WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 06:38 PM EDT

PDB ID	:	2MV7
BMRB ID	:	19516
Title	:	Solution NMR structure of DOT1L in complex with AF9 (DOT1L-AF9)
Authors	:	Kuntimaddi, A.; Bushweller, J.H.
Deposited on	:	2014-09-24

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

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

1 Overall quality at a glance ⓘ

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

The overall completeness of chemical shifts assignment is 87%.

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		19
Ramachandran outliers		2.5%
Sidechain outliers		7.5%

Worse   *Better*

▊ Percentile relative to all structures
▯ Percentile relative to all NMR structures
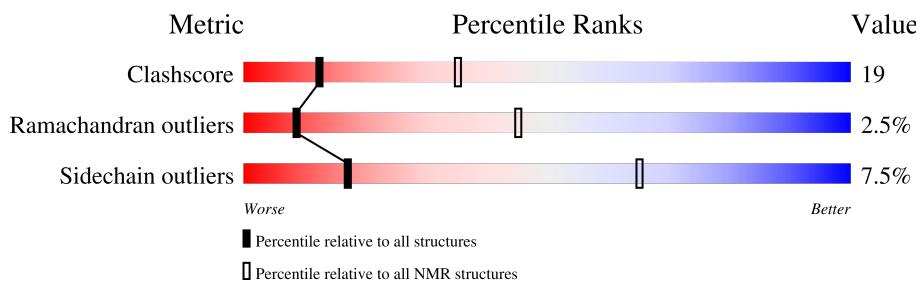
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	69	59% 29% · 10%
2	B	25	40% 12% 48%
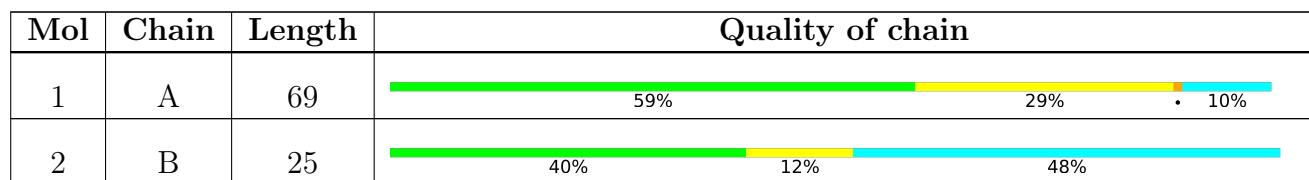
2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:501-A:562, B:878-B:890 (75)	0.39	1

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

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

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

Cluster number	Models
1	2, 4, 9
2	1, 10
3	5, 6
Single-model clusters	3; 7; 8

3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 1541 atoms, of which 782 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein AF-9.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	69	1147	358	575	100	112	2	0

- Molecule 2 is a protein called Histone-lysine N-methyltransferase, H3 lysine-79 specific.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	25	394	116	207	36	35	0

There is a discrepancy between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
B	876	THR	-	expression tag	UNP Q8TEK3

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Protein AF-9

Chain A:

- Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B:
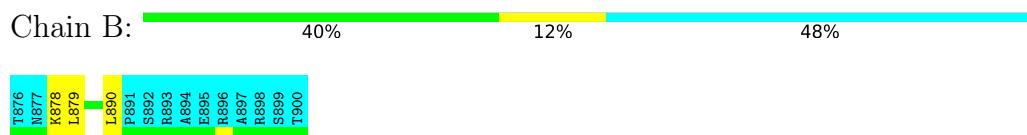
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Protein AF-9

Chain A:

- Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B:
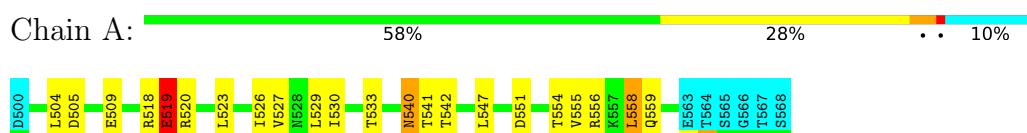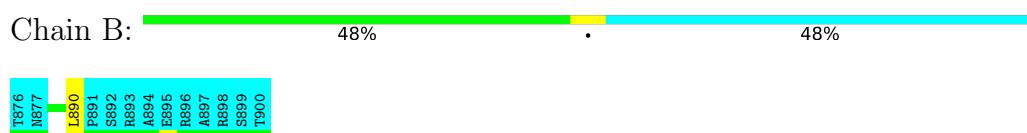
4.2.2   Score per residue for model 2

• Molecule 1: Protein AF-9

Chain A:

• Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B:
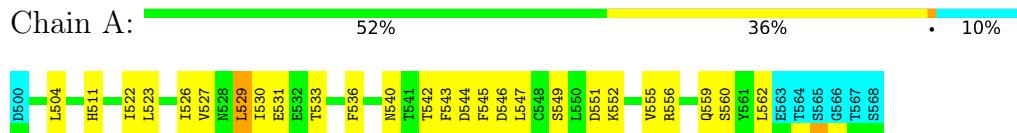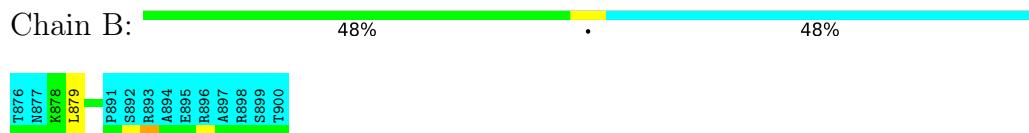
4.2.3   Score per residue for model 3

• Molecule 1: Protein AF-9

Chain A:

• Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B:
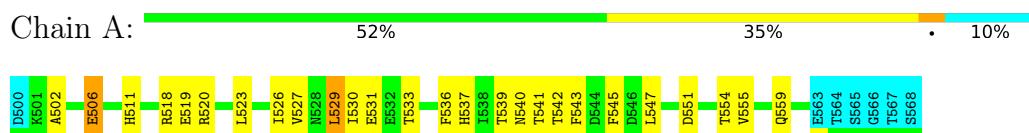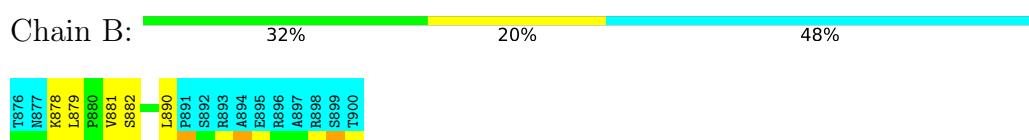
4.2.4   Score per residue for model 4

• Molecule 1: Protein AF-9

Chain A:

• Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B:

4.2.5 Score per residue for model 5

• Molecule 1: Protein AF-9

Chain A: 49% 36% · 10%

D500 L504 R518 E519 R520 L523 I526 V527 N528 L529 I530 H535 F536 T539 N540 T541 T542 F543 D544 F545 D546 L547 C548 S549 L550 D551 T554 V555 R556 K557 L558 Q559 S560 Y561 L562 E563 T564 S565 G566 T567 S568

• Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B: 44% 8% 48%

T876 N877 S887 L890 P891 S892 R893 A894 E895 R896 A897 R898 S899 T900
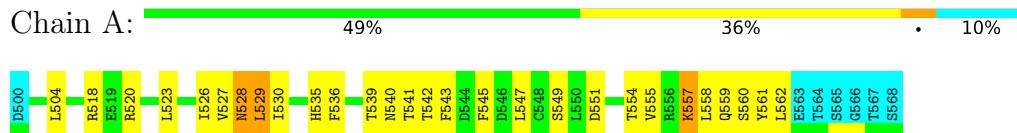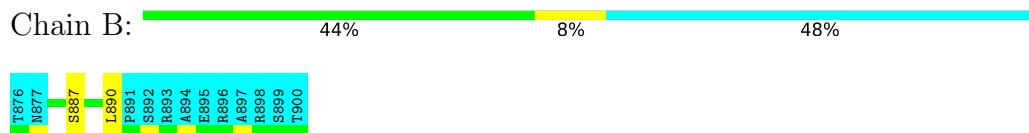
4.2.6 Score per residue for model 6

• Molecule 1: Protein AF-9

Chain A: 54% 33% · 10%

D500 L504 H511 T516 L517 R518 E519 R520 L523 V527 N528 L529 E532 T539 N540 T541 T542 D546 L547 C548 S549 L550 D551 T554 V555 L558 Q559 S560 Y561 L562 E563 T564 S565 G566 T567 S568

• Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B: 40% 8% · 48%

T876 N877 K878 L879 L890 P891 S892 R893 A894 E895 R896 A897 R898 S899 T900
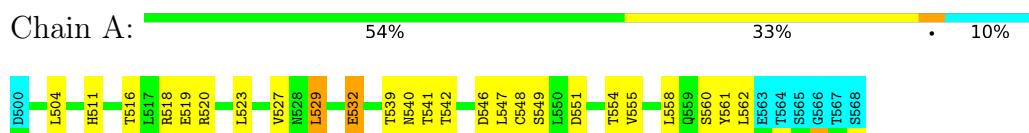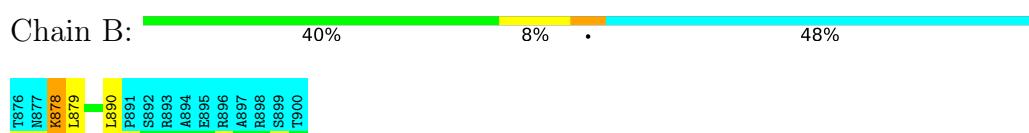
4.2.7 Score per residue for model 7

• Molecule 1: Protein AF-9

Chain A: 52% 32% 6% 10%

D500 Y503 L504 L510 H511 L523 V527 N528 L529 I530 T533 F536 H537 I538 T539 N540 T541 T542 F543 D544 F545 D546 L547 C548 S549 L550 D551 V555 R556 K557 L558 Q559 S560 E563 T564 S565 G566 T567 S568

• Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B: 44% 8% 48%

T876 N877 K878 L879 L890 P891 S892 R893 A894 E895 R896 A897 R898 S899 T900
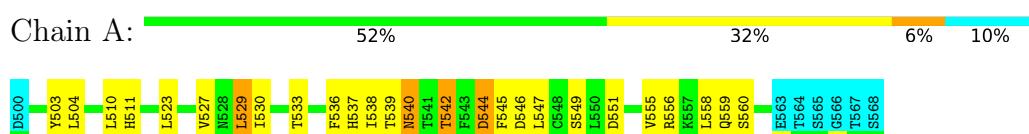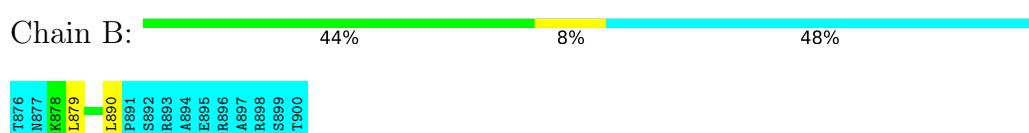
4.2.8 Score per residue for model 8

• Molecule 1: Protein AF-9

Chain A: 49% 36% • 10%

D500 Y503 L504 H511 R512 R513 R520 H521 I522 L523 Q524 Q525 I526 V527 N528 L529 I530 E531 E532 T533 G534 H535 T541 T542 F543 D544 L547 C548 S549 L550 D551 T554 V555 Q559 S560 Y561 L562 E563 T564 S565 G566 T567 S568

• Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B: 36% 12% • 48%

T876 N877 K878 L879 I883 L890 P891 S892 R893 A894 E895 R896 A897 R898 S899 T900
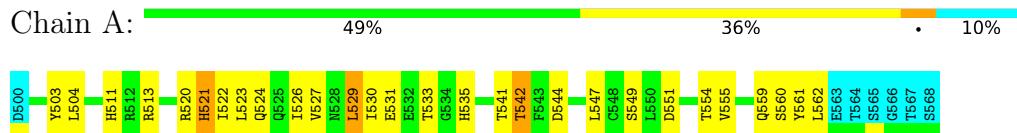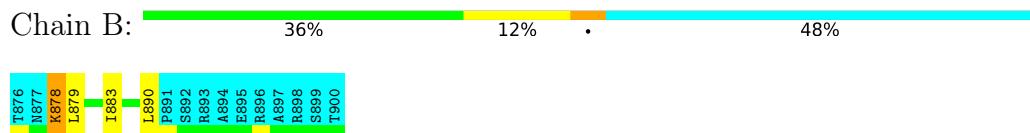
4.2.9 Score per residue for model 9

• Molecule 1: Protein AF-9

Chain A: 49% 36% • 10%

D500 L504 H511 M515 L523 Q524 Q525 I526 V527 N528 L529 I530 E531 G534 H535 T539 N540 T541 T542 F543 D544 L547 D551 K552 T553 T554 V555 R556 Q559 S560 Y561 L562 E563 T564 S565 G566 T567 S568

• Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B: 32% 16% • 48%

T876 N877 K878 L879 I883 P884 L885 V888 P891 S892 R893 A894 E895 R896 A897 R898 S899 T900
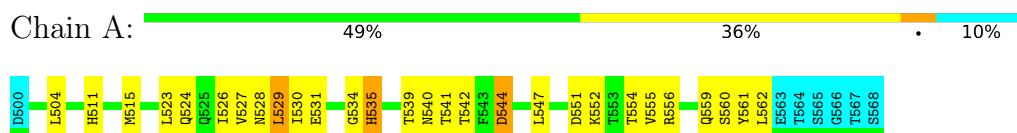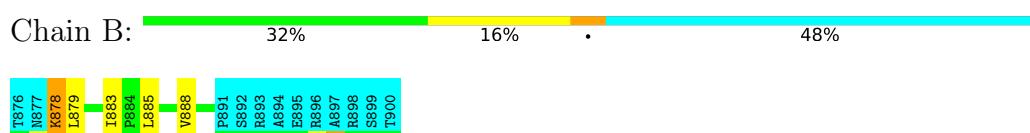
4.2.10 Score per residue for model 10

• Molecule 1: Protein AF-9

Chain A: 61% 22% 6% • 10%

D500 L504 R512 M515 R518 E519 R520 H521 I522 L523 I526 V527 N528 L529 T539 N540 T541 T542 L547 C548 D551 T554 V555 L558 E563 T564 S565 G566 T567 S568

• Molecule 2: Histone-lysine N-methyltransferase, H3 lysine-79 specific

Chain B: 52% 48%

T876 N877 P891 S892 R893 A894 E895 R896 A897 R898 S899 T900
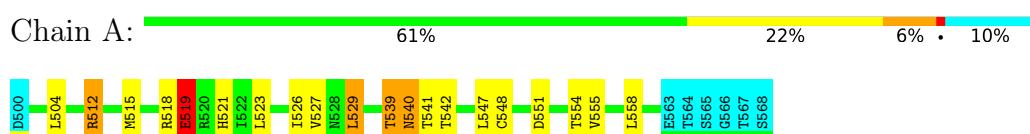
5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, SIMULATED AN-NEALING, SIMULATED ANNEALING.*

Of the 100 calculated structures, 10 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 2.34	refinement	
X-PLOR NIH 2.34	structure solution	
Sparky	structure solution	
Sparky	refinement	
MOLMOL	structure solution	

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	1150
Number of shifts mapped to atoms	1150
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6   Model quality ⓘ

6.1   Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	524	536	532	23±3
2	B	93	113	113	2±1
All	All	6170	6490	6450	239

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:530:ILE:HD12	1:A:531:GLU:N	0.62	2.09	2	2
1:A:523:LEU:O	1:A:527:VAL:HG23	0.62	1.95	6	10
1:A:556:ARG:NH1	1:A:559:GLN:HE22	0.58	1.96	7	2
1:A:547:LEU:N	1:A:547:LEU:HD22	0.58	2.13	8	9
1:A:534:GLY:O	1:A:535:HIS:CG	0.57	2.57	4	2
1:A:556:ARG:HH12	1:A:559:GLN:HE22	0.57	1.42	7	1
1:A:547:LEU:N	1:A:547:LEU:CD2	0.56	2.69	9	9
1:A:526:ILE:HD12	1:A:526:ILE:N	0.56	2.16	4	1
1:A:556:ARG:NH1	1:A:559:GLN:NE2	0.56	2.53	7	1
1:A:547:LEU:CD2	1:A:547:LEU:N	0.55	2.70	10	1
1:A:543:PHE:CE2	1:A:545:PHE:CD1	0.55	2.95	3	3
1:A:519:GLU:OE1	1:A:521:HIS:N	0.55	2.40	10	1
1:A:530:ILE:O	1:A:533:THR:N	0.54	2.40	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:890:LEU:N	2:B:890:LEU:CD2	0.54	2.71	8	4
1:A:504:LEU:HD12	1:A:504:LEU:N	0.53	2.18	1	8
1:A:520:ARG:NH1	1:A:524:GLN:NE2	0.53	2.57	8	1
1:A:557:LYS:N	1:A:557:LYS:CD	0.53	2.72	5	1
1:A:546:ASP:OD1	1:A:546:ASP:N	0.53	2.41	2	1
2:B:881:VAL:HG12	2:B:882:SER:N	0.53	2.18	3	1
1:A:535:HIS:CE1	1:A:549:SER:OG	0.53	2.62	5	1
1:A:518:ARG:O	1:A:520:ARG:N	0.53	2.42	6	3
1:A:551:ASP:O	1:A:554:THR:N	0.52	2.42	6	8
1:A:531:GLU:OE1	1:A:536:PHE:CE2	0.52	2.63	4	1
1:A:556:ARG:NH2	1:A:559:GLN:OE1	0.52	2.42	1	1
1:A:505:ASP:N	1:A:505:ASP:OD1	0.52	2.42	4	1
1:A:528:ASN:ND2	1:A:528:ASN:N	0.52	2.57	9	1
1:A:504:LEU:N	1:A:504:LEU:HD12	0.52	2.19	10	1
1:A:544:ASP:N	1:A:544:ASP:OD1	0.51	2.43	9	2
1:A:523:LEU:HD12	1:A:523:LEU:N	0.51	2.21	6	3
1:A:520:ARG:NH1	2:B:887:SER:O	0.51	2.44	5	1
1:A:531:GLU:OE2	1:A:536:PHE:CZ	0.50	2.64	3	1
1:A:548:CYS:O	1:A:548:CYS:SG	0.50	2.69	6	2
1:A:545:PHE:CD1	1:A:545:PHE:N	0.49	2.81	3	2
1:A:523:LEU:O	1:A:527:VAL:CG2	0.49	2.61	3	9
1:A:551:ASP:O	1:A:555:VAL:N	0.49	2.46	10	10
1:A:560:SER:O	1:A:562:LEU:N	0.49	2.45	8	5
1:A:544:ASP:OD1	1:A:545:PHE:N	0.49	2.46	4	1
1:A:537:HIS:CD2	1:A:537:HIS:N	0.49	2.81	7	1
1:A:551:ASP:OD1	1:A:552:LYS:N	0.48	2.47	2	1
1:A:560:SER:C	1:A:562:LEU:N	0.48	2.67	9	5
1:A:539:THR:CG2	1:A:542:THR:OG1	0.48	2.62	7	1
2:B:890:LEU:N	2:B:890:LEU:HD22	0.47	2.25	1	3
1:A:538:ILE:HG23	1:A:542:THR:O	0.47	2.10	7	1
1:A:535:HIS:ND1	1:A:549:SER:O	0.47	2.47	8	1
1:A:539:THR:OG1	1:A:540:ASN:ND2	0.47	2.47	10	1
1:A:555:VAL:CG1	1:A:559:GLN:OE1	0.47	2.62	4	2
1:A:504:LEU:HD12	1:A:504:LEU:H	0.47	1.70	1	6
1:A:535:HIS:CE1	1:A:549:SER:HG	0.47	2.28	5	1
1:A:528:ASN:N	1:A:528:ASN:HD22	0.46	2.08	9	1
1:A:511:HIS:CG	2:B:879:LEU:HD22	0.46	2.45	3	6
1:A:537:HIS:CG	1:A:537:HIS:O	0.46	2.69	3	1
1:A:519:GLU:CA	1:A:519:GLU:OE1	0.46	2.64	1	1
2:B:881:VAL:CG1	2:B:882:SER:N	0.46	2.79	3	1
1:A:526:ILE:N	1:A:526:ILE:CD1	0.46	2.79	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:536:PHE:CD1	1:A:536:PHE:C	0.46	2.90	7	3
1:A:504:LEU:H	1:A:504:LEU:CD1	0.45	2.23	1	8
1:A:539:THR:O	1:A:541:THR:N	0.45	2.49	9	6
1:A:534:GLY:O	1:A:535:HIS:CD2	0.45	2.69	4	1
1:A:515:MET:C	1:A:515:MET:SD	0.45	2.95	10	1
1:A:556:ARG:NH1	1:A:559:GLN:OE1	0.45	2.50	2	1
1:A:546:ASP:OD2	1:A:549:SER:N	0.45	2.49	7	1
1:A:526:ILE:O	1:A:529:LEU:N	0.45	2.50	2	6
1:A:501:LYS:CB	1:A:501:LYS:NZ	0.45	2.80	4	1
1:A:506:GLU:N	1:A:506:GLU:OE1	0.45	2.50	3	1
1:A:546:ASP:O	1:A:549:SER:OG	0.45	2.35	7	2
1:A:515:MET:SD	1:A:515:MET:C	0.45	2.95	9	1
1:A:530:ILE:O	1:A:533:THR:OG1	0.45	2.34	1	1
1:A:522:ILE:CD1	1:A:522:ILE:N	0.44	2.80	2	1
1:A:504:LEU:N	1:A:504:LEU:CD1	0.44	2.81	8	9
1:A:530:ILE:CD1	1:A:531:GLU:N	0.44	2.80	2	1
1:A:555:VAL:CG1	1:A:559:GLN:NE2	0.44	2.81	5	1
1:A:516:THR:O	1:A:518:ARG:NH1	0.44	2.47	6	1
1:A:522:ILE:O	1:A:524:GLN:N	0.44	2.51	4	1
1:A:522:ILE:C	1:A:524:GLN:N	0.43	2.71	4	1
1:A:540:ASN:C	1:A:540:ASN:HD22	0.43	2.15	1	2
1:A:523:LEU:N	1:A:523:LEU:CD1	0.43	2.82	6	3
2:B:878:LYS:NZ	2:B:878:LYS:CB	0.43	2.80	8	2
1:A:530:ILE:C	1:A:530:ILE:HD12	0.43	2.34	5	1
1:A:504:LEU:CD1	1:A:504:LEU:H	0.43	2.27	7	1
1:A:502:ALA:O	1:A:506:GLU:OE2	0.43	2.37	3	1
1:A:539:THR:OG1	1:A:540:ASN:N	0.43	2.52	7	1
1:A:509:GLU:N	1:A:509:GLU:CD	0.43	2.72	1	1
1:A:530:ILE:HG13	1:A:531:GLU:N	0.43	2.29	9	2
1:A:505:ASP:O	1:A:509:GLU:OE1	0.42	2.36	1	1
2:B:885:LEU:O	2:B:888:VAL:O	0.42	2.37	9	1
1:A:536:PHE:C	1:A:536:PHE:CD1	0.42	2.92	5	1
1:A:529:LEU:C	1:A:529:LEU:HD13	0.42	2.34	6	3
1:A:528:ASN:O	1:A:528:ASN:ND2	0.42	2.53	5	1
1:A:512:ARG:HE	1:A:512:ARG:CA	0.42	2.26	10	1
1:A:522:ILE:N	1:A:522:ILE:HD12	0.42	2.29	2	1
1:A:532:GLU:O	1:A:532:GLU:OE1	0.42	2.37	6	1
1:A:534:GLY:O	1:A:535:HIS:CB	0.42	2.67	4	2
1:A:545:PHE:N	1:A:545:PHE:CD1	0.42	2.88	4	1
1:A:510:LEU:N	1:A:510:LEU:CD2	0.42	2.83	7	1
1:A:506:GLU:N	1:A:506:GLU:CD	0.42	2.73	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:560:SER:C	1:A:562:LEU:H	0.41	2.18	6	2
1:A:521:HIS:ND1	1:A:521:HIS:N	0.41	2.60	8	1
1:A:530:ILE:HD12	1:A:530:ILE:C	0.41	2.36	3	1
1:A:541:THR:C	1:A:542:THR:OG1	0.41	2.59	8	1
1:A:540:ASN:C	1:A:540:ASN:ND2	0.41	2.74	1	1
1:A:526:ILE:HG23	1:A:558:LEU:HD21	0.41	1.93	1	1
1:A:529:LEU:HD13	1:A:529:LEU:C	0.41	2.35	3	2
1:A:530:ILE:O	1:A:531:GLU:C	0.40	2.60	2	1
1:A:557:LYS:O	1:A:561:TYR:CD2	0.40	2.74	5	1
1:A:523:LEU:CD1	1:A:523:LEU:H	0.40	2.30	6	1
1:A:522:ILE:N	1:A:522:ILE:CD1	0.40	2.85	8	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	62/69 (90%)	52±2 (84±3%)	8±2 (14±4%)	2±1 (3±2%)	8	43
2	B	13/25 (52%)	12±1 (88±5%)	1±0 (10±4%)	0±0 (2±3%)	14	59
All	All	750/940 (80%)	634 (85%)	97 (13%)	19 (3%)	9	45

All 6 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	540	ASN	7
1	A	519	GLU	4
1	A	561	TYR	3
1	A	535	HIS	2
2	B	878	LYS	2
1	A	523	LEU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	60/66 (91%)	55±1 (92±2%)	5±1 (8±2%)	14	61
2	B	12/22 (55%)	12±1 (98±5%)	0±1 (2±5%)	50	91
All	All	720/880 (82%)	666 (92%)	54 (8%)	17	65

All 23 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	529	LEU	10
1	A	542	THR	10
1	A	558	LEU	5
1	A	544	ASP	4
1	A	519	GLU	2
1	A	540	ASN	2
1	A	552	LYS	2
1	A	518	ARG	2
1	A	503	TYR	2
2	B	883	ILE	2
1	A	541	THR	1
1	A	549	SER	1
1	A	506	GLU	1
1	A	505	ASP	1
1	A	556	ARG	1
1	A	528	ASN	1
1	A	557	LYS	1
1	A	532	GLU	1
1	A	521	HIS	1
2	B	878	LYS	1
1	A	524	GLN	1
1	A	512	ARG	1
1	A	539	THR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *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	1150
Number of shifts mapped to atoms	1150
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	94	-0.29 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_\beta$	92	0.07 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	89	-0.32 ± 0.09	None needed (< 0.5 ppm)
^{15}N	89	0.01 ± 0.32	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 974 atoms were assigned a chemical shift out of a possible 1116. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	369/372 (99%)	149/149 (100%)	147/150 (98%)	73/73 (100%)
Sidechain	551/664 (83%)	376/435 (86%)	175/205 (85%)	0/24 (0%)

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	Total	**¹H**	**¹³C**	**¹⁵N**
Aromatic	54/80 (68%)	28/39 (72%)	26/33 (79%)	0/8 (0%)
Overall	974/1116 (87%)	553/623 (89%)	348/388 (90%)	73/105 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1150 atoms were assigned a chemical shift out of a possible 1342. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**¹H**	**¹³C**	**¹⁵N**
Backbone	455/466 (98%)	183/187 (98%)	183/188 (97%)	89/91 (98%)
Sidechain	641/796 (81%)	436/518 (84%)	205/244 (84%)	0/34 (0%)
Aromatic	54/80 (68%)	28/39 (72%)	26/33 (79%)	0/8 (0%)
Overall	1150/1342 (86%)	647/744 (87%)	414/465 (89%)	89/133 (67%)

7.1.4 Statistically unusual chemical shifts (i)

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

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	530	ILE	CG2	10.15	10.93 − 24.12	-5.6
1	B	881	VAL	HB	0.43	0.43 − 3.54	-5.0

7.1.5 Random Coil Index (RCI) plots (i)

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

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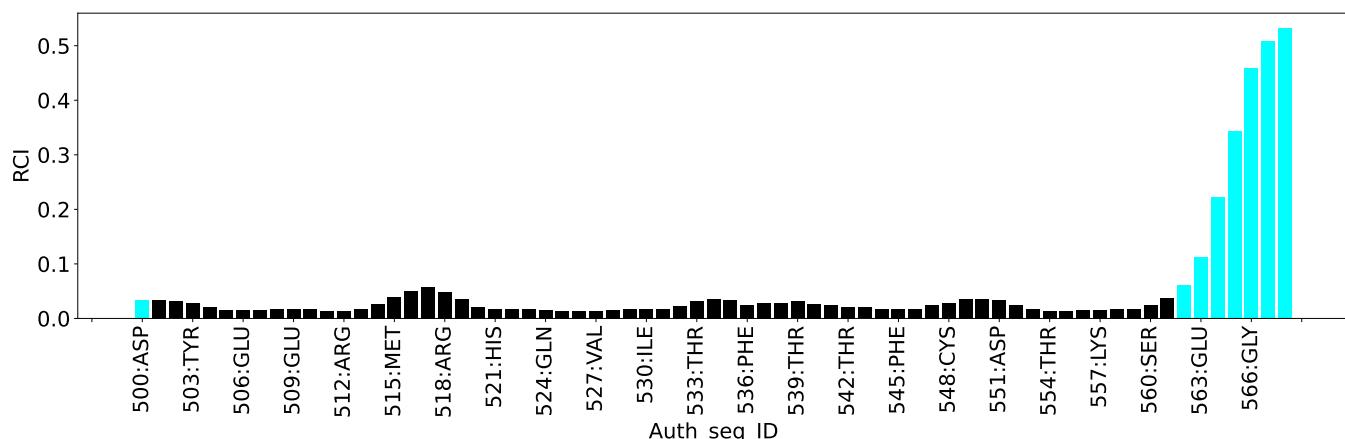
Random coil index (RCI) for chain B:
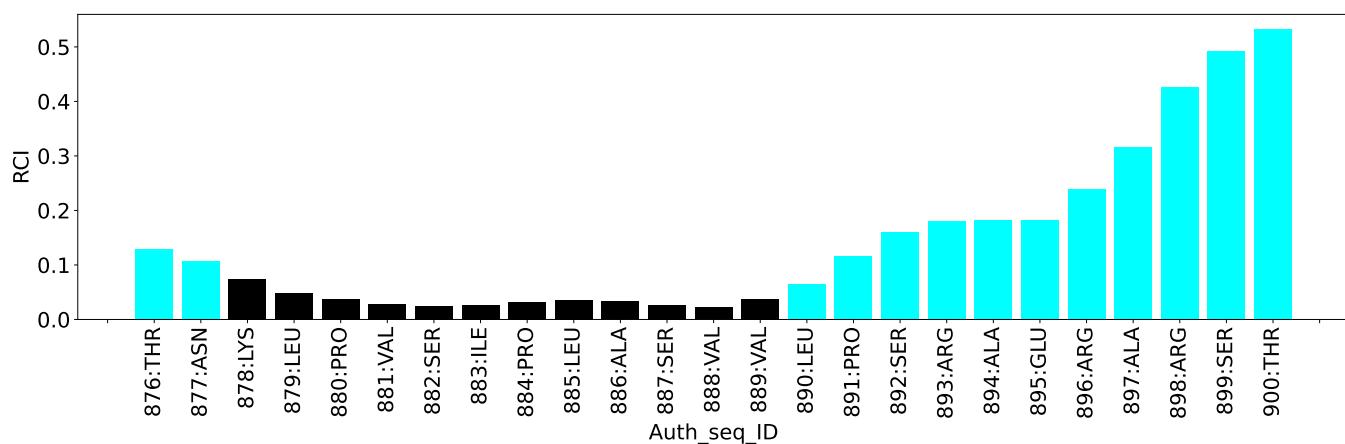
8 NMR restraints analysis ⓘ

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	1667
Intra-residue ($\lvert$i-j$\rvert$=0)	821
Sequential ($\lvert$i-j$\rvert$=1)	400
Medium range ($\lvert$i-j$\rvert$>1 and $\lvert$i-j$\rvert$<5)	216
Long range ($\lvert$i-j$\rvert$≥5)	96
Inter-chain	134
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	139
Number of unmapped restraints	0
Number of restraints per residue	19.2
Number of long range restraints per residue[1]	1.0

[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)	21.1	0.2
0.2-0.5 (Medium)	1.5	0.39
>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)	7.5	4.3
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)	821	49.3	16	1.9	1.0	2	0.2	0.1
Backbone-Backbone	107	6.4	1	0.9	0.1	0	0.0	0.0
Backbone-Sidechain	536	32.2	15	2.8	0.9	2	0.4	0.1
Sidechain-Sidechain	178	10.7	0	0.0	0.0	0	0.0	0.0
Sequential ($|i-j|$=1)	400	24.0	18	4.5	1.1	2	0.5	0.1
Backbone-Backbone	169	10.1	9	5.3	0.5	1	0.6	0.1
Backbone-Sidechain	211	12.7	9	4.3	0.5	1	0.5	0.1
Sidechain-Sidechain	20	1.2	0	0.0	0.0	0	0.0	0.0
Medium range ($|i-j|$>1 & $|i-j|$<5)	216	13.0	11	5.1	0.7	0	0.0	0.0
Backbone-Backbone	58	3.5	2	3.4	0.1	0	0.0	0.0
Backbone-Sidechain	110	6.6	5	4.5	0.3	0	0.0	0.0
Sidechain-Sidechain	48	2.9	4	8.3	0.2	0	0.0	0.0
Long range ($|i-j|\geq$5)	96	5.8	5	5.2	0.3	0	0.0	0.0
Backbone-Backbone	4	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	32	1.9	2	6.2	0.1	0	0.0	0.0
Sidechain-Sidechain	60	3.6	3	5.0	0.2	0	0.0	0.0
Inter-chain	134	8.0	14	10.4	0.8	0	0.0	0.0
Backbone-Backbone	13	0.8	3	23.1	0.2	0	0.0	0.0
Backbone-Sidechain	51	3.1	5	9.8	0.3	0	0.0	0.0
Sidechain-Sidechain	70	4.2	6	8.6	0.4	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1667	100.0	64	3.8	3.8	4	0.2	0.2
Backbone-Backbone	351	21.1	15	4.3	0.9	1	0.3	0.1
Backbone-Sidechain	940	56.4	36	3.8	2.2	3	0.3	0.2
Sidechain-Sidechain	376	22.6	13	3.5	0.8	0	0.0	0.0

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

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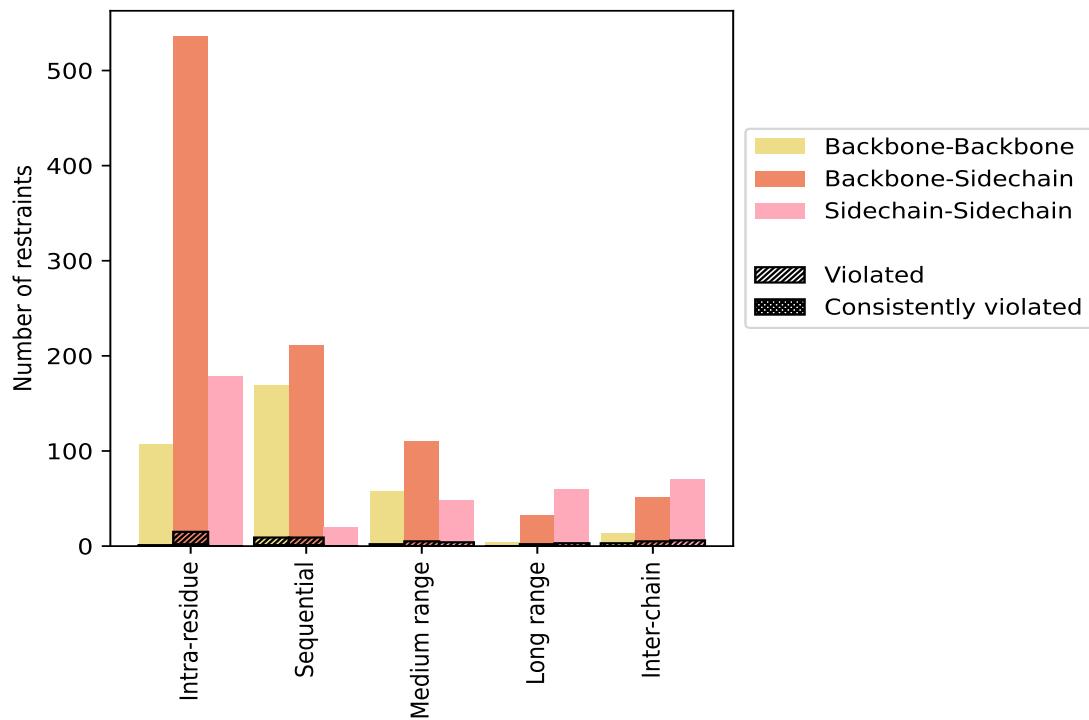
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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	4	5	2	3	3	17	0.16	0.3	0.05	0.14
2	5	7	4	3	3	22	0.15	0.2	0.03	0.15
3	6	8	2	2	8	26	0.14	0.25	0.03	0.13
4	5	7	2	2	4	20	0.15	0.22	0.03	0.15
5	8	6	1	1	5	21	0.15	0.2	0.03	0.15
6	6	9	0	2	4	21	0.16	0.3	0.04	0.15
7	7	7	4	1	4	23	0.15	0.2	0.03	0.15
8	6	7	2	4	4	23	0.17	0.39	0.07	0.14
9	4	12	6	2	3	27	0.15	0.2	0.03	0.15
10	5	10	3	3	5	26	0.16	0.24	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 ⓘ
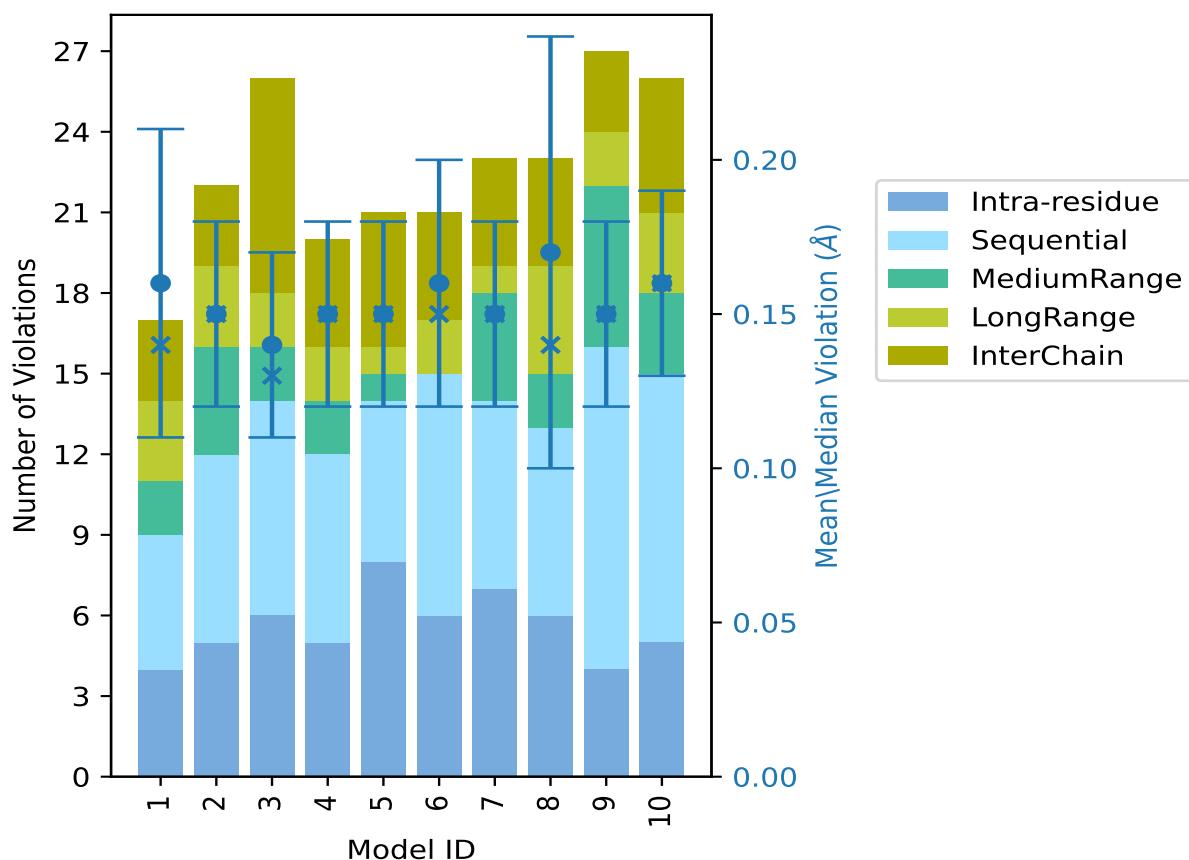
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

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, 1603(IR:805, SQ:382, MR:205, LR:91, IC:120) 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]	%
6	5	4	1	6	22	1	10.0
3	2	5	1	2	13	2	20.0
1	2	0	0	2	5	3	30.0
2	0	1	0	0	3	4	40.0

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Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	2	0	0	1	3	5	50.0
1	4	0	1	1	7	6	60.0
1	0	0	2	0	3	7	70.0
0	0	1	0	2	3	8	80.0
0	1	0	0	0	1	9	90.0
2	2	0	0	0	4	10	100.0

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

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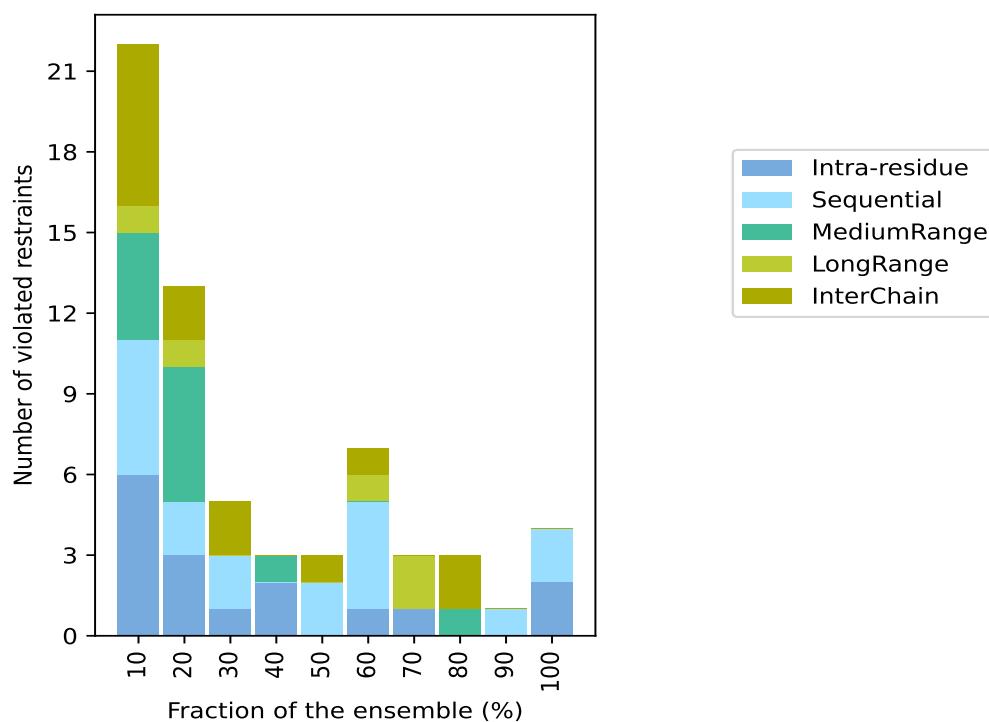
9.4   Most violated distance restraints in the ensemble ⓘ

9.4.1   Histogram : Distribution of mean distance violations ⓘ

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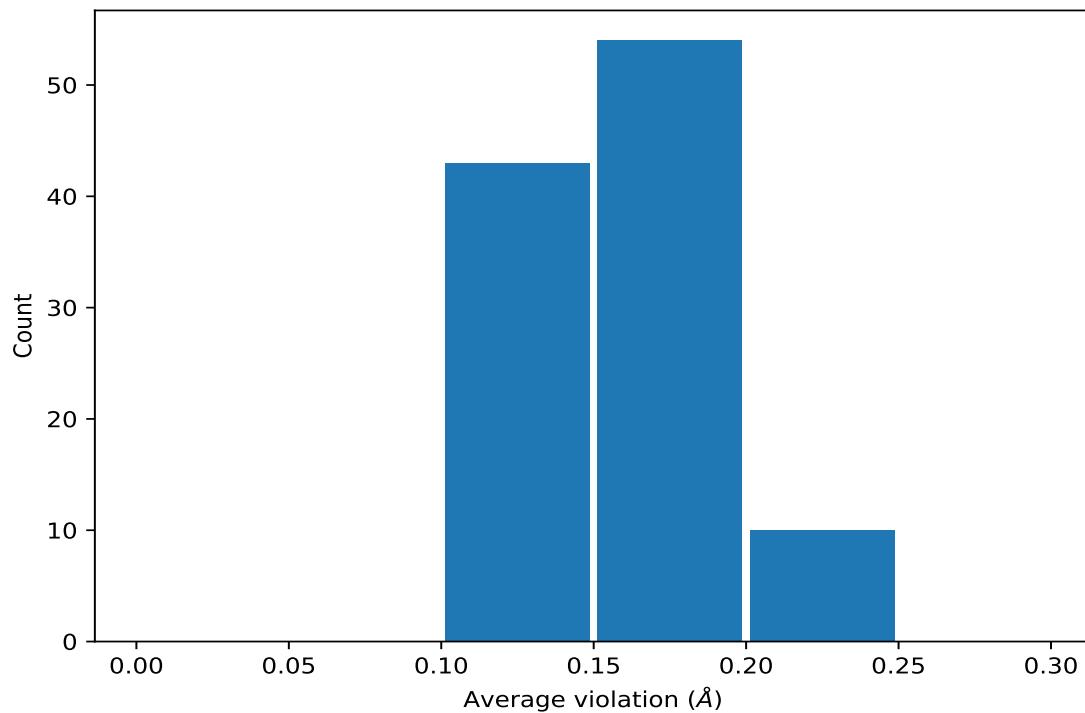
9.4.2   Table: Most violated distance restraints ⓘ

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	10	0.19	0.0	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	10	0.19	0.0	0.19
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	10	0.18	0.03	0.18
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	10	0.15	0.02	0.15
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	10	0.15	0.02	0.15
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	9	0.12	0.01	0.12
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD11	8	0.21	0.1	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD12	8	0.21	0.1	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD13	8	0.21	0.1	0.15
(1,1097)	1:A:517:LEU:H	1:A:515:MET:HA	8	0.16	0.03	0.17
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD11	8	0.16	0.04	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD12	8	0.16	0.04	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD13	8	0.16	0.04	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD11	8	0.16	0.04	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD12	8	0.16	0.04	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD13	8	0.16	0.04	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD11	8	0.16	0.04	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD12	8	0.16	0.04	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD13	8	0.16	0.04	0.13
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD21	7	0.16	0.03	0.15
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD22	7	0.16	0.03	0.15
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD23	7	0.16	0.03	0.15
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD11	7	0.15	0.02	0.14
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD12	7	0.15	0.02	0.14
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD13	7	0.15	0.02	0.14
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD11	7	0.15	0.02	0.14
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD12	7	0.15	0.02	0.14
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD13	7	0.15	0.02	0.14
(1,1509)	1:A:511:HIS:HD1	1:A:547:LEU:HG	7	0.14	0.02	0.14
(1,1509)	1:A:511:HIS:HD2	1:A:547:LEU:HG	7	0.14	0.02	0.14
(1,1009)	2:B:891:PRO:HG2	2:B:891:PRO:HA	6	0.2	0.0	0.2
(1,1009)	2:B:891:PRO:HG3	2:B:891:PRO:HA	6	0.2	0.0	0.2
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD11	6	0.17	0.02	0.17
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD12	6	0.17	0.02	0.17
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD13	6	0.17	0.02	0.17
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG21	6	0.16	0.02	0.16
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG22	6	0.16	0.02	0.16
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG23	6	0.16	0.02	0.16
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD11	6	0.16	0.03	0.16
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD12	6	0.16	0.03	0.16
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD13	6	0.16	0.03	0.16
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD11	6	0.16	0.03	0.16
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD12	6	0.16	0.03	0.16
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD13	6	0.16	0.03	0.16
(1,7)	2:B:879:LEU:H	2:B:878:LYS:H	6	0.14	0.02	0.14
(1,1502)	2:B:879:LEU:HD11	1:A:547:LEU:HG	6	0.13	0.02	0.14
(1,1502)	2:B:879:LEU:HD12	1:A:547:LEU:HG	6	0.13	0.02	0.14
(1,1502)	2:B:879:LEU:HD13	1:A:547:LEU:HG	6	0.13	0.02	0.14
(1,1042)	1:A:551:ASP:HA	1:A:552:LYS:HA	6	0.11	0.0	0.11
(1,1033)	2:B:890:LEU:HB2	2:B:889:VAL:HA	5	0.15	0.02	0.15
(1,1033)	2:B:890:LEU:HB3	2:B:889:VAL:HA	5	0.15	0.02	0.15
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG21	5	0.15	0.02	0.15
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG22	5	0.15	0.02	0.15
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG23	5	0.15	0.02	0.15
(1,756)	2:B:880:PRO:HA	1:A:546:ASP:HA	5	0.13	0.01	0.13
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG11	4	0.16	0.04	0.16
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG12	4	0.16	0.04	0.16
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG13	4	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,992)	1:A:530:ILE:HG12	1:A:530:ILE:HA	4	0.12	0.01	0.13
(1,992)	1:A:530:ILE:HG13	1:A:530:ILE:HA	4	0.12	0.01	0.13
(1,162)	1:A:517:LEU:HD21	1:A:517:LEU:H	4	0.12	0.0	0.12
(1,162)	1:A:517:LEU:HD22	1:A:517:LEU:H	4	0.12	0.0	0.12
(1,162)	1:A:517:LEU:HD23	1:A:517:LEU:H	4	0.12	0.0	0.12
(1,946)	1:A:541:THR:HA	1:A:541:THR:HB	3	0.2	0.0	0.2
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD21	3	0.15	0.02	0.15
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD22	3	0.15	0.02	0.15
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD23	3	0.15	0.02	0.15
(1,1197)	1:A:548:CYS:HB2	2:B:878:LYS:HA	3	0.14	0.02	0.16
(1,1197)	1:A:548:CYS:HB3	2:B:878:LYS:HA	3	0.14	0.02	0.16
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB1	3	0.13	0.02	0.14
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB2	3	0.13	0.02	0.14
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB3	3	0.13	0.02	0.14
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD11	3	0.12	0.01	0.12
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD12	3	0.12	0.01	0.12
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD13	3	0.12	0.01	0.12
(1,597)	1:A:512:ARG:H	1:A:512:ARG:HD2	2	0.22	0.08	0.22
(1,597)	1:A:512:ARG:H	1:A:512:ARG:HD3	2	0.22	0.08	0.22
(1,1154)	1:A:532:GLU:HG2	1:A:529:LEU:HA	2	0.2	0.0	0.2
(1,1154)	1:A:532:GLU:HG3	1:A:529:LEU:HA	2	0.2	0.0	0.2
(1,8)	2:B:877:ASN:HA	2:B:878:LYS:H	2	0.16	0.04	0.16
(1,762)	2:B:891:PRO:HD2	1:A:527:VAL:HG11	2	0.16	0.02	0.16
(1,762)	2:B:891:PRO:HD2	1:A:527:VAL:HG12	2	0.16	0.02	0.16
(1,762)	2:B:891:PRO:HD2	1:A:527:VAL:HG13	2	0.16	0.02	0.16
(1,762)	2:B:891:PRO:HD3	1:A:527:VAL:HG11	2	0.16	0.02	0.16
(1,762)	2:B:891:PRO:HD3	1:A:527:VAL:HG12	2	0.16	0.02	0.16
(1,762)	2:B:891:PRO:HD3	1:A:527:VAL:HG13	2	0.16	0.02	0.16
(1,935)	1:A:503:TYR:HE1	1:A:503:TYR:HA	2	0.14	0.01	0.14
(1,935)	1:A:503:TYR:HE2	1:A:503:TYR:HA	2	0.14	0.01	0.14
(1,1118)	1:A:560:SER:H	1:A:556:ARG:HA	2	0.13	0.02	0.13
(1,785)	1:A:524:GLN:HA	1:A:527:VAL:HG21	2	0.12	0.02	0.12
(1,785)	1:A:524:GLN:HA	1:A:527:VAL:HG22	2	0.12	0.02	0.12
(1,785)	1:A:524:GLN:HA	1:A:527:VAL:HG23	2	0.12	0.02	0.12
(1,977)	1:A:527:VAL:HG21	1:A:524:GLN:HA	2	0.12	0.02	0.12
(1,977)	1:A:527:VAL:HG22	1:A:524:GLN:HA	2	0.12	0.02	0.12
(1,977)	1:A:527:VAL:HG23	1:A:524:GLN:HA	2	0.12	0.02	0.12
(1,1080)	1:A:502:ALA:H	1:A:501:LYS:HA	2	0.12	0.01	0.12
(1,1569)	1:A:512:ARG:HB2	1:A:508:VAL:HG11	2	0.12	0.0	0.12
(1,1569)	1:A:512:ARG:HB2	1:A:508:VAL:HG12	2	0.12	0.0	0.12
(1,1569)	1:A:512:ARG:HB2	1:A:508:VAL:HG13	2	0.12	0.0	0.12
(1,1569)	1:A:512:ARG:HB3	1:A:508:VAL:HG11	2	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1569)	1:A:512:ARG:HB3	1:A:508:VAL:HG12	2	0.12	0.0	0.12
(1,1569)	1:A:512:ARG:HB3	1:A:508:VAL:HG13	2	0.12	0.0	0.12
(1,855)	1:A:562:LEU:HA	1:A:522:ILE:HD11	2	0.11	0.0	0.11
(1,855)	1:A:562:LEU:HA	1:A:522:ILE:HD12	2	0.11	0.0	0.11
(1,855)	1:A:562:LEU:HA	1:A:522:ILE:HD13	2	0.11	0.0	0.11
(1,954)	2:B:882:SER:HA	1:A:542:THR:HB	2	0.11	0.0	0.11
(1,1083)	1:A:563:GLU:H	1:A:563:GLU:HA	2	0.11	0.0	0.11

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

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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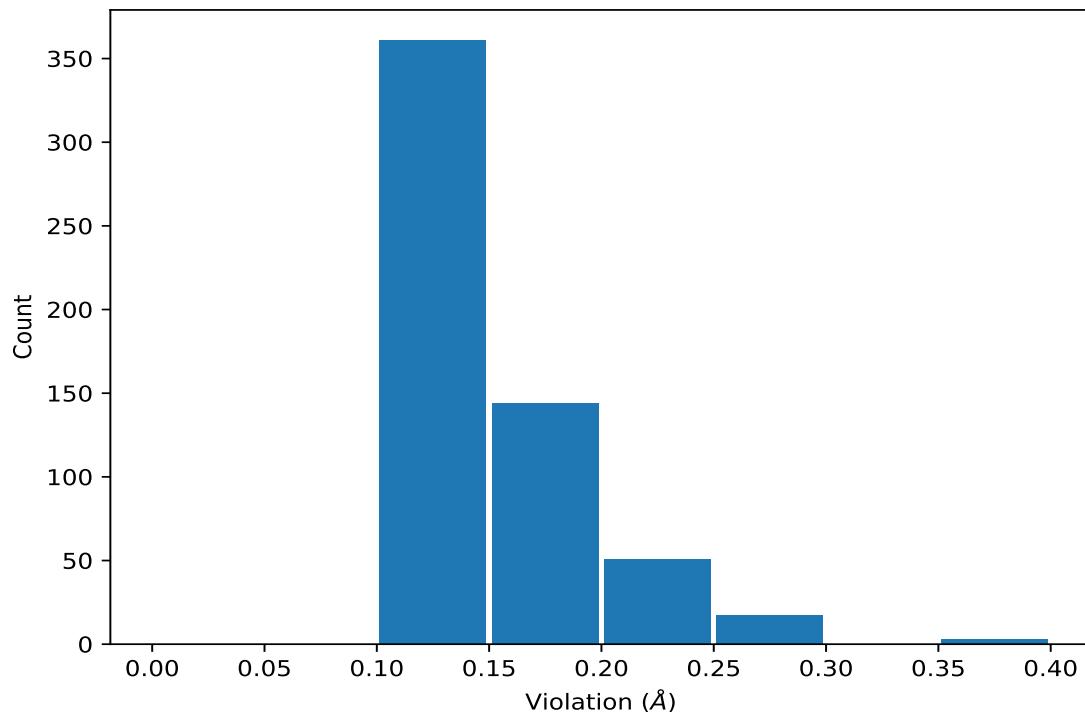
9.5.2 Table : All distance violations ⓘ

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD11	8	0.39
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD12	8	0.39
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD13	8	0.39
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD11	1	0.3
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD12	1	0.3
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD13	1	0.3
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD11	6	0.3
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD12	6	0.3
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD13	6	0.3
(1,597)	1:A:512:ARG:H	1:A:512:ARG:HD2	8	0.3
(1,597)	1:A:512:ARG:H	1:A:512:ARG:HD3	8	0.3
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD11	3	0.25
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD12	3	0.25
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD13	3	0.25
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD11	3	0.25
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD12	3	0.25
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD13	3	0.25
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD11	3	0.25
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD12	3	0.25
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD13	3	0.25
(1,1084)	1:A:564:THR:H	1:A:563:GLU:HA	10	0.24
(1,1412)	2:B:878:LYS:HA	2:B:878:LYS:HD2	8	0.23
(1,1412)	2:B:878:LYS:HA	2:B:878:LYS:HD3	8	0.23
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	1	0.22
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	4	0.22
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD11	8	0.22
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD12	8	0.22
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD13	8	0.22
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD11	8	0.22
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD12	8	0.22
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD13	8	0.22
(1,1027)	1:A:520:ARG:HD2	1:A:520:ARG:HA	6	0.22
(1,1027)	1:A:520:ARG:HD3	1:A:520:ARG:HA	6	0.22
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD11	6	0.21
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD12	6	0.21
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD13	6	0.21
(1,1154)	1:A:532:GLU:HG2	1:A:529:LEU:HA	10	0.21
(1,1154)	1:A:532:GLU:HG3	1:A:529:LEU:HA	10	0.21
(1,1097)	1:A:517:LEU:H	1:A:515:MET:HA	1	0.21
(1,1009)	2:B:891:PRO:HG2	2:B:891:PRO:HA	1	0.21
(1,1009)	2:B:891:PRO:HG3	2:B:891:PRO:HA	1	0.21
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	7	0.2
(1,946)	1:A:541:THR:HA	1:A:541:THR:HB	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:A:541:THR:HA	1:A:541:THR:HB	7	0.2
(1,946)	1:A:541:THR:HA	1:A:541:THR:HB	9	0.2
(1,8)	2:B:877:ASN:HA	2:B:878:LYS:H	9	0.2
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD21	6	0.2
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD22	6	0.2
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD23	6	0.2
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	3	0.2
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	3	0.2
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG11	4	0.2
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG12	4	0.2
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG13	4	0.2
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG11	10	0.2
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG12	10	0.2
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG13	10	0.2
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	7	0.2
(1,1154)	1:A:532:GLU:HG2	1:A:529:LEU:HA	9	0.2
(1,1154)	1:A:532:GLU:HG3	1:A:529:LEU:HA	9	0.2
(1,1132)	1:A:567:THR:HB	1:A:567:THR:HA	4	0.2
(1,1009)	2:B:891:PRO:HG2	2:B:891:PRO:HA	2	0.2
(1,1009)	2:B:891:PRO:HG3	2:B:891:PRO:HA	2	0.2
(1,1009)	2:B:891:PRO:HG2	2:B:891:PRO:HA	4	0.2
(1,1009)	2:B:891:PRO:HG3	2:B:891:PRO:HA	4	0.2
(1,1009)	2:B:891:PRO:HG2	2:B:891:PRO:HA	5	0.2
(1,1009)	2:B:891:PRO:HG3	2:B:891:PRO:HA	5	0.2
(1,1009)	2:B:891:PRO:HG2	2:B:891:PRO:HA	8	0.2
(1,1009)	2:B:891:PRO:HG3	2:B:891:PRO:HA	8	0.2
(1,1009)	2:B:891:PRO:HG2	2:B:891:PRO:HA	9	0.2
(1,1009)	2:B:891:PRO:HG3	2:B:891:PRO:HA	9	0.2
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	1	0.19
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	2	0.19
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	3	0.19
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	4	0.19
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	5	0.19
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	6	0.19
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	8	0.19
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	9	0.19
(1,949)	1:A:553:THR:HA	1:A:553:THR:HB	10	0.19
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD11	1	0.19
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD12	1	0.19
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD13	1	0.19
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD11	1	0.19
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD12	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD13	1	0.19
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD11	1	0.19
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD12	1	0.19
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD13	1	0.19
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD11	2	0.19
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD12	2	0.19
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD13	2	0.19
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD11	2	0.19
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD12	2	0.19
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD13	2	0.19
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD11	9	0.19
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD12	9	0.19
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD13	9	0.19
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG21	9	0.19
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG22	9	0.19
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG23	9	0.19
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	7	0.19
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	8	0.19
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	9	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	1	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	2	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	3	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	4	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	5	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	6	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	8	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	9	0.19
(1,1163)	1:A:553:THR:HB	1:A:553:THR:HA	10	0.19
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD11	5	0.18
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD12	5	0.18
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD13	5	0.18
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD11	5	0.18
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD12	5	0.18
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD13	5	0.18
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD11	5	0.18
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD12	5	0.18
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD13	5	0.18
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG21	7	0.18
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG22	7	0.18
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG23	7	0.18
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD21	5	0.18
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD22	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD23	5	0.18
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG21	8	0.18
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG22	8	0.18
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG23	8	0.18
(1,762)	2:B:891:PRO:HD2	1:A:527:VAL:HG11	3	0.18
(1,762)	2:B:891:PRO:HD2	1:A:527:VAL:HG12	3	0.18
(1,762)	2:B:891:PRO:HD2	1:A:527:VAL:HG13	3	0.18
(1,762)	2:B:891:PRO:HD3	1:A:527:VAL:HG11	3	0.18
(1,762)	2:B:891:PRO:HD3	1:A:527:VAL:HG12	3	0.18
(1,762)	2:B:891:PRO:HD3	1:A:527:VAL:HG13	3	0.18
(1,225)	1:A:535:HIS:H	1:A:534:GLY:H	2	0.18
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD11	9	0.18
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD12	9	0.18
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD13	9	0.18
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD11	9	0.18
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD12	9	0.18
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD13	9	0.18
(1,1509)	1:A:511:HIS:HD1	1:A:547:LEU:HG	10	0.18
(1,1509)	1:A:511:HIS:HD2	1:A:547:LEU:HG	10	0.18
(1,1336)	1:A:529:LEU:HD21	1:A:532:GLU:HB2	7	0.18
(1,1336)	1:A:529:LEU:HD21	1:A:532:GLU:HB3	7	0.18
(1,1336)	1:A:529:LEU:HD22	1:A:532:GLU:HB2	7	0.18
(1,1336)	1:A:529:LEU:HD22	1:A:532:GLU:HB3	7	0.18
(1,1336)	1:A:529:LEU:HD23	1:A:532:GLU:HB2	7	0.18
(1,1336)	1:A:529:LEU:HD23	1:A:532:GLU:HB3	7	0.18
(1,1097)	1:A:517:LEU:H	1:A:515:MET:HA	7	0.18
(1,1)	1:A:534:GLY:H	1:A:535:HIS:H	2	0.18
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD11	8	0.17
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD12	8	0.17
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD13	8	0.17
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD11	8	0.17
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD12	8	0.17
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD13	8	0.17
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG21	10	0.17
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG22	10	0.17
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG23	10	0.17
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD11	1	0.17
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD12	1	0.17
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD13	1	0.17
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD11	8	0.17
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD12	8	0.17
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD13	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD21	10	0.17
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD22	10	0.17
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD23	10	0.17
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD21	3	0.17
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD22	3	0.17
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD23	3	0.17
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG21	10	0.17
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG22	10	0.17
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG23	10	0.17
(1,7)	2:B:879:LEU:H	2:B:878:LYS:H	2	0.17
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	2	0.17
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	5	0.17
(1,1509)	1:A:511:HIS:HD1	1:A:547:LEU:HG	2	0.17
(1,1509)	1:A:511:HIS:HD2	1:A:547:LEU:HG	2	0.17
(1,1502)	2:B:879:LEU:HD11	1:A:547:LEU:HG	10	0.17
(1,1502)	2:B:879:LEU:HD12	1:A:547:LEU:HG	10	0.17
(1,1502)	2:B:879:LEU:HD13	1:A:547:LEU:HG	10	0.17
(1,1097)	1:A:517:LEU:H	1:A:515:MET:HA	3	0.17
(1,1097)	1:A:517:LEU:H	1:A:515:MET:HA	4	0.17
(1,1097)	1:A:517:LEU:H	1:A:515:MET:HA	10	0.17
(1,1033)	2:B:890:LEU:HB2	2:B:889:VAL:HA	7	0.17
(1,1033)	2:B:890:LEU:HB3	2:B:889:VAL:HA	7	0.17
(1,1033)	2:B:890:LEU:HB2	2:B:889:VAL:HA	10	0.17
(1,1033)	2:B:890:LEU:HB3	2:B:889:VAL:HA	10	0.17
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG21	7	0.16
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG22	7	0.16
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG23	7	0.16
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	10	0.16
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	10	0.16
(1,7)	2:B:879:LEU:H	2:B:878:LYS:H	5	0.16
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD11	2	0.16
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD12	2	0.16
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD13	2	0.16
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD11	2	0.16
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD12	2	0.16
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD13	2	0.16
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD11	4	0.16
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD12	4	0.16
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD13	4	0.16
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD11	4	0.16
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD12	4	0.16
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD13	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1197)	1:A:548:CYS:HB2	2:B:878:LYS:HA	5	0.16
(1,1197)	1:A:548:CYS:HB3	2:B:878:LYS:HA	5	0.16
(1,1197)	1:A:548:CYS:HB2	2:B:878:LYS:HA	10	0.16
(1,1197)	1:A:548:CYS:HB3	2:B:878:LYS:HA	10	0.16
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD11	2	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD12	2	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD13	2	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD11	7	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD12	7	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD13	7	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD11	9	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD12	9	0.15
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD13	9	0.15
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD11	9	0.15
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD12	9	0.15
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD13	9	0.15
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD11	9	0.15
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD12	9	0.15
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD13	9	0.15
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG21	3	0.15
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG22	3	0.15
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG23	3	0.15
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD11	10	0.15
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD12	10	0.15
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD13	10	0.15
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD21	5	0.15
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD22	5	0.15
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD23	5	0.15
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD21	7	0.15
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD22	7	0.15
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD23	7	0.15
(1,762)	2:B:891:PRO:HD2	1:A:527:VAL:HG11	5	0.15
(1,762)	2:B:891:PRO:HD2	1:A:527:VAL:HG12	5	0.15
(1,762)	2:B:891:PRO:HD2	1:A:527:VAL:HG13	5	0.15
(1,762)	2:B:891:PRO:HD3	1:A:527:VAL:HG11	5	0.15
(1,762)	2:B:891:PRO:HD3	1:A:527:VAL:HG12	5	0.15
(1,762)	2:B:891:PRO:HD3	1:A:527:VAL:HG13	5	0.15
(1,756)	2:B:880:PRO:HA	1:A:546:ASP:HA	2	0.15
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	4	0.15
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	4	0.15
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	6	0.15
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	7	0.15
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	7	0.15
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	9	0.15
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	9	0.15
(1,7)	2:B:879:LEU:H	2:B:878:LYS:H	10	0.15
(1,597)	1:A:512:ARG:H	1:A:512:ARG:HD2	6	0.15
(1,597)	1:A:512:ARG:H	1:A:512:ARG:HD3	6	0.15
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	6	0.15
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	6	0.15
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB1	6	0.15
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB2	6	0.15
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB3	6	0.15
(1,1509)	1:A:511:HIS:HD1	1:A:547:LEU:HG	4	0.15
(1,1509)	1:A:511:HIS:HD2	1:A:547:LEU:HG	4	0.15
(1,1118)	1:A:560:SER:H	1:A:556:ARG:HA	9	0.15
(1,1033)	2:B:890:LEU:HB2	2:B:889:VAL:HA	9	0.15
(1,1033)	2:B:890:LEU:HB3	2:B:889:VAL:HA	9	0.15
(1,977)	1:A:527:VAL:HG21	1:A:524:GLN:HA	9	0.14
(1,977)	1:A:527:VAL:HG22	1:A:524:GLN:HA	9	0.14
(1,977)	1:A:527:VAL:HG23	1:A:524:GLN:HA	9	0.14
(1,935)	1:A:503:TYR:HE1	1:A:503:TYR:HA	7	0.14
(1,935)	1:A:503:TYR:HE2	1:A:503:TYR:HA	7	0.14
(1,849)	1:A:523:LEU:H	1:A:526:ILE:HD11	2	0.14
(1,849)	1:A:523:LEU:H	1:A:526:ILE:HD12	2	0.14
(1,849)	1:A:523:LEU:H	1:A:526:ILE:HD13	2	0.14
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD11	3	0.14
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD12	3	0.14
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD13	3	0.14
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD11	3	0.14
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD12	3	0.14
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD13	3	0.14
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD11	6	0.14
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD12	6	0.14
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD13	6	0.14
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD11	6	0.14
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD12	6	0.14
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD13	6	0.14
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD11	7	0.14
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD12	7	0.14
(1,825)	1:A:531:GLU:HA	1:A:530:ILE:HD13	7	0.14
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD21	10	0.14
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD22	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD23	10	0.14
(1,785)	1:A:524:GLN:HA	1:A:527:VAL:HG21	9	0.14
(1,785)	1:A:524:GLN:HA	1:A:527:VAL:HG22	9	0.14
(1,785)	1:A:524:GLN:HA	1:A:527:VAL:HG23	9	0.14
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG21	1	0.14
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG22	1	0.14
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG23	1	0.14
(1,756)	2:B:880:PRO:HA	1:A:546:ASP:HA	9	0.14
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	2	0.14
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	2	0.14
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	8	0.14
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	8	0.14
(1,742)	1:A:518:ARG:HD2	1:A:518:ARG:HA	10	0.14
(1,742)	1:A:518:ARG:HD3	1:A:518:ARG:HA	10	0.14
(1,598)	1:A:518:ARG:HA	1:A:518:ARG:HD2	10	0.14
(1,598)	1:A:518:ARG:HA	1:A:518:ARG:HD3	10	0.14
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	8	0.14
(1,1634)	1:A:504:LEU:H	1:A:504:LEU:HD21	3	0.14
(1,1634)	1:A:504:LEU:H	1:A:504:LEU:HD22	3	0.14
(1,1634)	1:A:504:LEU:H	1:A:504:LEU:HD23	3	0.14
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	3	0.14
(1,16)	2:B:880:PRO:HA	2:B:879:LEU:H	10	0.14
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB1	5	0.14
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB2	5	0.14
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB3	5	0.14
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD11	1	0.14
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD12	1	0.14
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD13	1	0.14
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD11	1	0.14
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD12	1	0.14
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD13	1	0.14
(1,1509)	1:A:511:HIS:HD1	1:A:547:LEU:HG	6	0.14
(1,1509)	1:A:511:HIS:HD2	1:A:547:LEU:HG	6	0.14
(1,1502)	2:B:879:LEU:HD11	1:A:547:LEU:HG	5	0.14
(1,1502)	2:B:879:LEU:HD12	1:A:547:LEU:HG	5	0.14
(1,1502)	2:B:879:LEU:HD13	1:A:547:LEU:HG	5	0.14
(1,1502)	2:B:879:LEU:HD11	1:A:547:LEU:HG	7	0.14
(1,1502)	2:B:879:LEU:HD12	1:A:547:LEU:HG	7	0.14
(1,1502)	2:B:879:LEU:HD13	1:A:547:LEU:HG	7	0.14
(1,1490)	1:A:514:LEU:HB2	2:B:881:VAL:HG21	3	0.14
(1,1490)	1:A:514:LEU:HB2	2:B:881:VAL:HG22	3	0.14
(1,1490)	1:A:514:LEU:HB2	2:B:881:VAL:HG23	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1490)	1:A:514:LEU:HB3	2:B:881:VAL:HG21	3	0.14
(1,1490)	1:A:514:LEU:HB3	2:B:881:VAL:HG22	3	0.14
(1,1490)	1:A:514:LEU:HB3	2:B:881:VAL:HG23	3	0.14
(1,1097)	1:A:517:LEU:H	1:A:515:MET:HA	2	0.14
(1,1033)	2:B:890:LEU:HB2	2:B:889:VAL:HA	4	0.14
(1,1033)	2:B:890:LEU:HB3	2:B:889:VAL:HA	4	0.14
(1,992)	1:A:530:ILE:HG12	1:A:530:ILE:HA	3	0.13
(1,992)	1:A:530:ILE:HG13	1:A:530:ILE:HA	3	0.13
(1,992)	1:A:530:ILE:HG12	1:A:530:ILE:HA	4	0.13
(1,992)	1:A:530:ILE:HG13	1:A:530:ILE:HA	4	0.13
(1,992)	1:A:530:ILE:HG12	1:A:530:ILE:HA	5	0.13
(1,992)	1:A:530:ILE:HG13	1:A:530:ILE:HA	5	0.13
(1,935)	1:A:503:TYR:HE1	1:A:503:TYR:HA	3	0.13
(1,935)	1:A:503:TYR:HE2	1:A:503:TYR:HA	3	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD11	2	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD12	2	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD13	2	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD11	2	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD12	2	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD13	2	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD11	2	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD12	2	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD13	2	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD11	4	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD12	4	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD13	4	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD11	4	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD12	4	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD13	4	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD11	4	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD12	4	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD13	4	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD11	6	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD12	6	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD13	6	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD11	6	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD12	6	0.13
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD13	6	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD11	6	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD12	6	0.13
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD13	6	0.13
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD11	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD12	3	0.13
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD13	3	0.13
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD11	7	0.13
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD12	7	0.13
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD13	7	0.13
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD11	7	0.13
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD12	7	0.13
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD13	7	0.13
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG21	9	0.13
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG22	9	0.13
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG23	9	0.13
(1,8)	2:B:877:ASN:HA	2:B:878:LYS:H	6	0.13
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD21	6	0.13
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD22	6	0.13
(1,797)	1:A:512:ARG:H	2:B:879:LEU:HD23	6	0.13
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD21	8	0.13
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD22	8	0.13
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD23	8	0.13
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG21	6	0.13
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG22	6	0.13
(1,773)	1:A:529:LEU:H	1:A:530:ILE:HG23	6	0.13
(1,756)	2:B:880:PRO:HA	1:A:546:ASP:HA	3	0.13
(1,756)	2:B:880:PRO:HA	1:A:546:ASP:HA	8	0.13
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	5	0.13
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	5	0.13
(1,7)	2:B:879:LEU:H	2:B:878:LYS:H	3	0.13
(1,7)	2:B:879:LEU:H	2:B:878:LYS:H	4	0.13
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	4	0.13
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	9	0.13
(1,162)	1:A:517:LEU:HD21	1:A:517:LEU:H	5	0.13
(1,162)	1:A:517:LEU:HD22	1:A:517:LEU:H	5	0.13
(1,162)	1:A:517:LEU:HD23	1:A:517:LEU:H	5	0.13
(1,1509)	1:A:511:HIS:HD1	1:A:547:LEU:HG	1	0.13
(1,1509)	1:A:511:HIS:HD2	1:A:547:LEU:HG	1	0.13
(1,1502)	2:B:879:LEU:HD11	1:A:547:LEU:HG	3	0.13
(1,1502)	2:B:879:LEU:HD12	1:A:547:LEU:HG	3	0.13
(1,1502)	2:B:879:LEU:HD13	1:A:547:LEU:HG	3	0.13
(1,1080)	1:A:502:ALA:H	1:A:501:LYS:HA	9	0.13
(1,1033)	2:B:890:LEU:HB2	2:B:889:VAL:HA	2	0.13
(1,1033)	2:B:890:LEU:HB3	2:B:889:VAL:HA	2	0.13
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD11	7	0.12
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD12	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD13	7	0.12
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD11	7	0.12
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD12	7	0.12
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD13	7	0.12
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD11	7	0.12
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD12	7	0.12
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD13	7	0.12
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD11	4	0.12
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD12	4	0.12
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD13	4	0.12
(1,856)	1:A:521:HIS:HA	1:A:522:ILE:HD11	3	0.12
(1,856)	1:A:521:HIS:HA	1:A:522:ILE:HD12	3	0.12
(1,856)	1:A:521:HIS:HA	1:A:522:ILE:HD13	3	0.12
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD11	10	0.12
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD12	10	0.12
(1,847)	1:A:561:TYR:HE1	1:A:526:ILE:HD13	10	0.12
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD11	10	0.12
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD12	10	0.12
(1,847)	1:A:561:TYR:HE2	1:A:526:ILE:HD13	10	0.12
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG21	6	0.12
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG22	6	0.12
(1,842)	1:A:523:LEU:H	1:A:522:ILE:HG23	6	0.12
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD21	2	0.12
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD22	2	0.12
(1,796)	2:B:879:LEU:H	2:B:879:LEU:HD23	2	0.12
(1,756)	2:B:880:PRO:HA	1:A:546:ASP:HA	4	0.12
(1,754)	1:A:547:LEU:HB2	1:A:546:ASP:HA	1	0.12
(1,754)	1:A:547:LEU:HB3	1:A:546:ASP:HA	1	0.12
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	2	0.12
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	5	0.12
(1,162)	1:A:517:LEU:HD21	1:A:517:LEU:H	1	0.12
(1,162)	1:A:517:LEU:HD22	1:A:517:LEU:H	1	0.12
(1,162)	1:A:517:LEU:HD23	1:A:517:LEU:H	1	0.12
(1,162)	1:A:517:LEU:HD21	1:A:517:LEU:H	6	0.12
(1,162)	1:A:517:LEU:HD22	1:A:517:LEU:H	6	0.12
(1,162)	1:A:517:LEU:HD23	1:A:517:LEU:H	6	0.12
(1,162)	1:A:517:LEU:HD21	1:A:517:LEU:H	7	0.12
(1,162)	1:A:517:LEU:HD22	1:A:517:LEU:H	7	0.12
(1,162)	1:A:517:LEU:HD23	1:A:517:LEU:H	7	0.12
(1,1569)	1:A:512:ARG:HB2	1:A:508:VAL:HG11	3	0.12
(1,1569)	1:A:512:ARG:HB2	1:A:508:VAL:HG12	3	0.12
(1,1569)	1:A:512:ARG:HB2	1:A:508:VAL:HG13	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1569)	1:A:512:ARG:HB3	1:A:508:VAL:HG11	3	0.12
(1,1569)	1:A:512:ARG:HB3	1:A:508:VAL:HG12	3	0.12
(1,1569)	1:A:512:ARG:HB3	1:A:508:VAL:HG13	3	0.12
(1,1520)	1:A:507:LEU:HA	1:A:550:LEU:HD11	8	0.12
(1,1520)	1:A:507:LEU:HA	1:A:550:LEU:HD12	8	0.12
(1,1520)	1:A:507:LEU:HA	1:A:550:LEU:HD13	8	0.12
(1,1509)	1:A:511:HIS:HD1	1:A:547:LEU:HG	5	0.12
(1,1509)	1:A:511:HIS:HD2	1:A:547:LEU:HG	5	0.12
(1,1509)	1:A:511:HIS:HD1	1:A:547:LEU:HG	8	0.12
(1,1509)	1:A:511:HIS:HD2	1:A:547:LEU:HG	8	0.12
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG11	2	0.12
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG12	2	0.12
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG13	2	0.12
(1,1097)	1:A:517:LEU:H	1:A:515:MET:HA	8	0.12
(1,1097)	1:A:517:LEU:H	1:A:515:MET:HA	9	0.12
(1,1042)	1:A:551:ASP:HA	1:A:552:LYS:HA	3	0.12
(1,1042)	1:A:551:ASP:HA	1:A:552:LYS:HA	9	0.12
(1,992)	1:A:530:ILE:HG12	1:A:530:ILE:HA	2	0.11
(1,992)	1:A:530:ILE:HG13	1:A:530:ILE:HA	2	0.11
(1,977)	1:A:527:VAL:HG21	1:A:524:GLN:HA	7	0.11
(1,977)	1:A:527:VAL:HG22	1:A:524:GLN:HA	7	0.11
(1,977)	1:A:527:VAL:HG23	1:A:524:GLN:HA	7	0.11
(1,954)	2:B:882:SER:HA	1:A:542:THR:HB	1	0.11
(1,954)	2:B:882:SER:HA	1:A:542:THR:HB	6	0.11
(1,908)	2:B:885:LEU:HB2	1:A:542:THR:HA	10	0.11
(1,908)	2:B:885:LEU:HB3	1:A:542:THR:HA	10	0.11
(1,891)	1:A:545:PHE:H	2:B:882:SER:HA	3	0.11
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD11	3	0.11
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD12	3	0.11
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD13	3	0.11
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD11	4	0.11
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD12	4	0.11
(1,878)	2:B:890:LEU:HA	1:A:538:ILE:HD13	4	0.11
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD11	9	0.11
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD12	9	0.11
(1,866)	1:A:527:VAL:HG11	2:B:883:ILE:HD13	9	0.11
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD11	9	0.11
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD12	9	0.11
(1,866)	1:A:527:VAL:HG12	2:B:883:ILE:HD13	9	0.11
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD11	9	0.11
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD12	9	0.11
(1,866)	1:A:527:VAL:HG13	2:B:883:ILE:HD13	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD11	9	0.11
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD12	9	0.11
(1,858)	1:A:523:LEU:H	1:A:522:ILE:HD13	9	0.11
(1,855)	1:A:562:LEU:HA	1:A:522:ILE:HD11	1	0.11
(1,855)	1:A:562:LEU:HA	1:A:522:ILE:HD12	1	0.11
(1,855)	1:A:562:LEU:HA	1:A:522:ILE:HD13	1	0.11
(1,855)	1:A:562:LEU:HA	1:A:522:ILE:HD11	3	0.11
(1,855)	1:A:562:LEU:HA	1:A:522:ILE:HD12	3	0.11
(1,855)	1:A:562:LEU:HA	1:A:522:ILE:HD13	3	0.11
(1,853)	1:A:519:GLU:HG2	1:A:522:ILE:HD11	8	0.11
(1,853)	1:A:519:GLU:HG2	1:A:522:ILE:HD12	8	0.11
(1,853)	1:A:519:GLU:HG2	1:A:522:ILE:HD13	8	0.11
(1,853)	1:A:519:GLU:HG3	1:A:522:ILE:HD11	8	0.11
(1,853)	1:A:519:GLU:HG3	1:A:522:ILE:HD12	8	0.11
(1,853)	1:A:519:GLU:HG3	1:A:522:ILE:HD13	8	0.11
(1,852)	1:A:525:GLN:HG2	1:A:522:ILE:HD11	2	0.11
(1,852)	1:A:525:GLN:HG2	1:A:522:ILE:HD12	2	0.11
(1,852)	1:A:525:GLN:HG2	1:A:522:ILE:HD13	2	0.11
(1,852)	1:A:525:GLN:HG3	1:A:522:ILE:HD11	2	0.11
(1,852)	1:A:525:GLN:HG3	1:A:522:ILE:HD12	2	0.11
(1,852)	1:A:525:GLN:HG3	1:A:522:ILE:HD13	2	0.11
(1,785)	1:A:524:GLN:HA	1:A:527:VAL:HG21	7	0.11
(1,785)	1:A:524:GLN:HA	1:A:527:VAL:HG22	7	0.11
(1,785)	1:A:524:GLN:HA	1:A:527:VAL:HG23	7	0.11
(1,7)	2:B:879:LEU:H	2:B:878:LYS:H	9	0.11
(1,509)	2:B:881:VAL:HB	1:A:543:PHE:HE1	8	0.11
(1,509)	2:B:881:VAL:HB	1:A:543:PHE:HE2	8	0.11
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	1	0.11
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	7	0.11
(1,400)	2:B:888:VAL:H	2:B:889:VAL:H	10	0.11
(1,265)	2:B:882:SER:HA	1:A:545:PHE:H	3	0.11
(1,1569)	1:A:512:ARG:HB2	1:A:508:VAL:HG11	9	0.11
(1,1569)	1:A:512:ARG:HB2	1:A:508:VAL:HG12	9	0.11
(1,1569)	1:A:512:ARG:HB2	1:A:508:VAL:HG13	9	0.11
(1,1569)	1:A:512:ARG:HB3	1:A:508:VAL:HG11	9	0.11
(1,1569)	1:A:512:ARG:HB3	1:A:508:VAL:HG12	9	0.11
(1,1569)	1:A:512:ARG:HB3	1:A:508:VAL:HG13	9	0.11
(1,1565)	2:B:888:VAL:H	2:B:889:VAL:HG21	6	0.11
(1,1565)	2:B:888:VAL:H	2:B:889:VAL:HG22	6	0.11
(1,1565)	2:B:888:VAL:H	2:B:889:VAL:HG23	6	0.11
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB1	8	0.11
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB2	8	0.11

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| Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1552)	2:B:885:LEU:H	2:B:886:ALA:HB3	8	0.11
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD11	10	0.11
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD12	10	0.11
(1,1519)	1:A:559:GLN:HG2	1:A:550:LEU:HD13	10	0.11
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD11	10	0.11
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD12	10	0.11
(1,1519)	1:A:559:GLN:HG3	1:A:550:LEU:HD13	10	0.11
(1,1514)	2:B:881:VAL:HB	1:A:514:LEU:HD11	10	0.11
(1,1514)	2:B:881:VAL:HB	1:A:514:LEU:HD12	10	0.11
(1,1514)	2:B:881:VAL:HB	1:A:514:LEU:HD13	10	0.11
(1,1502)	2:B:879:LEU:HD11	1:A:547:LEU:HG	4	0.11
(1,1502)	2:B:879:LEU:HD12	1:A:547:LEU:HG	4	0.11
(1,1502)	2:B:879:LEU:HD13	1:A:547:LEU:HG	4	0.11
(1,1502)	2:B:879:LEU:HD11	1:A:547:LEU:HG	8	0.11
(1,1502)	2:B:879:LEU:HD12	1:A:547:LEU:HG	8	0.11
(1,1502)	2:B:879:LEU:HD13	1:A:547:LEU:HG	8	0.11
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG11	5	0.11
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG12	5	0.11
(1,1488)	2:B:883:ILE:H	2:B:881:VAL:HG13	5	0.11
(1,1197)	1:A:548:CYS:HB2	2:B:878:LYS:HA	7	0.11
(1,1197)	1:A:548:CYS:HB3	2:B:878:LYS:HA	7	0.11
(1,1118)	1:A:560:SER:H	1:A:556:ARG:HA	1	0.11
(1,1083)	1:A:563:GLU:H	1:A:563:GLU:HA	5	0.11
(1,1083)	1:A:563:GLU:H	1:A:563:GLU:HA	7	0.11
(1,1080)	1:A:502:ALA:H	1:A:501:LYS:HA	3	0.11
(1,1042)	1:A:551:ASP:HA	1:A:552:LYS:HA	4	0.11
(1,1042)	1:A:551:ASP:HA	1:A:552:LYS:HA	5	0.11
(1,1042)	1:A:551:ASP:HA	1:A:552:LYS:HA	8	0.11
(1,1042)	1:A:551:ASP:HA	1:A:552:LYS:HA	10	0.11

10 Dihedral-angle violation analysis ⓘ

10.1 Summary of dihedral-angle violations ⓘ

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	$\%^1$	Violated[3]			Consistently Violated[4]		
			Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
PSI	69	49.6	7	10.1	5.0	1	1.4	0.7
PHI	70	50.4	7	10.0	5.0	1	1.4	0.7
Total	139	100.0	14	10.1	10.1	2	1.4	1.4

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations ⓘ
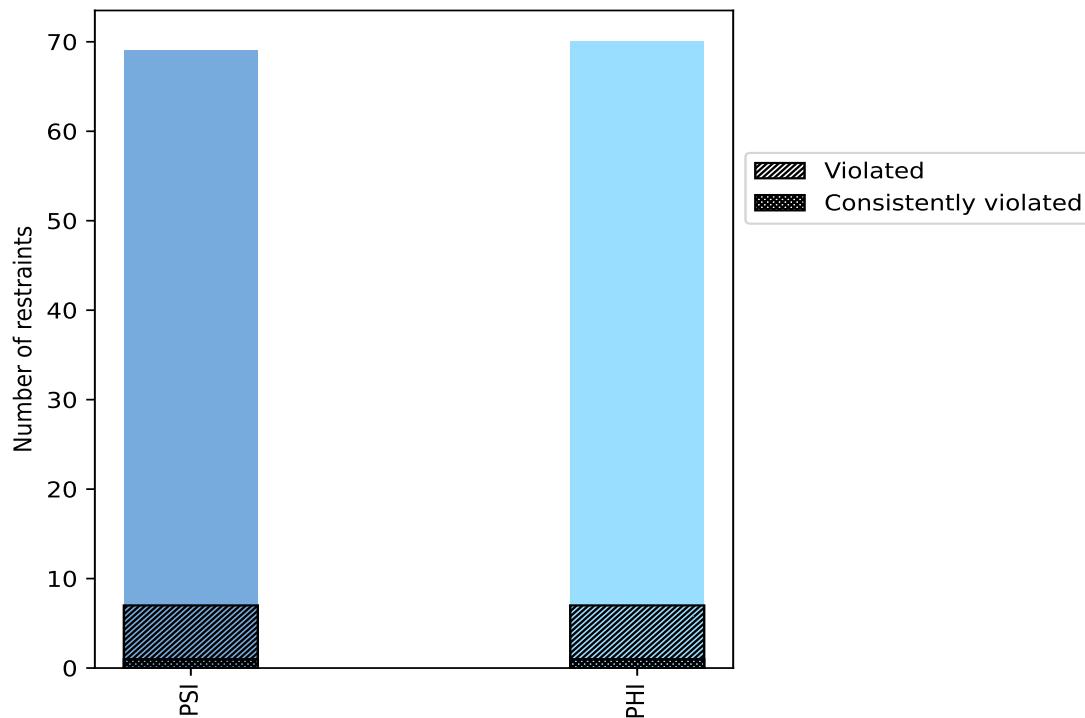

Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2   Dihedral-angle violation statistics for each model ⓘ

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	4	4	8	1.69	2.5	0.47	1.55
2	3	4	7	2.03	3.2	0.79	1.6
3	3	5	8	1.7	2.7	0.45	1.6
4	2	4	6	1.62	2.1	0.29	1.6
5	3	6	9	1.58	2.9	0.56	1.4
6	3	7	10	2.07	3.6	0.61	2.0
7	4	4	8	2.31	4.3	1.0	2.0
8	3	3	6	2.07	3.0	0.67	2.1
9	3	3	6	1.65	2.4	0.47	1.4
10	4	3	7	1.56	2.6	0.5	1.4

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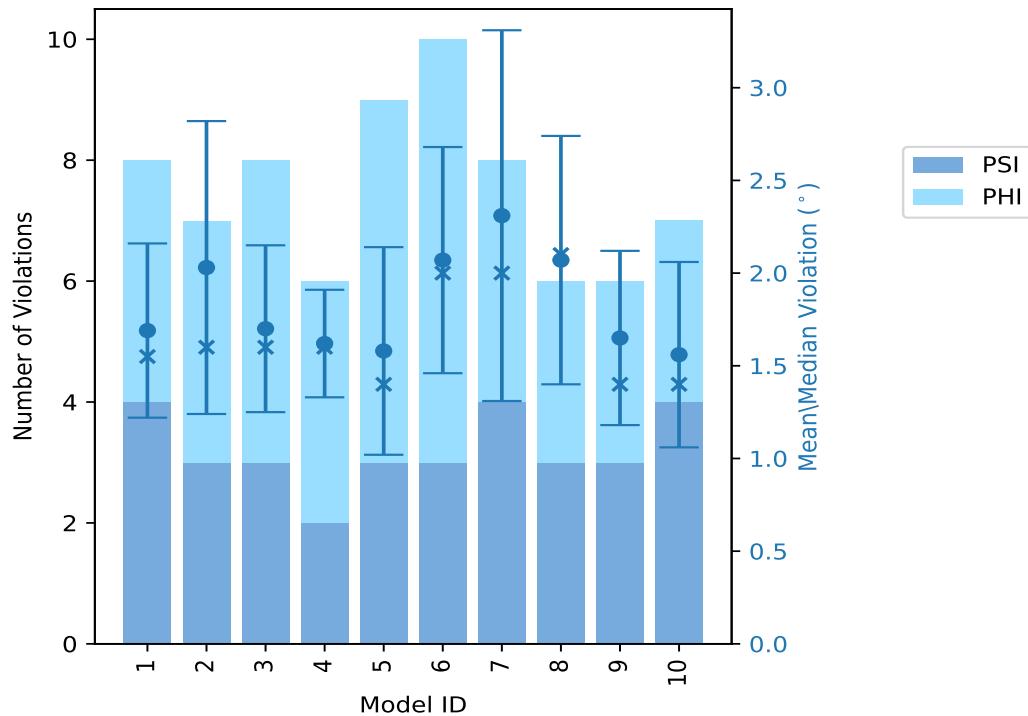
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble (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	
PSI	PHI	Total	Count[1]	%
1	0	1	1	10.0
3	1	4	2	20.0
0	2	2	3	30.0
0	0	0	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
1	1	2	7	70.0
1	0	1	8	80.0
0	2	2	9	90.0
1	1	2	10	100.0

[1] Number of models with violations

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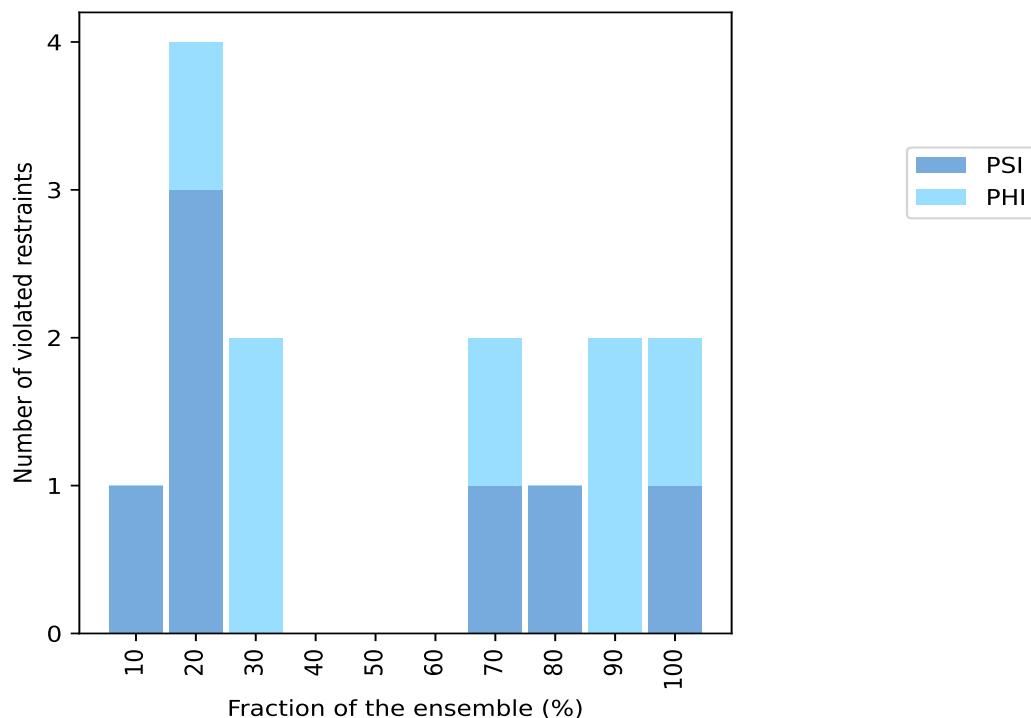
10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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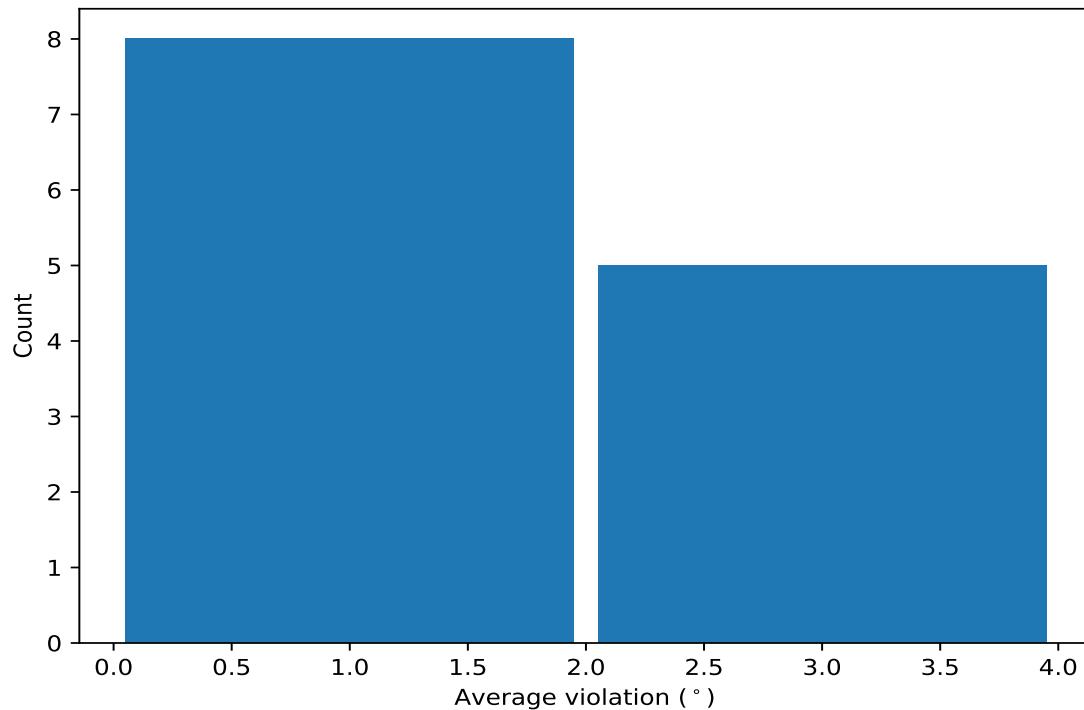
10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	10	2.44	0.5	2.65
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	10	2.26	0.62	2.2
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	9	1.68	0.47	1.6
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	9	1.33	0.24	1.3
(1,117)	2:B:879:LEU:N	2:B:879:LEU:CA	2:B:879:LEU:C	2:B:880:PRO:N	8	1.59	0.34	1.5
(1,129)	2:B:885:LEU:N	2:B:885:LEU:CA	2:B:885:LEU:C	2:B:886:ALA:N	7	1.57	0.4	1.5
(1,3)	1:A:502:ALA:C	1:A:503:TYR:N	1:A:503:TYR:CA	1:A:503:TYR:C	7	1.53	0.33	1.5
(1,82)	1:A:546:ASP:C	1:A:547:LEU:N	1:A:547:LEU:CA	1:A:547:LEU:C	3	2.03	1.11	1.4
(1,11)	1:A:506:GLU:C	1:A:507:LEU:N	1:A:507:LEU:CA	1:A:507:LEU:C	3	1.6	0.14	1.5
(1,55)	1:A:530:ILE:N	1:A:530:ILE:CA	1:A:530:ILE:C	1:A:531:GLU:N	2	2.3	0.0	2.3
(1,31)	1:A:516:THR:C	1:A:517:LEU:N	1:A:517:LEU:CA	1:A:517:LEU:C	2	2.05	0.25	2.05
(1,121)	2:B:881:VAL:N	2:B:881:VAL:CA	2:B:881:VAL:C	2:B:882:SER:N	2	1.5	0.2	1.5
(1,49)	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	1:A:528:ASN:N	2	1.1	0.0	1.1

[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.
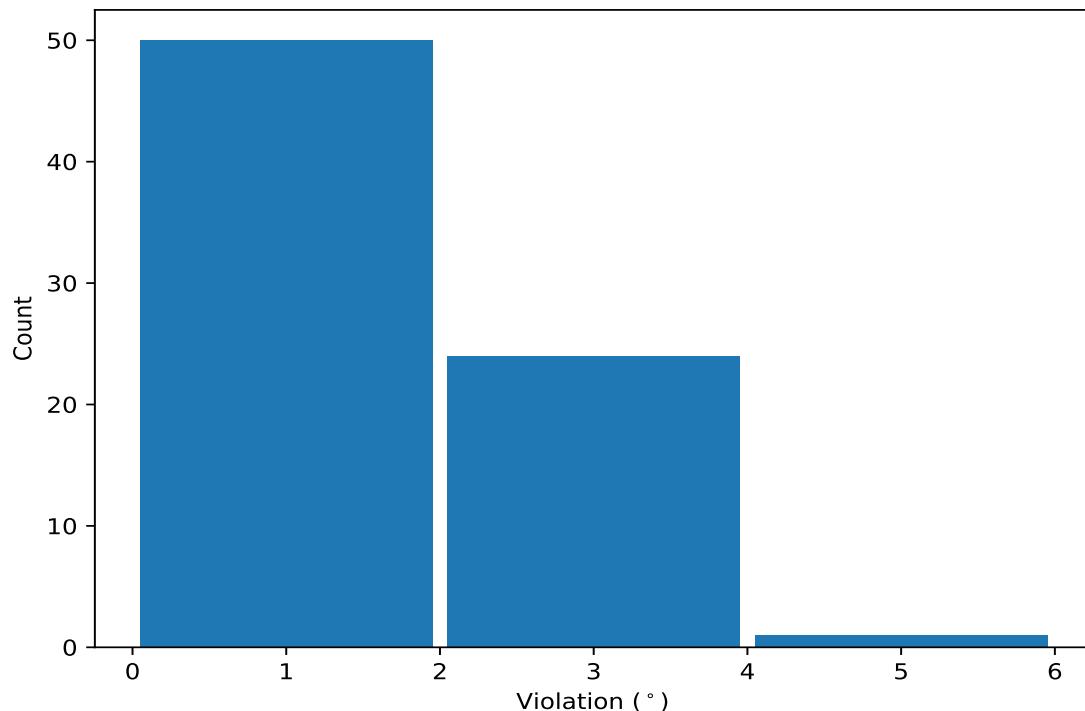
10.5.2　Table: All violated dihedral-angle restraints ⓘ

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 (°)
(1,139)	2:B:890:LEU:N	2:B:890:LEU:CA	2:B:890:LEU:C	2:B:891:PRO:N	7	4.3
(1,82)	1:A:546:ASP:C	1:A:547:LEU:N	1:A:547:LEU:CA	1:A:547:LEU:C	6	3.6
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	2	3.2
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	7	3.1
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	7	3.0
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	8	3.0
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	2	2.9
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	5	2.9
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	3	2.7
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	8	2.7
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	2	2.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	10	2.6
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	1	2.5
(1,117)	2:B:879:LEU:N	2:B:879:LEU:CA	2:B:879:LEU:C	2:B:880:PRO:N	9	2.4
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	6	2.3
(1,55)	1:A:530:ILE:N	1:A:530:ILE:CA	1:A:530:ILE:C	1:A:531:GLU:N	1	2.3
(1,55)	1:A:530:ILE:N	1:A:530:ILE:CA	1:A:530:ILE:C	1:A:531:GLU:N	6	2.3
(1,31)	1:A:516:THR:C	1:A:517:LEU:N	1:A:517:LEU:CA	1:A:517:LEU:C	6	2.3
(1,129)	2:B:885:LEU:N	2:B:885:LEU:CA	2:B:885:LEU:C	2:B:886:ALA:N	8	2.3
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	7	2.2
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	9	2.2
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	4	2.1
(1,3)	1:A:502:ALA:C	1:A:503:TYR:N	1:A:503:TYR:CA	1:A:503:TYR:C	6	2.1
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	3	2.0
(1,129)	2:B:885:LEU:N	2:B:885:LEU:CA	2:B:885:LEU:C	2:B:886:ALA:N	5	2.0
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	8	1.9
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	1	1.9
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	6	1.9
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	4	1.8
(1,31)	1:A:516:THR:C	1:A:517:LEU:N	1:A:517:LEU:CA	1:A:517:LEU:C	5	1.8
(1,3)	1:A:502:ALA:C	1:A:503:TYR:N	1:A:503:TYR:CA	1:A:503:TYR:C	10	1.8
(1,11)	1:A:506:GLU:C	1:A:507:LEU:N	1:A:507:LEU:CA	1:A:507:LEU:C	7	1.8
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	4	1.7
(1,48)	1:A:526:ILE:C	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	6	1.7
(1,3)	1:A:502:ALA:C	1:A:503:TYR:N	1:A:503:TYR:CA	1:A:503:TYR:C	3	1.7
(1,121)	2:B:881:VAL:N	2:B:881:VAL:CA	2:B:881:VAL:C	2:B:882:SER:N	10	1.7
(1,117)	2:B:879:LEU:N	2:B:879:LEU:CA	2:B:879:LEU:C	2:B:880:PRO:N	3	1.7
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	1	1.6
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	5	1.6
(1,117)	2:B:879:LEU:N	2:B:879:LEU:CA	2:B:879:LEU:C	2:B:880:PRO:N	2	1.6
(1,117)	2:B:879:LEU:N	2:B:879:LEU:CA	2:B:879:LEU:C	2:B:880:PRO:N	6	1.6
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	9	1.5
(1,3)	1:A:502:ALA:C	1:A:503:TYR:N	1:A:503:TYR:CA	1:A:503:TYR:C	4	1.5
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	3	1.5
(1,129)	2:B:885:LEU:N	2:B:885:LEU:CA	2:B:885:LEU:C	2:B:886:ALA:N	2	1.5
(1,129)	2:B:885:LEU:N	2:B:885:LEU:CA	2:B:885:LEU:C	2:B:886:ALA:N	3	1.5
(1,11)	1:A:506:GLU:C	1:A:507:LEU:N	1:A:507:LEU:CA	1:A:507:LEU:C	1	1.5
(1,11)	1:A:506:GLU:C	1:A:507:LEU:N	1:A:507:LEU:CA	1:A:507:LEU:C	6	1.5
(1,82)	1:A:546:ASP:C	1:A:547:LEU:N	1:A:547:LEU:CA	1:A:547:LEU:C	3	1.4
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	6	1.4
(1,71)	1:A:541:THR:N	1:A:541:THR:CA	1:A:541:THR:C	1:A:542:THR:N	10	1.4
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	5	1.4
(1,129)	2:B:885:LEU:N	2:B:885:LEU:CA	2:B:885:LEU:C	2:B:886:ALA:N	7	1.4
(1,117)	2:B:879:LEU:N	2:B:879:LEU:CA	2:B:879:LEU:C	2:B:880:PRO:N	1	1.4
(1,117)	2:B:879:LEU:N	2:B:879:LEU:CA	2:B:879:LEU:C	2:B:880:PRO:N	4	1.4
(1,117)	2:B:879:LEU:N	2:B:879:LEU:CA	2:B:879:LEU:C	2:B:880:PRO:N	7	1.4
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	9	1.3
(1,3)	1:A:502:ALA:C	1:A:503:TYR:N	1:A:503:TYR:CA	1:A:503:TYR:C	2	1.3
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	7	1.3
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	9	1.3
(1,121)	2:B:881:VAL:N	2:B:881:VAL:CA	2:B:881:VAL:C	2:B:882:SER:N	8	1.3
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	5	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,3)	1:A:502:ALA:C	1:A:503:TYR:N	1:A:503:TYR:CA	1:A:503:TYR:C	8	1.2
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	1	1.2
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	4	1.2
(1,129)	2:B:885:LEU:N	2:B:885:LEU:CA	2:B:885:LEU:C	2:B:886:ALA:N	9	1.2
(1,117)	2:B:879:LEU:N	2:B:879:LEU:CA	2:B:879:LEU:C	2:B:880:PRO:N	10	1.2
(1,82)	1:A:546:ASP:C	1:A:547:LEU:N	1:A:547:LEU:CA	1:A:547:LEU:C	5	1.1
(1,72)	1:A:541:THR:C	1:A:542:THR:N	1:A:542:THR:CA	1:A:542:THR:C	3	1.1
(1,49)	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	1:A:528:ASN:N	1	1.1
(1,49)	1:A:527:VAL:N	1:A:527:VAL:CA	1:A:527:VAL:C	1:A:528:ASN:N	5	1.1
(1,3)	1:A:502:ALA:C	1:A:503:TYR:N	1:A:503:TYR:CA	1:A:503:TYR:C	5	1.1
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	2	1.1
(1,136)	2:B:888:VAL:C	2:B:889:VAL:N	2:B:889:VAL:CA	2:B:889:VAL:C	10	1.1
(1,129)	2:B:885:LEU:N	2:B:885:LEU:CA	2:B:885:LEU:C	2:B:886:ALA:N	10	1.1