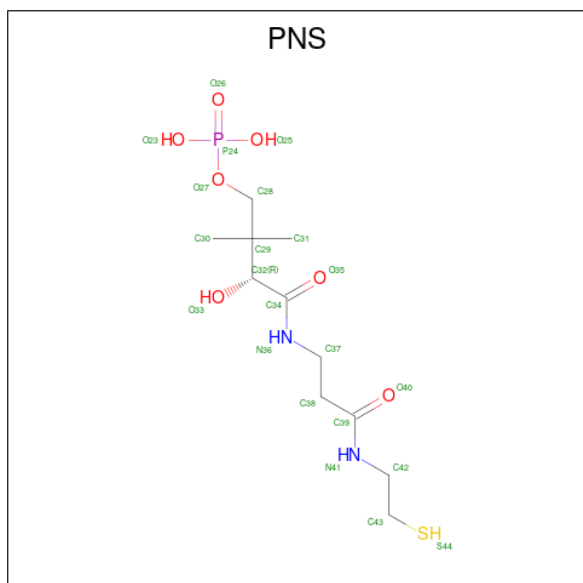
Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
2	A	1	42	11	21	2	6	1	1

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.
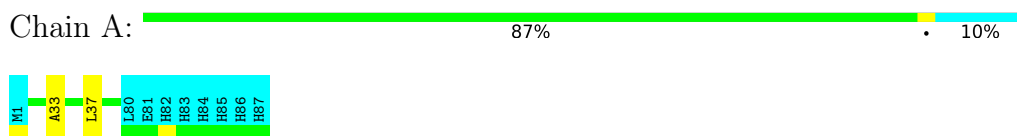
• Molecule 1: Putative acyl carrier protein

Chain A:

86% · 10%
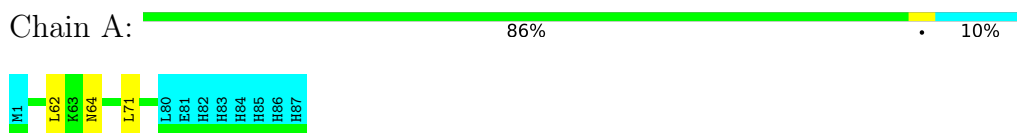
4.2 Scores per residue for each member of the ensemble

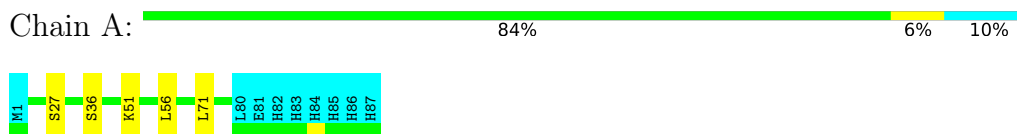Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1
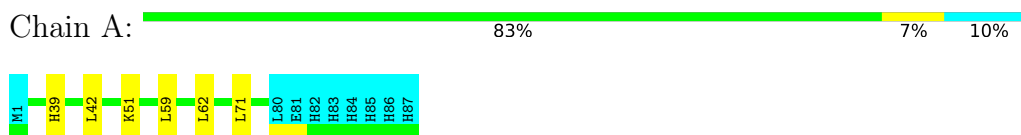
• Molecule 1: Putative acyl carrier protein

Chain A:

87% · 10%

4.2.2 Score per residue for model 2

• Molecule 1: Putative acyl carrier protein

Chain A:

84% 6% 10%

4.2.3 Score per residue for model 3

• Molecule 1: Putative acyl carrier protein

Chain A:

83%   7%   10%

M1 H39 L42 K51 L59 L62 L71 L80 E81 H82 H83 H84 H85 H86 H87

4.2.4 Score per residue for model 4

• Molecule 1: Putative acyl carrier protein

Chain A:

78%   11%   10%

M1 L22 T23 R24 E25 D35 S36 K51 L56 V65 D70 K74 L80 E81 H82 H83 H84 H85 H86 H87

4.2.5 Score per residue for model 5

• Molecule 1: Putative acyl carrier protein

Chain A:

82%   6% · 10%

M1 I43 E47 Q60 K61 L62 D70 L71 K74 L80 E81 H82 H83 H84 H85 H86 H87

4.2.6 Score per residue for model 6

• Molecule 1: Putative acyl carrier protein

Chain A:

77%   13%   10%

M1 E25 S36 Y50 F54 A55 L56 L59 L62 D70 L71 K74 K79 L80 E81 H82 H83 H84 H85 H86 H87

4.2.7 Score per residue for model 7

• Molecule 1: Putative acyl carrier protein

Chain A:

83%   6% · 10%

M1 S27 A28 N29 I43 L59 N64 L80 E81 H82 H83 H84 H85 H86 H87

4.2.8 Score per residue for model 8

• Molecule 1: Putative acyl carrier protein

Chain A:

4.2.9 Score per residue for model 9
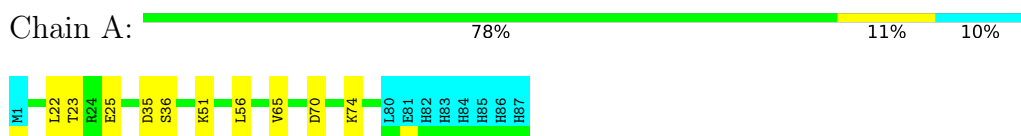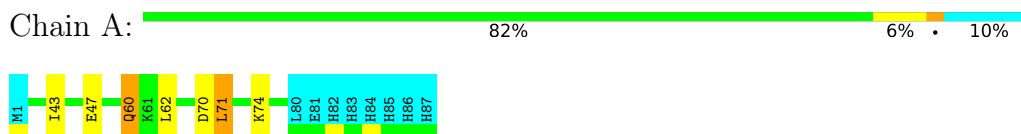
• Molecule 1: Putative acyl carrier protein
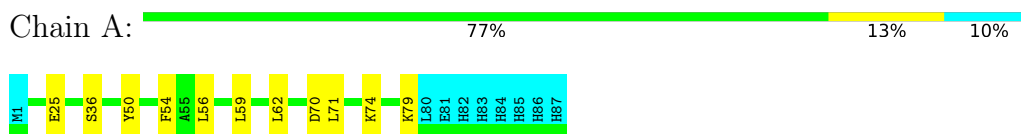
Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: Putative acyl carrier protein

Chain A:

4.2.11 Score per residue for model 11

• Molecule 1: Putative acyl carrier protein

Chain A:
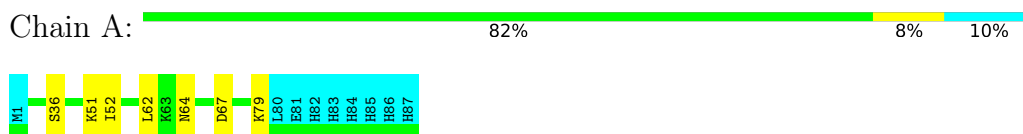
4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: Putative acyl carrier protein

Chain A:
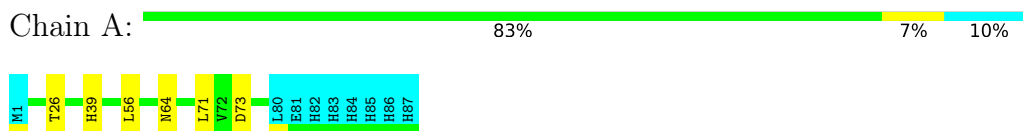
4.2.13 Score per residue for model 13

• Molecule 1: Putative acyl carrier protein

Chain A:
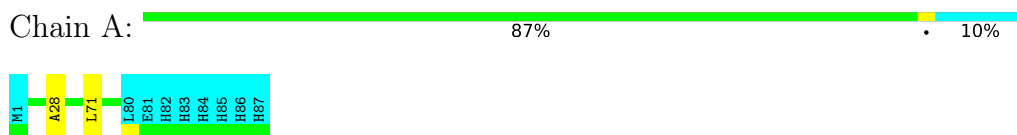
4.2.14 Score per residue for model 14

• Molecule 1: Putative acyl carrier protein

Chain A:
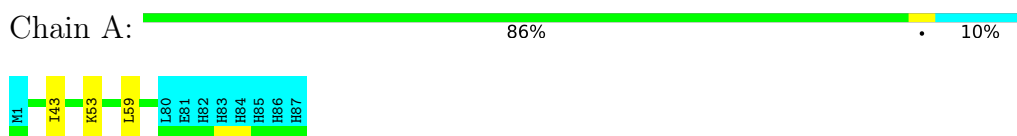
4.2.15 Score per residue for model 15

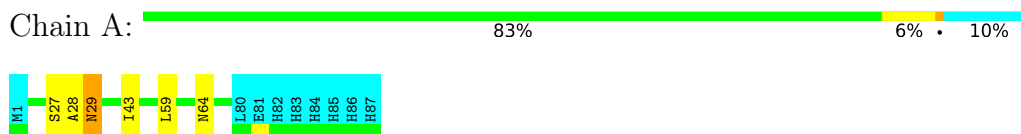• Molecule 1: Putative acyl carrier protein

Chain A:
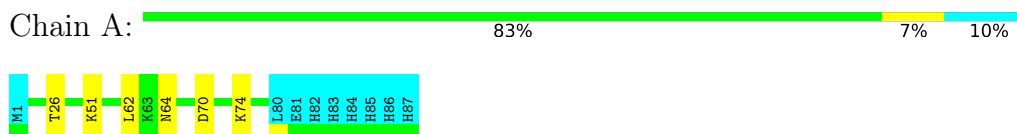
4.2.16 Score per residue for model 16

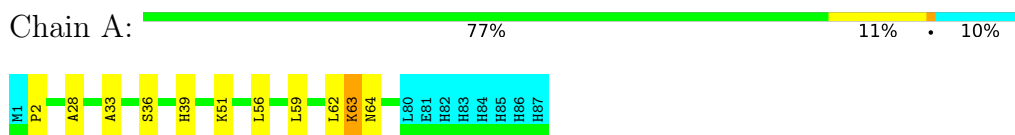• Molecule 1: Putative acyl carrier protein

Chain A:
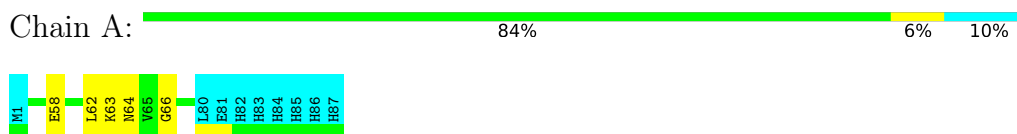
4.2.17 Score per residue for model 17
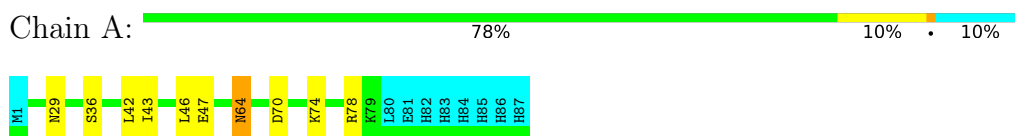
• Molecule 1: Putative acyl carrier protein

Chain A:

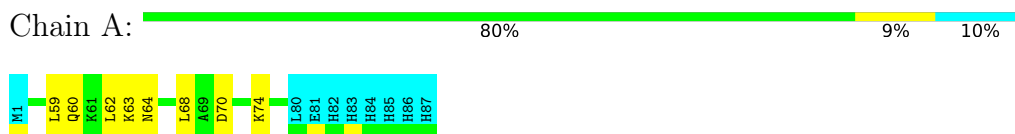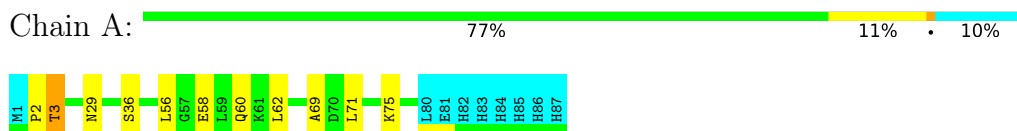#### 4.2.18 Score per residue for model 18

• Molecule 1: Putative acyl carrier protein

Chain A:

76%   14%   10%

M1 P2 T3 L22 S36 E58 L62 K63 N64 V65 A69 D70 L71 K74 R78 K79 L80 E81 H82 H83 H84 H85 H86 H87
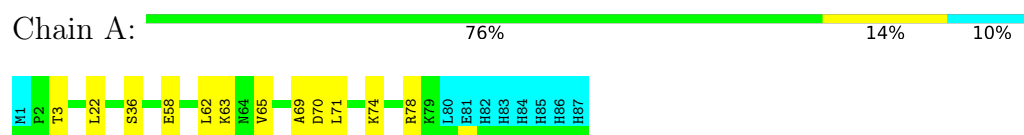
4.2.19 Score per residue for model 19

• Molecule 1: Putative acyl carrier protein

Chain A:

76%   14%   10%

M1 S36 K51 I52 K53 F54 L59 L62 K63 N64 D70 L71 K74 K75 L80 E81 H82 H83 H84 H85 H86 H87
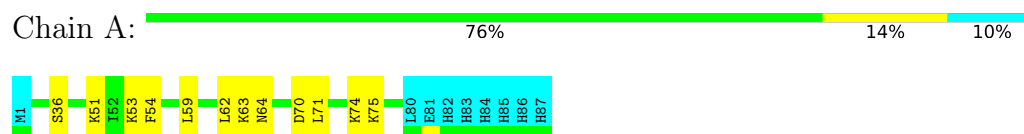
4.2.20 Score per residue for model 20

• Molecule 1: Putative acyl carrier protein

Chain A:

80%   7%   •   10%

M1 P2 T3 L59 Q60 N64 D70 L71 V72 D73 K74 L80 E81 H82 H83 H84 H85 H86 H87
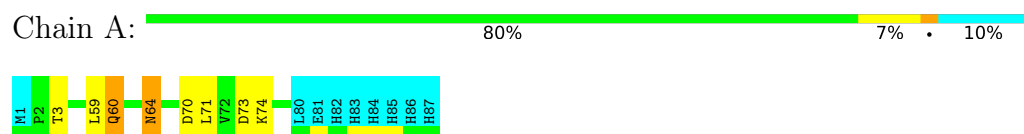
5 Refinement protocol and experimental data overview ⓘ

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

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

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.25
CNS	refinement	1.3
PSVS	refinement	1.4
PdbStat	structure solution	5.4
CYANA	structure solution	2.1
FMCGUI	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	1103
Number of shifts mapped to atoms	1103
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PNS

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	0.86±0.01	0±0/630 (0.0± 0.0%)	0.60±0.02	0±0/853 (0.0± 0.0%)
All	All	0.86	2/12600 (0.0%)	0.60	0/17060 (0.0%)

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	0.1±0.2
All	All	0	1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	36	SER	CB-OG	5.25	1.49	1.42	2	2

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	28	ALA	Peptide	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	620	635	634	3±1
2	A	21	21	21	1±1
All	All	12820	13120	13100	54

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:59:LEU:HD13	1:A:62:LEU:HD12	0.56	1.76	19	5
1:A:43:ILE:HG12	1:A:59:LEU:HD11	0.53	1.80	7	1
1:A:64:ASN:HA	2:A:88:PNS:H432	0.51	1.83	9	1
1:A:52:ILE:HA	1:A:79:LYS:HE3	0.50	1.84	11	1
1:A:54:PHE:CD1	1:A:59:LEU:HD21	0.49	2.43	19	1
1:A:54:PHE:HB3	1:A:75:LYS:HE3	0.48	1.84	19	1
1:A:3:THR:HB	1:A:69:ALA:HB1	0.47	1.86	18	2
1:A:39:HIS:NE2	2:A:88:PNS:H312	0.47	2.24	12	2
1:A:62:LEU:HD11	1:A:71:LEU:HG	0.45	1.87	19	2
1:A:62:LEU:HD22	1:A:67:ASP:HB3	0.45	1.89	11	1
1:A:60:GLN:HE21	1:A:60:GLN:HA	0.44	1.72	20	2
1:A:22:LEU:HD13	1:A:65:VAL:HG11	0.44	1.87	4	1
1:A:70:ASP:O	1:A:74:LYS:HG2	0.44	2.13	18	9
2:A:88:PNS:H36	2:A:88:PNS:H303	0.44	1.72	11	1
1:A:28:ALA:H	2:A:88:PNS:H422	0.44	1.73	13	1
1:A:64:ASN:ND2	1:A:66:GLY:H	0.43	2.10	16	1
1:A:3:THR:HG22	1:A:73:ASP:HB2	0.43	1.89	20	1
2:A:88:PNS:H36	2:A:88:PNS:H313	0.43	1.74	12	1
1:A:71:LEU:O	1:A:75:LYS:HG2	0.43	2.12	17	1
1:A:68:LEU:HD21	2:A:88:PNS:S44	0.43	2.54	10	1
1:A:43:ILE:O	1:A:47:GLU:HG2	0.43	2.14	9	2
1:A:43:ILE:HG12	1:A:59:LEU:HD22	0.43	1.89	14	1
1:A:28:ALA:HB2	2:A:88:PNS:H422	0.43	1.90	8	1
1:A:27:SER:HB2	1:A:29:ASN:HB3	0.42	1.90	7	1
1:A:58:GLU:O	1:A:62:LEU:HG	0.42	2.14	17	3
1:A:64:ASN:HD22	1:A:64:ASN:N	0.42	2.12	20	1
1:A:63:LYS:HA	2:A:88:PNS:H381	0.42	1.92	18	2
1:A:27:SER:HA	2:A:88:PNS:S44	0.41	2.55	2	1
1:A:22:LEU:HD22	1:A:65:VAL:HG11	0.41	1.91	18	1
1:A:62:LEU:HD21	1:A:71:LEU:HG	0.41	1.91	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:74:LYS:O	1:A:78:ARG:HG2	0.41	2.16	9	1
1:A:62:LEU:O	2:A:88:PNS:H381	0.41	2.14	15	1
1:A:42:LEU:O	1:A:46:LEU:HG	0.40	2.17	9	1
1:A:50:TYR:O	1:A:79:LYS:HE3	0.40	2.17	6	1

6.3   Torsion angles ⓘ

6.3.1   Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	78/87 (90%)	72±1 (93±2%)	5±2 (7±2%)	0±1 (1±1%)	29	74
All	All	1560/1740 (90%)	1444 (93%)	107 (7%)	9 (1%)	29	74

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	33	ALA	2
1	A	29	ASN	2
1	A	2	PRO	2
1	A	26	THR	2
1	A	3	THR	1

6.3.2   Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	70/79 (89%)	67±2 (96±2%)	3±2 (4±2%)	34	82
All	All	1400/1580 (89%)	1343 (96%)	57 (4%)	34	82

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All 18 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	64	ASN	9
1	A	51	LYS	7
1	A	71	LEU	7
1	A	36	SER	7
1	A	56	LEU	6
1	A	60	GLN	4
1	A	63	LYS	4
1	A	25	GLU	2
1	A	53	LYS	2
1	A	37	LEU	1
1	A	42	LEU	1
1	A	23	THR	1
1	A	35	ASP	1
1	A	54	PHE	1
1	A	39	HIS	1
1	A	29	ASN	1
1	A	73	ASP	1
1	A	59	LEU	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard

deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	PNS	A	88	1	13,20,21	0.81±0.07	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	PNS	A	88	1	18,26,29	0.66±0.08	0±0 (0±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PNS	A	88	1	-	0±0,24,26,27	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	88	PNS	C31-C29-C32	2.42	113.02	108.82	10	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PNS A 88

Bond lengths

Bond angles

Torsions

Rings
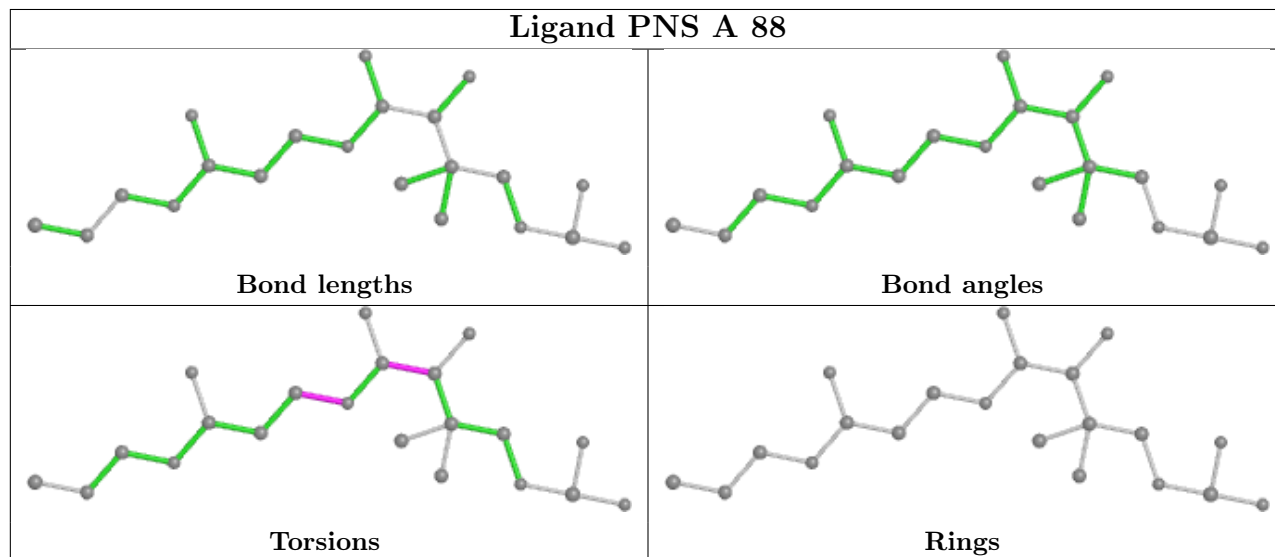
6.7 Other polymers ⓘ

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 94% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping ⓘ

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	1103
Number of shifts mapped to atoms	1103
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	81	-0.35 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	79	-0.06 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	74	-0.46 ± 0.21	None needed (< 0.5 ppm)
^{15}N	78	0.81 ± 0.28	Should be applied

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 94%, i.e. 1034 atoms were assigned a chemical shift out of a possible 1095. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	380/388 (98%)	155/156 (99%)	150/156 (96%)	75/76 (99%)
Sidechain	595/640 (93%)	404/417 (97%)	184/202 (91%)	7/21 (33%)

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	Total	**^{1}H**	**^{13}C**	**^{15}N**
Aromatic	59/67 (88%)	29/33 (88%)	27/29 (93%)	3/5 (60%)
Overall	1034/1095 (94%)	588/606 (97%)	361/387 (93%)	85/102 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1070 atoms were assigned a chemical shift out of a possible 1236. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	394/433 (91%)	161/174 (93%)	155/174 (89%)	78/85 (92%)
Sidechain	617/688 (90%)	419/449 (93%)	191/218 (88%)	7/21 (33%)
Aromatic	59/115 (51%)	29/57 (51%)	27/41 (66%)	3/17 (18%)
Overall	1070/1236 (87%)	609/680 (90%)	373/433 (86%)	88/123 (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	26	THR	HG1	5.99	0.08 − 2.19	23.0
1	A	8	THR	HG1	5.48	0.08 − 2.19	20.6
1	A	28	ALA	HB1	0.01	0.14 − 2.58	-5.5
1	A	28	ALA	HB2	0.01	0.14 − 2.58	-5.5
1	A	28	ALA	HB3	0.01	0.14 − 2.58	-5.5

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:
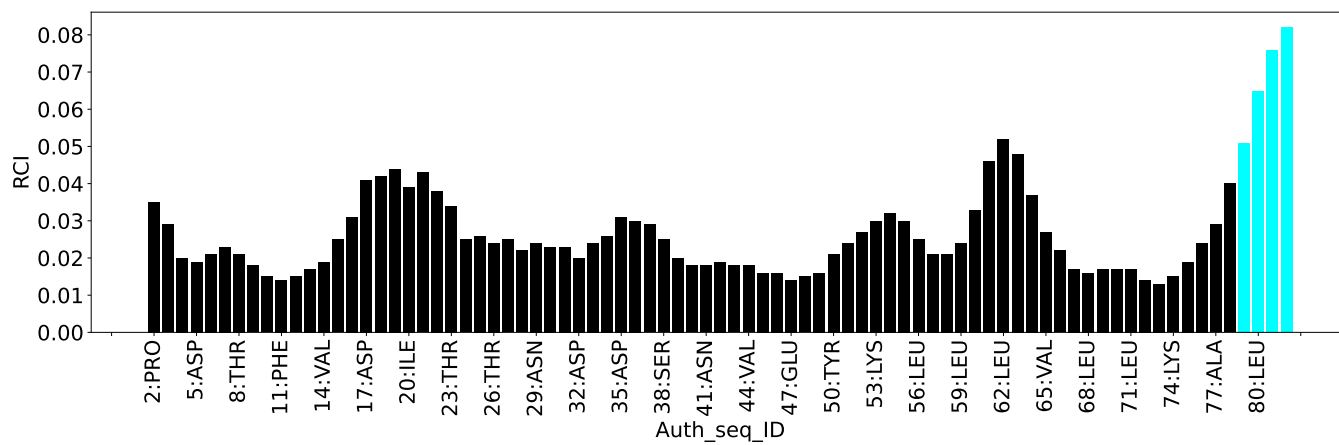
8   NMR restraints analysis ⓘ

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	1165
Intra-residue ($|i-j|$=0)	315
Sequential ($|i-j|$=1)	249
Medium range ($|i-j|$>1 and $|i-j|$<5)	286
Long range ($|i-j|$≥5)	263
Inter-chain	0
Hydrogen bond restraints	52
Disulfide bond restraints	0
Total dihedral-angle restraints	102
Number of unmapped restraints	0
Number of restraints per residue	14.6
Number of long range restraints per residue[1]	3.0

[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)	6.3	0.2
0.2-0.5 (Medium)	2.4	0.41
>0.5 (Large)	None	None

8.2.2　Average number of dihedral-angle violations per model ⓘ

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.4	6.7
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)	315	27.0	7	2.2	0.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	247	21.2	7	2.8	0.6	0	0.0	0.0
Sidechain-Sidechain	68	5.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	249	21.4	4	1.6	0.3	0	0.0	0.0
Backbone-Backbone	72	6.2	1	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	171	14.7	3	1.8	0.3	0	0.0	0.0
Sidechain-Sidechain	6	0.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	286	24.5	11	3.8	0.9	0	0.0	0.0
Backbone-Backbone	85	7.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	128	11.0	5	3.9	0.4	0	0.0	0.0
Sidechain-Sidechain	73	6.3	6	8.2	0.5	0	0.0	0.0
Long range (|i-j|≥5)	263	22.6	19	7.2	1.6	0	0.0	0.0
Backbone-Backbone	10	0.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	83	7.1	2	2.4	0.2	0	0.0	0.0
Sidechain-Sidechain	170	14.6	17	10.0	1.5	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	52	4.5	6	11.5	0.5	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1165	100.0	47	4.0	4.0	0	0.0	0.0
Backbone-Backbone	219	18.8	7	3.2	0.6	0	0.0	0.0
Backbone-Sidechain	629	54.0	17	2.7	1.5	0	0.0	0.0
Sidechain-Sidechain	317	27.2	23	7.3	2.0	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 ⓘ
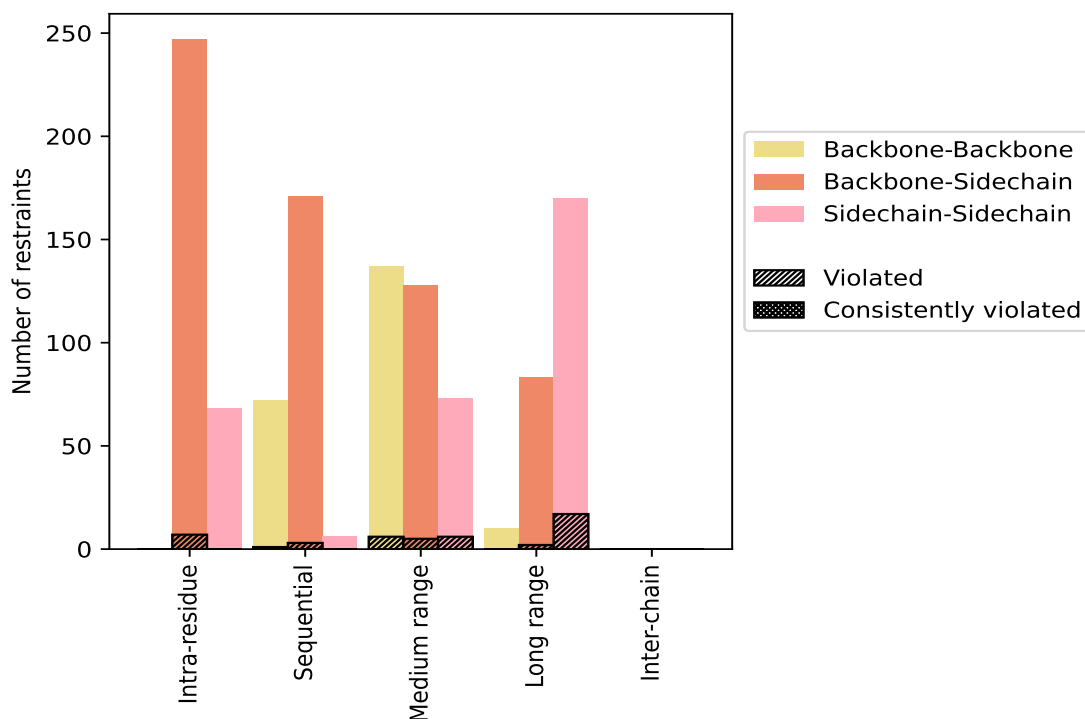
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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	2	1	3	2	0	8	0.15	0.2	0.03	0.15
2	2	1	3	1	0	7	0.14	0.21	0.03	0.13
3	1	0	4	3	0	8	0.18	0.35	0.08	0.16
4	2	0	6	9	0	17	0.17	0.28	0.06	0.15
5	2	1	1	6	0	10	0.17	0.33	0.07	0.15
6	1	0	2	3	0	6	0.19	0.26	0.06	0.2
7	2	2	3	4	0	11	0.17	0.41	0.09	0.14
8	1	1	4	4	0	10	0.14	0.29	0.05	0.12
9	1	0	5	3	0	9	0.2	0.3	0.07	0.21
10	0	1	4	3	0	8	0.16	0.31	0.06	0.14
11	2	0	8	3	0	13	0.17	0.3	0.07	0.14

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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	0	2	1	0	4	0.14	0.15	0.0	0.14
13	2	1	2	0	0	5	0.15	0.26	0.05	0.13
14	3	1	1	3	0	8	0.14	0.18	0.02	0.13
15	3	1	2	2	0	8	0.15	0.24	0.04	0.14
16	2	1	3	2	0	8	0.18	0.28	0.06	0.16
17	2	2	2	3	0	9	0.2	0.29	0.06	0.22
18	1	1	1	0	0	3	0.13	0.14	0.01	0.13
19	1	0	8	4	0	13	0.19	0.29	0.06	0.22
20	3	1	2	4	0	10	0.19	0.29	0.07	0.16

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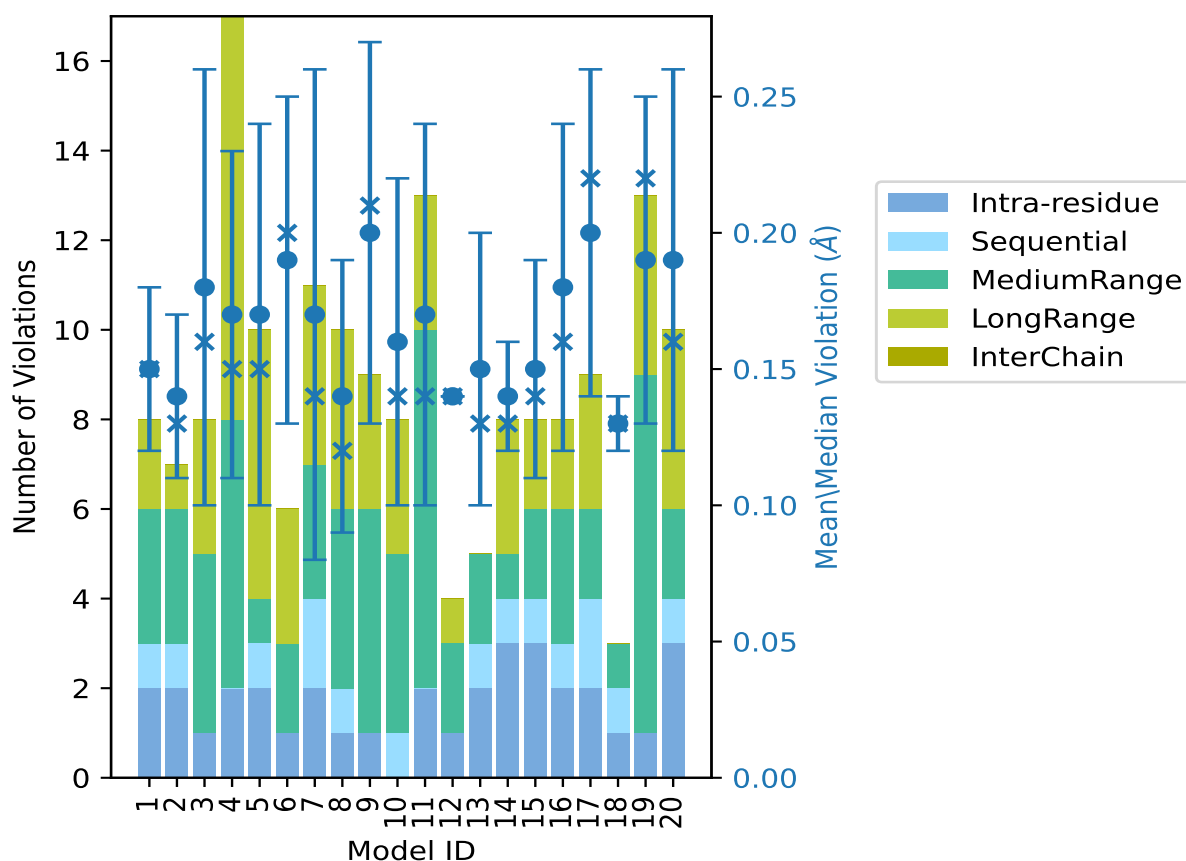
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

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, 1072(IR:308, SQ:245, MR:275, LR:244, 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]	%
5	2	3	10	0	20	1	5.0
0	1	1	2	0	4	2	10.0
0	0	2	3	0	5	3	15.0
0	0	3	0	0	3	4	20.0
0	0	0	1	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	1	0	1	9	45.0
0	0	0	1	0	1	10	50.0
0	1	0	0	0	1	11	55.0
1	0	0	0	0	1	12	60.0
0	0	1	1	0	2	13	65.0
0	0	1	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
1	0	0	0	0	1	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

[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

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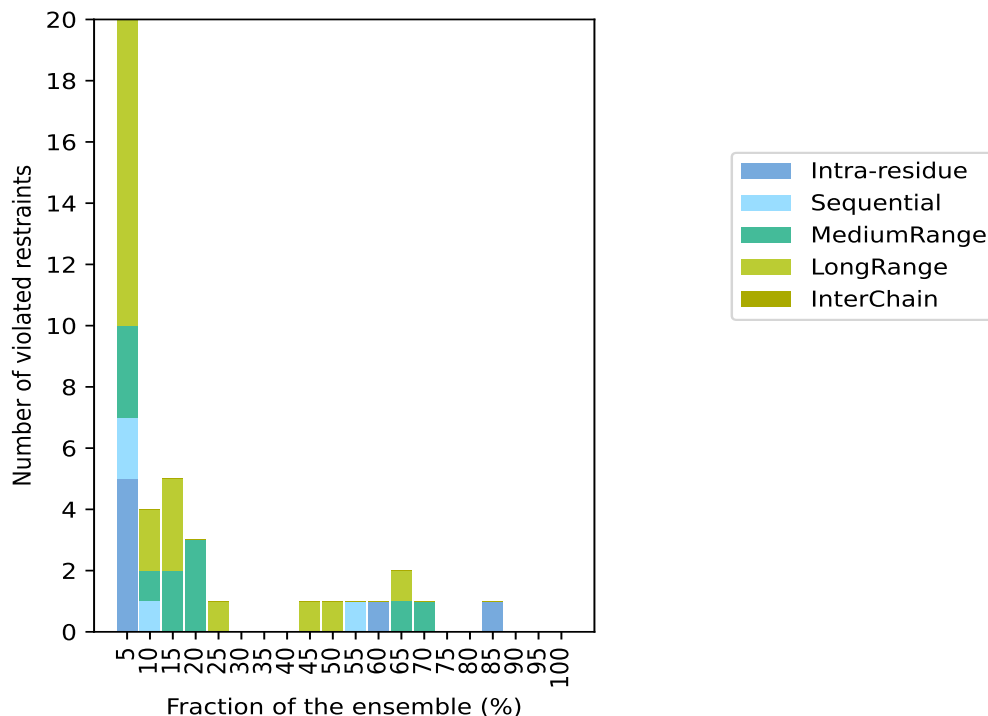
9.4 Most violated distance restraints in the ensemble ⓘ

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
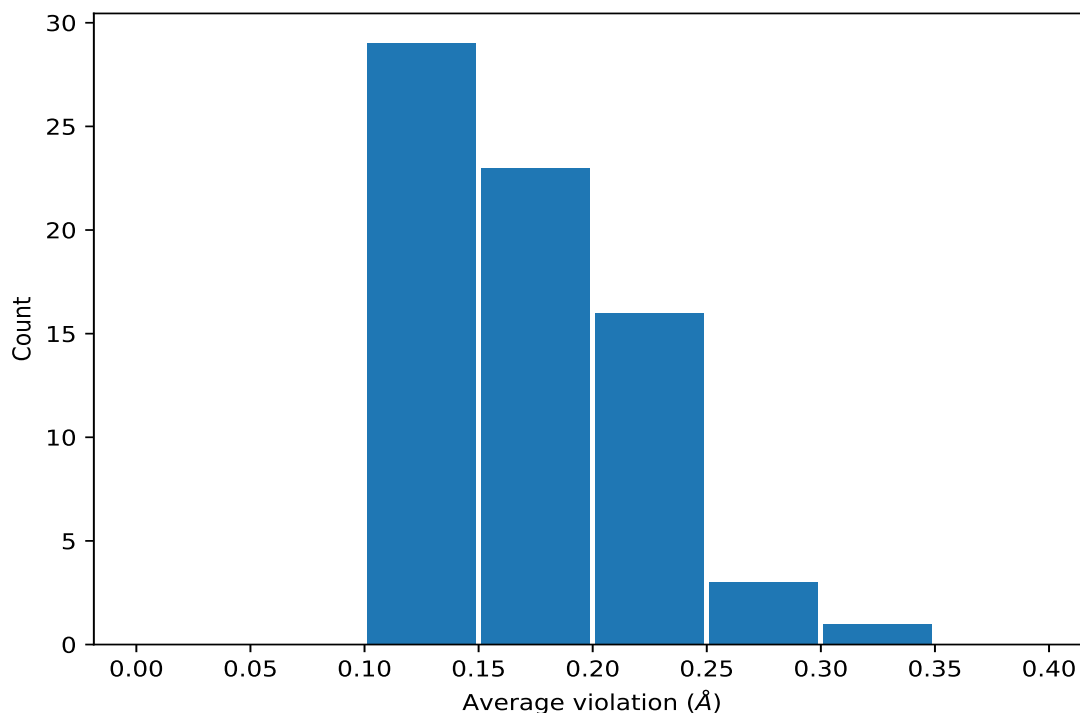
9.4.2   Table: Most violated distance restraints ⓘ

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)
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	17	0.12	0.01	0.12
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	14	0.27	0.04	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	14	0.27	0.04	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	14	0.27	0.04	0.26
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	13	0.23	0.07	0.25
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	13	0.23	0.07	0.25
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	13	0.23	0.07	0.25
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	13	0.16	0.03	0.16
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	13	0.16	0.03	0.16
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	13	0.16	0.03	0.16
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	13	0.16	0.03	0.16
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	13	0.16	0.03	0.16
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	13	0.16	0.03	0.16
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	12	0.12	0.01	0.12
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	11	0.13	0.01	0.14
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	10	0.2	0.06	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	10	0.14	0.02	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	9	0.16	0.05	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	9	0.16	0.05	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	9	0.16	0.05	0.14
(2,650)	1:A:47:GLU:HG2	1:A:52:ILE:H	5	0.13	0.02	0.11
(2,650)	1:A:47:GLU:HG3	1:A:52:ILE:H	5	0.13	0.02	0.11
(2,560)	1:A:42:LEU:HD21	1:A:46:LEU:HG	4	0.2	0.07	0.2
(2,560)	1:A:42:LEU:HD22	1:A:46:LEU:HG	4	0.2	0.07	0.2
(2,560)	1:A:42:LEU:HD23	1:A:46:LEU:HG	4	0.2	0.07	0.2
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD21	4	0.12	0.01	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD22	4	0.12	0.01	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD23	4	0.12	0.01	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD21	4	0.12	0.01	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD22	4	0.12	0.01	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD23	4	0.12	0.01	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD21	4	0.12	0.01	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD22	4	0.12	0.01	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD23	4	0.12	0.01	0.12
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB2	4	0.12	0.02	0.12
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB3	4	0.12	0.02	0.12
(2,21)	1:A:3:THR:HG21	1:A:72:VAL:HB	3	0.21	0.04	0.22
(2,21)	1:A:3:THR:HG22	1:A:72:VAL:HB	3	0.21	0.04	0.22
(2,21)	1:A:3:THR:HG23	1:A:72:VAL:HB	3	0.21	0.04	0.22
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD11	3	0.19	0.03	0.19
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD12	3	0.19	0.03	0.19
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD13	3	0.19	0.03	0.19
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD11	3	0.19	0.03	0.19
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD12	3	0.19	0.03	0.19
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD13	3	0.19	0.03	0.19
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD11	3	0.19	0.03	0.19
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD12	3	0.19	0.03	0.19
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD13	3	0.19	0.03	0.19
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD11	3	0.17	0.05	0.19
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD12	3	0.17	0.05	0.19
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD13	3	0.17	0.05	0.19
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD21	3	0.15	0.02	0.16
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD22	3	0.15	0.02	0.16
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD23	3	0.15	0.02	0.16
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD21	3	0.15	0.02	0.16
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD22	3	0.15	0.02	0.16
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD23	3	0.15	0.02	0.16
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD11	3	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD12	3	0.15	0.02	0.15
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD13	3	0.15	0.02	0.15
(2,425)	1:A:28:ALA:H	1:A:29:ASN:H	2	0.34	0.06	0.34
(2,3)	1:A:2:PRO:HD2	1:A:69:ALA:HB1	2	0.2	0.06	0.2
(2,3)	1:A:2:PRO:HD2	1:A:69:ALA:HB2	2	0.2	0.06	0.2
(2,3)	1:A:2:PRO:HD2	1:A:69:ALA:HB3	2	0.2	0.06	0.2
(2,3)	1:A:2:PRO:HD3	1:A:69:ALA:HB1	2	0.2	0.06	0.2
(2,3)	1:A:2:PRO:HD3	1:A:69:ALA:HB2	2	0.2	0.06	0.2
(2,3)	1:A:2:PRO:HD3	1:A:69:ALA:HB3	2	0.2	0.06	0.2
(2,1049)	1:A:75:LYS:HA	1:A:78:ARG:HD2	2	0.19	0.07	0.19
(2,1049)	1:A:75:LYS:HA	1:A:78:ARG:HD3	2	0.19	0.07	0.19
(1,51)	1:A:78:ARG:H	1:A:74:LYS:O	2	0.14	0.02	0.14
(2,653)	1:A:47:GLU:HG3	1:A:54:PHE:HD1	2	0.13	0.02	0.13
(2,653)	1:A:47:GLU:HG3	1:A:54:PHE:HD2	2	0.13	0.02	0.13

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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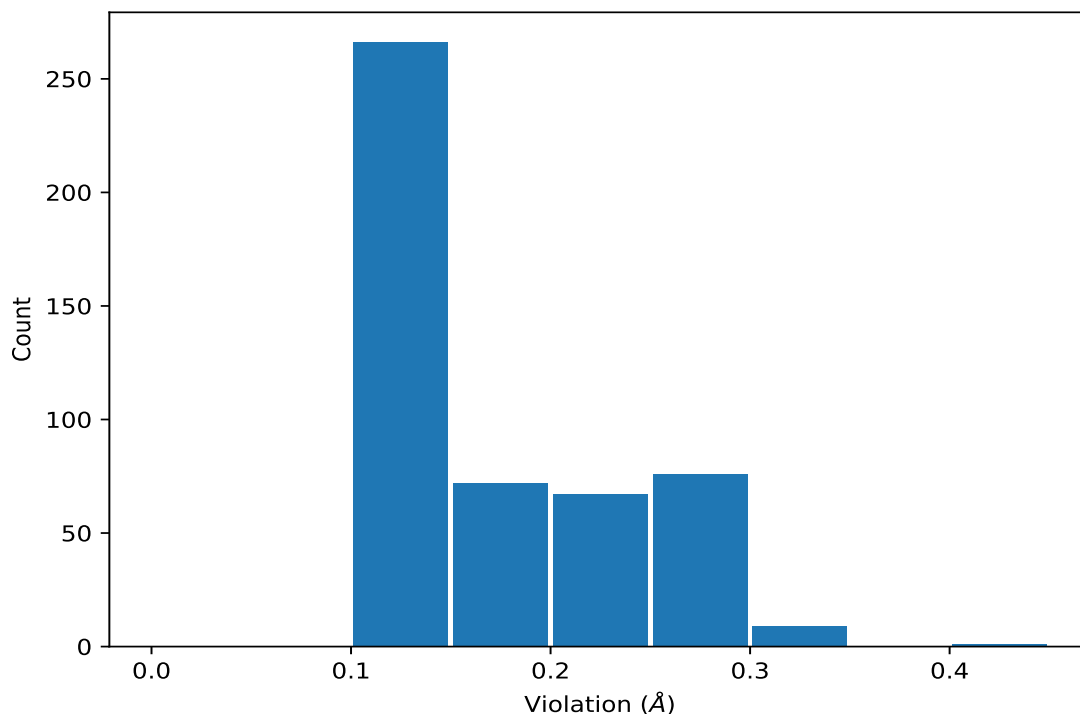
9.5.2 Table : All distance violations ⓘ

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)
(2,425)	1:A:28:ALA:H	1:A:29:ASN:H	7	0.41
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	3	0.35
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	3	0.35
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	3	0.35
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	5	0.33
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	5	0.33
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	5	0.33
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	10	0.31
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	10	0.31
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	10	0.31
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	9	0.3
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	9	0.3
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	9	0.3
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	11	0.3
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	11	0.3
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	11	0.3
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	17	0.29
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	17	0.29
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	17	0.29
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	19	0.29
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	19	0.29
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	19	0.29
(2,840)	1:A:59:LEU:H	1:A:59:LEU:HG	20	0.29
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	8	0.29
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	8	0.29
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	8	0.29
(2,560)	1:A:42:LEU:HD21	1:A:46:LEU:HG	9	0.29
(2,560)	1:A:42:LEU:HD22	1:A:46:LEU:HG	9	0.29
(2,560)	1:A:42:LEU:HD23	1:A:46:LEU:HG	9	0.29
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	7	0.28
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	7	0.28
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	7	0.28
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	16	0.28
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	16	0.28
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	16	0.28
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	20	0.28
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	20	0.28
(2,425)	1:A:28:ALA:H	1:A:29:ASN:H	17	0.28
(2,34)	1:A:4:LEU:HD11	1:A:22:LEU:HD11	4	0.28
(2,34)	1:A:4:LEU:HD11	1:A:22:LEU:HD12	4	0.28
(2,34)	1:A:4:LEU:HD11	1:A:22:LEU:HD13	4	0.28
(2,34)	1:A:4:LEU:HD12	1:A:22:LEU:HD11	4	0.28
(2,34)	1:A:4:LEU:HD12	1:A:22:LEU:HD12	4	0.28
(2,34)	1:A:4:LEU:HD12	1:A:22:LEU:HD13	4	0.28
(2,34)	1:A:4:LEU:HD13	1:A:22:LEU:HD11	4	0.28
(2,34)	1:A:4:LEU:HD13	1:A:22:LEU:HD12	4	0.28
(2,34)	1:A:4:LEU:HD13	1:A:22:LEU:HD13	4	0.28
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	16	0.27
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	16	0.27
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	16	0.27
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	4	0.27
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	4	0.27
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	4	0.27
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	11	0.27
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	11	0.27
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	11	0.27
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	11	0.27
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	19	0.27
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	6	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	6	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	6	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	13	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	13	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	13	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	19	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	19	0.26
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	19	0.26
(2,3)	1:A:2:PRO:HD2	1:A:69:ALA:HB1	5	0.26
(2,3)	1:A:2:PRO:HD2	1:A:69:ALA:HB2	5	0.26
(2,3)	1:A:2:PRO:HD2	1:A:69:ALA:HB3	5	0.26
(2,3)	1:A:2:PRO:HD3	1:A:69:ALA:HB1	5	0.26
(2,3)	1:A:2:PRO:HD3	1:A:69:ALA:HB2	5	0.26
(2,3)	1:A:2:PRO:HD3	1:A:69:ALA:HB3	5	0.26
(2,1103)	1:A:80:LEU:HD11	1:A:81:GLU:H	20	0.26
(2,1103)	1:A:80:LEU:HD12	1:A:81:GLU:H	20	0.26
(2,1103)	1:A:80:LEU:HD13	1:A:81:GLU:H	20	0.26
(2,1049)	1:A:75:LYS:HA	1:A:78:ARG:HD2	3	0.26
(2,1049)	1:A:75:LYS:HA	1:A:78:ARG:HD3	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:A:79:LYS:H	1:A:75:LYS:O	6	0.26
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	20	0.25
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	20	0.25
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	20	0.25
(2,21)	1:A:3:THR:HG21	1:A:72:VAL:HB	19	0.25
(2,21)	1:A:3:THR:HG22	1:A:72:VAL:HB	19	0.25
(2,21)	1:A:3:THR:HG23	1:A:72:VAL:HB	19	0.25
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	4	0.24
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	4	0.24
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	4	0.24
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	9	0.24
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	9	0.24
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	9	0.24
(2,560)	1:A:42:LEU:HD21	1:A:46:LEU:HG	4	0.24
(2,560)	1:A:42:LEU:HD22	1:A:46:LEU:HG	4	0.24
(2,560)	1:A:42:LEU:HD23	1:A:46:LEU:HG	4	0.24
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	15	0.24
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	17	0.24
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	6	0.23
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD11	9	0.22
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD12	9	0.22
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD13	9	0.22
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD11	9	0.22
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD12	9	0.22
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD13	9	0.22
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD11	9	0.22
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD12	9	0.22
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD13	9	0.22
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	7	0.22
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	7	0.22
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	7	0.22
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	17	0.22
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	17	0.22
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	17	0.22
(2,796)	1:A:54:PHE:HZ	1:A:72:VAL:HG21	19	0.22
(2,796)	1:A:54:PHE:HZ	1:A:72:VAL:HG22	19	0.22
(2,796)	1:A:54:PHE:HZ	1:A:72:VAL:HG23	19	0.22
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD11	19	0.22
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD12	19	0.22
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD13	19	0.22
(2,21)	1:A:3:THR:HG21	1:A:72:VAL:HB	17	0.22
(2,21)	1:A:3:THR:HG22	1:A:72:VAL:HB	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:A:3:THR:HG23	1:A:72:VAL:HB	17	0.22
(2,161)	1:A:10:ILE:HG21	1:A:42:LEU:HD21	4	0.22
(2,161)	1:A:10:ILE:HG21	1:A:42:LEU:HD22	4	0.22
(2,161)	1:A:10:ILE:HG21	1:A:42:LEU:HD23	4	0.22
(2,161)	1:A:10:ILE:HG22	1:A:42:LEU:HD21	4	0.22
(2,161)	1:A:10:ILE:HG22	1:A:42:LEU:HD22	4	0.22
(2,161)	1:A:10:ILE:HG22	1:A:42:LEU:HD23	4	0.22
(2,161)	1:A:10:ILE:HG23	1:A:42:LEU:HD21	4	0.22
(2,161)	1:A:10:ILE:HG23	1:A:42:LEU:HD22	4	0.22
(2,161)	1:A:10:ILE:HG23	1:A:42:LEU:HD23	4	0.22
(1,29)	1:A:59:LEU:H	1:A:55:ALA:O	19	0.22
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	2	0.21
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	2	0.21
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	2	0.21
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	5	0.21
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	5	0.21
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	5	0.21
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	5	0.21
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	5	0.21
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	5	0.21
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	11	0.21
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	11	0.21
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	11	0.21
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	11	0.21
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	11	0.21
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	11	0.21
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	9	0.21
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	9	0.21
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	9	0.21
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD11	1	0.2
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD12	1	0.2
(2,807)	1:A:56:LEU:HA	1:A:59:LEU:HD13	1	0.2
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD11	16	0.19
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD12	16	0.19
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD13	16	0.19
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD11	16	0.19
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD12	16	0.19
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD13	16	0.19
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD11	16	0.19
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD12	16	0.19
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD13	16	0.19
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	1	0.19
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	1	0.19
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	1	0.19
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	1	0.19
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	1	0.19
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD11	11	0.19
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD12	11	0.19
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD13	11	0.19
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	3	0.18
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	3	0.18
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	3	0.18
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	3	0.18
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	3	0.18
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	3	0.18
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	16	0.18
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	16	0.18
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	16	0.18
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	16	0.18
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	16	0.18
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	16	0.18
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	17	0.18
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	17	0.18
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	17	0.18
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	17	0.18
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	17	0.18
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	17	0.18
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD11	20	0.18
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD12	20	0.18
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD13	20	0.18
(2,1111)	1:A:81:GLU:H	1:A:81:GLU:HG2	14	0.18
(2,1111)	1:A:81:GLU:H	1:A:81:GLU:HG3	14	0.18
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	1	0.18
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD21	6	0.17
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD22	6	0.17
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD23	6	0.17
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD21	6	0.17
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD22	6	0.17
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD23	6	0.17
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	3	0.17
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	5	0.17
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	14	0.16
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	14	0.16
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD21	8	0.16
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD22	8	0.16
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD23	8	0.16
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD21	8	0.16
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD22	8	0.16
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD23	8	0.16
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	4	0.16
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	4	0.16
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	4	0.16
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	4	0.16
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	4	0.16
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	4	0.16
(2,650)	1:A:47:GLU:HG2	1:A:52:ILE:H	4	0.16
(2,650)	1:A:47:GLU:HG3	1:A:52:ILE:H	4	0.16
(2,21)	1:A:3:THR:HG21	1:A:72:VAL:HB	10	0.16
(2,21)	1:A:3:THR:HG22	1:A:72:VAL:HB	10	0.16
(2,21)	1:A:3:THR:HG23	1:A:72:VAL:HB	10	0.16
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	9	0.16
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	3	0.16
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD11	4	0.15
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD12	4	0.15
(2,835)	1:A:59:LEU:HD21	1:A:68:LEU:HD13	4	0.15
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD11	4	0.15
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD12	4	0.15
(2,835)	1:A:59:LEU:HD22	1:A:68:LEU:HD13	4	0.15
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD11	4	0.15
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD12	4	0.15
(2,835)	1:A:59:LEU:HD23	1:A:68:LEU:HD13	4	0.15
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	14	0.15
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	14	0.15
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	14	0.15
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	14	0.15
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	14	0.15
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	14	0.15
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	15	0.15
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	15	0.15
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	15	0.15
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	15	0.15
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	15	0.15
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	15	0.15
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD11	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD12	10	0.15
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD13	10	0.15
(2,653)	1:A:47:GLU:HG3	1:A:54:PHE:HD1	5	0.15
(2,653)	1:A:47:GLU:HG3	1:A:54:PHE:HD2	5	0.15
(2,650)	1:A:47:GLU:HG2	1:A:52:ILE:H	8	0.15
(2,650)	1:A:47:GLU:HG3	1:A:52:ILE:H	8	0.15
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	1	0.15
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	7	0.15
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	10	0.15
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	15	0.15
(2,560)	1:A:42:LEU:HD21	1:A:46:LEU:HG	11	0.15
(2,560)	1:A:42:LEU:HD22	1:A:46:LEU:HG	11	0.15
(2,560)	1:A:42:LEU:HD23	1:A:46:LEU:HG	11	0.15
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB2	2	0.15
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB3	2	0.15
(2,3)	1:A:2:PRO:HD2	1:A:69:ALA:HB1	7	0.15
(2,3)	1:A:2:PRO:HD2	1:A:69:ALA:HB2	7	0.15
(2,3)	1:A:2:PRO:HD2	1:A:69:ALA:HB3	7	0.15
(2,3)	1:A:2:PRO:HD3	1:A:69:ALA:HB1	7	0.15
(2,3)	1:A:2:PRO:HD3	1:A:69:ALA:HB2	7	0.15
(2,3)	1:A:2:PRO:HD3	1:A:69:ALA:HB3	7	0.15
(2,1108)	1:A:80:LEU:H	1:A:80:LEU:HG	13	0.15
(2,1104)	1:A:80:LEU:H	1:A:80:LEU:HB3	4	0.15
(1,51)	1:A:78:ARG:H	1:A:74:LYS:O	12	0.15
(2,966)	1:A:69:ALA:HA	1:A:72:VAL:HG21	15	0.14
(2,966)	1:A:69:ALA:HA	1:A:72:VAL:HG22	15	0.14
(2,966)	1:A:69:ALA:HA	1:A:72:VAL:HG23	15	0.14
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	12	0.14
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	12	0.14
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	12	0.14
(2,790)	1:A:54:PHE:HE1	1:A:71:LEU:HG	19	0.14
(2,790)	1:A:54:PHE:HE2	1:A:71:LEU:HG	19	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	5	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	5	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	5	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	6	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	6	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	6	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	7	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	7	0.14
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	7	0.14
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	12	0.14
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	18	0.14
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	1	0.14
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	2	0.14
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	5	0.14
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD21	4	0.14
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD22	4	0.14
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD23	4	0.14
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD21	4	0.14
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD22	4	0.14
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD23	4	0.14
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD21	4	0.14
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD22	4	0.14
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD23	4	0.14
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	4	0.14
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	11	0.14
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	15	0.14
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	19	0.14
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	12	0.14
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	1	0.13
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	1	0.13
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	1	0.13
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG21	10	0.13
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG22	10	0.13
(2,955)	1:A:68:LEU:HG	1:A:72:VAL:HG23	10	0.13
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD21	20	0.13
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD22	20	0.13
(2,789)	1:A:54:PHE:HE1	1:A:71:LEU:HD23	20	0.13
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD21	20	0.13
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD22	20	0.13
(2,789)	1:A:54:PHE:HE2	1:A:71:LEU:HD23	20	0.13
(2,752)	1:A:52:ILE:HG21	1:A:79:LYS:HE2	4	0.13
(2,752)	1:A:52:ILE:HG21	1:A:79:LYS:HE3	4	0.13
(2,752)	1:A:52:ILE:HG22	1:A:79:LYS:HE2	4	0.13
(2,752)	1:A:52:ILE:HG22	1:A:79:LYS:HE3	4	0.13
(2,752)	1:A:52:ILE:HG23	1:A:79:LYS:HE2	4	0.13
(2,752)	1:A:52:ILE:HG23	1:A:79:LYS:HE3	4	0.13
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	3	0.13
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	3	0.13
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	3	0.13
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	8	0.13
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	8	0.13
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	10	0.13
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	10	0.13
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	10	0.13
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	2	0.13
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	16	0.13
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	17	0.13
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	13	0.13
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	15	0.13
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	16	0.13
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	14	0.13
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	18	0.13
(2,5)	1:A:2:PRO:HD2	1:A:72:VAL:HG21	14	0.13
(2,5)	1:A:2:PRO:HD2	1:A:72:VAL:HG22	14	0.13
(2,5)	1:A:2:PRO:HD2	1:A:72:VAL:HG23	14	0.13
(2,5)	1:A:2:PRO:HD3	1:A:72:VAL:HG21	14	0.13
(2,5)	1:A:2:PRO:HD3	1:A:72:VAL:HG22	14	0.13
(2,5)	1:A:2:PRO:HD3	1:A:72:VAL:HG23	14	0.13
(2,462)	1:A:32:ASP:HB2	1:A:33:ALA:H	8	0.13
(2,462)	1:A:32:ASP:HB3	1:A:33:ALA:H	8	0.13
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	10	0.13
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	16	0.13
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	20	0.13
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	7	0.12
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	7	0.12
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	7	0.12
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	7	0.12
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	7	0.12
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	7	0.12
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	8	0.12
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	8	0.12
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	8	0.12
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	8	0.12
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	8	0.12
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	8	0.12
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	10	0.12
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	10	0.12
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	10	0.12
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	10	0.12
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	10	0.12
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	10	0.12
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD11	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD12	8	0.12
(2,75)	1:A:7:LEU:HA	1:A:10:ILE:HD13	8	0.12
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	1	0.12
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	5	0.12
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	7	0.12
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	15	0.12
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	19	0.12
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	2	0.12
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	8	0.12
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	17	0.12
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	20	0.12
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	13	0.12
(2,560)	1:A:42:LEU:HD21	1:A:46:LEU:HG	19	0.12
(2,560)	1:A:42:LEU:HD22	1:A:46:LEU:HG	19	0.12
(2,560)	1:A:42:LEU:HD23	1:A:46:LEU:HG	19	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD21	9	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD22	9	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD23	9	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD21	9	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD22	9	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD23	9	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD21	9	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD22	9	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD23	9	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD21	11	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD22	11	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD23	11	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD21	11	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD22	11	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD23	11	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD21	11	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD22	11	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD23	11	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD21	19	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD22	19	0.12
(2,559)	1:A:42:LEU:HD21	1:A:46:LEU:HD23	19	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD21	19	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD22	19	0.12
(2,559)	1:A:42:LEU:HD22	1:A:46:LEU:HD23	19	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD21	19	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD22	19	0.12
(2,559)	1:A:42:LEU:HD23	1:A:46:LEU:HD23	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,485)	1:A:34:TRP:HZ2	1:A:42:LEU:HD11	9	0.12
(2,485)	1:A:34:TRP:HZ2	1:A:42:LEU:HD12	9	0.12
(2,485)	1:A:34:TRP:HZ2	1:A:42:LEU:HD13	9	0.12
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB2	19	0.12
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB3	19	0.12
(2,1072)	1:A:76:LEU:HD21	1:A:79:LYS:HD2	11	0.12
(2,1072)	1:A:76:LEU:HD21	1:A:79:LYS:HD3	11	0.12
(2,1072)	1:A:76:LEU:HD22	1:A:79:LYS:HD2	11	0.12
(2,1072)	1:A:76:LEU:HD22	1:A:79:LYS:HD3	11	0.12
(2,1072)	1:A:76:LEU:HD23	1:A:79:LYS:HD2	11	0.12
(2,1072)	1:A:76:LEU:HD23	1:A:79:LYS:HD3	11	0.12
(2,1049)	1:A:75:LYS:HA	1:A:78:ARG:HD2	8	0.12
(2,1049)	1:A:75:LYS:HA	1:A:78:ARG:HD3	8	0.12
(1,51)	1:A:78:ARG:H	1:A:74:LYS:O	2	0.12
(2,900)	1:A:63:LYS:H	1:A:63:LYS:HG2	15	0.11
(2,900)	1:A:63:LYS:H	1:A:63:LYS:HG3	15	0.11
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD21	2	0.11
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD22	2	0.11
(2,783)	1:A:54:PHE:HD1	1:A:71:LEU:HD23	2	0.11
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD21	2	0.11
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD22	2	0.11
(2,783)	1:A:54:PHE:HD2	1:A:71:LEU:HD23	2	0.11
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD11	4	0.11
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD12	4	0.11
(2,740)	1:A:54:PHE:HB2	1:A:59:LEU:HD13	4	0.11
(2,734)	1:A:52:ILE:HD11	1:A:75:LYS:HD2	1	0.11
(2,734)	1:A:52:ILE:HD11	1:A:75:LYS:HD3	1	0.11
(2,734)	1:A:52:ILE:HD12	1:A:75:LYS:HD2	1	0.11
(2,734)	1:A:52:ILE:HD12	1:A:75:LYS:HD3	1	0.11
(2,734)	1:A:52:ILE:HD13	1:A:75:LYS:HD2	1	0.11
(2,734)	1:A:52:ILE:HD13	1:A:75:LYS:HD3	1	0.11
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	4	0.11
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	14	0.11
(2,669)	1:A:48:VAL:H	1:A:48:VAL:HB	20	0.11
(2,653)	1:A:47:GLU:HG3	1:A:54:PHE:HD1	7	0.11
(2,653)	1:A:47:GLU:HG3	1:A:54:PHE:HD2	7	0.11
(2,650)	1:A:47:GLU:HG2	1:A:52:ILE:H	5	0.11
(2,650)	1:A:47:GLU:HG3	1:A:52:ILE:H	5	0.11
(2,650)	1:A:47:GLU:HG2	1:A:52:ILE:H	11	0.11
(2,650)	1:A:47:GLU:HG3	1:A:52:ILE:H	11	0.11
(2,650)	1:A:47:GLU:HG2	1:A:52:ILE:H	20	0.11
(2,650)	1:A:47:GLU:HG3	1:A:52:ILE:H	20	0.11

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| Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	3	0.11
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	5	0.11
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	6	0.11
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	7	0.11
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	9	0.11
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	11	0.11
(2,601)	1:A:44:VAL:H	1:A:44:VAL:HB	14	0.11
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	16	0.11
(2,596)	1:A:44:VAL:HB	1:A:45:SER:H	17	0.11
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD11	3	0.11
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD12	3	0.11
(2,522)	1:A:39:HIS:HE1	1:A:42:LEU:HD13	3	0.11
(2,49)	1:A:4:LEU:HD21	1:A:24:ARG:H	14	0.11
(2,49)	1:A:4:LEU:HD22	1:A:24:ARG:H	14	0.11
(2,49)	1:A:4:LEU:HD23	1:A:24:ARG:H	14	0.11
(2,472)	1:A:34:TRP:HD1	1:A:39:HIS:HB2	4	0.11
(2,472)	1:A:34:TRP:HD1	1:A:39:HIS:HB3	4	0.11
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB2	4	0.11
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB3	4	0.11
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB2	11	0.11
(2,413)	1:A:27:SER:H	1:A:30:ASP:HB3	11	0.11
(2,17)	1:A:3:THR:HG21	1:A:7:LEU:HD11	18	0.11
(2,17)	1:A:3:THR:HG21	1:A:7:LEU:HD12	18	0.11
(2,17)	1:A:3:THR:HG21	1:A:7:LEU:HD13	18	0.11
(2,17)	1:A:3:THR:HG22	1:A:7:LEU:HD11	18	0.11
(2,17)	1:A:3:THR:HG22	1:A:7:LEU:HD12	18	0.11
(2,17)	1:A:3:THR:HG22	1:A:7:LEU:HD13	18	0.11
(2,17)	1:A:3:THR:HG23	1:A:7:LEU:HD11	18	0.11
(2,17)	1:A:3:THR:HG23	1:A:7:LEU:HD12	18	0.11
(2,17)	1:A:3:THR:HG23	1:A:7:LEU:HD13	18	0.11
(1,41)	1:A:73:ASP:H	1:A:69:ALA:O	7	0.11
(1,19)	1:A:46:LEU:H	1:A:42:LEU:O	13	0.11
(1,17)	1:A:45:SER:H	1:A:41:ASN:O	8	0.11
(1,1)	1:A:34:TRP:HE1	1:A:39:HIS:ND1	4	0.11

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	51	50.0	9	17.6	8.8	0	0.0	0.0
PHI	51	50.0	3	5.9	2.9	0	0.0	0.0
Total	102	100.0	12	11.8	11.8	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 (i)
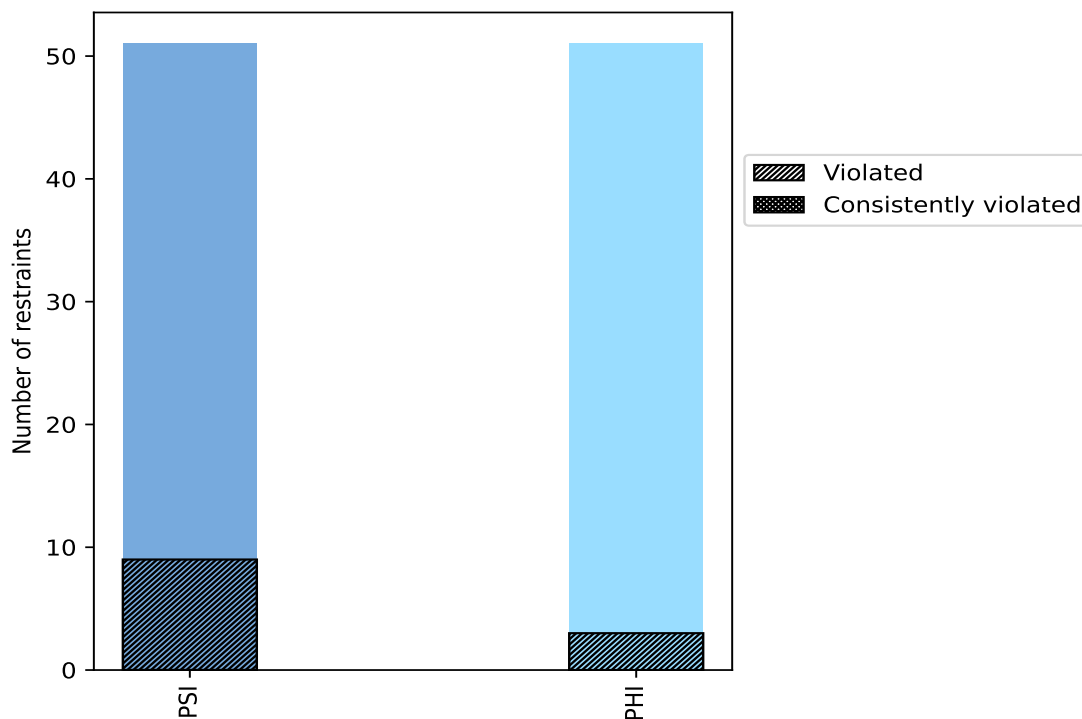
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (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 (°)
	PSI	PHI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	2	0	2	1.35	1.5	0.15	1.35
3	2	0	2	1.4	1.4	0.0	1.4
4	0	0	0	0.0	0.0	0.0	0.0
5	1	0	1	2.7	2.7	0.0	2.7
6	1	0	1	1.3	1.3	0.0	1.3
7	0	2	2	2.1	2.7	0.6	2.1
8	4	0	4	2.9	3.6	0.54	2.95
9	1	1	2	1.45	1.6	0.15	1.45
10	1	0	1	2.2	2.2	0.0	2.2
11	1	1	2	2.6	2.9	0.3	2.6
12	1	0	1	3.1	3.1	0.0	3.1
13	1	0	1	2.3	2.3	0.0	2.3
14	1	0	1	3.4	3.4	0.0	3.4
15	3	1	4	3.8	6.7	2.07	3.4
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	1	1	2	2.15	3.1	0.95	2.15
20	1	0	1	3.1	3.1	0.0	3.1

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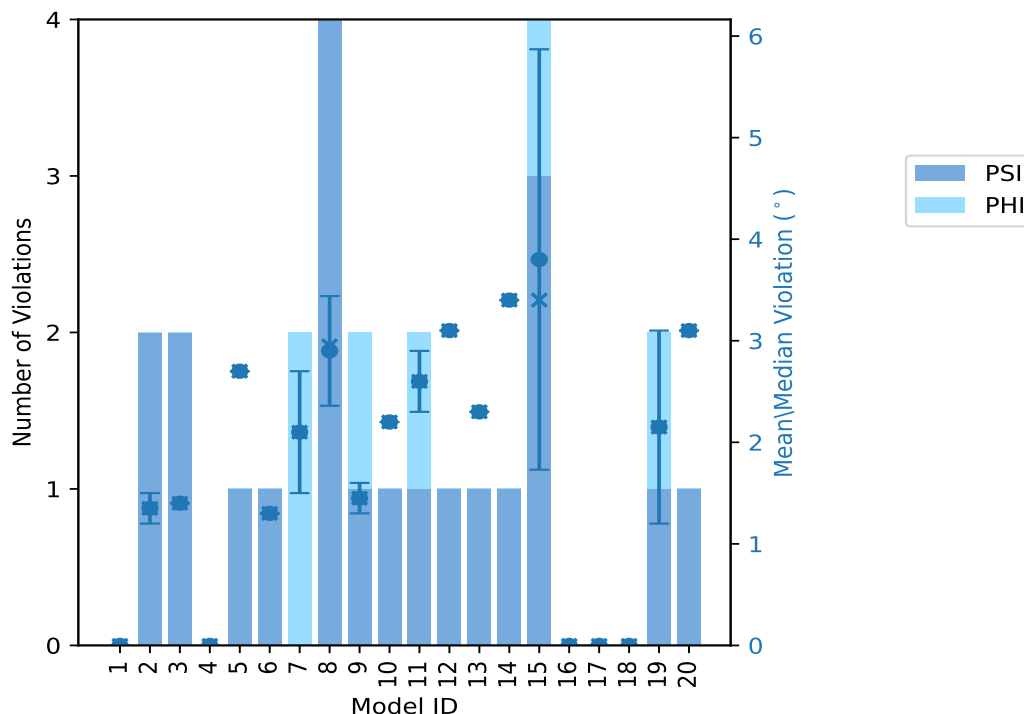
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

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

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

[1] Number of models with violations

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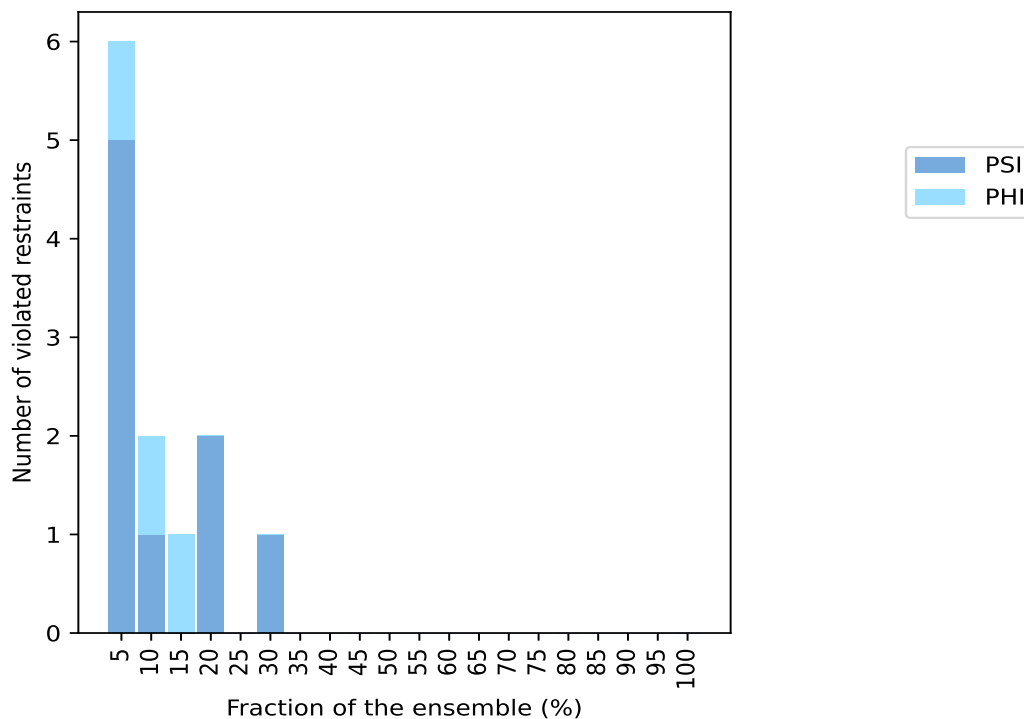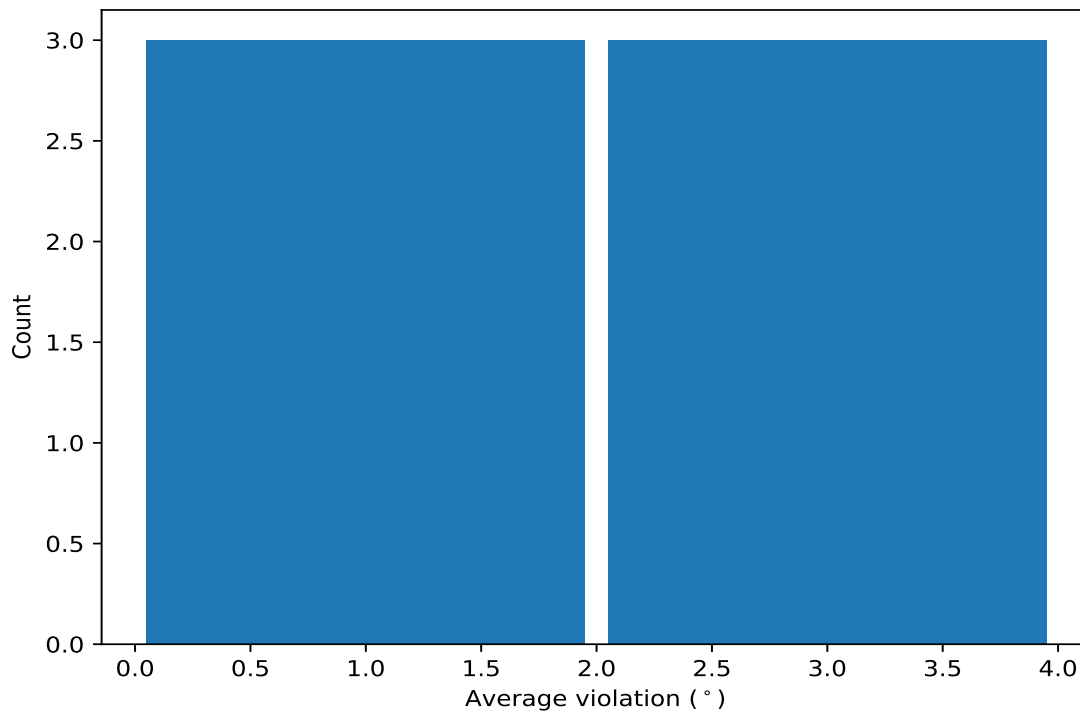

10.4 Most violated dihedral-angle restraints in the ensemble (i)

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 ⓘ

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
(1,102)	1:A:79:LYS:N	1:A:79:LYS:CA	1:A:79:LYS:C	1:A:80:LEU:N	6	3.42	1.6	3.1
(1,26)	1:A:15:PHE:N	1:A:15:PHE:CA	1:A:15:PHE:C	1:A:16:ASP:N	4	2.42	0.41	2.3
(1,24)	1:A:14:VAL:N	1:A:14:VAL:CA	1:A:14:VAL:C	1:A:15:PHE:N	4	1.95	0.53	1.85
(1,52)	1:A:51:LYS:C	1:A:52:ILE:N	1:A:52:ILE:CA	1:A:52:ILE:C	3	1.97	0.81	1.5
(1,69)	1:A:62:LEU:C	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	2	3.85	0.95	3.85
(1,57)	1:A:54:PHE:N	1:A:54:PHE:CA	1:A:54:PHE:C	1:A:55:ALA:N	2	1.25	0.05	1.25

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

10.5   All violated dihedral-angle restraints ⓘ

10.5.1   Histogram : Distribution of violations ⓘ

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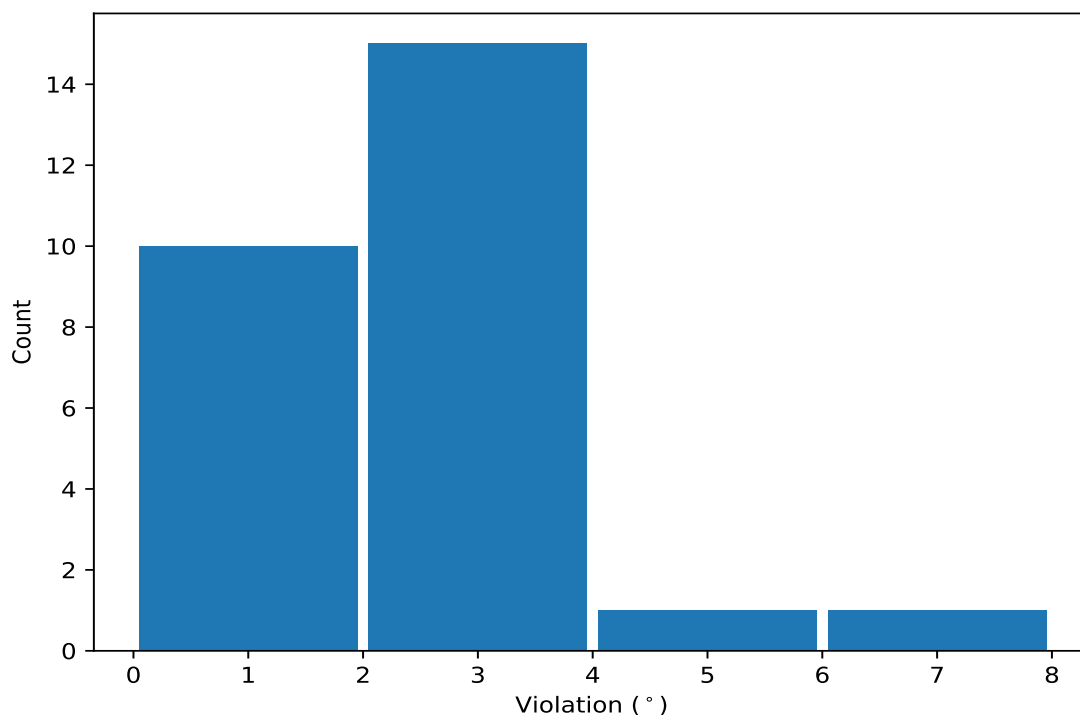
10.5.2   Table: All violated dihedral-angle restraints ⓘ

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,102)	1:A:79:LYS:N	1:A:79:LYS:CA	1:A:79:LYS:C	1:A:80:LEU:N	15	6.7
(1,69)	1:A:62:LEU:C	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	15	4.8
(1,20)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:GLN:N	8	3.6
(1,102)	1:A:79:LYS:N	1:A:79:LYS:CA	1:A:79:LYS:C	1:A:80:LEU:N	14	3.4
(1,52)	1:A:51:LYS:C	1:A:52:ILE:N	1:A:52:ILE:CA	1:A:52:ILE:C	19	3.1
(1,26)	1:A:15:PHE:N	1:A:15:PHE:CA	1:A:15:PHE:C	1:A:16:ASP:N	8	3.1
(1,102)	1:A:79:LYS:N	1:A:79:LYS:CA	1:A:79:LYS:C	1:A:80:LEU:N	12	3.1
(1,102)	1:A:79:LYS:N	1:A:79:LYS:CA	1:A:79:LYS:C	1:A:80:LEU:N	20	3.1
(1,69)	1:A:62:LEU:C	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	11	2.9
(1,102)	1:A:79:LYS:N	1:A:79:LYS:CA	1:A:79:LYS:C	1:A:80:LEU:N	8	2.8
(1,3)	1:A:3:THR:C	1:A:4:LEU:N	1:A:4:LEU:CA	1:A:4:LEU:C	7	2.7
(1,24)	1:A:14:VAL:N	1:A:14:VAL:CA	1:A:14:VAL:C	1:A:15:PHE:N	5	2.7
(1,26)	1:A:15:PHE:N	1:A:15:PHE:CA	1:A:15:PHE:C	1:A:16:ASP:N	11	2.3
(1,26)	1:A:15:PHE:N	1:A:15:PHE:CA	1:A:15:PHE:C	1:A:16:ASP:N	13	2.3
(1,24)	1:A:14:VAL:N	1:A:14:VAL:CA	1:A:14:VAL:C	1:A:15:PHE:N	10	2.2
(1,55)	1:A:53:LYS:N	1:A:53:LYS:CA	1:A:53:LYS:C	1:A:54:PHE:N	8	2.1
(1,26)	1:A:15:PHE:N	1:A:15:PHE:CA	1:A:15:PHE:C	1:A:16:ASP:N	15	2.0
(1,98)	1:A:77:ALA:N	1:A:77:ALA:CA	1:A:77:ALA:C	1:A:78:ARG:N	15	1.7
(1,84)	1:A:70:ASP:N	1:A:70:ASP:CA	1:A:70:ASP:C	1:A:71:LEU:N	9	1.6
(1,52)	1:A:51:LYS:C	1:A:52:ILE:N	1:A:52:ILE:CA	1:A:52:ILE:C	7	1.5
(1,24)	1:A:14:VAL:N	1:A:14:VAL:CA	1:A:14:VAL:C	1:A:15:PHE:N	2	1.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:A:14:VAL:N	1:A:14:VAL:CA	1:A:14:VAL:C	1:A:15:PHE:N	3	1.4
(1,102)	1:A:79:LYS:N	1:A:79:LYS:CA	1:A:79:LYS:C	1:A:80:LEU:N	3	1.4
(1,57)	1:A:54:PHE:N	1:A:54:PHE:CA	1:A:54:PHE:C	1:A:55:ALA:N	6	1.3
(1,52)	1:A:51:LYS:C	1:A:52:ILE:N	1:A:52:ILE:CA	1:A:52:ILE:C	9	1.3
(1,57)	1:A:54:PHE:N	1:A:54:PHE:CA	1:A:54:PHE:C	1:A:55:ALA:N	19	1.2
(1,2)	1:A:3:THR:N	1:A:3:THR:CA	1:A:3:THR:C	1:A:4:LEU:N	2	1.2