W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB NMR Structure Validation Report (i)

Dec 24, 2024 – 03:15 PM EST

PDB ID	:	2LCW
BMRB ID	:	17635
Title	:	solution structure of FUS/TLS RRM domain
Authors	:	Liu, X.; Ren, J.; Niu, C.; Gong, W.; Feng, W.
Deposited on	:	2011-05-10

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

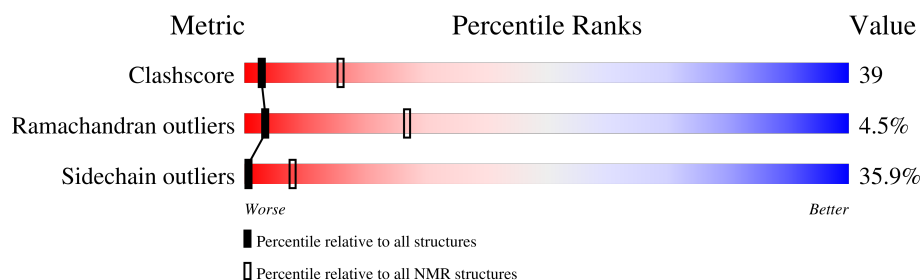|		
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 91%.

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		39
Ramachandran outliers		4.5%
Sidechain outliers		35.9%

Worse *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	116	20%　34%　12%　28%　7%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

2　Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:284-A:325,　A:335-A:368 (76)	0.57	17

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 4 clusters. No single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 1626 atoms, of which 799 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA-binding protein FUS.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	108	1626	513	799	146	167	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	expression tag	UNP P35637
A	387	GLU	-	expression tag	UNP P35637
A	388	HIS	-	expression tag	UNP P35637
A	389	HIS	-	expression tag	UNP P35637
A	390	HIS	-	expression tag	UNP P35637
A	391	HIS	-	expression tag	UNP P35637
A	392	HIS	-	expression tag	UNP P35637
A	393	HIS	-	expression tag	UNP P35637

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: RNA-binding protein FUS
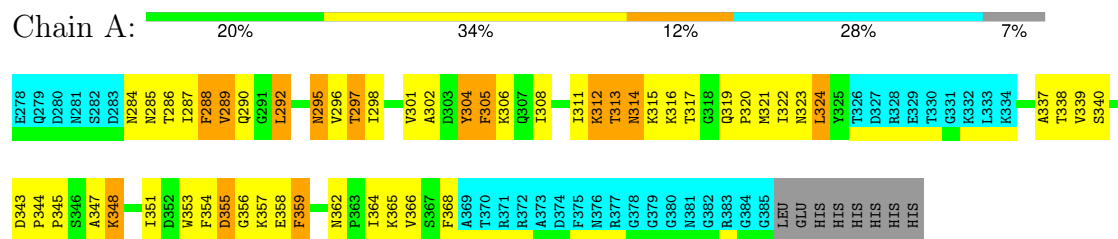
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: RNA-binding protein FUS
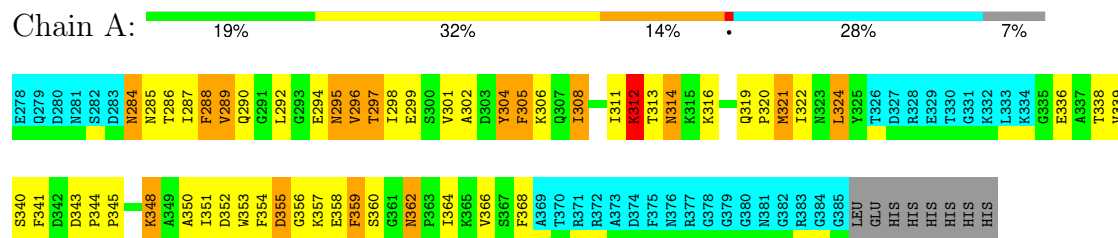
4.2.2 Score per residue for model 2

• Molecule 1: RNA-binding protein FUS

4.2.3 Score per residue for model 3

• Molecule 1: RNA-binding protein FUS

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: RNA-binding protein FUS

Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: RNA-binding protein FUS

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: RNA-binding protein FUS

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: RNA-binding protein FUS

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: RNA-binding protein FUS

Chain A:
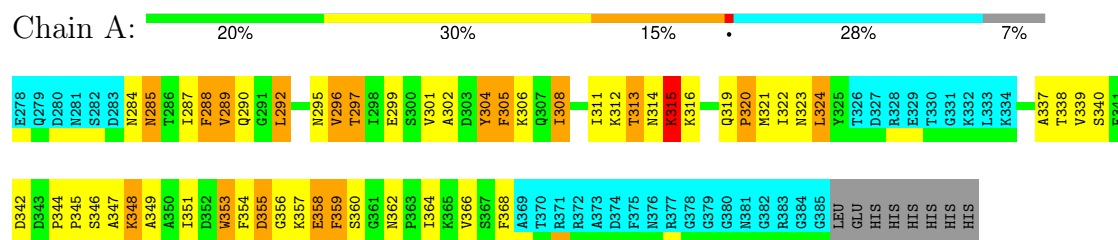
4.2.9 Score per residue for model 9

• Molecule 1: RNA-binding protein FUS

Chain A:
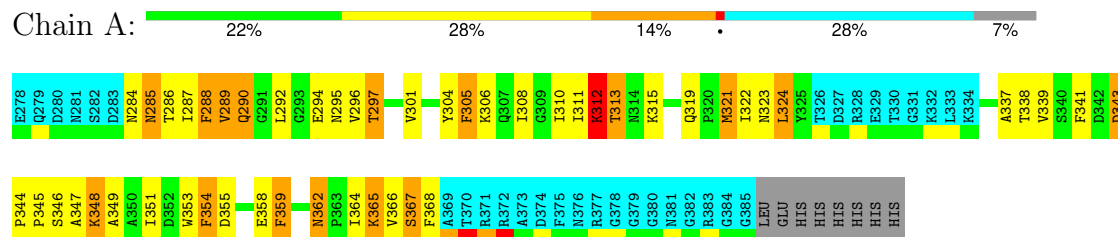
4.2.10 Score per residue for model 10

• Molecule 1: RNA-binding protein FUS
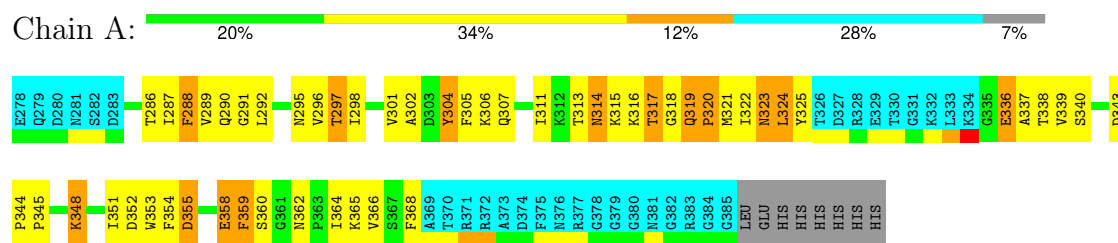
4.2.11 Score per residue for model 11

• Molecule 1: RNA-binding protein FUS
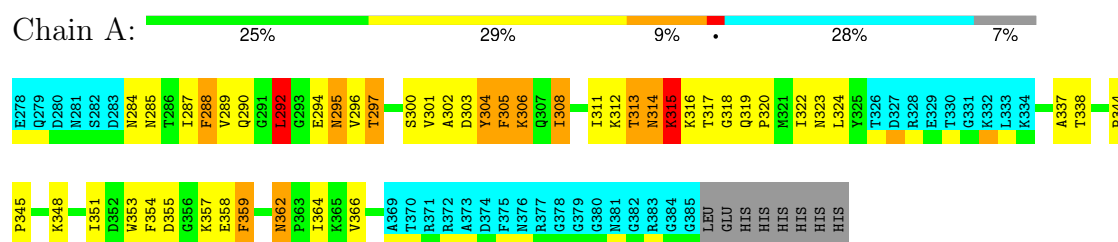
4.2.12 Score per residue for model 12

• Molecule 1: RNA-binding protein FUS
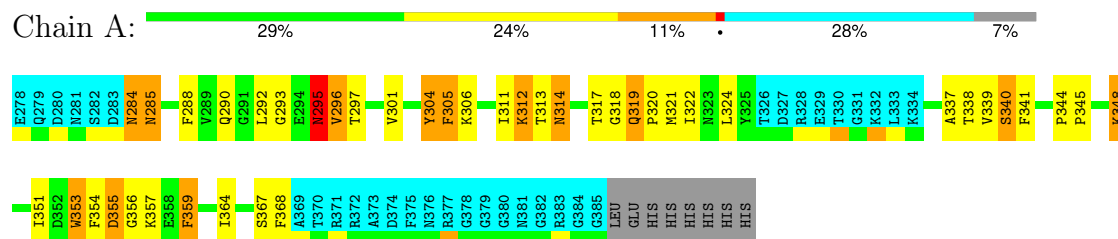
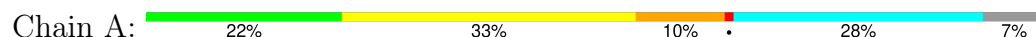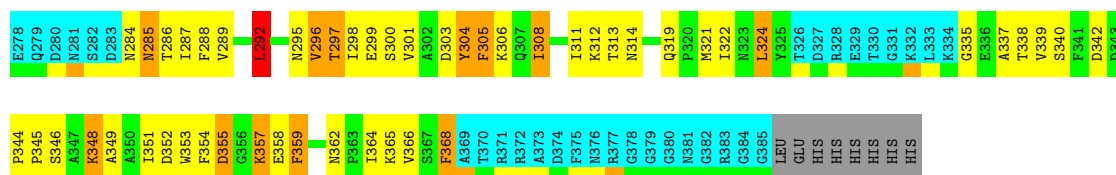### 4.2.13 Score per residue for model 13

• Molecule 1: RNA-binding protein FUS
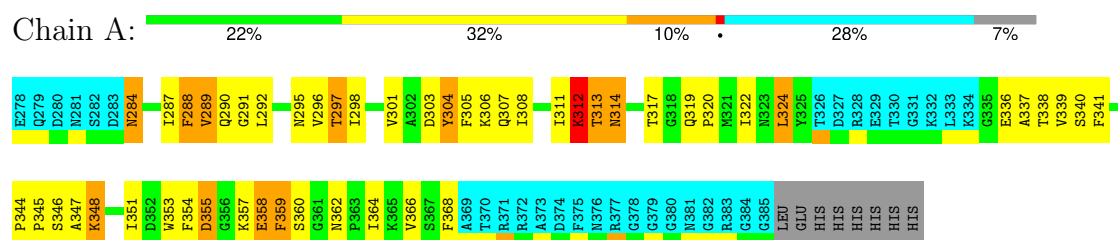
4.2.14 Score per residue for model 14

• Molecule 1: RNA-binding protein FUS

Chain A:
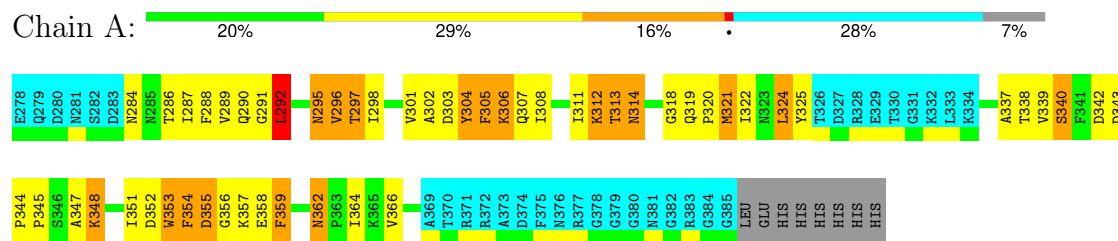
4.2.15 Score per residue for model 15

• Molecule 1: RNA-binding protein FUS

Chain A:
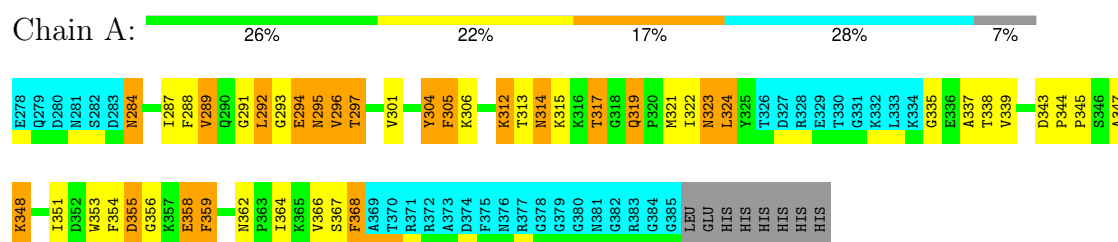
4.2.16 Score per residue for model 16

• Molecule 1: RNA-binding protein FUS

Chain A:
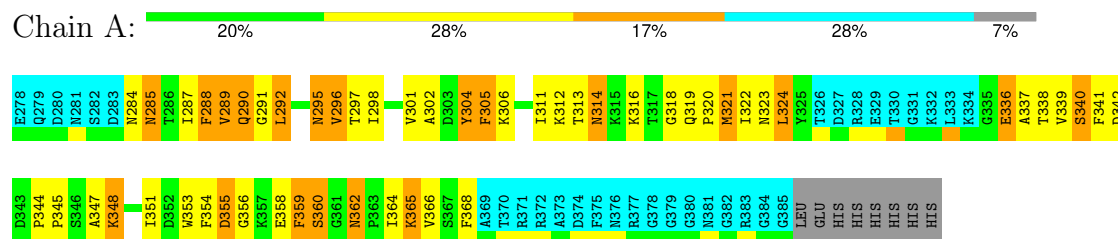
4.2.17 Score per residue for model 17 (medoid)

• Molecule 1: RNA-binding protein FUS

Chain A:
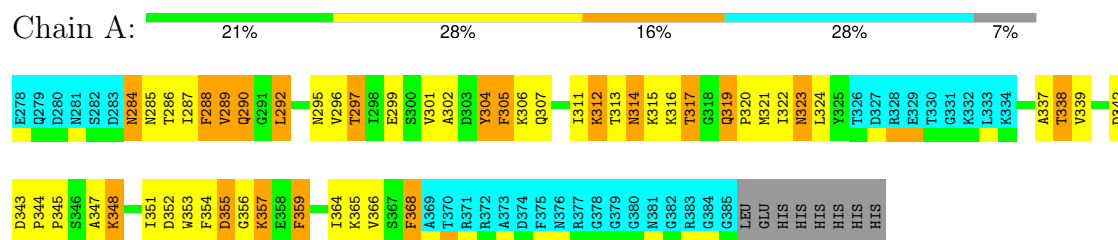
4.2.18 Score per residue for model 18

• Molecule 1: RNA-binding protein FUS

Chain A:
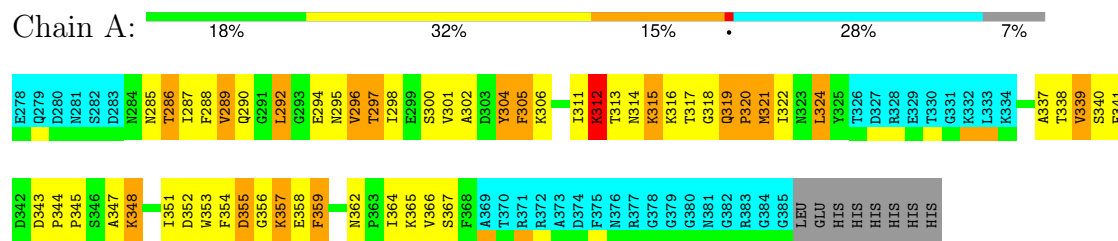
4.2.19 Score per residue for model 19

• Molecule 1: RNA-binding protein FUS

Chain A:

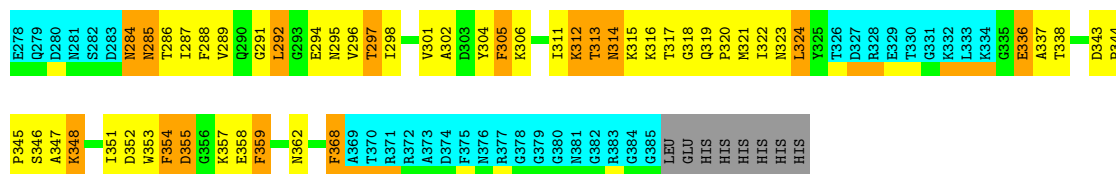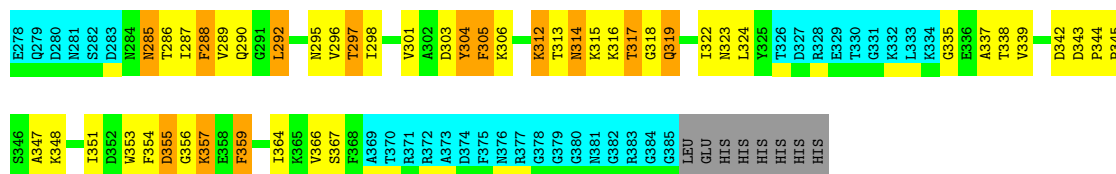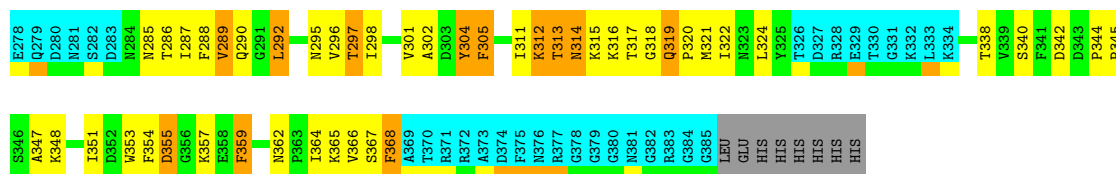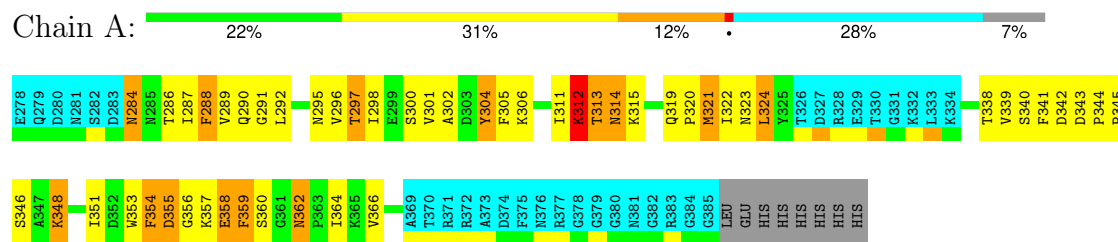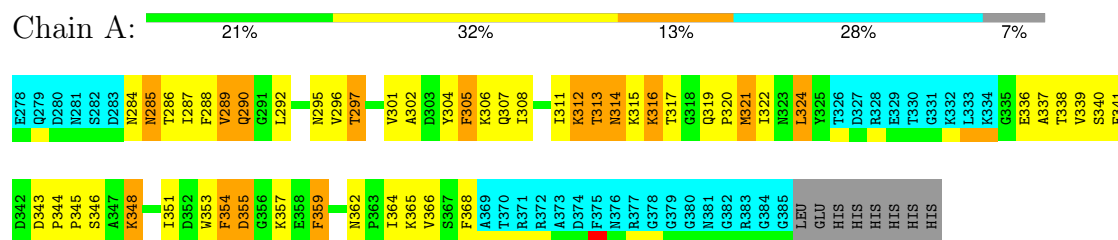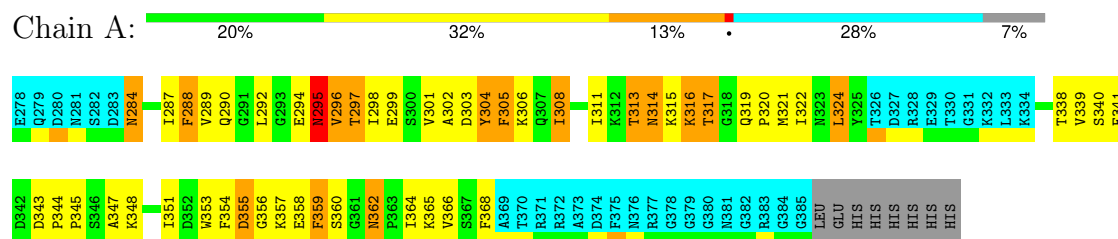### 4.2.20 Score per residue for model 20

• Molecule 1: RNA-binding protein FUS

Chain A:
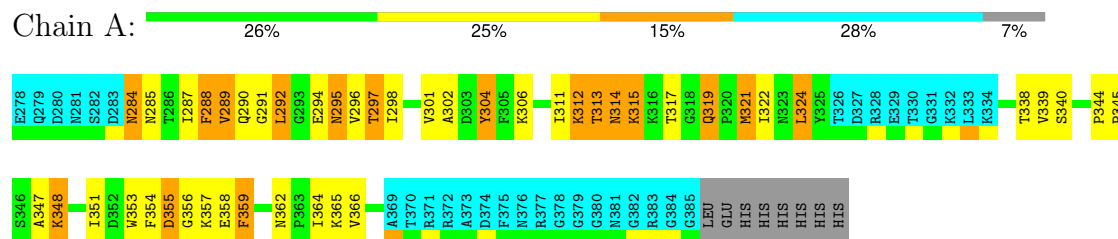
5 Refinement protocol and experimental data overview ⓘ

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy and the least restraint violations*.

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

Software name	Classification	Version
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1220
Number of shifts mapped to atoms	1220
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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	587	575	575	46±7
All	All	11740	11500	11500	910

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:296:VAL:HG22	1:A:324:LEU:HD23	1.05	1.24	10	1
1:A:296:VAL:HG12	1:A:324:LEU:HD23	0.91	1.35	3	1
1:A:287:ILE:HD12	1:A:366:VAL:HG13	0.84	1.48	7	12
1:A:297:THR:O	1:A:301:VAL:HG23	0.80	1.76	9	20
1:A:311:ILE:HG23	1:A:340:SER:O	0.79	1.78	16	12
1:A:289:VAL:HG13	1:A:366:VAL:HG22	0.79	1.54	13	8
1:A:316:LYS:HD3	1:A:317:THR:HG23	0.79	1.53	7	1
1:A:348:LYS:HA	1:A:351:ILE:HD12	0.78	1.56	3	20
1:A:305:PHE:CD2	1:A:339:VAL:HG21	0.78	2.14	18	2
1:A:292:LEU:HD12	1:A:295:ASN:ND2	0.78	1.94	12	1
1:A:296:VAL:HG12	1:A:324:LEU:HD22	0.75	1.56	6	2
1:A:292:LEU:HD21	1:A:359:PHE:CE2	0.75	2.16	13	1
1:A:301:VAL:HG11	1:A:339:VAL:CG2	0.75	2.12	1	9
1:A:285:ASN:O	1:A:347:ALA:HB2	0.75	1.82	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:ILE:HD11	1:A:324:LEU:HD11	0.75	1.56	3	4
1:A:296:VAL:O	1:A:324:LEU:HD13	0.75	1.82	4	3
1:A:287:ILE:HD12	1:A:366:VAL:CG1	0.74	2.12	5	10
1:A:291:GLY:C	1:A:292:LEU:HD13	0.74	2.02	3	2
1:A:287:ILE:HD11	1:A:305:PHE:CE2	0.73	2.18	2	3
1:A:291:GLY:O	1:A:364:ILE:HG22	0.73	1.83	10	6
1:A:322:ILE:HG23	1:A:338:THR:O	0.73	1.83	4	10
1:A:314:ASN:ND2	1:A:317:THR:OG1	0.72	2.23	12	2
1:A:292:LEU:HD21	1:A:336:GLU:HA	0.72	1.59	3	1
1:A:298:ILE:CD1	1:A:324:LEU:HD11	0.72	2.15	1	4
1:A:292:LEU:HD12	1:A:296:VAL:HG22	0.72	1.60	6	3
1:A:305:PHE:O	1:A:311:ILE:HD11	0.70	1.85	17	4
1:A:324:LEU:HD23	1:A:337:ALA:CB	0.70	2.16	18	4
1:A:292:LEU:HD22	1:A:359:PHE:CD2	0.70	2.20	15	3
1:A:358:GLU:HA	1:A:362:ASN:O	0.69	1.87	10	15
1:A:296:VAL:HG12	1:A:296:VAL:O	0.69	1.85	19	3
1:A:288:PHE:CE1	1:A:338:THR:HG22	0.68	2.23	16	6
1:A:287:ILE:HD12	1:A:366:VAL:HG11	0.68	1.64	18	2
1:A:351:ILE:HD13	1:A:368:PHE:CE1	0.68	2.24	9	1
1:A:289:VAL:CG1	1:A:364:ILE:HD12	0.67	2.20	9	3
1:A:322:ILE:HG12	1:A:339:VAL:HG23	0.67	1.66	18	1
1:A:288:PHE:CD1	1:A:338:THR:HG22	0.66	2.26	10	9
1:A:316:LYS:CD	1:A:317:THR:HG23	0.66	2.19	7	1
1:A:305:PHE:HB3	1:A:311:ILE:HD11	0.66	1.67	3	3
1:A:323:ASN:O	1:A:337:ALA:HB1	0.66	1.90	11	8
1:A:351:ILE:HG23	1:A:366:VAL:O	0.66	1.90	13	1
1:A:287:ILE:CG2	1:A:347:ALA:HB1	0.65	2.21	5	6
1:A:296:VAL:CG1	1:A:324:LEU:HD22	0.65	2.22	6	3
1:A:292:LEU:CD2	1:A:292:LEU:N	0.65	2.60	14	1
1:A:322:ILE:HG12	1:A:339:VAL:HG22	0.64	1.69	9	9
1:A:354:PHE:HB3	1:A:364:ILE:HD11	0.63	1.69	15	1
1:A:314:ASN:HD21	1:A:317:THR:HG23	0.62	1.54	3	2
1:A:301:VAL:HG11	1:A:339:VAL:HG21	0.61	1.72	10	3
1:A:296:VAL:CG1	1:A:337:ALA:HB2	0.61	2.25	3	2
1:A:354:PHE:O	1:A:356:GLY:N	0.61	2.34	12	10
1:A:292:LEU:HD12	1:A:359:PHE:CD2	0.61	2.30	3	3
1:A:292:LEU:HD13	1:A:292:LEU:N	0.61	2.10	16	3
1:A:354:PHE:HB2	1:A:366:VAL:HG21	0.61	1.72	8	10
1:A:353:TRP:CD1	1:A:353:TRP:C	0.61	2.74	12	20
1:A:296:VAL:HG13	1:A:324:LEU:HD22	0.60	1.72	18	1
1:A:302:ALA:HA	1:A:311:ILE:HD13	0.60	1.73	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:ILE:HD13	1:A:324:LEU:HD21	0.60	1.73	13	1
1:A:298:ILE:HD12	1:A:298:ILE:N	0.60	2.11	19	1
1:A:288:PHE:CD1	1:A:288:PHE:O	0.60	2.55	4	4
1:A:314:ASN:OD1	1:A:317:THR:OG1	0.60	2.19	13	1
1:A:296:VAL:HG22	1:A:324:LEU:HD13	0.60	1.74	12	1
1:A:288:PHE:CZ	1:A:338:THR:HG21	0.59	2.32	3	5
1:A:296:VAL:HG13	1:A:296:VAL:O	0.59	1.97	1	9
1:A:359:PHE:CD1	1:A:364:ILE:HG21	0.59	2.33	8	2
1:A:313:THR:HA	1:A:320:PRO:HA	0.59	1.74	19	8
1:A:289:VAL:HG13	1:A:366:VAL:CG2	0.59	2.26	13	2
1:A:298:ILE:HG23	1:A:322:ILE:HD12	0.59	1.74	10	6
1:A:313:THR:HG23	1:A:319:GLN:C	0.58	2.18	15	4
1:A:324:LEU:HD23	1:A:337:ALA:HB1	0.58	1.74	17	5
1:A:298:ILE:HG23	1:A:322:ILE:HB	0.58	1.75	4	3
1:A:314:ASN:OD1	1:A:321:MET:CG	0.58	2.52	6	7
1:A:301:VAL:HG11	1:A:339:VAL:HG22	0.58	1.74	2	4
1:A:358:GLU:CA	1:A:362:ASN:O	0.57	2.51	10	12
1:A:292:LEU:CB	1:A:296:VAL:HG22	0.57	2.29	7	1
1:A:298:ILE:HD12	1:A:324:LEU:HD21	0.57	1.75	19	1
1:A:351:ILE:HD13	1:A:368:PHE:CD2	0.57	2.35	5	1
1:A:296:VAL:CG2	1:A:337:ALA:HB2	0.57	2.30	8	2
1:A:287:ILE:HD11	1:A:305:PHE:CZ	0.57	2.35	5	3
1:A:288:PHE:CD2	1:A:338:THR:HG22	0.57	2.35	5	1
1:A:359:PHE:HD2	1:A:364:ILE:HG21	0.56	1.60	6	3
1:A:292:LEU:HD22	1:A:292:LEU:N	0.56	2.15	3	2
1:A:324:LEU:HD12	1:A:324:LEU:N	0.56	2.15	16	3
1:A:353:TRP:CD1	1:A:354:PHE:CD1	0.56	2.93	3	5
1:A:292:LEU:HD12	1:A:295:ASN:HD21	0.56	1.61	12	1
1:A:354:PHE:O	1:A:355:ASP:C	0.56	2.44	1	19
1:A:292:LEU:HD22	1:A:292:LEU:H	0.56	1.61	3	2
1:A:292:LEU:HD22	1:A:296:VAL:CB	0.56	2.30	13	1
1:A:351:ILE:HD11	1:A:368:PHE:CD1	0.56	2.36	15	1
1:A:359:PHE:N	1:A:362:ASN:O	0.56	2.38	3	15
1:A:305:PHE:CZ	1:A:354:PHE:CE2	0.56	2.94	8	6
1:A:292:LEU:HD12	1:A:292:LEU:N	0.56	2.16	19	1
1:A:359:PHE:HB2	1:A:364:ILE:HD13	0.56	1.76	18	1
1:A:296:VAL:O	1:A:297:THR:HG23	0.56	2.01	12	3
1:A:308:ILE:HG23	1:A:341:PHE:CE2	0.55	2.36	19	2
1:A:296:VAL:HG22	1:A:324:LEU:HD22	0.55	1.77	14	1
1:A:292:LEU:HD22	1:A:335:GLY:O	0.55	2.00	2	2
1:A:284:ASN:OD1	1:A:368:PHE:CD1	0.55	2.59	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:351:ILE:CD1	1:A:368:PHE:CE1	0.55	2.89	7	4
1:A:324:LEU:N	1:A:324:LEU:HD23	0.55	2.17	2	2
1:A:302:ALA:HB1	1:A:320:PRO:HG2	0.55	1.77	1	5
1:A:292:LEU:HD22	1:A:296:VAL:HB	0.55	1.78	13	1
1:A:311:ILE:HD13	1:A:339:VAL:CG1	0.55	2.31	19	1
1:A:344:PRO:N	1:A:345:PRO:HD2	0.54	2.17	4	20
1:A:304:TYR:CE1	1:A:359:PHE:CZ	0.54	2.95	16	12
1:A:314:ASN:ND2	1:A:319:GLN:O	0.54	2.41	15	2
1:A:301:VAL:O	1:A:305:PHE:HB2	0.54	2.01	12	15
1:A:302:ALA:HA	1:A:311:ILE:HD12	0.54	1.78	14	2
1:A:289:VAL:HG13	1:A:364:ILE:HD12	0.54	1.79	9	2
1:A:288:PHE:HD1	1:A:338:THR:HG22	0.54	1.63	12	1
1:A:354:PHE:CB	1:A:366:VAL:HG21	0.54	2.33	8	5
1:A:351:ILE:O	1:A:355:ASP:CB	0.54	2.56	11	8
1:A:291:GLY:C	1:A:292:LEU:HD23	0.54	2.23	15	1
1:A:304:TYR:CZ	1:A:305:PHE:CD1	0.53	2.97	15	4
1:A:353:TRP:CE3	1:A:354:PHE:CZ	0.53	2.96	2	6
1:A:312:LYS:O	1:A:321:MET:N	0.53	2.41	18	8
1:A:304:TYR:CZ	1:A:305:PHE:CE1	0.53	2.97	2	3
1:A:353:TRP:CZ3	1:A:354:PHE:CZ	0.53	2.96	8	5
1:A:305:PHE:CZ	1:A:354:PHE:CD2	0.53	2.95	11	3
1:A:305:PHE:CE1	1:A:354:PHE:CE2	0.53	2.97	1	10
1:A:308:ILE:HG21	1:A:354:PHE:CE2	0.53	2.39	11	1
1:A:301:VAL:CG1	1:A:339:VAL:HG21	0.53	2.34	13	5
1:A:315:LYS:N	1:A:315:LYS:HD2	0.53	2.19	11	1
1:A:305:PHE:CE1	1:A:354:PHE:CZ	0.53	2.96	12	2
1:A:304:TYR:CE2	1:A:359:PHE:CZ	0.53	2.97	20	2
1:A:292:LEU:N	1:A:292:LEU:HD23	0.52	2.19	20	1
1:A:314:ASN:OD1	1:A:318:GLY:N	0.52	2.42	18	1
1:A:288:PHE:CE1	1:A:338:THR:HG21	0.52	2.40	3	3
1:A:351:ILE:O	1:A:355:ASP:HB3	0.52	2.04	9	9
1:A:353:TRP:CD1	1:A:354:PHE:CD2	0.52	2.97	9	1
1:A:304:TYR:CZ	1:A:359:PHE:CE2	0.52	2.98	17	2
1:A:295:ASN:O	1:A:296:VAL:C	0.52	2.48	2	4
1:A:289:VAL:HG12	1:A:364:ILE:HB	0.52	1.80	13	2
1:A:288:PHE:CE2	1:A:367:SER:CB	0.52	2.93	9	1
1:A:301:VAL:HB	1:A:322:ILE:HD13	0.52	1.81	16	3
1:A:308:ILE:HD11	1:A:349:ALA:O	0.52	2.05	9	3
1:A:314:ASN:O	1:A:318:GLY:N	0.52	2.40	11	8
1:A:287:ILE:HG23	1:A:347:ALA:HB1	0.52	1.81	15	3
1:A:292:LEU:CD1	1:A:296:VAL:HG13	0.52	2.35	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:296:VAL:CG2	1:A:324:LEU:HD23	0.51	2.16	10	1
1:A:298:ILE:HG21	1:A:319:GLN:HE22	0.51	1.65	19	1
1:A:304:TYR:CE1	1:A:305:PHE:CD2	0.51	2.98	6	2
1:A:295:ASN:O	1:A:295:ASN:CG	0.51	2.47	20	1
1:A:305:PHE:CE1	1:A:354:PHE:CE1	0.51	2.98	9	1
1:A:304:TYR:CE1	1:A:305:PHE:CD1	0.51	2.99	2	3
1:A:314:ASN:HB3	1:A:317:THR:OG1	0.50	2.06	11	1
1:A:321:MET:O	1:A:340:SER:OG	0.50	2.29	18	2
1:A:298:ILE:N	1:A:298:ILE:CD1	0.50	2.74	19	1
1:A:288:PHE:HD2	1:A:338:THR:HG22	0.50	1.65	5	1
1:A:311:ILE:HD13	1:A:339:VAL:HG13	0.50	1.83	19	1
1:A:304:TYR:CE1	1:A:359:PHE:CE2	0.50	2.99	2	4
1:A:289:VAL:HA	1:A:365:LYS:O	0.50	2.07	16	1
1:A:292:LEU:HD23	1:A:295:ASN:HD21	0.50	1.66	19	1
1:A:290:GLN:O	1:A:364:ILE:HA	0.50	2.06	6	5
1:A:292:LEU:HD22	1:A:359:PHE:HD2	0.49	1.66	18	1
1:A:311:ILE:HB	1:A:320:PRO:HB3	0.49	1.84	19	6
1:A:292:LEU:HD12	1:A:359:PHE:HD2	0.49	1.66	3	2
1:A:304:TYR:CE2	1:A:305:PHE:CE1	0.49	3.01	11	1
1:A:359:PHE:CD2	1:A:364:ILE:HG21	0.49	2.43	1	6
1:A:287:ILE:CD1	1:A:305:PHE:CZ	0.49	2.96	19	7
1:A:284:ASN:O	1:A:285:ASN:ND2	0.49	2.45	2	1
1:A:301:VAL:HG22	1:A:359:PHE:HZ	0.49	1.68	14	2
1:A:313:THR:HA	1:A:320:PRO:CA	0.49	2.36	19	1
1:A:314:ASN:ND2	1:A:317:THR:HG23	0.49	2.21	3	1
1:A:284:ASN:ND2	1:A:368:PHE:CD1	0.49	2.80	17	2
1:A:285:ASN:HA	1:A:347:ALA:HB2	0.48	1.84	4	2
1:A:296:VAL:HG22	1:A:324:LEU:CD2	0.48	2.38	15	1
1:A:288:PHE:CD2	1:A:290:GLN:OE1	0.48	2.66	4	3
1:A:314:ASN:OD1	1:A:316:LYS:HB2	0.48	2.08	19	1
1:A:288:PHE:CE1	1:A:338:THR:CG2	0.48	2.96	14	9
1:A:351:ILE:O	1:A:355:ASP:HB2	0.48	2.07	2	7
1:A:348:LYS:CD	1:A:348:LYS:C	0.48	2.82	16	3
1:A:287:ILE:HD13	1:A:341:PHE:HE2	0.48	1.67	6	1
1:A:319:GLN:HG2	1:A:320:PRO:N	0.48	2.22	18	2
1:A:296:VAL:HG23	1:A:337:ALA:HB2	0.48	1.86	8	1
1:A:287:ILE:HG12	1:A:339:VAL:HG12	0.48	1.86	18	1
1:A:317:THR:HG22	1:A:319:GLN:H	0.47	1.68	10	2
1:A:288:PHE:CE2	1:A:290:GLN:CG	0.47	2.97	13	1
1:A:317:THR:HG21	1:A:319:GLN:HG2	0.47	1.86	19	1
1:A:296:VAL:O	1:A:296:VAL:CG1	0.47	2.56	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:339:VAL:CG1	1:A:341:PHE:CE1	0.47	2.97	7	1
1:A:288:PHE:CZ	1:A:338:THR:CG2	0.47	2.98	15	4
1:A:343:ASP:OD1	1:A:343:ASP:N	0.47	2.48	9	1
1:A:289:VAL:CG2	1:A:339:VAL:HG23	0.47	2.40	1	2
1:A:314:ASN:OD1	1:A:319:GLN:O	0.47	2.32	17	1
1:A:347:ALA:HB3	1:A:368:PHE:CE1	0.47	2.44	3	2
1:A:351:ILE:HD13	1:A:368:PHE:CD1	0.47	2.45	9	1
1:A:289:VAL:HG22	1:A:366:VAL:HG22	0.47	1.85	11	1
1:A:285:ASN:ND2	1:A:341:PHE:CB	0.47	2.78	16	1
1:A:298:ILE:HD13	1:A:324:LEU:HD11	0.47	1.87	18	1
1:A:323:ASN:O	1:A:324:LEU:HD23	0.47	2.10	4	1
1:A:308:ILE:HD13	1:A:350:ALA:HA	0.47	1.87	1	1
1:A:301:VAL:O	1:A:305:PHE:CB	0.47	2.63	10	3
1:A:314:ASN:OD1	1:A:316:LYS:N	0.46	2.49	10	1
1:A:304:TYR:CZ	1:A:359:PHE:CZ	0.46	3.02	11	1
1:A:312:LYS:HB2	1:A:340:SER:CB	0.46	2.40	1	1
1:A:292:LEU:CD2	1:A:359:PHE:CE1	0.46	2.98	8	1
1:A:312:LYS:CE	1:A:341:PHE:O	0.46	2.64	9	1
1:A:290:GLN:N	1:A:290:GLN:CD	0.46	2.68	4	1
1:A:322:ILE:HG12	1:A:339:VAL:HG13	0.46	1.86	4	1
1:A:292:LEU:CD2	1:A:359:PHE:CD2	0.46	2.98	10	2
1:A:301:VAL:HG22	1:A:359:PHE:CZ	0.46	2.45	13	4
1:A:317:THR:OG1	1:A:319:GLN:HG3	0.46	2.11	20	2
1:A:295:ASN:ND2	1:A:295:ASN:C	0.46	2.68	15	1
1:A:359:PHE:HD1	1:A:364:ILE:HG21	0.46	1.68	8	2
1:A:356:GLY:HA2	1:A:364:ILE:O	0.46	2.11	6	2
1:A:313:THR:CA	1:A:320:PRO:HA	0.46	2.40	19	2
1:A:353:TRP:CZ2	1:A:354:PHE:CE1	0.45	3.04	8	1
1:A:311:ILE:CG2	1:A:320:PRO:CB	0.45	2.94	14	3
1:A:305:PHE:CE1	1:A:354:PHE:CD2	0.45	3.04	11	1
1:A:298:ILE:CD1	1:A:324:LEU:HD21	0.45	2.41	19	1
1:A:319:GLN:NE2	1:A:320:PRO:O	0.45	2.50	19	1
1:A:296:VAL:CG2	1:A:337:ALA:CB	0.45	2.95	2	1
1:A:292:LEU:CD2	1:A:359:PHE:CD1	0.45	2.98	8	1
1:A:351:ILE:CD1	1:A:368:PHE:CE2	0.45	2.99	16	1
1:A:287:ILE:HD13	1:A:341:PHE:CE2	0.45	2.47	18	2
1:A:284:ASN:ND2	1:A:368:PHE:CE1	0.45	2.84	2	1
1:A:354:PHE:HB3	1:A:357:LYS:HG2	0.45	1.89	17	3
1:A:292:LEU:CD1	1:A:359:PHE:CE2	0.45	3.00	7	1
1:A:324:LEU:HB3	1:A:337:ALA:HB2	0.44	1.88	2	1
1:A:314:ASN:O	1:A:315:LYS:CB	0.44	2.65	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:287:ILE:CD1	1:A:305:PHE:CE2	0.44	3.00	10	1
1:A:313:THR:HG23	1:A:319:GLN:CA	0.44	2.42	17	1
1:A:351:ILE:HD12	1:A:368:PHE:CE1	0.44	2.47	7	1
1:A:314:ASN:OD1	1:A:317:THR:N	0.44	2.44	10	1
1:A:285:ASN:N	1:A:285:ASN:ND2	0.44	2.63	12	1
1:A:292:LEU:N	1:A:292:LEU:HD22	0.44	2.25	14	1
1:A:292:LEU:HG	1:A:296:VAL:HG22	0.44	1.89	7	1
1:A:323:ASN:O	1:A:337:ALA:CB	0.44	2.66	8	3
1:A:292:LEU:HD13	1:A:295:ASN:ND2	0.44	2.28	11	1
1:A:288:PHE:CG	1:A:290:GLN:OE1	0.44	2.70	4	1
1:A:296:VAL:CG1	1:A:324:LEU:CB	0.44	2.96	6	2
1:A:351:ILE:CD1	1:A:368:PHE:CD1	0.44	3.00	15	1
1:A:296:VAL:HG13	1:A:324:LEU:CB	0.44	2.43	18	1
1:A:314:ASN:HB2	1:A:321:MET:CG	0.44	2.43	5	2
1:A:288:PHE:CD1	1:A:338:THR:CG2	0.44	3.00	7	1
1:A:298:ILE:HD12	1:A:322:ILE:O	0.44	2.12	16	1
1:A:353:TRP:CD1	1:A:357:LYS:HG3	0.44	2.47	11	1
1:A:302:ALA:O	1:A:306:LYS:HB3	0.44	2.13	14	1
1:A:296:VAL:CG2	1:A:337:ALA:HB3	0.43	2.43	2	1
1:A:294:GLU:O	1:A:294:GLU:HG3	0.43	2.13	3	1
1:A:354:PHE:CD2	1:A:357:LYS:HD3	0.43	2.48	12	1
1:A:288:PHE:CE2	1:A:367:SER:HB2	0.43	2.49	9	1
1:A:296:VAL:O	1:A:297:THR:CG2	0.43	2.67	16	1
1:A:324:LEU:HD23	1:A:337:ALA:HB2	0.43	1.86	18	1
1:A:284:ASN:OD1	1:A:368:PHE:CZ	0.43	2.71	3	1
1:A:314:ASN:OD1	1:A:321:MET:HG3	0.43	2.13	6	1
1:A:292:LEU:HD22	1:A:359:PHE:CE2	0.43	2.48	5	1
1:A:314:ASN:OD1	1:A:321:MET:CB	0.43	2.67	1	1
1:A:292:LEU:N	1:A:292:LEU:CD2	0.43	2.82	12	2
1:A:296:VAL:CG1	1:A:324:LEU:HD23	0.43	2.26	3	1
1:A:295:ASN:ND2	1:A:296:VAL:N	0.43	2.67	16	1
1:A:288:PHE:CE2	1:A:367:SER:HB3	0.43	2.48	9	1
1:A:304:TYR:OH	1:A:364:ILE:HD13	0.42	2.13	1	1
1:A:292:LEU:N	1:A:292:LEU:CD1	0.42	2.82	19	1
1:A:354:PHE:HB2	1:A:366:VAL:CG2	0.42	2.43	8	1
1:A:359:PHE:HB2	1:A:364:ILE:CG2	0.42	2.44	9	1
1:A:292:LEU:HD12	1:A:296:VAL:HG13	0.42	1.90	6	1
1:A:290:GLN:NE2	1:A:336:GLU:HB2	0.42	2.29	16	1
1:A:298:ILE:CD1	1:A:322:ILE:O	0.42	2.66	1	1
1:A:314:ASN:OD1	1:A:314:ASN:N	0.42	2.53	6	1
1:A:314:ASN:O	1:A:316:LYS:N	0.42	2.52	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:296:VAL:HG22	1:A:324:LEU:HB3	0.42	1.92	8	1
1:A:285:ASN:HD22	1:A:347:ALA:HB2	0.42	1.74	16	1
1:A:289:VAL:O	1:A:290:GLN:NE2	0.42	2.52	19	2
1:A:314:ASN:ND2	1:A:317:THR:N	0.42	2.66	20	2
1:A:292:LEU:CD1	1:A:359:PHE:CD2	0.42	3.03	2	1
1:A:314:ASN:C	1:A:316:LYS:N	0.42	2.73	11	1
1:A:286:THR:OG1	1:A:340:SER:HA	0.42	2.14	18	1
1:A:284:ASN:ND2	1:A:284:ASN:N	0.42	2.68	6	1
1:A:289:VAL:HG21	1:A:305:PHE:CE2	0.42	2.50	11	1
1:A:295:ASN:O	1:A:297:THR:N	0.42	2.52	16	2
1:A:292:LEU:HD23	1:A:296:VAL:CG2	0.42	2.45	3	1
1:A:317:THR:HG21	1:A:319:GLN:CD	0.42	2.35	10	1
1:A:351:ILE:HD13	1:A:368:PHE:CZ	0.42	2.50	16	1
1:A:313:THR:OG1	1:A:319:GLN:N	0.42	2.53	19	1
1:A:287:ILE:CD1	1:A:366:VAL:HG13	0.42	2.35	7	1
1:A:288:PHE:CE1	1:A:290:GLN:OE1	0.42	2.72	9	1
1:A:311:ILE:CG2	1:A:320:PRO:HB3	0.42	2.45	18	2
1:A:339:VAL:HG12	1:A:341:PHE:CZ	0.41	2.50	7	1
1:A:339:VAL:HG12	1:A:341:PHE:CE1	0.41	2.49	7	1
1:A:290:GLN:O	1:A:365:LYS:N	0.41	2.53	9	1
1:A:317:THR:CG2	1:A:319:GLN:CG	0.41	2.98	19	1
1:A:348:LYS:C	1:A:348:LYS:HD3	0.41	2.36	10	1
1:A:351:ILE:O	1:A:355:ASP:CG	0.41	2.58	19	1
1:A:339:VAL:CG1	1:A:341:PHE:CZ	0.41	3.03	7	2
1:A:301:VAL:HG11	1:A:339:VAL:HG23	0.41	1.92	12	1
1:A:284:ASN:N	1:A:284:ASN:ND2	0.41	2.68	1	1
1:A:301:VAL:CG1	1:A:339:VAL:CG2	0.41	2.98	13	2
1:A:344:PRO:N	1:A:345:PRO:CD	0.41	2.84	7	2
1:A:343:ASP:OD1	1:A:346:SER:CB	0.41	2.68	9	1
1:A:306:LYS:O	1:A:306:LYS:CG	0.41	2.68	11	1
1:A:339:VAL:HG11	1:A:341:PHE:CZ	0.41	2.50	12	1
1:A:314:ASN:ND2	1:A:321:MET:HG2	0.41	2.30	2	1
1:A:348:LYS:C	1:A:348:LYS:CD	0.41	2.89	2	2
1:A:314:ASN:ND2	1:A:317:THR:H	0.41	2.13	5	1
1:A:312:LYS:HB3	1:A:340:SER:CB	0.41	2.46	6	1
1:A:351:ILE:HG23	1:A:355:ASP:HB2	0.41	1.91	8	1
1:A:311:ILE:O	1:A:313:THR:N	0.41	2.53	9	1
1:A:312:LYS:O	1:A:321:MET:HB2	0.41	2.16	12	1
1:A:315:LYS:CD	1:A:315:LYS:N	0.41	2.84	18	1
1:A:311:ILE:CB	1:A:320:PRO:HB3	0.41	2.45	3	2
1:A:296:VAL:HG13	1:A:324:LEU:CD2	0.41	2.45	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:284:ASN:O	1:A:285:ASN:CB	0.41	2.68	2	1
1:A:313:THR:HG22	1:A:318:GLY:C	0.41	2.36	3	1
1:A:312:LYS:N	1:A:340:SER:O	0.41	2.53	6	1
1:A:353:TRP:CE2	1:A:354:PHE:CE1	0.41	3.09	8	1
1:A:288:PHE:CD1	1:A:288:PHE:C	0.41	2.93	9	1
1:A:341:PHE:CD2	1:A:347:ALA:HA	0.41	2.51	9	1
1:A:289:VAL:CG1	1:A:366:VAL:HG22	0.41	2.36	13	1
1:A:291:GLY:O	1:A:364:ILE:CG2	0.41	2.66	14	1
1:A:314:ASN:ND2	1:A:317:THR:CB	0.41	2.84	15	1
1:A:295:ASN:ND2	1:A:359:PHE:CD1	0.41	2.89	1	1
1:A:323:ASN:O	1:A:337:ALA:CA	0.41	2.69	9	2
1:A:292:LEU:HD12	1:A:296:VAL:CG2	0.41	2.39	6	1
1:A:296:VAL:HG12	1:A:324:LEU:HB3	0.41	1.93	7	1
1:A:296:VAL:HG23	1:A:324:LEU:HB3	0.41	1.92	12	1
1:A:290:GLN:NE2	1:A:336:GLU:CB	0.41	2.84	16	1
1:A:297:THR:O	1:A:301:VAL:CG2	0.41	2.69	18	1
1:A:292:LEU:HD22	1:A:335:GLY:C	0.40	2.35	4	1
1:A:285:ASN:OD1	1:A:344:PRO:CD	0.40	2.69	7	1
1:A:287:ILE:HD13	1:A:305:PHE:CE2	0.40	2.51	10	1
1:A:312:LYS:CG	1:A:341:PHE:O	0.40	2.69	13	1
1:A:311:ILE:HG22	1:A:320:PRO:CB	0.40	2.46	14	1
1:A:287:ILE:CD1	1:A:366:VAL:CG1	0.40	2.99	7	1
1:A:292:LEU:HB3	1:A:295:ASN:ND2	0.40	2.31	20	1
1:A:292:LEU:HD13	1:A:364:ILE:HG22	0.40	1.93	2	1
1:A:292:LEU:CG	1:A:296:VAL:HG22	0.40	2.46	7	1
1:A:288:PHE:O	1:A:288:PHE:CG	0.40	2.75	13	2
1:A:296:VAL:CG2	1:A:324:LEU:CB	0.40	3.00	9	1
1:A:323:ASN:O	1:A:337:ALA:HA	0.40	2.16	9	1
1:A:306:LYS:O	1:A:306:LYS:CD	0.40	2.69	11	1
1:A:296:VAL:HG13	1:A:324:LEU:HB3	0.40	1.93	18	1
1:A:302:ALA:HB1	1:A:320:PRO:CG	0.40	2.46	19	1
1:A:353:TRP:CD1	1:A:357:LYS:HD2	0.40	2.51	2	1
1:A:302:ALA:CA	1:A:311:ILE:HD13	0.40	2.44	6	1
1:A:302:ALA:O	1:A:306:LYS:CG	0.40	2.69	7	1
1:A:288:PHE:CZ	1:A:325:TYR:OH	0.40	2.73	14	1
1:A:312:LYS:O	1:A:321:MET:CB	0.40	2.70	15	1
1:A:314:ASN:CG	1:A:317:THR:OG1	0.40	2.59	17	1
1:A:313:THR:OG1	1:A:314:ASN:N	0.40	2.55	19	1
1:A:304:TYR:OH	1:A:359:PHE:CE1	0.40	2.71	19	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	76/116 (66%)	61±2 (80±2%)	12±2 (16±3%)	3±1 (5±2%)	3	27
All	All	1520/2320 (66%)	1215 (80%)	236 (16%)	69 (5%)	3	27

All 13 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	355	ASP	18
1	A	312	LYS	15
1	A	296	VAL	9
1	A	292	LEU	6
1	A	284	ASN	5
1	A	320	PRO	4
1	A	315	LYS	3
1	A	285	ASN	2
1	A	354	PHE	2
1	A	295	ASN	2
1	A	343	ASP	1
1	A	293	GLY	1
1	A	360	SER	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	64/95 (67%)	41±3 (64±5%)	23±3 (36±5%)	1	8
All	All	1280/1900 (67%)	820 (64%)	460 (36%)	1	8

All 49 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	304	TYR	20
1	A	359	PHE	20
1	A	295	ASN	19
1	A	319	GLN	19
1	A	297	THR	18
1	A	306	LYS	18
1	A	313	THR	18
1	A	305	PHE	17
1	A	289	VAL	16
1	A	314	ASN	16
1	A	324	LEU	16
1	A	348	LYS	16
1	A	357	LYS	14
1	A	315	LYS	14
1	A	288	PHE	12
1	A	292	LEU	11
1	A	312	LYS	11
1	A	343	ASP	11
1	A	284	ASN	10
1	A	285	ASN	10
1	A	290	GLN	10
1	A	316	LYS	10
1	A	321	MET	10
1	A	365	LYS	10
1	A	342	ASP	8
1	A	308	ILE	7
1	A	352	ASP	7
1	A	360	SER	7
1	A	362	ASN	7
1	A	368	PHE	7
1	A	336	GLU	6
1	A	303	ASP	6
1	A	346	SER	6
1	A	367	SER	6
1	A	299	GLU	5
1	A	317	THR	5
1	A	358	GLU	5
1	A	307	GLN	5
1	A	294	GLU	5
1	A	300	SER	4
1	A	323	ASN	4
1	A	354	PHE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	353	TRP	3
1	A	340	SER	3
1	A	341	PHE	1
1	A	310	ILE	1
1	A	338	THR	1
1	A	286	THR	1
1	A	339	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1220
Number of shifts mapped to atoms	1220
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	108	-0.52 ± 0.19	Should be checked
$^{13}C_\beta$	94	0.04 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	107	0.71 ± 0.27	Should be applied
^{15}N	103	0.50 ± 0.43	None needed (imprecise)

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 91%, i.e. 911 atoms were assigned a chemical shift out of a possible 998. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	378/379 (100%)	155/155 (100%)	151/152 (99%)	72/72 (100%)
Sidechain	492/529 (93%)	323/343 (94%)	160/170 (94%)	9/16 (56%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	41/90 (46%)	22/44 (50%)	18/45 (40%)	1/1 (100%)
Overall	911/998 (91%)	500/542 (92%)	329/367 (90%)	82/89 (92%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1220 atoms were assigned a chemical shift out of a possible 1397. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	537/546 (98%)	219/226 (97%)	215/216 (100%)	103/104 (99%)
Sidechain	641/751 (85%)	415/479 (87%)	213/235 (91%)	13/37 (35%)
Aromatic	42/100 (42%)	23/49 (47%)	18/50 (36%)	1/1 (100%)
Overall	1220/1397 (87%)	657/754 (87%)	446/501 (89%)	117/142 (82%)

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	353	TRP	HD1	5.24	5.46 – 8.81	-5.7

7.1.5   Random Coil Index (RCI) plots (i)

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

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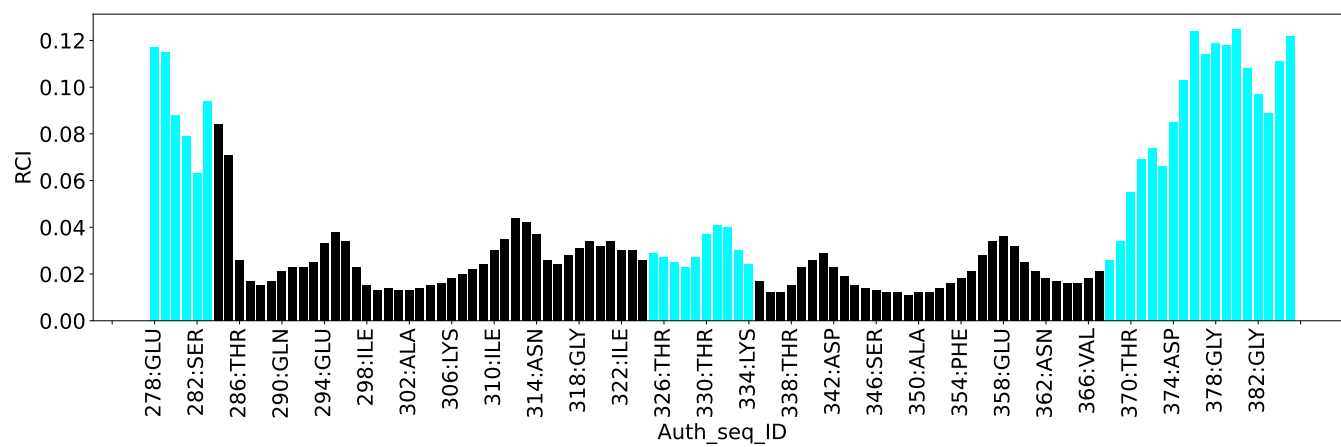
8   NMR restraints analysis ⓘ

8.1   Conformationally restricting restraints ⓘ

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

Description	Value
Total distance restraints	1676
Intra-residue ($\|i\text{-}j\|$=0)	719
Sequential ($\|i\text{-}j\|$=1)	425
Medium range ($\|i\text{-}j\|$>1 and $\|i\text{-}j\|$<5)	186
Long range ($\|i\text{-}j\|$≥5)	328
Inter-chain	0
Hydrogen bond restraints	18
Disulfide bond restraints	0
Total dihedral-angle restraints	94
Number of unmapped restraints	0
Number of restraints per residue	15.3
Number of long range restraints per residue[1]	2.9

[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)	8.6	0.2
0.2-0.5 (Medium)	0.4	0.28
>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)	0.8	1.86
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

9.1 Summary of distance violations ⓘ

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	719	42.9	13	1.8	0.8	0	0.0	0.0
Backbone-Backbone	108	6.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	395	23.6	13	3.3	0.8	0	0.0	0.0
Sidechain-Sidechain	216	12.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	425	25.4	12	2.8	0.7	1	0.2	0.1
Backbone-Backbone	181	10.8	5	2.8	0.3	1	0.6	0.1
Backbone-Sidechain	217	12.9	7	3.2	0.4	0	0.0	0.0
Sidechain-Sidechain	27	1.6	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	186	11.1	10	5.4	0.6	0	0.0	0.0
Backbone-Backbone	74	4.4	8	10.8	0.5	0	0.0	0.0
Backbone-Sidechain	79	4.7	2	2.5	0.1	0	0.0	0.0
Sidechain-Sidechain	33	2.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	328	19.6	12	3.7	0.7	0	0.0	0.0
Backbone-Backbone	58	3.5	3	5.2	0.2	0	0.0	0.0
Backbone-Sidechain	162	9.7	3	1.9	0.2	0	0.0	0.0
Sidechain-Sidechain	108	6.4	6	5.6	0.4	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	18	1.1	4	22.2	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1676	100.0	51	3.0	3.0	1	0.1	0.1
Backbone-Backbone	421	25.1	16	3.8	1.0	1	0.2	0.1
Backbone-Sidechain	871	52.0	29	3.3	1.7	0	0.0	0.0
Sidechain-Sidechain	384	22.9	6	1.6	0.4	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 ⓘ
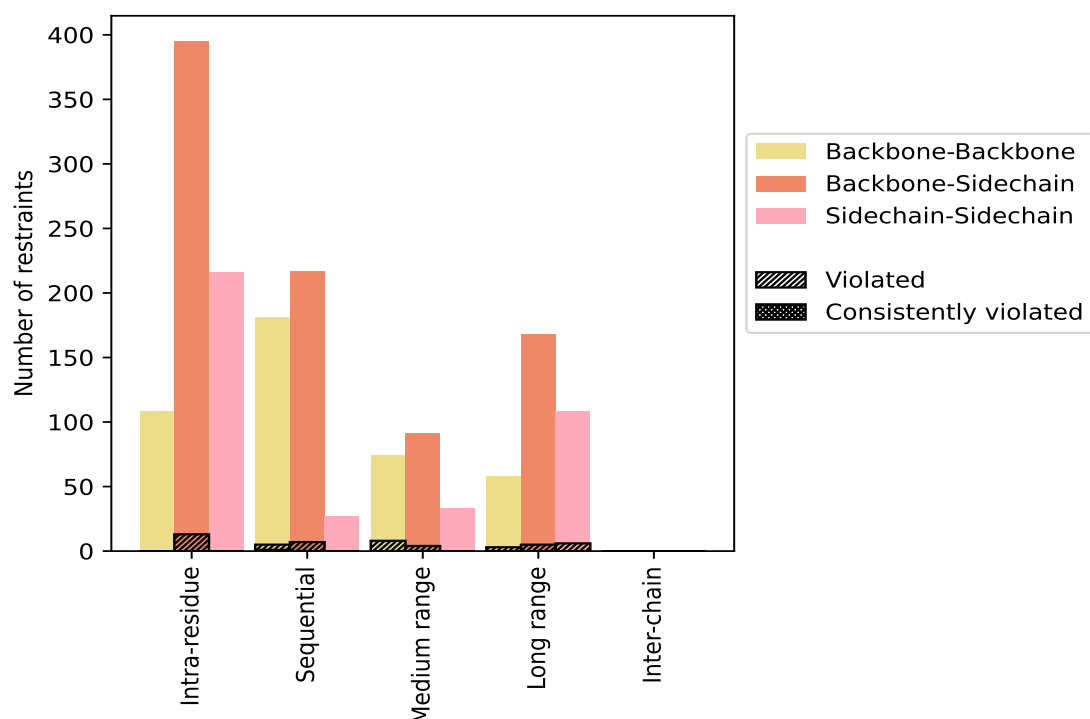
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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	1	3	0	3	0	7	0.16	0.23	0.05	0.15
2	1	6	3	4	0	14	0.14	0.24	0.04	0.13
3	3	3	1	4	0	11	0.12	0.14	0.01	0.12
4	1	5	1	3	0	10	0.14	0.17	0.02	0.14
5	2	4	1	1	0	8	0.16	0.18	0.03	0.17
6	5	3	0	3	0	11	0.15	0.23	0.04	0.16
7	1	4	2	2	0	9	0.13	0.15	0.02	0.13
8	1	3	2	3	0	9	0.13	0.18	0.03	0.14
9	1	2	1	6	0	10	0.13	0.17	0.02	0.12
10	3	4	4	3	0	14	0.15	0.24	0.04	0.15

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Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	3	2	2	3	0	10	0.13	0.17	0.02	0.12
12	3	5	2	4	0	14	0.15	0.28	0.05	0.13
13	1	3	1	3	0	8	0.15	0.19	0.02	0.15
14	1	5	1	3	0	10	0.13	0.21	0.03	0.12
15	2	3	1	1	0	7	0.14	0.18	0.02	0.13
16	6	3	2	4	0	15	0.13	0.17	0.02	0.13
17	1	3	3	2	0	9	0.14	0.19	0.03	0.14
18	0	3	2	3	0	8	0.15	0.2	0.04	0.15
19	3	3	3	2	0	11	0.15	0.22	0.04	0.14
20	3	3	1	3	0	10	0.14	0.2	0.03	0.14

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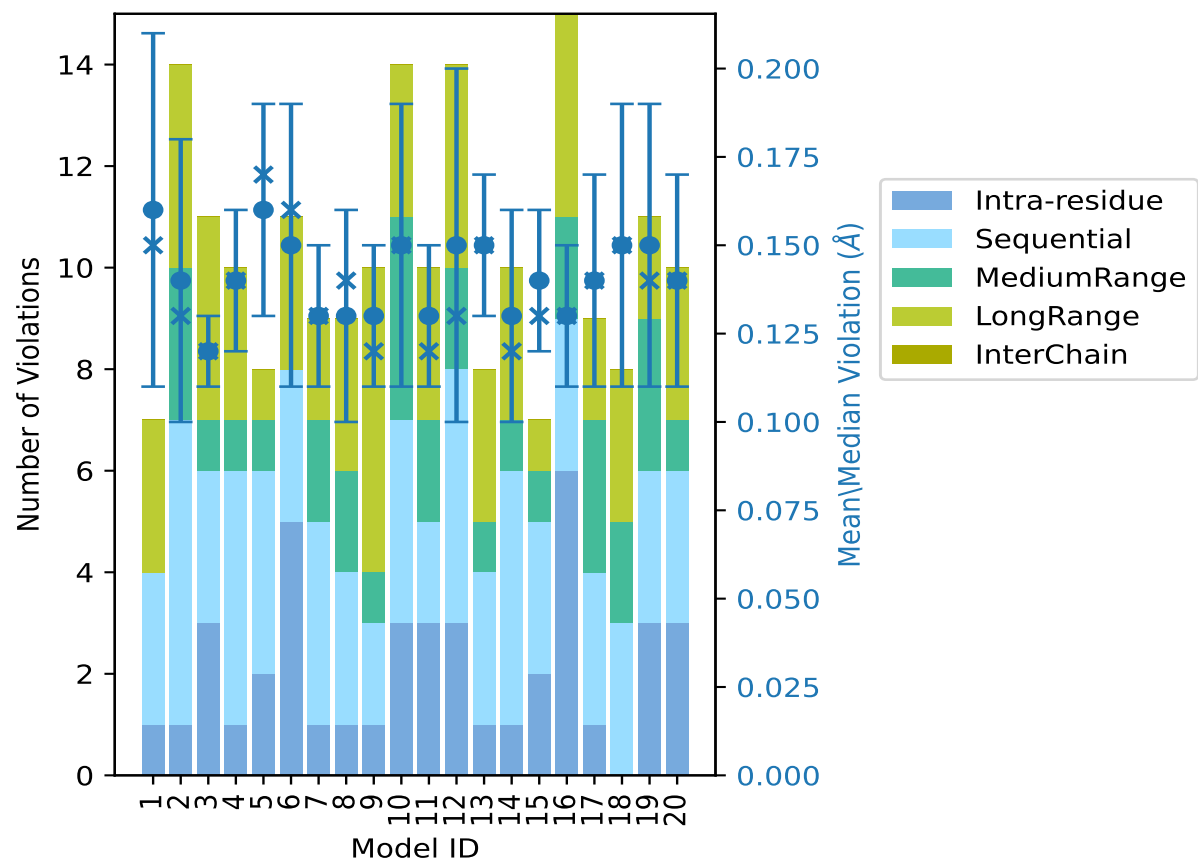
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis
on the right

9.3   Distance violation statistics for the ensemble (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, 1611(IR:706, SQ:413, MR:176, LR:316, 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]	%
2	5	1	5	0	13	1	5.0
6	2	3	3	0	14	2	10.0
3	2	4	1	0	10	3	15.0
0	0	1	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	1	0	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
1	0	0	2	0	3	9	45.0
1	0	0	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	1	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	1	0	0	0	1	17	85.0
0	1	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	1	0	0	0	1	20	100.0

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

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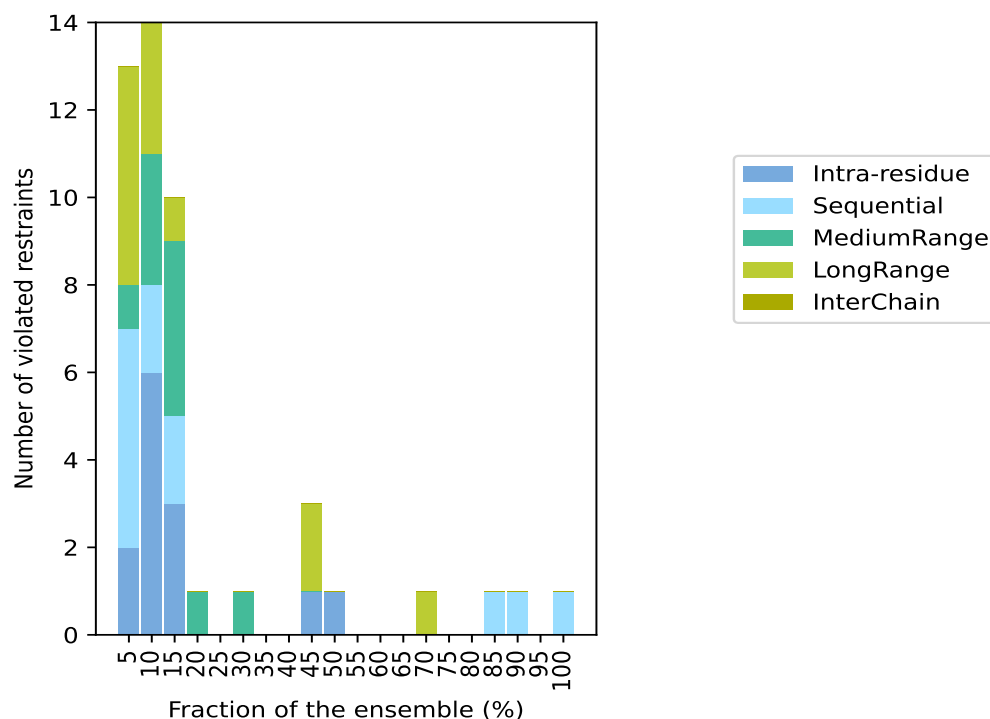
9.4 Most violated distance restraints in the ensemble ⓘ

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
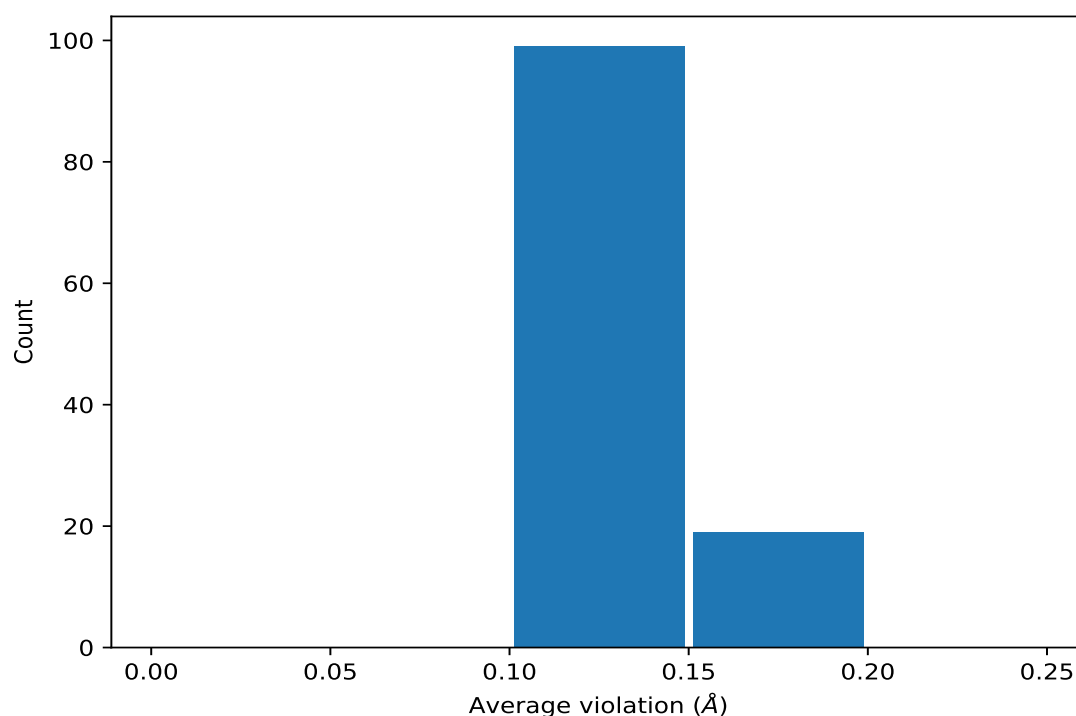
9.4.2 Table: Most violated distance restraints ⓘ

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)
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	20	0.15	0.01	0.15
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	18	0.18	0.03	0.18
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	17	0.12	0.02	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	14	0.15	0.04	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	14	0.15	0.04	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	14	0.15	0.04	0.14
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	10	0.15	0.02	0.16
(2,12)	1:340:A:SER:H	1:321:A:MET:O	10	0.12	0.02	0.12
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	9	0.16	0.02	0.15
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	9	0.14	0.02	0.13
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	9	0.13	0.02	0.13
(1,395)	1:317:A:THR:HB	1:319:A:GLN:H	6	0.19	0.05	0.19
(2,17)	1:367:A:SER:H	1:288:A:PHE:O	4	0.11	0.0	0.11
(1,198)	1:298:A:ILE:HA	1:301:A:VAL:H	4	0.1	0.0	0.11
(1,351)	1:313:A:THR:HB	1:313:A:THR:H	3	0.13	0.03	0.12
(1,401)	1:317:A:THR:H	1:319:A:GLN:H	3	0.13	0.03	0.13
(1,392)	1:316:A:LYS:H	1:319:A:GLN:H	3	0.13	0.01	0.13
(1,132)	1:291:A:GLY:H	1:293:A:GLY:H	3	0.12	0.01	0.12
(1,691)	1:355:A:ASP:H	1:356:A:GLY:H	3	0.12	0.03	0.11
(1,114)	1:290:A:GLN:HA	1:290:A:GLN:HE22	3	0.12	0.01	0.12
(1,101)	1:289:A:VAL:HB	1:337:A:ALA:H	3	0.12	0.02	0.11
(1,567)	1:344:A:PRO:HA	1:347:A:ALA:H	3	0.12	0.01	0.11
(1,352)	1:313:A:THR:HB	1:314:A:ASN:H	3	0.11	0.01	0.11
(1,1558)	1:370:A:THR:HA	1:370:A:THR:HB	3	0.1	0.0	0.1
(1,491)	1:329:A:GLU:H	1:331:A:GLY:H	2	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,511)	1:333:A:LEU:HD11	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,511)	1:333:A:LEU:HD12	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,511)	1:333:A:LEU:HD13	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,511)	1:333:A:LEU:HD21	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,511)	1:333:A:LEU:HD22	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,511)	1:333:A:LEU:HD23	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,1310)	1:333:A:LEU:HD11	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,1310)	1:333:A:LEU:HD12	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,1310)	1:333:A:LEU:HD13	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,1310)	1:333:A:LEU:HD21	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,1310)	1:333:A:LEU:HD22	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,1310)	1:333:A:LEU:HD23	1:333:A:LEU:H	2	0.17	0.0	0.17
(1,136)	1:292:A:LEU:HB2	1:293:A:GLY:H	2	0.17	0.01	0.17
(1,136)	1:292:A:LEU:HB3	1:293:A:GLY:H	2	0.17	0.01	0.17
(1,427)	1:322:A:ILE:HB	1:340:A:SER:H	2	0.16	0.04	0.16
(1,205)	1:298:A:ILE:HG12	1:298:A:ILE:H	2	0.15	0.04	0.15
(1,177)	1:296:A:VAL:HB	1:296:A:VAL:H	2	0.14	0.01	0.14
(1,1311)	1:333:A:LEU:HG	1:333:A:LEU:H	2	0.14	0.04	0.14
(1,642)	1:351:A:ILE:HG12	1:352:A:ASP:H	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD11	1:337:A:ALA:HB1	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD11	1:337:A:ALA:HB2	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD11	1:337:A:ALA:HB3	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD12	1:337:A:ALA:HB1	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD12	1:337:A:ALA:HB2	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD12	1:337:A:ALA:HB3	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD13	1:337:A:ALA:HB1	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD13	1:337:A:ALA:HB2	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD13	1:337:A:ALA:HB3	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD21	1:337:A:ALA:HB1	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD21	1:337:A:ALA:HB2	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD21	1:337:A:ALA:HB3	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD22	1:337:A:ALA:HB1	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD22	1:337:A:ALA:HB2	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD22	1:337:A:ALA:HB3	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD23	1:337:A:ALA:HB1	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD23	1:337:A:ALA:HB2	2	0.12	0.02	0.12
(1,1254)	1:324:A:LEU:HD23	1:337:A:ALA:HB3	2	0.12	0.02	0.12
(1,372)	1:314:A:ASN:HD22	1:317:A:THR:H	2	0.12	0.02	0.12
(1,589)	1:347:A:ALA:HA	1:350:A:ALA:H	2	0.12	0.01	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD11	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD12	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD13	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)
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD21	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD22	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD23	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD11	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD12	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD13	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD21	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD22	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD23	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD11	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD12	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD13	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD21	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD22	2	0.12	0.0	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD23	2	0.12	0.0	0.12
(2,4)	1:304:A:TYR:H	1:300:A:SER:O	2	0.11	0.01	0.11
(2,15)	1:359:A:PHE:H	1:362:A:ASN:O	2	0.11	0.0	0.11
(1,946)	1:296:A:VAL:HA	1:296:A:VAL:HB	2	0.1	0.0	0.1

[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.
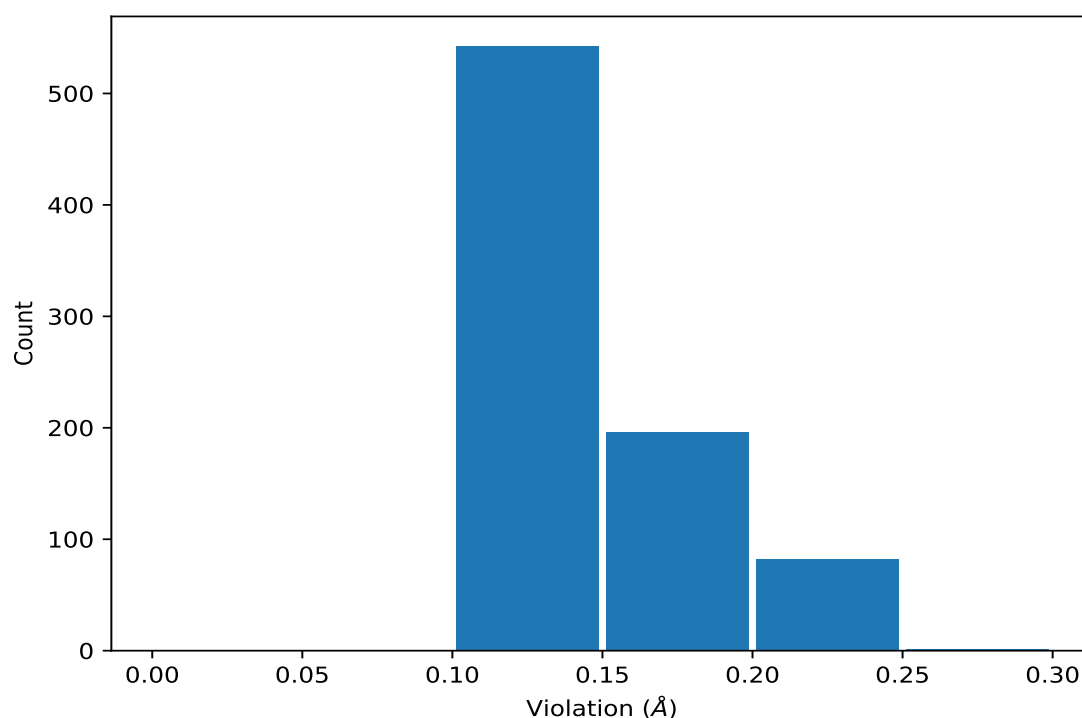
9.5.2 Table : All distance violations ⓘ

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)
(1,395)	1:317:A:THR:HB	1:319:A:GLN:H	12	0.28
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	2	0.24
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	2	0.24
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	2	0.24
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	2	0.24
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	2	0.24
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	2	0.24
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	2	0.24
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	2	0.24
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	2	0.24
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	2	0.24
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	2	0.24
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	2	0.24
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	2	0.24
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	2	0.24
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	2	0.24
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	2	0.24
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	2	0.24
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	2	0.24
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	2	0.24
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	2	0.24
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	2	0.24
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	2	0.24
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	2	0.24
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	2	0.24
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	2	0.24
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	2	0.24
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	2	0.24
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	2	0.24
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	2	0.24
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	2	0.24
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	2	0.24
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	2	0.24
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	2	0.24
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	2	0.24
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	2	0.24
(1,395)	1:317:A:THR:HB	1:319:A:GLN:H	10	0.24
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	1	0.23
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	1	0.23
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	1	0.23
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	1	0.23
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	1	0.23
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	1	0.23
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	1	0.23
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	1	0.23
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	1	0.23
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	1	0.23
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	1	0.23
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	1	0.23
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	1	0.23
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	1	0.23
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	1	0.23
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	1	0.23
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	1	0.23
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	1	0.23
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	1	0.23
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	1	0.23
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	1	0.23
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	1	0.23
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	1	0.23
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	1	0.23
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	1	0.23
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	1	0.23
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	1	0.23
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	1	0.23
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	1	0.23
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	1	0.23
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	1	0.23
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	1	0.23
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	1	0.23
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	1	0.23
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	1	0.23
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	1	0.23
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	6	0.23
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	19	0.22
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	14	0.21
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	20	0.2
(1,679)	1:354:A:PHE:HD1	1:354:A:PHE:H	12	0.2
(1,679)	1:354:A:PHE:HD2	1:354:A:PHE:H	12	0.2
(1,491)	1:329:A:GLU:H	1:331:A:GLY:H	10	0.2
(1,427)	1:322:A:ILE:HB	1:340:A:SER:H	18	0.2
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	13	0.19
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	17	0.19
(1,395)	1:317:A:THR:HB	1:319:A:GLN:H	18	0.19
(1,395)	1:317:A:THR:HB	1:319:A:GLN:H	19	0.19
(1,205)	1:298:A:ILE:HG12	1:298:A:ILE:H	19	0.19
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	2	0.18
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	5	0.18
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	8	0.18
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	12	0.18
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	15	0.18
(1,519)	1:334:A:LYS:H	1:336:A:GLU:H	10	0.18
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	5	0.18
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	5	0.18
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	6	0.18
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	18	0.18
(1,136)	1:292:A:LEU:HB2	1:293:A:GLY:H	5	0.18
(1,136)	1:292:A:LEU:HB3	1:293:A:GLY:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	8	0.17
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	12	0.17
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	20	0.17
(1,1311)	1:333:A:LEU:HG	1:333:A:LEU:H	9	0.17
(1,1310)	1:333:A:LEU:HD11	1:333:A:LEU:H	6	0.17
(1,1310)	1:333:A:LEU:HD12	1:333:A:LEU:H	6	0.17
(1,1310)	1:333:A:LEU:HD13	1:333:A:LEU:H	6	0.17
(1,1310)	1:333:A:LEU:HD21	1:333:A:LEU:H	6	0.17
(1,1310)	1:333:A:LEU:HD22	1:333:A:LEU:H	6	0.17
(1,1310)	1:333:A:LEU:HD23	1:333:A:LEU:H	6	0.17
(1,1310)	1:333:A:LEU:HD11	1:333:A:LEU:H	16	0.17
(1,1310)	1:333:A:LEU:HD12	1:333:A:LEU:H	16	0.17
(1,1310)	1:333:A:LEU:HD13	1:333:A:LEU:H	16	0.17
(1,1310)	1:333:A:LEU:HD21	1:333:A:LEU:H	16	0.17
(1,1310)	1:333:A:LEU:HD22	1:333:A:LEU:H	16	0.17
(1,1310)	1:333:A:LEU:HD23	1:333:A:LEU:H	16	0.17
(1,796)	1:370:A:THR:HB	1:370:A:THR:H	15	0.17
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	4	0.17
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	10	0.17
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	11	0.17
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	19	0.17
(1,511)	1:333:A:LEU:HD11	1:333:A:LEU:H	6	0.17
(1,511)	1:333:A:LEU:HD12	1:333:A:LEU:H	6	0.17
(1,511)	1:333:A:LEU:HD13	1:333:A:LEU:H	6	0.17
(1,511)	1:333:A:LEU:HD21	1:333:A:LEU:H	6	0.17
(1,511)	1:333:A:LEU:HD22	1:333:A:LEU:H	6	0.17
(1,511)	1:333:A:LEU:HD23	1:333:A:LEU:H	6	0.17
(1,511)	1:333:A:LEU:HD11	1:333:A:LEU:H	16	0.17
(1,511)	1:333:A:LEU:HD12	1:333:A:LEU:H	16	0.17
(1,511)	1:333:A:LEU:HD13	1:333:A:LEU:H	16	0.17
(1,511)	1:333:A:LEU:HD21	1:333:A:LEU:H	16	0.17
(1,511)	1:333:A:LEU:HD22	1:333:A:LEU:H	16	0.17
(1,511)	1:333:A:LEU:HD23	1:333:A:LEU:H	16	0.17
(1,401)	1:317:A:THR:H	1:319:A:GLN:H	17	0.17
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	14	0.17
(1,351)	1:313:A:THR:HB	1:313:A:THR:H	6	0.17
(2,12)	1:340:A:SER:H	1:321:A:MET:O	13	0.16
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	5	0.16
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	15	0.16
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	10	0.16
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	10	0.16
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	10	0.16
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	10	0.16
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	10	0.16
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	10	0.16
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	10	0.16
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	10	0.16
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	10	0.16
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	10	0.16
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	10	0.16
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	10	0.16
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	10	0.16
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	10	0.16
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	10	0.16
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	10	0.16
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	10	0.16
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	10	0.16
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	10	0.16
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	10	0.16
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	10	0.16
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	10	0.16
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	10	0.16
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	10	0.16
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	10	0.16
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	10	0.16
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	10	0.16
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	10	0.16
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	10	0.16
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	10	0.16
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	10	0.16
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	10	0.16
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	10	0.16
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	10	0.16
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	10	0.16
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	10	0.16
(1,691)	1:355:A:ASP:H	1:356:A:GLY:H	11	0.16
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	2	0.16
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	16	0.16
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	1	0.16
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	5	0.16
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	6	0.16
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	9	0.16
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	13	0.16
(1,395)	1:317:A:THR:HB	1:319:A:GLN:H	4	0.16
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	20	0.16
(1,136)	1:292:A:LEU:HB2	1:293:A:GLY:H	2	0.16
(1,136)	1:292:A:LEU:HB3	1:293:A:GLY:H	2	0.16
(2,12)	1:340:A:SER:H	1:321:A:MET:O	19	0.15
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	2	0.15
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	10	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	12	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	12	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	12	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	12	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	12	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	12	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	12	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	12	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	12	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	12	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	12	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	12	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	12	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	12	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	12	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	12	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	12	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	12	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	12	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	12	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	12	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	12	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	12	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	12	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	12	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	12	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	12	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	12	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	12	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	12	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	12	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	12	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	12	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	12	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	12	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	13	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	13	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	13	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	13	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	13	0.15
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	13	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	13	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	13	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	13	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	13	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	13	0.15
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	13	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	13	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	13	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	13	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	13	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	13	0.15
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	13	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	13	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	13	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	13	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	13	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	13	0.15
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	13	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	13	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	13	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	13	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	13	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	13	0.15
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	13	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	13	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	13	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	13	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	13	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	13	0.15
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	13	0.15
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	16	0.15
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	7	0.15
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	10	0.15
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	18	0.15
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	2	0.15
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	4	0.15
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	7	0.15
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	14	0.15
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	17	0.15
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	18	0.15
(1,491)	1:329:A:GLU:H	1:331:A:GLY:H	17	0.15
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	1	0.15
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	7	0.15
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	12	0.15
(2,12)	1:340:A:SER:H	1:321:A:MET:O	9	0.14
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	16	0.14
(1,1254)	1:324:A:LEU:HD11	1:337:A:ALA:HB1	17	0.14
(1,1254)	1:324:A:LEU:HD11	1:337:A:ALA:HB2	17	0.14
(1,1254)	1:324:A:LEU:HD11	1:337:A:ALA:HB3	17	0.14
(1,1254)	1:324:A:LEU:HD12	1:337:A:ALA:HB1	17	0.14
(1,1254)	1:324:A:LEU:HD12	1:337:A:ALA:HB2	17	0.14
(1,1254)	1:324:A:LEU:HD12	1:337:A:ALA:HB3	17	0.14
(1,1254)	1:324:A:LEU:HD13	1:337:A:ALA:HB1	17	0.14
(1,1254)	1:324:A:LEU:HD13	1:337:A:ALA:HB2	17	0.14
(1,1254)	1:324:A:LEU:HD13	1:337:A:ALA:HB3	17	0.14
(1,1254)	1:324:A:LEU:HD21	1:337:A:ALA:HB1	17	0.14
(1,1254)	1:324:A:LEU:HD21	1:337:A:ALA:HB2	17	0.14
(1,1254)	1:324:A:LEU:HD21	1:337:A:ALA:HB3	17	0.14
(1,1254)	1:324:A:LEU:HD22	1:337:A:ALA:HB1	17	0.14
(1,1254)	1:324:A:LEU:HD22	1:337:A:ALA:HB2	17	0.14
(1,1254)	1:324:A:LEU:HD22	1:337:A:ALA:HB3	17	0.14
(1,1254)	1:324:A:LEU:HD23	1:337:A:ALA:HB1	17	0.14
(1,1254)	1:324:A:LEU:HD23	1:337:A:ALA:HB2	17	0.14
(1,1254)	1:324:A:LEU:HD23	1:337:A:ALA:HB3	17	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	4	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	4	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	4	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	4	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	4	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	4	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	4	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	4	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	4	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	4	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	4	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	4	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	4	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	4	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	4	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	4	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	4	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	4	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	4	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	4	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	4	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	4	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	4	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	4	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	4	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	4	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	4	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	4	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	4	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	4	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	4	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	4	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	4	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	4	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	4	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	8	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	8	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	8	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	8	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	8	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	8	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	8	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	8	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	8	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	8	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	8	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	8	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	8	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	8	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	8	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	8	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	8	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	8	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	8	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	8	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	8	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	8	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	8	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	8	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	8	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	8	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	8	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	8	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	8	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	8	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	8	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	8	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	8	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	8	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	8	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	9	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	9	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	9	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	9	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	9	0.14
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	9	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	9	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	9	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	9	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	9	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	9	0.14
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	9	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	9	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	9	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	9	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	9	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	9	0.14
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	9	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	9	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	9	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	9	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	9	0.14
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	9	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	9	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	9	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	9	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	9	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	9	0.14
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	9	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	9	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	9	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	9	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	9	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	9	0.14
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	9	0.14
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	3	0.14
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	6	0.14
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	10	0.14
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	13	0.14
(1,642)	1:351:A:ILE:HG12	1:352:A:ASP:H	14	0.14
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	3	0.14
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	8	0.14
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	16	0.14
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	20	0.14
(1,392)	1:316:A:LYS:H	1:319:A:GLN:H	20	0.14
(1,372)	1:314:A:ASN:HD22	1:317:A:THR:H	8	0.14
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	11	0.14
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	13	0.14
(1,177)	1:296:A:VAL:HB	1:296:A:VAL:H	19	0.14
(1,132)	1:291:A:GLY:H	1:293:A:GLY:H	5	0.14
(1,101)	1:289:A:VAL:HB	1:337:A:ALA:H	4	0.14
(2,12)	1:340:A:SER:H	1:321:A:MET:O	11	0.13
(2,12)	1:340:A:SER:H	1:321:A:MET:O	16	0.13
(1,933)	1:292:A:LEU:HD11	1:364:A:ILE:HG21	2	0.13
(1,933)	1:292:A:LEU:HD11	1:364:A:ILE:HG22	2	0.13
(1,933)	1:292:A:LEU:HD11	1:364:A:ILE:HG23	2	0.13
(1,933)	1:292:A:LEU:HD12	1:364:A:ILE:HG21	2	0.13
(1,933)	1:292:A:LEU:HD12	1:364:A:ILE:HG22	2	0.13
(1,933)	1:292:A:LEU:HD12	1:364:A:ILE:HG23	2	0.13
(1,933)	1:292:A:LEU:HD13	1:364:A:ILE:HG21	2	0.13
(1,933)	1:292:A:LEU:HD13	1:364:A:ILE:HG22	2	0.13
(1,933)	1:292:A:LEU:HD13	1:364:A:ILE:HG23	2	0.13
(1,933)	1:292:A:LEU:HD21	1:364:A:ILE:HG21	2	0.13
(1,933)	1:292:A:LEU:HD21	1:364:A:ILE:HG22	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:292:A:LEU:HD21	1:364:A:ILE:HG23	2	0.13
(1,933)	1:292:A:LEU:HD22	1:364:A:ILE:HG21	2	0.13
(1,933)	1:292:A:LEU:HD22	1:364:A:ILE:HG22	2	0.13
(1,933)	1:292:A:LEU:HD22	1:364:A:ILE:HG23	2	0.13
(1,933)	1:292:A:LEU:HD23	1:364:A:ILE:HG21	2	0.13
(1,933)	1:292:A:LEU:HD23	1:364:A:ILE:HG22	2	0.13
(1,933)	1:292:A:LEU:HD23	1:364:A:ILE:HG23	2	0.13
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	2	0.13
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	6	0.13
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	3	0.13
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	15	0.13
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	17	0.13
(1,589)	1:347:A:ALA:HA	1:350:A:ALA:H	16	0.13
(1,567)	1:344:A:PRO:HA	1:347:A:ALA:H	7	0.13
(1,518)	1:334:A:LYS:H	1:335:A:GLY:H	10	0.13
(1,401)	1:317:A:THR:H	1:319:A:GLN:H	15	0.13
(1,392)	1:316:A:LYS:H	1:319:A:GLN:H	11	0.13
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	7	0.13
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	20	0.13
(1,177)	1:296:A:VAL:HB	1:296:A:VAL:H	16	0.13
(1,130)	1:291:A:GLY:H	1:292:A:LEU:HG	4	0.13
(1,114)	1:290:A:GLN:HA	1:290:A:GLN:HE22	3	0.13
(2,4)	1:304:A:TYR:H	1:300:A:SER:O	14	0.12
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	6	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD11	2	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD12	2	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD13	2	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD21	2	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD22	2	0.12
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD23	2	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD11	2	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD12	2	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD13	2	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD21	2	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD22	2	0.12
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD23	2	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD11	2	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD12	2	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD13	2	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD21	2	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD22	2	0.12
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD23	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	3	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	3	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	3	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	3	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	3	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	3	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	3	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	3	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	3	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	3	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	3	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	3	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	3	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	3	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	3	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	3	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	3	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	3	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	3	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	3	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	3	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	3	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	3	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	3	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	3	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	3	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	3	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	3	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	3	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	3	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	3	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	3	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	3	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	3	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	3	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	3	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	14	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	14	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	14	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	14	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	14	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	14	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	14	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	14	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	14	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	14	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	14	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	14	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	14	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	14	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	14	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	14	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	14	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	14	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	14	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	14	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	14	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	14	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	14	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	14	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	14	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	14	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	14	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	14	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	14	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	14	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	14	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	14	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	14	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	14	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	14	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	17	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	17	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	17	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	17	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	17	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	17	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	17	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	17	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	17	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	17	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	17	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	17	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	17	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	17	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	17	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	17	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	17	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	17	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	17	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	17	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	17	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	17	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	17	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	17	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	17	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	17	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	17	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	17	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	17	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	17	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	17	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	17	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	17	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	17	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	17	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	20	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	20	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	20	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	20	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	20	0.12
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	20	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	20	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	20	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	20	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	20	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	20	0.12
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	20	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	20	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	20	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	20	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	20	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	20	0.12
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	20	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	20	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	20	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	20	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	20	0.12
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	20	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	20	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	20	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	20	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	20	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	20	0.12
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	20	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	20	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	20	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	20	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	20	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	20	0.12
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	20	0.12
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	9	0.12
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	4	0.12
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	9	0.12
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	18	0.12
(1,624)	1:350:A:ALA:H	1:351:A:ILE:HA	15	0.12
(1,427)	1:322:A:ILE:HB	1:340:A:SER:H	4	0.12
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	3	0.12
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	16	0.12
(1,361)	1:314:A:ASN:HA	1:319:A:GLN:H	3	0.12
(1,352)	1:313:A:THR:HB	1:314:A:ASN:H	7	0.12
(1,351)	1:313:A:THR:HB	1:313:A:THR:H	11	0.12
(1,318)	1:310:A:ILE:HG13	1:342:A:ASP:H	9	0.12
(1,132)	1:291:A:GLY:H	1:293:A:GLY:H	2	0.12
(1,114)	1:290:A:GLN:HA	1:290:A:GLN:HE22	11	0.12
(2,17)	1:367:A:SER:H	1:288:A:PHE:O	9	0.11
(2,17)	1:367:A:SER:H	1:288:A:PHE:O	16	0.11
(2,15)	1:359:A:PHE:H	1:362:A:ASN:O	2	0.11
(2,12)	1:340:A:SER:H	1:321:A:MET:O	1	0.11
(2,12)	1:340:A:SER:H	1:321:A:MET:O	10	0.11
(2,12)	1:340:A:SER:H	1:321:A:MET:O	12	0.11
(1,1639)	1:353:A:TRP:HA	1:353:A:TRP:HE3	14	0.11
(1,1558)	1:370:A:THR:HA	1:370:A:THR:HB	3	0.11
(1,1480)	1:357:A:LYS:HB2	1:358:A:GLU:H	2	0.11
(1,1480)	1:357:A:LYS:HB3	1:358:A:GLU:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD11	1	0.11
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD12	1	0.11
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD13	1	0.11
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD21	1	0.11
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD22	1	0.11
(1,1271)	1:326:A:THR:HG21	1:333:A:LEU:HD23	1	0.11
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD11	1	0.11
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD12	1	0.11
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD13	1	0.11
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD21	1	0.11
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD22	1	0.11
(1,1271)	1:326:A:THR:HG22	1:333:A:LEU:HD23	1	0.11
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD11	1	0.11
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD12	1	0.11
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD13	1	0.11
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD21	1	0.11
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD22	1	0.11
(1,1271)	1:326:A:THR:HG23	1:333:A:LEU:HD23	1	0.11
(1,1254)	1:324:A:LEU:HD11	1:337:A:ALA:HB1	12	0.11
(1,1254)	1:324:A:LEU:HD11	1:337:A:ALA:HB2	12	0.11
(1,1254)	1:324:A:LEU:HD11	1:337:A:ALA:HB3	12	0.11
(1,1254)	1:324:A:LEU:HD12	1:337:A:ALA:HB1	12	0.11
(1,1254)	1:324:A:LEU:HD12	1:337:A:ALA:HB2	12	0.11
(1,1254)	1:324:A:LEU:HD12	1:337:A:ALA:HB3	12	0.11
(1,1254)	1:324:A:LEU:HD13	1:337:A:ALA:HB1	12	0.11
(1,1254)	1:324:A:LEU:HD13	1:337:A:ALA:HB2	12	0.11
(1,1254)	1:324:A:LEU:HD13	1:337:A:ALA:HB3	12	0.11
(1,1254)	1:324:A:LEU:HD21	1:337:A:ALA:HB1	12	0.11
(1,1254)	1:324:A:LEU:HD21	1:337:A:ALA:HB2	12	0.11
(1,1254)	1:324:A:LEU:HD21	1:337:A:ALA:HB3	12	0.11
(1,1254)	1:324:A:LEU:HD22	1:337:A:ALA:HB1	12	0.11
(1,1254)	1:324:A:LEU:HD22	1:337:A:ALA:HB2	12	0.11
(1,1254)	1:324:A:LEU:HD22	1:337:A:ALA:HB3	12	0.11
(1,1254)	1:324:A:LEU:HD23	1:337:A:ALA:HB1	12	0.11
(1,1254)	1:324:A:LEU:HD23	1:337:A:ALA:HB2	12	0.11
(1,1254)	1:324:A:LEU:HD23	1:337:A:ALA:HB3	12	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	11	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	11	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	11	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	11	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	11	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	11	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	11	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	11	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	11	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	11	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	11	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	11	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	11	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	11	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	11	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	11	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	11	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	11	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	11	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	11	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	11	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	11	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	11	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	11	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	11	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	11	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	11	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	11	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	11	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	11	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	11	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	11	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	11	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	11	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	11	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG11	15	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG12	15	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG13	15	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG21	15	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG22	15	0.11
(1,1018)	1:301:A:VAL:HG11	1:339:A:VAL:HG23	15	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG11	15	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG12	15	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG13	15	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG21	15	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG22	15	0.11
(1,1018)	1:301:A:VAL:HG12	1:339:A:VAL:HG23	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG11	15	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG12	15	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG13	15	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG21	15	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG22	15	0.11
(1,1018)	1:301:A:VAL:HG13	1:339:A:VAL:HG23	15	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG11	15	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG12	15	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG13	15	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG21	15	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG22	15	0.11
(1,1018)	1:301:A:VAL:HG21	1:339:A:VAL:HG23	15	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG11	15	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG12	15	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG13	15	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG21	15	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG22	15	0.11
(1,1018)	1:301:A:VAL:HG22	1:339:A:VAL:HG23	15	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG11	15	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG12	15	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG13	15	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG21	15	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG22	15	0.11
(1,1018)	1:301:A:VAL:HG23	1:339:A:VAL:HG23	15	0.11
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	19	0.11
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	20	0.11
(1,709)	1:357:A:LYS:HB2	1:358:A:GLU:H	2	0.11
(1,709)	1:357:A:LYS:HB3	1:358:A:GLU:H	2	0.11
(1,691)	1:355:A:ASP:H	1:356:A:GLY:H	14	0.11
(1,680)	1:354:A:PHE:H	1:355:A:ASP:H	3	0.11
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	1	0.11
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	19	0.11
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	20	0.11
(1,642)	1:351:A:ILE:HG12	1:352:A:ASP:H	8	0.11
(1,589)	1:347:A:ALA:HA	1:350:A:ALA:H	7	0.11
(1,567)	1:344:A:PRO:HA	1:347:A:ALA:H	12	0.11
(1,567)	1:344:A:PRO:HA	1:347:A:ALA:H	16	0.11
(1,395)	1:317:A:THR:HB	1:319:A:GLN:H	3	0.11
(1,392)	1:316:A:LYS:H	1:319:A:GLN:H	19	0.11
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	6	0.11
(1,370)	1:314:A:ASN:HD21	1:314:A:ASN:H	19	0.11
(1,352)	1:313:A:THR:HB	1:314:A:ASN:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:313:A:THR:HB	1:313:A:THR:H	13	0.11
(1,205)	1:298:A:ILE:HG12	1:298:A:ILE:H	10	0.11
(1,198)	1:298:A:ILE:HA	1:301:A:VAL:H	13	0.11
(1,198)	1:298:A:ILE:HA	1:301:A:VAL:H	18	0.11
(1,148)	1:293:A:GLY:H	1:294:A:GLU:H	12	0.11
(1,132)	1:291:A:GLY:H	1:293:A:GLY:H	19	0.11
(1,114)	1:290:A:GLN:HA	1:290:A:GLN:HE22	4	0.11
(1,101)	1:289:A:VAL:HB	1:337:A:ALA:H	9	0.11
(2,17)	1:367:A:SER:H	1:288:A:PHE:O	3	0.1
(2,17)	1:367:A:SER:H	1:288:A:PHE:O	11	0.1
(2,15)	1:359:A:PHE:H	1:362:A:ASN:O	17	0.1
(2,12)	1:340:A:SER:H	1:321:A:MET:O	7	0.1
(2,12)	1:340:A:SER:H	1:321:A:MET:O	8	0.1
(2,4)	1:304:A:TYR:H	1:300:A:SER:O	10	0.1
(1,1558)	1:370:A:THR:HA	1:370:A:THR:HB	10	0.1
(1,1558)	1:370:A:THR:HA	1:370:A:THR:HB	12	0.1
(1,1465)	1:354:A:PHE:HB2	1:366:A:VAL:HG11	8	0.1
(1,1465)	1:354:A:PHE:HB2	1:366:A:VAL:HG12	8	0.1
(1,1465)	1:354:A:PHE:HB2	1:366:A:VAL:HG13	8	0.1
(1,1465)	1:354:A:PHE:HB2	1:366:A:VAL:HG21	8	0.1
(1,1465)	1:354:A:PHE:HB2	1:366:A:VAL:HG22	8	0.1
(1,1465)	1:354:A:PHE:HB2	1:366:A:VAL:HG23	8	0.1
(1,1465)	1:354:A:PHE:HB3	1:366:A:VAL:HG11	8	0.1
(1,1465)	1:354:A:PHE:HB3	1:366:A:VAL:HG12	8	0.1
(1,1465)	1:354:A:PHE:HB3	1:366:A:VAL:HG13	8	0.1
(1,1465)	1:354:A:PHE:HB3	1:366:A:VAL:HG21	8	0.1
(1,1465)	1:354:A:PHE:HB3	1:366:A:VAL:HG22	8	0.1
(1,1465)	1:354:A:PHE:HB3	1:366:A:VAL:HG23	8	0.1
(1,1311)	1:333:A:LEU:HG	1:333:A:LEU:H	16	0.1
(1,1157)	1:311:A:ILE:HG21	1:320:A:PRO:HB2	14	0.1
(1,1157)	1:311:A:ILE:HG21	1:320:A:PRO:HB3	14	0.1
(1,1157)	1:311:A:ILE:HG22	1:320:A:PRO:HB2	14	0.1
(1,1157)	1:311:A:ILE:HG22	1:320:A:PRO:HB3	14	0.1
(1,1157)	1:311:A:ILE:HG23	1:320:A:PRO:HB2	14	0.1
(1,1157)	1:311:A:ILE:HG23	1:320:A:PRO:HB3	14	0.1
(1,946)	1:296:A:VAL:HA	1:296:A:VAL:HB	17	0.1
(1,946)	1:296:A:VAL:HA	1:296:A:VAL:HB	20	0.1
(1,716)	1:357:A:LYS:H	1:364:A:ILE:H	18	0.1
(1,691)	1:355:A:ASP:H	1:356:A:GLY:H	12	0.1
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	5	0.1
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	7	0.1
(1,668)	1:353:A:TRP:HE1	1:354:A:PHE:H	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,401)	1:317:A:THR:H	1:319:A:GLN:H	2	0.1
(1,372)	1:314:A:ASN:HD22	1:317:A:THR:H	11	0.1
(1,352)	1:313:A:THR:HB	1:314:A:ASN:H	14	0.1
(1,198)	1:298:A:ILE:HA	1:301:A:VAL:H	8	0.1
(1,198)	1:298:A:ILE:HA	1:301:A:VAL:H	9	0.1
(1,101)	1:289:A:VAL:HB	1:337:A:ALA:H	6	0.1
(1,37)	1:285:A:ASN:HA	1:347:A:ALA:H	16	0.1

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	47	50.0	4	8.5	4.3	0	0.0	0.0
PHI	47	50.0	6	12.8	6.4	0	0.0	0.0
Total	94	100.0	10	10.6	10.6	0	0.0	0.0

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

### 10.1.1 Bar chart : Distribution of dihedral-angles and violations ⓘ
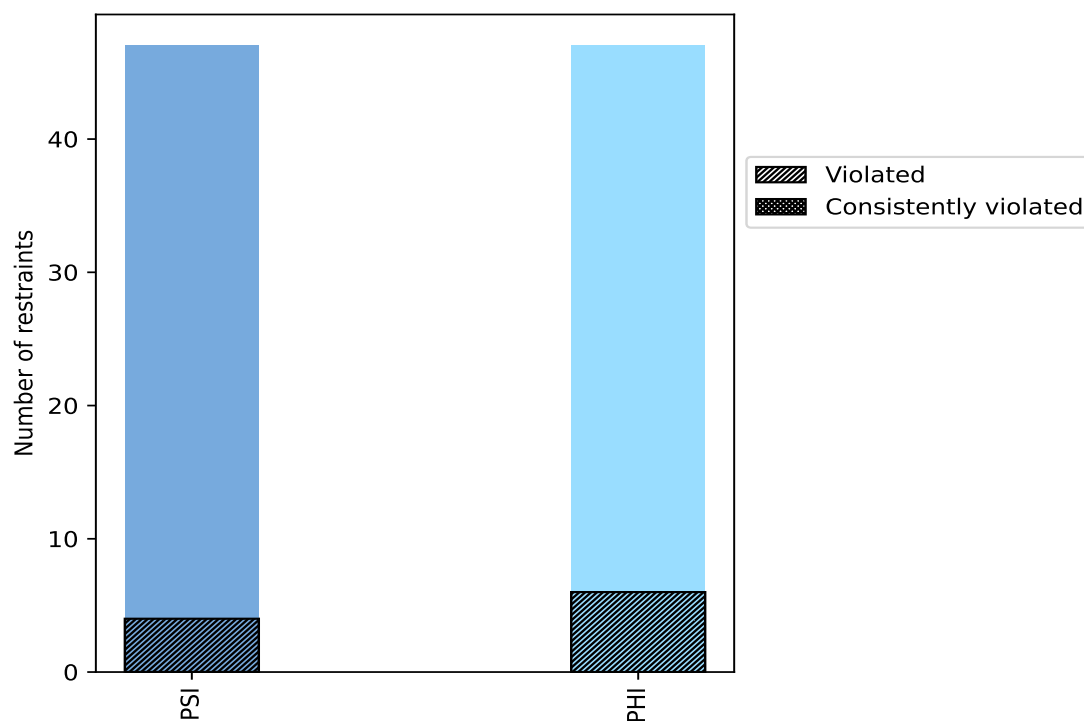
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	2	1	3	1.1	1.19	0.07	1.1
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	1	0	1	1.18	1.18	0.0	1.18
5	0	1	1	1.86	1.86	0.0	1.86
6	0	1	1	1.02	1.02	0.0	1.02
7	0	1	1	1.54	1.54	0.0	1.54
8	0	0	0	0.0	0.0	0.0	0.0
9	0	1	1	1.0	1.0	0.0	1.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	1	1	1.2	1.2	0.0	1.2
15	0	0	0	0.0	0.0	0.0	0.0
16	2	1	3	1.24	1.42	0.13	1.16
17	0	1	1	1.12	1.12	0.0	1.12
18	0	1	1	1.38	1.38	0.0	1.38
19	1	1	2	1.5	1.8	0.3	1.5
20	1	1	2	1.34	1.58	0.24	1.34

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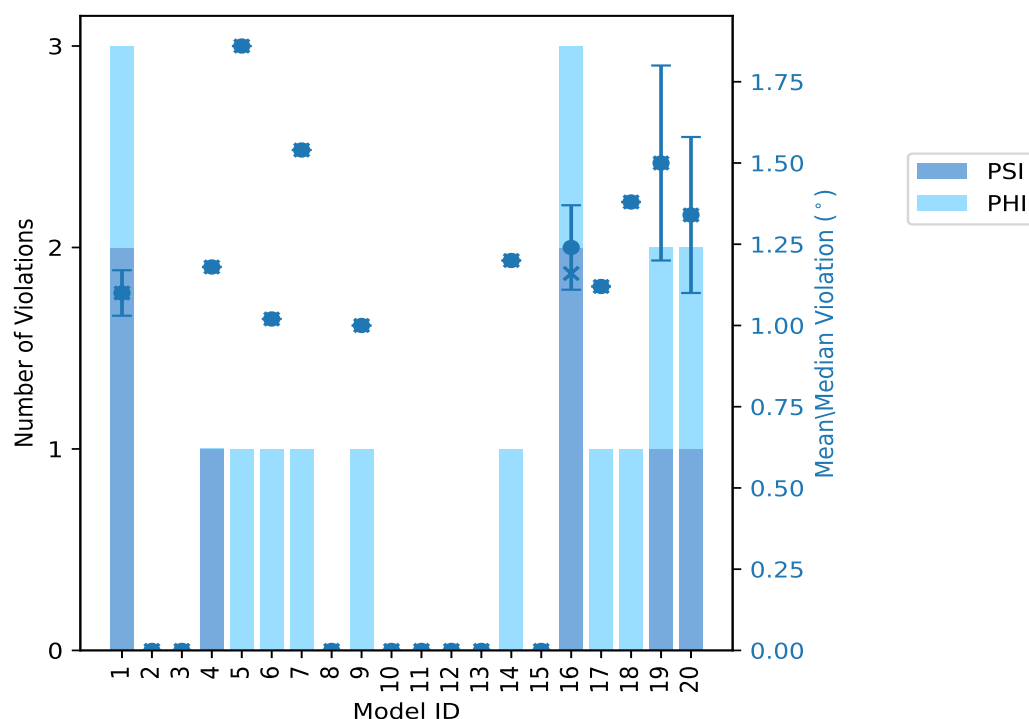
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

| Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	5	6	1	5.0
3	0	3	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	1	1	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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

[1] Number of models with violations

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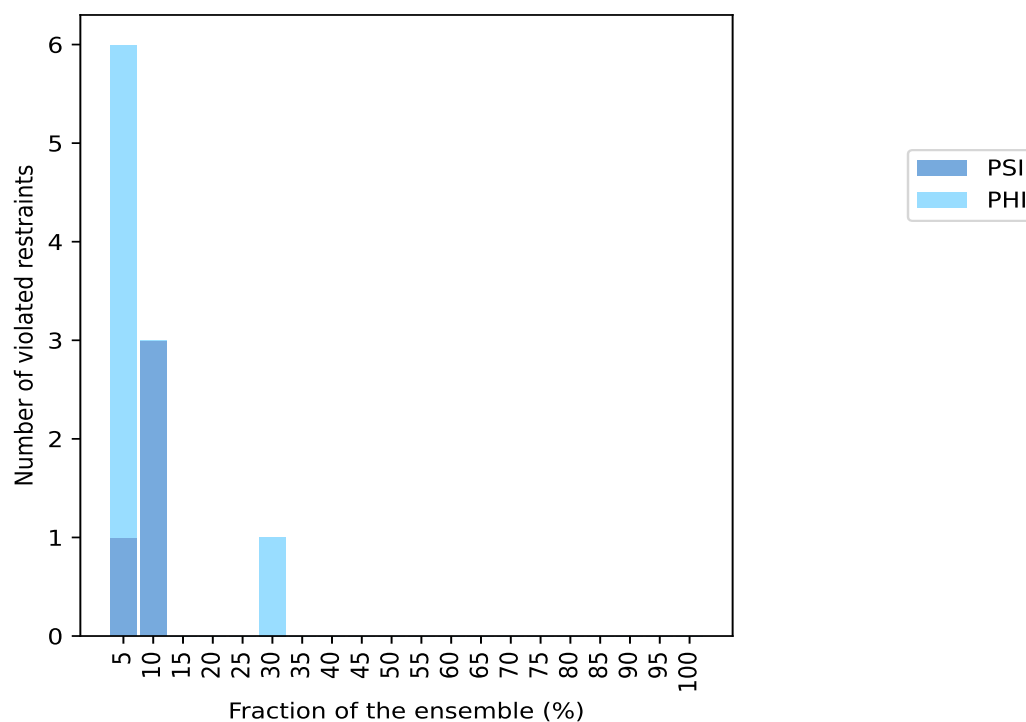
10.4   Most violated dihedral-angle restraints in the ensemble ⓘ

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
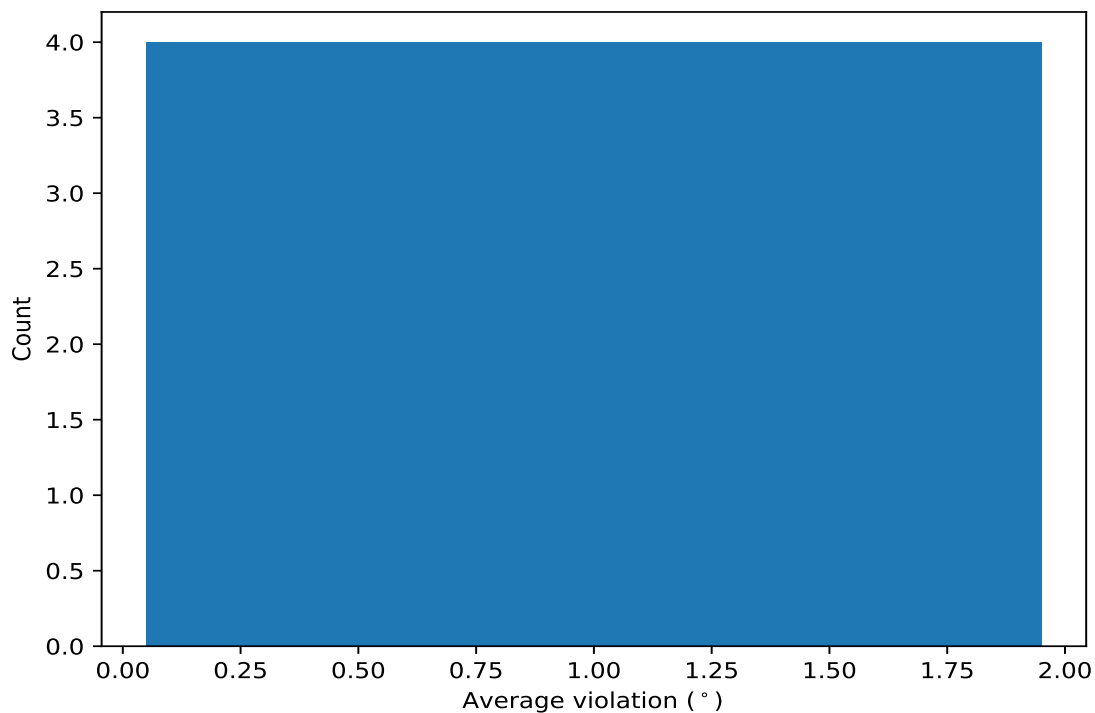
10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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.
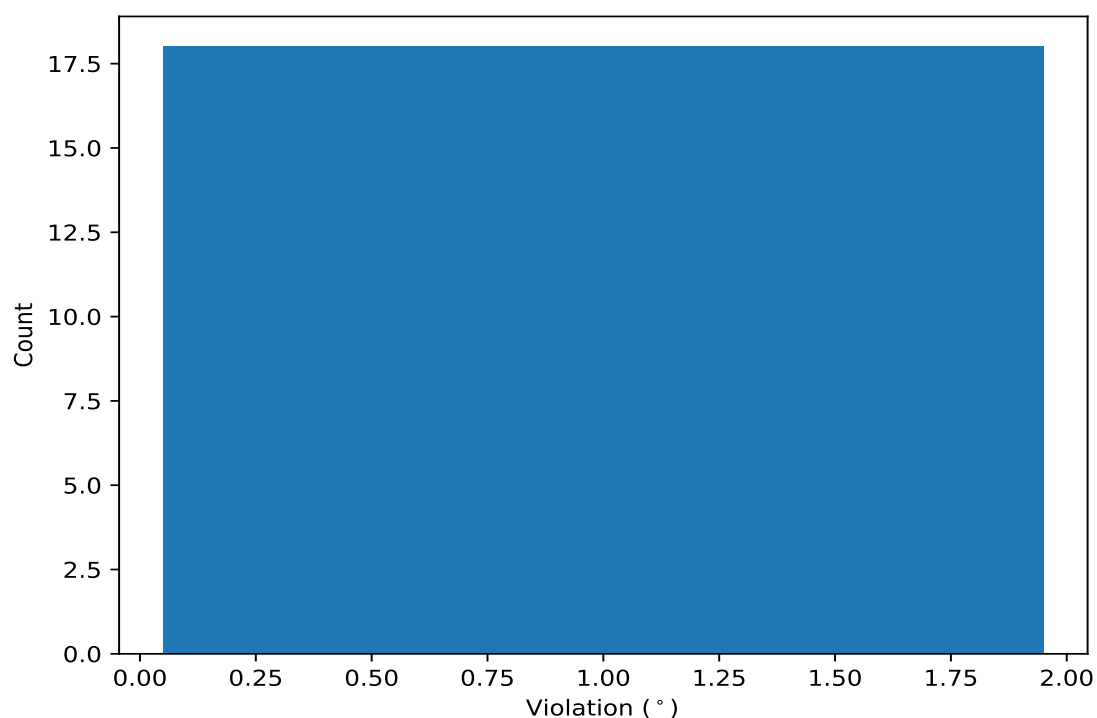
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,18)	1:318:A:GLY:C	1:319:A:GLN:N	1:319:A:GLN:CA	1:319:A:GLN:C	6	1.41	0.27	1.37
(1,54)	1:297:A:THR:N	1:297:A:THR:CA	1:297:A:THR:C	1:298:A:ILE:N	2	1.61	0.19	1.61
(1,88)	1:359:A:PHE:N	1:359:A:PHE:CA	1:359:A:PHE:C	1:360:A:SER:N	2	1.13	0.03	1.13
(1,53)	1:290:A:GLN:N	1:290:A:GLN:CA	1:290:A:GLN:C	1:291:A:GLY:N	2	1.1	0.08	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 (°)
(1,18)	1:318:A:GLY:C	1:319:A:GLN:N	1:319:A:GLN:CA	1:319:A:GLN:C	5	1.86
(1,54)	1:297:A:THR:N	1:297:A:THR:CA	1:297:A:THR:C	1:298:A:ILE:N	19	1.8
(1,18)	1:318:A:GLY:C	1:319:A:GLN:N	1:319:A:GLN:CA	1:319:A:GLN:C	20	1.58
(1,18)	1:318:A:GLY:C	1:319:A:GLN:N	1:319:A:GLN:CA	1:319:A:GLN:C	7	1.54
(1,54)	1:297:A:THR:N	1:297:A:THR:CA	1:297:A:THR:C	1:298:A:ILE:N	16	1.42
(1,21)	1:321:A:MET:C	1:322:A:ILE:N	1:322:A:ILE:CA	1:322:A:ILE:C	18	1.38
(1,8)	1:297:A:THR:C	1:298:A:ILE:N	1:298:A:ILE:CA	1:298:A:ILE:C	19	1.21
(1,18)	1:318:A:GLY:C	1:319:A:GLN:N	1:319:A:GLN:CA	1:319:A:GLN:C	14	1.2
(1,9)	1:298:A:ILE:C	1:299:A:GLU:N	1:299:A:GLU:CA	1:299:A:GLU:C	1	1.19
(1,53)	1:290:A:GLN:N	1:290:A:GLN:CA	1:290:A:GLN:C	1:291:A:GLY:N	4	1.18
(1,88)	1:359:A:PHE:N	1:359:A:PHE:CA	1:359:A:PHE:C	1:360:A:SER:N	16	1.16
(1,18)	1:318:A:GLY:C	1:319:A:GLN:N	1:319:A:GLN:CA	1:319:A:GLN:C	16	1.14
(1,18)	1:318:A:GLY:C	1:319:A:GLN:N	1:319:A:GLN:CA	1:319:A:GLN:C	17	1.12
(1,88)	1:359:A:PHE:N	1:359:A:PHE:CA	1:359:A:PHE:C	1:360:A:SER:N	20	1.1
(1,55)	1:298:A:ILE:N	1:298:A:ILE:CA	1:298:A:ILE:C	1:299:A:GLU:N	1	1.1
(1,53)	1:290:A:GLN:N	1:290:A:GLN:CA	1:290:A:GLN:C	1:291:A:GLY:N	1	1.02
(1,25)	1:326:A:THR:C	1:327:A:ASP:N	1:327:A:ASP:CA	1:327:A:ASP:C	6	1.02
(1,16)	1:311:A:ILE:C	1:312:A:LYS:N	1:312:A:LYS:CA	1:312:A:LYS:C	9	1.0