Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1HEH
BMRB ID	:	4900
Title	:	C-terminal xylan binding domain from Cellulomonas fimi xylanase 11A
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Deposited on	:	2000-11-22

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 (i) 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 (1)) were used in the production of this report:

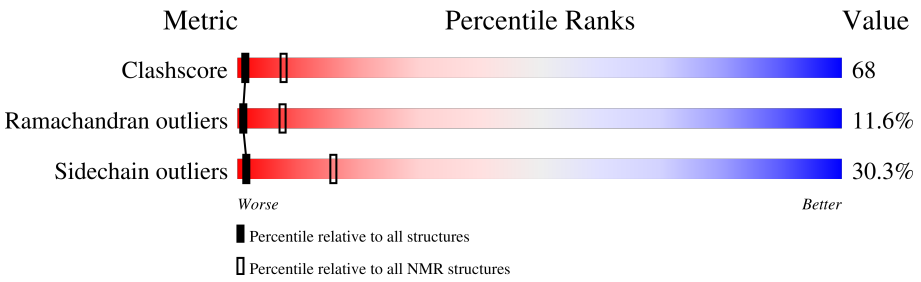
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 62%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	C	88	24% 51% 20% 5%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1185 atoms, of which 570 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ENDO-1,4-BETA-XYLANASE D.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	C	88	1185	372	570	109	132	2	0

4 Residue-property plots (i)

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: ENDO-1,4-BETA-XYLANASE D

Chain C: 24% 51% 20% 5%

T557 G558 S559 C560 S561 V562 S563 A564 V565 R566 G567 E568 E569 W570 A571 D572 R573 F574 N575 V576 T577 Y578 S579 V580 S581 G582 S583 S584 S585 W586 V587 V588 T589 L590 G591 L592 N593 G594 G595 Q596 S597 S600 S601 W602 N603 A604 A605 L606 T607 G608 S609 S610 V613 T614 A615 R616 P617 N618

G619 S620 G621 N622 S623 F624 G625 V626 T627 F628 Y629 K630 N631 G632 S633 S634 A635 T636 P637 G638 A639 T640 C641 A642 T643 G644

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *HYBRID DISTANCE GEOMETRY/ SIMULATED ANNEALING*.

Of the 50 calculated structures, 1 were deposited, based on the following criterion: *?*.

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

Software name	**Classification**	**Version**
X-PLOR	refinement	3.1
Felix	structure solution	97.0

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	622
Number of shifts mapped to atoms	622
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	62%

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

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	C	0	3
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	C	566	ARG	Sidechain
1	C	573	ARG	Sidechain
1	C	616	ARG	Sidechain

6.2 Too-close contacts (i)

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	C	615	570	567	80
All	All	615	570	567	80

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 68.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:C:588:VAL:HG23	1:C:640:THR:O	1.04	1.52

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:C:580:VAL:HG21	1:C:586:TRP:CZ2	0.99	1.92
1:C:592:LEU:HD13	1:C:596:GLN:O	0.88	1.68
1:C:580:VAL:HG21	1:C:586:TRP:CH2	0.86	2.05
1:C:607:THR:O	1:C:613:VAL:HG22	0.85	1.71
1:C:601:SER:OG	1:C:606:LEU:HD21	0.80	1.77
1:C:636:THR:HG22	1:C:637:PRO:HD2	0.79	1.54
1:C:588:VAL:CG2	1:C:640:THR:O	0.77	2.33
1:C:586:TRP:CE3	1:C:615:ALA:HB3	0.74	2.17
1:C:580:VAL:CG2	1:C:586:TRP:CH2	0.72	2.72
1:C:565:VAL:O	1:C:576:VAL:HG13	0.67	1.89
1:C:588:VAL:HG21	1:C:639:ALA:HB1	0.67	1.67
1:C:603:ASN:O	1:C:604:ALA:HB2	0.66	1.91
1:C:586:TRP:CE3	1:C:615:ALA:CB	0.64	2.81
1:C:574:PHE:CZ	1:C:628:PHE:CB	0.63	2.81
1:C:559:SER:OG	1:C:643:THR:HG23	0.62	1.95
1:C:560:CYS:SG	1:C:562:VAL:CG1	0.61	2.89
1:C:636:THR:HG22	1:C:637:PRO:CD	0.61	2.26
1:C:565:VAL:O	1:C:576:VAL:CG1	0.60	2.49
1:C:588:VAL:CG2	1:C:589:THR:N	0.60	2.65
1:C:606:LEU:HD23	1:C:606:LEU:N	0.59	2.11
1:C:580:VAL:CG2	1:C:586:TRP:CZ2	0.58	2.79
1:C:588:VAL:HG22	1:C:589:THR:N	0.58	2.12
1:C:562:VAL:CG1	1:C:641:CYS:SG	0.58	2.92
1:C:562:VAL:HG11	1:C:641:CYS:SG	0.57	2.39
1:C:588:VAL:O	1:C:614:THR:HG23	0.57	2.00
1:C:601:SER:HB3	1:C:626:VAL:HG22	0.56	1.77
1:C:574:PHE:CE1	1:C:628:PHE:HB2	0.55	2.37
1:C:603:ASN:O	1:C:604:ALA:CB	0.54	2.56
1:C:586:TRP:O	1:C:587:VAL:CG2	0.54	2.56
1:C:636:THR:CG2	1:C:637:PRO:HD2	0.54	2.32
1:C:602:TRP:O	1:C:603:ASN:CB	0.53	2.57
1:C:559:SER:CB	1:C:643:THR:HG23	0.53	2.34
1:C:574:PHE:CZ	1:C:628:PHE:HB2	0.53	2.39
1:C:627:THR:O	1:C:628:PHE:CG	0.52	2.61
1:C:619:GLY:O	1:C:620:SER:CB	0.52	2.58
1:C:574:PHE:CZ	1:C:628:PHE:HB3	0.52	2.40
1:C:613:VAL:CG1	1:C:614:THR:N	0.51	2.74
1:C:559:SER:N	1:C:643:THR:CG2	0.50	2.74
1:C:587:VAL:O	1:C:587:VAL:HG12	0.50	2.05
1:C:588:VAL:O	1:C:614:THR:HA	0.50	2.07
1:C:580:VAL:HG11	1:C:583:SER:HB2	0.49	1.83
1:C:566:ARG:O	1:C:567:GLY:O	0.49	2.30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:C:583:SER:O	1:C:584:SER:C	0.48	2.51
1:C:570:TRP:CZ3	1:C:575:ASN:HB2	0.48	2.44
1:C:586:TRP:C	1:C:587:VAL:HG23	0.48	2.29
1:C:588:VAL:HG23	1:C:640:THR:N	0.48	2.23
1:C:606:LEU:N	1:C:606:LEU:CD2	0.47	2.76
1:C:567:GLY:O	1:C:568:GLU:O	0.47	2.33
1:C:588:VAL:CG2	1:C:640:THR:N	0.47	2.78
1:C:568:GLU:O	1:C:575:ASN:HB3	0.46	2.11
1:C:624:PHE:CD1	1:C:624:PHE:C	0.46	2.89
1:C:593:ASN:O	1:C:594:GLY:O	0.46	2.33
1:C:574:PHE:CE1	1:C:636:THR:HG22	0.46	2.46
1:C:602:TRP:O	1:C:603:ASN:HB2	0.45	2.11
1:C:561:SER:CB	1:C:581:SER:HB2	0.45	2.41
1:C:567:GLY:O	1:C:568:GLU:C	0.45	2.54
1:C:601:SER:OG	1:C:606:LEU:CD2	0.45	2.60
1:C:609:SER:O	1:C:610:SER:CB	0.44	2.66
1:C:559:SER:CA	1:C:643:THR:CG2	0.44	2.96
1:C:563:SER:O	1:C:578:TYR:HA	0.43	2.12
1:C:588:VAL:HG23	1:C:640:THR:C	0.43	2.29
1:C:630:LYS:O	1:C:631:ASN:C	0.43	2.56
1:C:586:TRP:C	1:C:587:VAL:CG2	0.42	2.87
1:C:605:ALA:C	1:C:606:LEU:HD23	0.42	2.34
1:C:607:THR:O	1:C:613:VAL:HA	0.42	2.14
1:C:559:SER:CA	1:C:643:THR:HG23	0.42	2.44
1:C:627:THR:HG22	1:C:628:PHE:N	0.42	2.30
1:C:630:LYS:HB3	1:C:633:SER:OG	0.42	2.15
1:C:574:PHE:CZ	1:C:637:PRO:HD3	0.42	2.50
1:C:595:GLY:O	1:C:596:GLN:C	0.42	2.57
1:C:633:SER:O	1:C:634:SER:OG	0.42	2.33
1:C:580:VAL:HB	1:C:622:ASN:O	0.41	2.15
1:C:572:ASP:O	1:C:630:LYS:HG3	0.41	2.16
1:C:634:SER:O	1:C:635:ALA:C	0.41	2.57
1:C:575:ASN:ND2	1:C:627:THR:HA	0.41	2.30
1:C:624:PHE:CD1	1:C:624:PHE:O	0.41	2.74
1:C:570:TRP:HB2	1:C:573:ARG:O	0.41	2.16
1:C:607:THR:O	1:C:613:VAL:CG2	0.41	2.58
1:C:618:ASN:OD1	1:C:618:ASN:C	0.40	2.58

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	C	86/88 (98%)	57 (66%)	19 (22%)	10 (12%)	1 7
All	All	86/88 (98%)	57 (66%)	19 (22%)	10 (12%)	1 7

All 10 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	C	558	GLY
1	C	567	GLY
1	C	568	GLU
1	C	587	VAL
1	C	592	LEU
1	C	594	GLY
1	C	604	ALA
1	C	610	SER
1	C	620	SER
1	C	634	SER

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	C	66/66 (100%)	46 (70%)	20 (30%)	1 16
All	All	66/66 (100%)	46 (70%)	20 (30%)	1 16

All 20 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	C	559	SER
1	C	560	CYS
1	C	566	ARG
1	C	573	ARG
1	C	581	SER
1	C	584	SER
1	C	585	SER
1	C	589	THR
1	C	590	LEU
1	C	597	SER
1	C	600	SER
1	C	603	ASN
1	C	606	LEU
1	C	609	SER
1	C	610	SER
1	C	620	SER
1	C	623	SER
1	C	630	LYS
1	C	636	THR
1	C	640	THR

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 62% for the well-defined parts and 62% 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 (i)

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	622
Number of shifts mapped to atoms	622
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	83	-0.52 ± 0.64	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 62%, i.e. 619 atoms were assigned a chemical shift out of a possible 1001. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	269/450 (60%)	186/188 (99%)	0/176 (0%)	83/86 (97%)
Sidechain	306/467 (66%)	295/307 (96%)	0/142 (0%)	11/18 (61%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	44/84 (52%)	41/41 (100%)	0/40 (0%)	3/3 (100%)
Overall	619/1001 (62%)	522/536 (97%)	0/358 (0%)	97/107 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 62%, i.e. 619 atoms were assigned a chemical shift out of a possible 1001. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	269/450 (60%)	186/188 (99%)	0/176 (0%)	83/86 (97%)
Sidechain	306/467 (66%)	295/307 (96%)	0/142 (0%)	11/18 (61%)
Aromatic	44/84 (52%)	41/41 (100%)	0/40 (0%)	3/3 (100%)
Overall	619/1001 (62%)	522/536 (97%)	0/358 (0%)	97/107 (91%)

7.1.4 Statistically unusual chemical shifts (i)

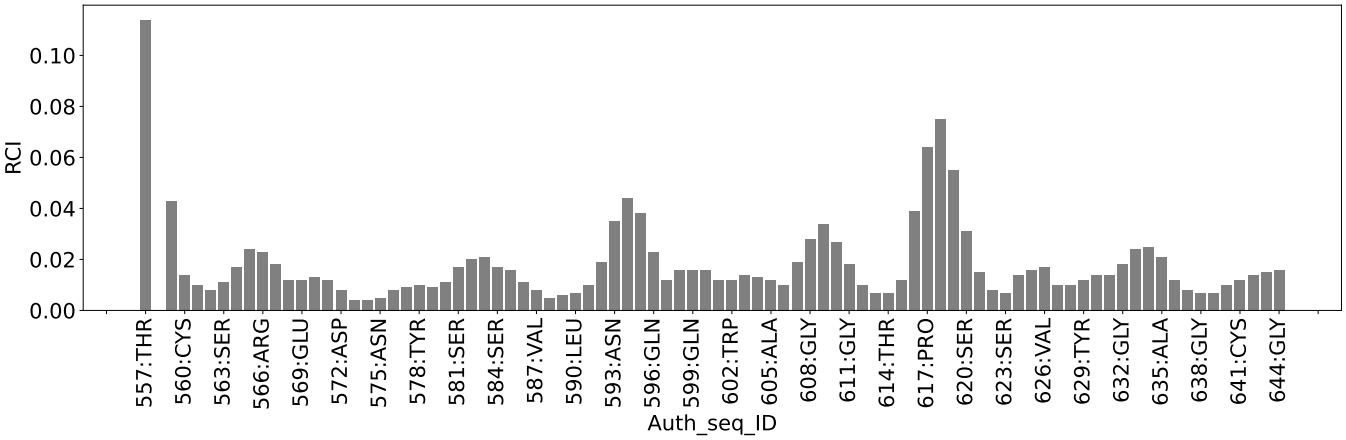
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	C	627	THR	HG1	5.69	0.08 – 2.19	21.6
1	C	637	PRO	HG2	0.07	0.41 – 3.45	-6.1
1	C	599	GLN	HB2	0.56	0.80 – 3.29	-6.0
1	C	578	TYR	HB2	0.86	1.09 – 4.72	-5.6

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain C:


RCI
0.00
0.02
0.04
0.06
0.08
0.10
557:THR
560:CYS
563:SER
566:ARG
569:GLU
572:ASP
575:ASN
578:TYR
581:SER
584:SER
587:VAL
590:LEU
593:ASN
596:GLN
599:GLN
602:TRP
605:ALA
608:GLY
611:GLY
614:THR
617:PRO
620:SER
623:SER
626:VAL
629:TYR
632:GLY
635:ALA
638:GLY
641:CYS
644:GLY
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	935
Intra-residue (|i-j|=0)	307
Sequential (|i-j|=1)	246
Medium range (|i-j|>1 and |i-j|<5)	72
Long range (|i-j|≥5)	258
Inter-chain	0
Hydrogen bond restraints	52
Disulfide bond restraints	0
Total dihedral-angle restraints	94
Number of unmapped restraints	0
Number of restraints per residue	11.7
Number of long range restraints per residue[1]	3.5

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

8.2 Residual restraint violations (i)

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 (i)

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)	11.0	0.2
0.2-0.5 (Medium)	1.0	0.21
>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)	3.0	3.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

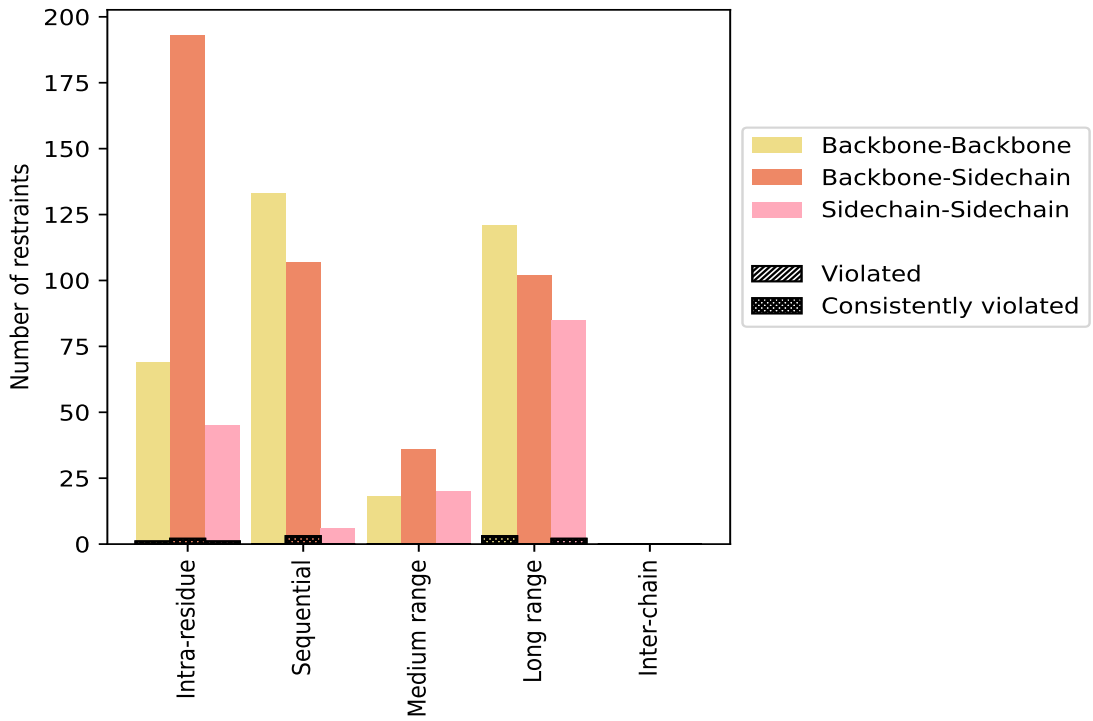
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	307	32.8	4	1.3	0.4	4	1.3	0.4
Backbone-Backbone	69	7.4	1	1.4	0.1	1	1.4	0.1
Backbone-Sidechain	193	20.6	2	1.0	0.2	2	1.0	0.2
Sidechain-Sidechain	45	4.8	1	2.2	0.1	1	2.2	0.1
Sequential (|i-j|=1)	246	26.3	3	1.2	0.3	3	1.2	0.3
Backbone-Backbone	133	14.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	107	11.4	3	2.8	0.3	3	2.8	0.3
Sidechain-Sidechain	6	0.6	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	72	7.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	16	1.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	36	3.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	20	2.1	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	258	27.6	3	1.2	0.3	3	1.2	0.3
Backbone-Backbone	71	7.6	1	1.4	0.1	1	1.4	0.1
Backbone-Sidechain	102	10.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	85	9.1	2	2.4	0.2	2	2.4	0.2
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	5.6	2	3.8	0.2	2	3.8	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	935	100.0	12	1.3	1.3	12	1.3	1.3
Backbone-Backbone	341	36.5	4	1.2	0.4	4	1.2	0.4
Backbone-Sidechain	438	46.8	5	1.1	0.5	5	1.1	0.5
Sidechain-Sidechain	156	16.7	3	1.9	0.3	3	1.9	0.3

[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

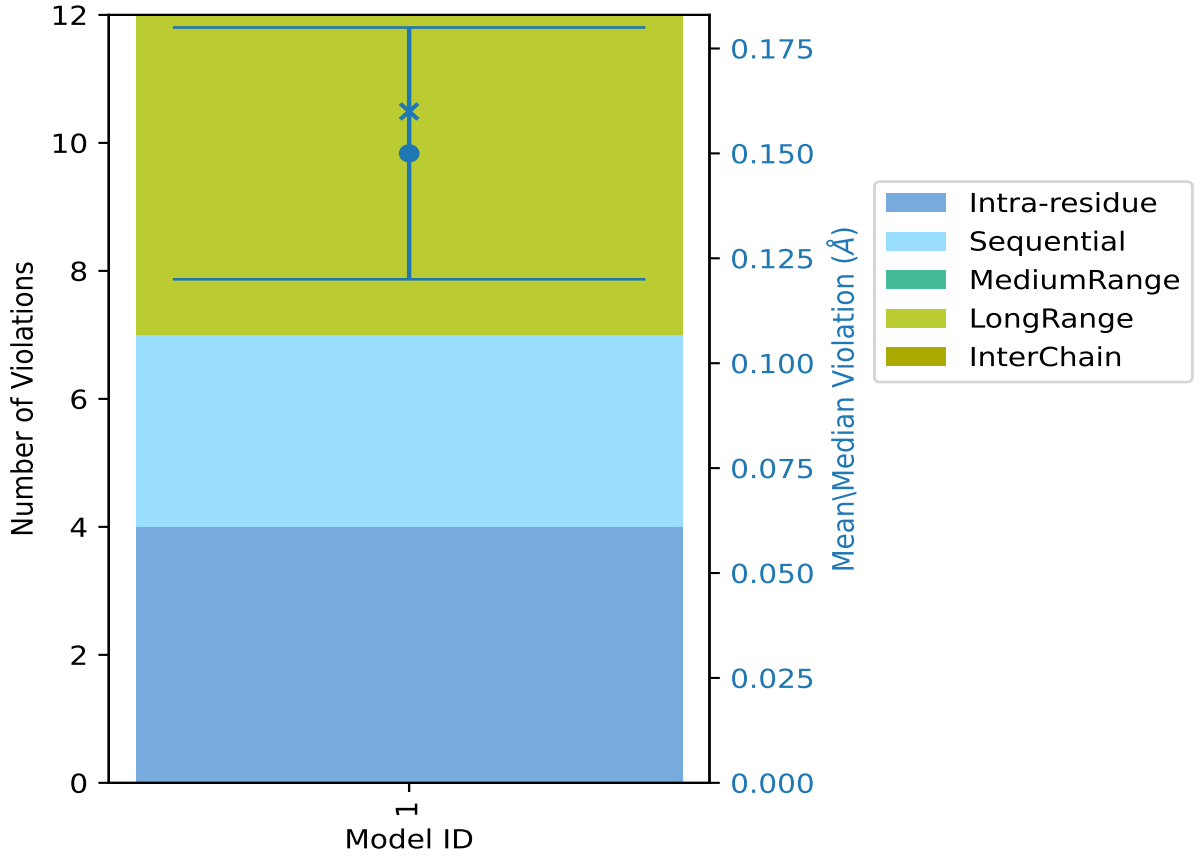
9.2 Distance violation statistics for each model (i)

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	4	3	0	5	0	12	0.15	0.21	0.03	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 (i)



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

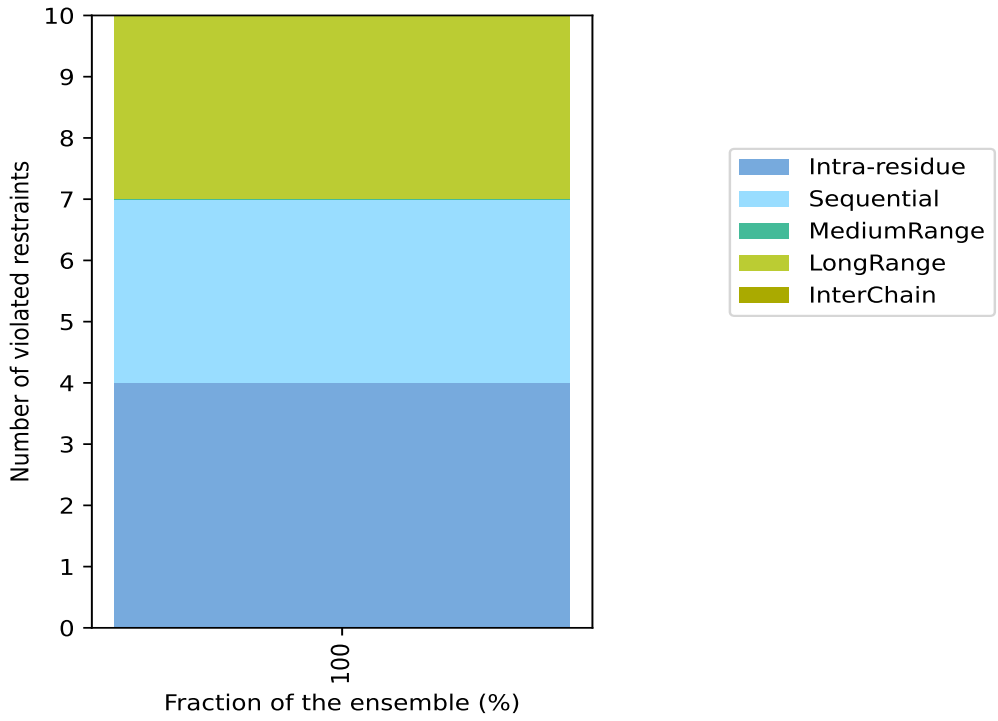
9.3 Distance violation statistics for the ensemble (i)

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, 873(IR:303, SQ:243, MR:72, LR:255, 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	3	0	3	0	10	1	100.0

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

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



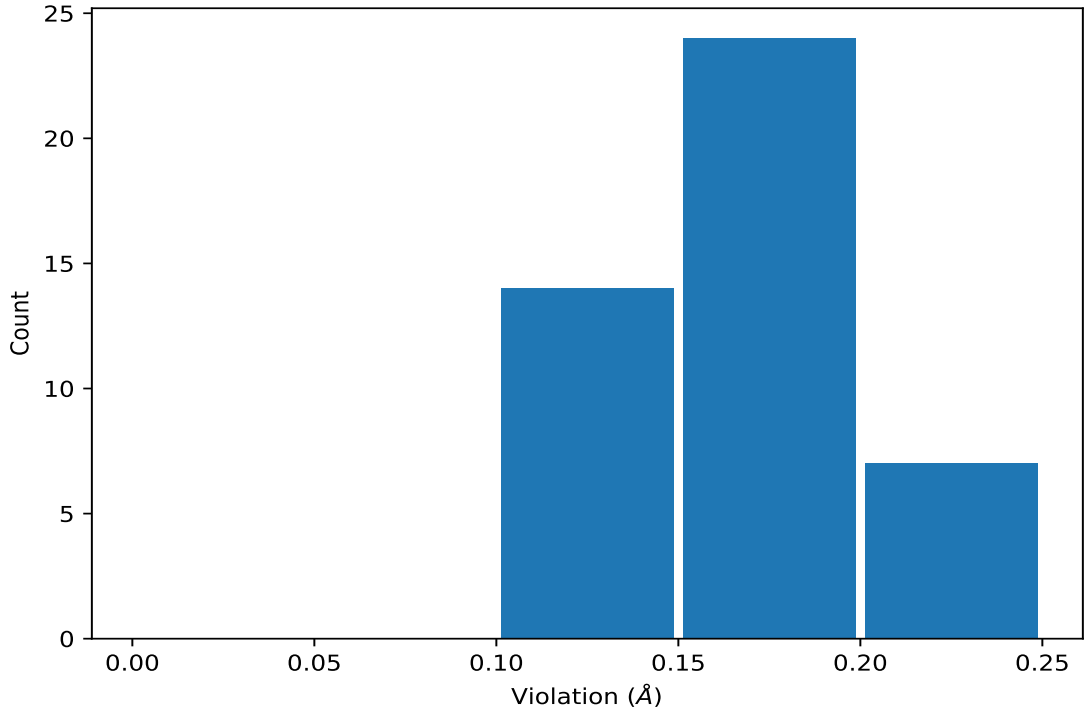
9.4 Most violated distance restraints in the ensemble (i)

No violations found

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)
(1,521)	1:C:592:LEU:H	1:C:592:LEU:HB3	1	0.21
(1,778)	1:C:640:THR:HB	1:C:588:VAL:HG11	1	0.2
(1,778)	1:C:640:THR:HB	1:C:588:VAL:HG12	1	0.2
(1,778)	1:C:640:THR:HB	1:C:588:VAL:HG13	1	0.2
(1,778)	1:C:640:THR:HB	1:C:588:VAL:HG21	1	0.2
(1,778)	1:C:640:THR:HB	1:C:588:VAL:HG22	1	0.2
(1,778)	1:C:640:THR:HB	1:C:588:VAL:HG23	1	0.2
(1,868)	1:C:606:LEU:HD11	1:C:606:LEU:HB2	1	0.19
(1,868)	1:C:606:LEU:HD11	1:C:606:LEU:HB3	1	0.19
(1,868)	1:C:606:LEU:HD11	1:C:606:LEU:HG	1	0.19
(1,868)	1:C:606:LEU:HD12	1:C:606:LEU:HB2	1	0.19
(1,868)	1:C:606:LEU:HD12	1:C:606:LEU:HB3	1	0.19
(1,868)	1:C:606:LEU:HD12	1:C:606:LEU:HG	1	0.19
(1,868)	1:C:606:LEU:HD13	1:C:606:LEU:HB2	1	0.19
(1,868)	1:C:606:LEU:HD13	1:C:606:LEU:HB3	1	0.19
(1,868)	1:C:606:LEU:HD13	1:C:606:LEU:HG	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:C:606:LEU:HD21	1:C:606:LEU:HB2	1	0.19
(1,868)	1:C:606:LEU:HD21	1:C:606:LEU:HB3	1	0.19
(1,868)	1:C:606:LEU:HD21	1:C:606:LEU:HG	1	0.19
(1,868)	1:C:606:LEU:HD22	1:C:606:LEU:HB2	1	0.19
(1,868)	1:C:606:LEU:HD22	1:C:606:LEU:HB3	1	0.19
(1,868)	1:C:606:LEU:HD22	1:C:606:LEU:HG	1	0.19
(1,868)	1:C:606:LEU:HD23	1:C:606:LEU:HB2	1	0.19
(1,868)	1:C:606:LEU:HD23	1:C:606:LEU:HB3	1	0.19
(1,868)	1:C:606:LEU:HD23	1:C:606:LEU:HG	1	0.19
(1,855)	1:C:636:THR:H	1:C:636:THR:HA	1	0.18
(1,855)	1:C:636:THR:H	1:C:636:THR:HB	1	0.18
(1,716)	1:C:613:VAL:H	1:C:613:VAL:HG11	1	0.17
(1,716)	1:C:613:VAL:H	1:C:613:VAL:HG12	1	0.17
(1,716)	1:C:613:VAL:H	1:C:613:VAL:HG13	1	0.17
(2,9)	1:C:589:THR:H	1:C:640:THR:O	1	0.16
(1,456)	1:C:641:CYS:H	1:C:640:THR:HB	1	0.15
(1,568)	1:C:577:THR:H	1:C:567:GLY:HA2	1	0.13
(1,568)	1:C:577:THR:H	1:C:567:GLY:HA3	1	0.13
(1,567)	1:C:577:THR:H	1:C:576:VAL:HB	1	0.12
(1,168)	1:C:586:TRP:HE1	1:C:615:ALA:HB1	1	0.12
(1,168)	1:C:586:TRP:HE1	1:C:615:ALA:HB2	1	0.12
(1,168)	1:C:586:TRP:HE1	1:C:615:ALA:HB3	1	0.12
(2,13)	1:C:615:ALA:H	1:C:588:VAL:O	1	0.11
(1,779)	1:C:588:VAL:HG11	1:C:589:THR:HA	1	0.11
(1,779)	1:C:588:VAL:HG12	1:C:589:THR:HA	1	0.11
(1,779)	1:C:588:VAL:HG13	1:C:589:THR:HA	1	0.11
(1,779)	1:C:588:VAL:HG21	1:C:589:THR:HA	1	0.11
(1,779)	1:C:588:VAL:HG22	1:C:589:THR:HA	1	0.11
(1,779)	1:C:588:VAL:HG23	1:C:589:THR:HA	1	0.11

10 Dihedral-angle violation analysis (i)

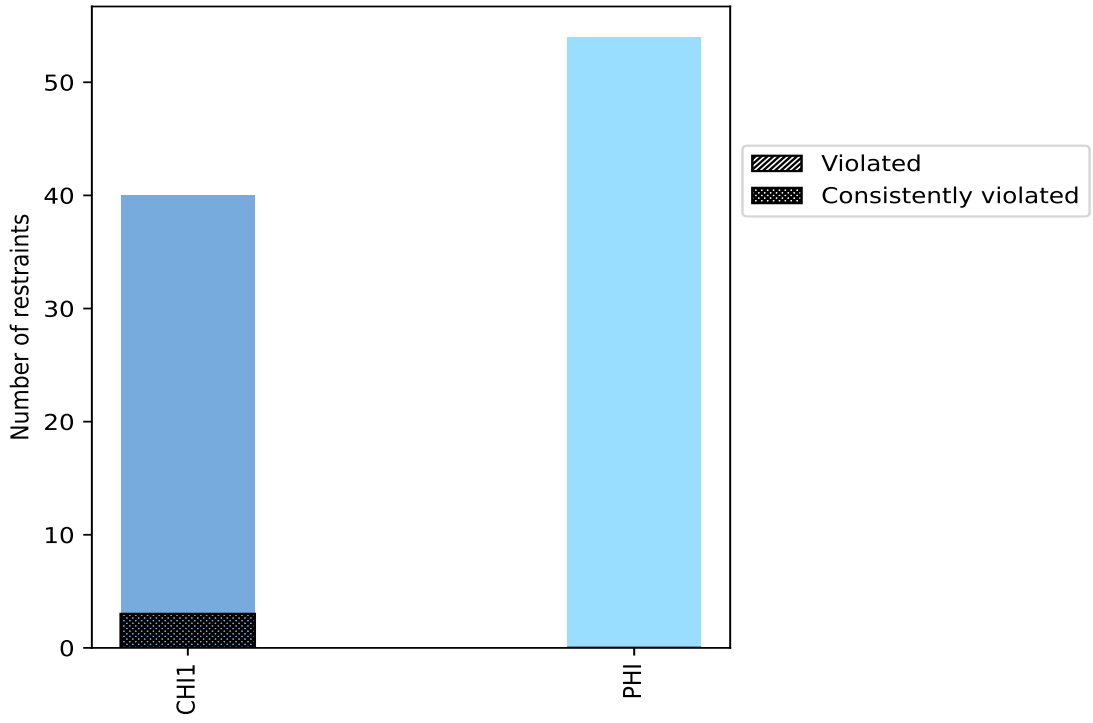
10.1 Summary of dihedral-angle violations (i)

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]
CHI1	40	42.6	3	7.5	3.2	3	7.5	3.2
PHI	54	57.4	0	0.0	0.0	0	0.0	0.0
Total	94	100.0	3	3.2	3.2	3	3.2	3.2

[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)



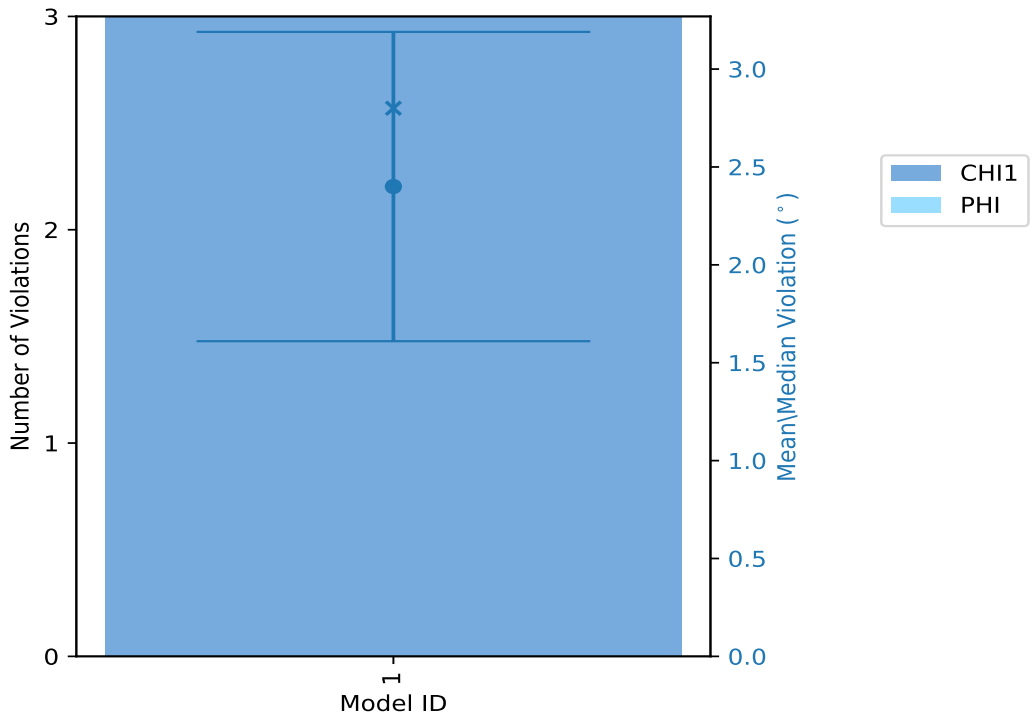
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	CHI1	PHI	Total				
1	3	0	3	2.4	3.1	0.79	2.8

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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

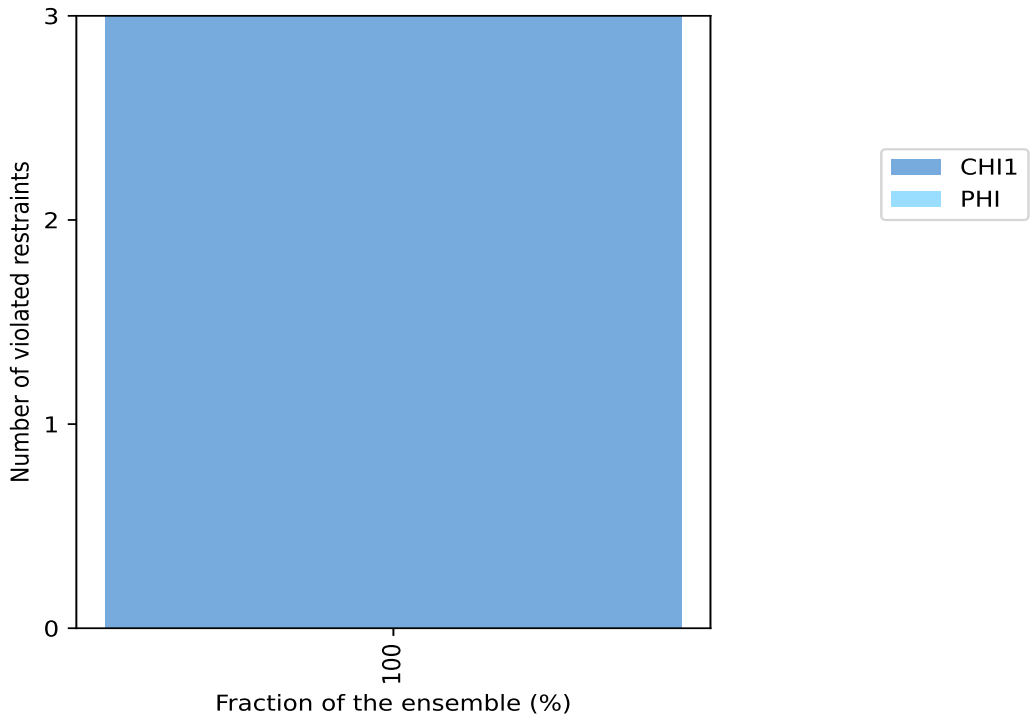
10.3 Dihedral-angle violation statistics for the ensemble (i)

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	
CHI1	PHI	Total	Count[1]	%
3	0	3	1	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)

No violations found

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.
Data insufficient to plot histogram

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 (°)
(1,93)	1:C:641:CYS:N	1:C:641:CYS:CA	1:C:641:CYS:CB	1:C:641:CYS:SG	1	3.1
(1,68)	1:C:586:TRP:N	1:C:586:TRP:CA	1:C:586:TRP:CB	1:C:586:TRP:CG	1	2.8
(1,80)	1:C:613:VAL:N	1:C:613:VAL:CA	1:C:613:VAL:CB	1:C:613:VAL:CG1	1	1.3