



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 01:16 PM UTC

PDB ID : 2JNU / pdb_00002jnu
BMRB ID : 15128
Title : Solution structure of the RGS domain of human RGS14
Authors : Dowler, E.F.; Diehl, A.; Bray, J.; Elkins, J.; Soundararajan, M.; Doyle, D.A.; Gileadi, C.; Phillips, C.; Schoch, G.A.; Yang, X.; Brockmann, C.; Leidert, M.; Rehbein, K.; Schmieder, P.; Kuhne, R.; Higman, V.A.; Sundstrom, M.; Arrowsmith, C.; Weigelt, J.; Edwards, A.; Oschkinat, H.; Ball, L.J.; Structural Genomics Consortium (SGC)
Deposited on : 2007-02-02

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

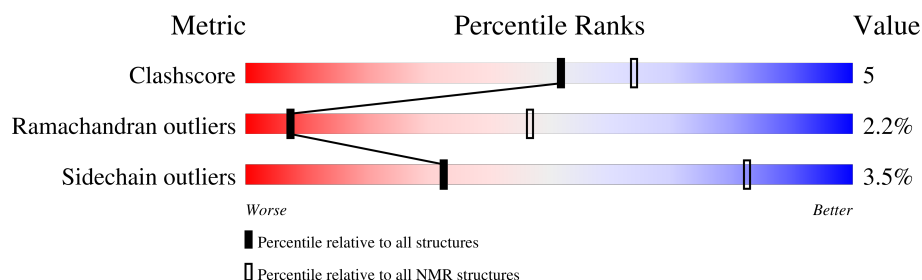
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	154	

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:130 (123)	1.10	5

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2203 atoms, of which 1084 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Regulator of G-protein signaling 14.

Mol	Chain	Residues	Atoms						Trace
1	A	136	Total	C	H	N	O	S	0
			2203	718	1084	185	211	5	

There are 2 discrepancies between the modelled and reference sequences:

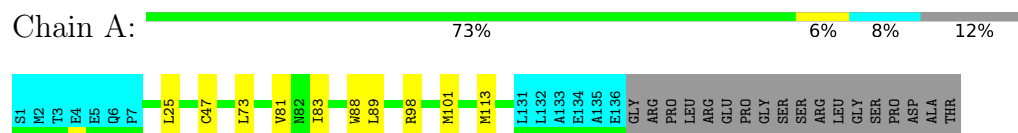
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	cloning artifact	UNP O43566
A	2	MET	-	cloning artifact	UNP O43566

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: Regulator of G-protein signaling 14

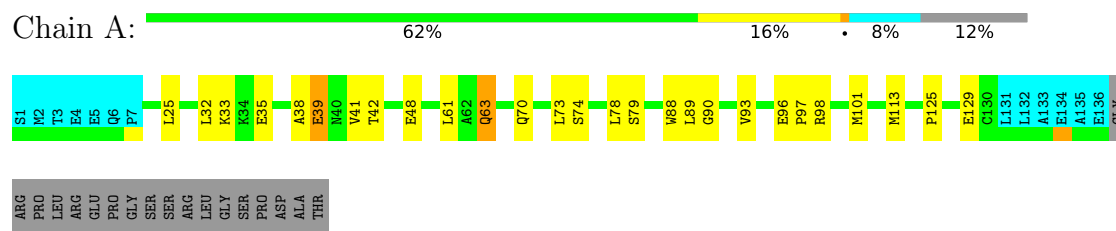


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

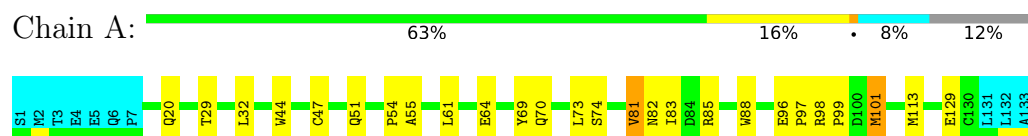
4.2.1 Score per residue for model 1

- Molecule 1: Regulator of G-protein signaling 14



4.2.2 Score per residue for model 2

- Molecule 1: Regulator of G-protein signaling 14



PRO
LEU
ARG
GLU
PRO
GLY
SER
SER
ARG
LEU
GLY
SER
PRO
ASP
ALA
THR

4.2.3 Score per residue for model 3

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 60% 18% 8% 12%

S1 M2 T3 E4 E5 E6 E7 Q20 L25 A26 E30 F36 E39 M40 V41 K45 P54 A55 Q59 E71 F72 L73 S74 S76 Q76 A77 L78 W88 L89 G90 E91 R98 P99 D100 M101 Q106 L107 Q108 I109 F110 M113 R128 E129 C130 L131 L132

A133 E134 A135 E136 GLY ARG PRO LEU ARG GLU PRO GLY SER SER ARG LEU GLY SER ASP ALA THR

4.2.4 Score per residue for model 4

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 69% 10% 8% 12%

S1 M2 T3 E4 E5 E6 E7 Q20 L25 F31 E39 K45 A46 C47 L73 S79 W88 L89 G90 V93 M101 F102 R103 I109 L126 L131 L132 A133 E134 A135 E136 GLY ARG PRO LEU ARG GLU PRO GLY SER SER ARG LEU GLY ASP

ALA
THR

4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 64% 14% 8% 12%

S1 M2 T3 E4 E5 E6 E7 V8 L13 L25 T29 L32 K33 E39 M40 W44 C47 Y69 L73 I83 W88 L89 R98 M101 F102 Q106 Q108 I109 M113 P125 G130 L131 L132 A133 E134 A135 E136 GLY ARG PRO LEU ARG

GLU PRO GLY SER SER ARG LEU GLY SER PRO ASP ALA THR

4.2.6 Score per residue for model 6

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 73% 7% 8% 12%



4.2.7 Score per residue for model 7

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 69% 9% 8% 12%



ALA
THR

4.2.8 Score per residue for model 8

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 67% 13% 8% 12%



GLY
SER
PRO
ASP
ALA
THR

4.2.9 Score per residue for model 9

- Molecule 1: Regulator of G-protein signaling 14

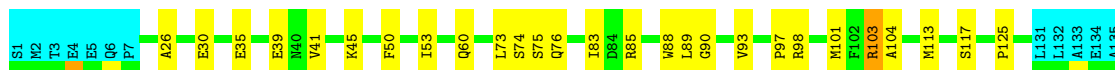
Chain A: 71% 8% 8% 12%

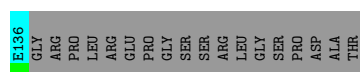


4.2.10 Score per residue for model 10

- Molecule 1: Regulator of G-protein signaling 14

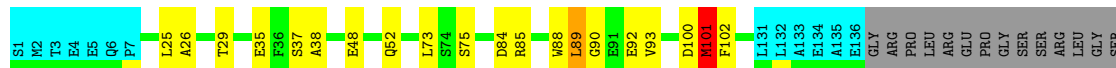
Chain A: 62% 17% 8% 12%





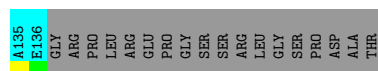
4.2.11 Score per residue for model 11

- Molecule 1: Regulator of G-protein signaling 14



4.2.12 Score per residue for model 12

- Molecule 1: Regulator of G-protein signaling 14



4.2.13 Score per residue for model 13

- Molecule 1: Regulator of G-protein signaling 14



4.2.14 Score per residue for model 14

- Molecule 1: Regulator of G-protein signaling 14

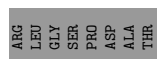
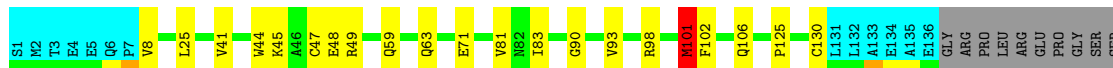




4.2.15 Score per residue for model 15

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 66% 13% 8% 12%



4.2.16 Score per residue for model 16

- Molecule 1: Regulator of G-protein signaling 14

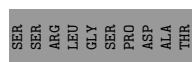
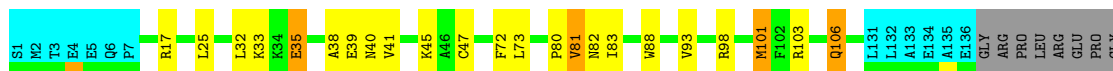
Chain A: 71% 7% 8% 12%



4.2.17 Score per residue for model 17

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 65% 12% 8% 12%



4.2.18 Score per residue for model 18

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 67% 12% 8% 12%



LEU
GLY
SER
PRO
ASP
ALA
THR

4.2.19 Score per residue for model 19

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 62% 16% 8% 12%

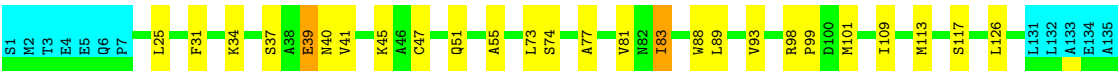


GLY
ARG
PRO
LEU
ARG
GLU
PRO
GLY
SER
SER
ARG
LEU
GLY
SER
PRO
ASP
ALA
THR

4.2.20 Score per residue for model 20

- Molecule 1: Regulator of G-protein signaling 14

Chain A: 63% 16% 8% 12%



E136
GLY
ARG
PRO
LEU
ARG
GLU
PRO
GLY
SER
SER
ARG
LEU
GLY
SER
PRO
ASP
ALA
THR

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
X-PLOR NIH	structure solution	2.14
X-PLOR NIH	refinement	2.14
CNSSOLVE	refinement	1.1

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	1729
Number of shifts mapped to atoms	1575
Number of unparsed shifts	0
Number of shifts with mapping errors	154
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1020	990	990	11±4
All	All	20400	19800	19800	216

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:MET:SD	1:A:102:PHE:N	0.76	2.58	13	3
1:A:89:LEU:HD13	1:A:89:LEU:H	0.66	1.50	7	1
1:A:70:GLN:HA	1:A:74:SER:HB2	0.65	1.68	18	3
1:A:8:VAL:HG11	1:A:130:CYS:SG	0.64	2.33	14	1
1:A:101:MET:SD	1:A:102:PHE:CG	0.63	2.92	13	1
1:A:89:LEU:HD22	1:A:101:MET:SD	0.62	2.34	9	1
1:A:93:VAL:HG23	1:A:101:MET:SD	0.62	2.33	19	1
1:A:97:PRO:HA	1:A:101:MET:SD	0.61	2.35	10	1
1:A:83:ILE:HG12	1:A:84:ASP:H	0.61	1.56	12	1
1:A:32:LEU:HG	1:A:38:ALA:HA	0.60	1.73	18	1
1:A:8:VAL:HG21	1:A:130:CYS:SG	0.60	2.37	5	2
1:A:47:CYS:SG	1:A:106:GLN:HB2	0.60	2.36	7	1
1:A:40:ASN:ND2	1:A:113:MET:SD	0.59	2.76	5	1
1:A:98:ARG:HG2	1:A:101:MET:HG2	0.57	1.75	7	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:TRP:O	1:A:47:CYS:SG	0.57	2.61	8	2
1:A:89:LEU:H	1:A:89:LEU:HD23	0.57	1.59	6	2
1:A:89:LEU:HD13	1:A:101:MET:SD	0.57	2.40	20	1
1:A:40:ASN:HB3	1:A:113:MET:SD	0.56	2.41	8	1
1:A:100:ASP:C	1:A:101:MET:SD	0.56	2.89	11	1
1:A:101:MET:HA	1:A:101:MET:HE3	0.55	1.79	8	1
1:A:73:LEU:HD13	1:A:88:TRP:CZ2	0.54	2.38	10	11
1:A:41:VAL:O	1:A:45:LYS:HG2	0.54	2.03	3	1
1:A:93:VAL:HG13	1:A:101:MET:SD	0.53	2.44	17	1
1:A:63:GLN:HE21	1:A:63:GLN:HA	0.53	1.64	1	1
1:A:47:CYS:SG	1:A:102:PHE:HB2	0.52	2.44	18	2
1:A:89:LEU:N	1:A:89:LEU:HD13	0.52	2.19	11	1
1:A:98:ARG:HG2	1:A:101:MET:SD	0.51	2.46	3	1
1:A:93:VAL:HA	1:A:101:MET:HE3	0.51	1.81	14	1
1:A:32:LEU:HD21	1:A:40:ASN:HD21	0.51	1.65	18	4
1:A:89:LEU:HD12	1:A:89:LEU:H	0.50	1.65	1	2
1:A:41:VAL:O	1:A:45:LYS:HG3	0.50	2.07	10	6
1:A:74:SER:O	1:A:76:GLN:N	0.50	2.44	10	2
1:A:39:GLU:HG2	1:A:79:SER:HB2	0.50	1.84	4	2
1:A:113:MET:HB2	1:A:117:SER:OG	0.50	2.07	7	1
1:A:100:ASP:O	1:A:102:PHE:N	0.50	2.44	11	1
1:A:47:CYS:HB3	1:A:101:MET:HE2	0.49	1.84	16	1
1:A:61:LEU:HB3	1:A:97:PRO:HB2	0.49	1.85	12	3
1:A:126:LEU:O	1:A:126:LEU:HD23	0.49	2.08	4	1
1:A:128:ARG:HG3	1:A:129:GLU:HG3	0.49	1.85	3	1
1:A:16:GLU:H	1:A:16:GLU:CD	0.49	2.15	8	1
1:A:35:GLU:H	1:A:35:GLU:CD	0.49	2.16	17	2
1:A:29:THR:O	1:A:33:LYS:HB3	0.48	2.08	5	1
1:A:81:VAL:HG23	1:A:83:ILE:HG12	0.48	1.83	15	1
1:A:44:TRP:NE1	1:A:106:GLN:HE21	0.48	2.06	5	2
1:A:98:ARG:HG2	1:A:101:MET:HE2	0.48	1.86	9	1
1:A:72:PHE:HA	1:A:79:SER:O	0.48	2.09	12	1
1:A:26:ALA:O	1:A:29:THR:HG22	0.48	2.09	11	1
1:A:47:CYS:HB3	1:A:106:GLN:HG2	0.47	1.85	15	1
1:A:48:GLU:O	1:A:52:GLN:HG2	0.47	2.09	11	1
1:A:113:MET:HB3	1:A:117:SER:HB2	0.47	1.85	18	1
1:A:101:MET:HG2	1:A:102:PHE:N	0.47	2.24	11	1
1:A:128:ARG:HG3	1:A:129:GLU:N	0.47	2.24	3	1
1:A:89:LEU:O	1:A:92:GLU:HG2	0.47	2.09	11	1
1:A:37:SER:O	1:A:40:ASN:ND2	0.47	2.48	20	1
1:A:54:PRO:O	1:A:99:PRO:HG3	0.47	2.10	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:HD13	1:A:88:TRP:CH2	0.47	2.45	5	2
1:A:44:TRP:HA	1:A:106:GLN:OE1	0.47	2.09	9	2
1:A:103:ARG:HD3	1:A:104:ALA:N	0.47	2.25	10	1
1:A:88:TRP:CZ3	1:A:90:GLY:HA2	0.47	2.45	19	1
1:A:93:VAL:HG22	1:A:101:MET:HE3	0.47	1.86	10	1
1:A:38:ALA:O	1:A:41:VAL:HG22	0.47	2.10	18	2
1:A:90:GLY:O	1:A:93:VAL:HG12	0.46	2.10	15	6
1:A:99:PRO:O	1:A:100:ASP:HB2	0.46	2.10	19	1
1:A:26:ALA:O	1:A:30:GLU:HG2	0.46	2.10	14	2
1:A:72:PHE:O	1:A:81:VAL:HG22	0.46	2.11	12	1
1:A:19:LEU:HD12	1:A:25:LEU:HG	0.46	1.87	18	1
1:A:113:MET:HE2	1:A:113:MET:HA	0.46	1.86	2	1
1:A:88:TRP:HE1	1:A:105:GLN:HG2	0.46	1.69	16	1
1:A:113:MET:HB3	1:A:117:SER:OG	0.46	2.10	6	1
1:A:84:ASP:CG	1:A:85:ARG:N	0.45	2.74	11	2
1:A:33:LYS:O	1:A:33:LYS:HD3	0.45	2.12	17	1
1:A:98:ARG:HG2	1:A:101:MET:HB2	0.45	1.88	19	1
1:A:89:LEU:H	1:A:89:LEU:HD22	0.45	1.72	4	1
1:A:55:ALA:HB2	1:A:99:PRO:HG3	0.45	1.88	19	2
1:A:96:GLU:HG3	1:A:98:ARG:HH21	0.45	1.71	2	1
1:A:89:LEU:N	1:A:89:LEU:HD12	0.45	2.27	3	1
1:A:11:TRP:HB3	1:A:18:LEU:HD12	0.45	1.89	6	1
1:A:74:SER:OG	1:A:77:ALA:HB2	0.45	2.11	20	1
1:A:8:VAL:HA	1:A:11:TRP:CE2	0.45	2.46	18	1
1:A:26:ALA:O	1:A:30:GLU:HG3	0.45	2.11	7	2
1:A:45:LYS:O	1:A:48:GLU:HG3	0.45	2.12	15	1
1:A:50:PHE:HZ	1:A:101:MET:SD	0.45	2.35	10	1
1:A:54:PRO:O	1:A:55:ALA:HB2	0.44	2.12	16	2
1:A:83:ILE:HG13	1:A:105:GLN:HG3	0.44	1.88	12	1
1:A:39:GLU:CD	1:A:39:GLU:H	0.44	2.20	10	1
1:A:83:ILE:HD13	1:A:83:ILE:H	0.44	1.72	20	1
1:A:44:TRP:NE1	1:A:106:GLN:NE2	0.44	2.66	13	2
1:A:29:THR:HA	1:A:32:LEU:HB3	0.44	1.88	2	1
1:A:103:ARG:HA	1:A:106:GLN:HG2	0.44	1.89	17	1
1:A:93:VAL:HG22	1:A:101:MET:SD	0.44	2.53	17	2
1:A:45:LYS:HB3	1:A:45:LYS:NZ	0.44	2.28	4	1
1:A:108:GLN:HE21	1:A:108:GLN:HA	0.44	1.73	16	1
1:A:84:ASP:O	1:A:86:GLN:N	0.44	2.50	7	1
1:A:48:GLU:HG3	1:A:51:GLN:HE21	0.44	1.73	18	1
1:A:89:LEU:HD12	1:A:89:LEU:N	0.43	2.28	1	1
1:A:70:GLN:HA	1:A:74:SER:OG	0.43	2.12	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:HD11	1:A:64:GLU:HG3	0.43	1.90	19	1
1:A:50:PHE:CZ	1:A:101:MET:SD	0.43	3.12	10	1
1:A:71:GLU:HA	1:A:78:LEU:HD13	0.43	1.90	8	1
1:A:113:MET:SD	1:A:117:SER:HB2	0.43	2.53	10	2
1:A:41:VAL:HG12	1:A:113:MET:SD	0.43	2.54	1	2
1:A:30:GLU:O	1:A:34:LYS:HG3	0.43	2.14	6	1
1:A:51:GLN:NE2	1:A:101:MET:SD	0.43	2.87	2	1
1:A:106:GLN:O	1:A:109:ILE:HG22	0.43	2.12	3	1
1:A:48:GLU:O	1:A:51:GLN:HG2	0.43	2.13	12	1
1:A:113:MET:HB2	1:A:117:SER:HB3	0.43	1.89	19	1
1:A:31:PHE:CD1	1:A:31:PHE:N	0.43	2.85	4	1
1:A:108:GLN:HA	1:A:111:ASN:HD21	0.43	1.74	13	1
1:A:113:MET:HB3	1:A:117:SER:HB3	0.43	1.90	10	1
1:A:31:PHE:HB2	1:A:126:LEU:HD12	0.43	1.90	20	1
1:A:47:CYS:O	1:A:51:GLN:HG2	0.43	2.14	20	2
1:A:77:ALA:O	1:A:78:LEU:HB2	0.43	2.14	19	1
1:A:54:PRO:O	1:A:99:PRO:HB3	0.43	2.14	2	1
1:A:36:PHE:O	1:A:39:GLU:HG3	0.43	2.13	3	1
1:A:20:GLN:HE21	1:A:20:GLN:HA	0.43	1.74	4	1
1:A:17:ARG:HA	1:A:17:ARG:NE	0.42	2.28	17	1
1:A:39:GLU:N	1:A:39:GLU:CD	0.42	2.77	5	1
1:A:28:PHE:O	1:A:32:LEU:HB2	0.42	2.14	9	1
1:A:83:ILE:HD13	1:A:83:ILE:N	0.42	2.28	20	1
1:A:47:CYS:SG	1:A:48:GLU:N	0.42	2.92	8	1
1:A:72:PHE:O	1:A:80:PRO:HA	0.42	2.15	17	1
1:A:88:TRP:NE1	1:A:105:GLN:NE2	0.42	2.68	5	1
1:A:46:ALA:O	1:A:50:PHE:HB2	0.42	2.15	8	1
1:A:85:ARG:HA	1:A:88:TRP:HB2	0.42	1.91	10	1
1:A:82:ASN:O	1:A:84:ASP:N	0.42	2.53	12	1
1:A:110:PHE:O	1:A:114:LYS:HB2	0.42	2.14	12	1
1:A:50:PHE:CD1	1:A:101:MET:HE3	0.42	2.50	13	1
1:A:70:GLN:O	1:A:77:ALA:HA	0.42	2.14	13	1
1:A:108:GLN:HA	1:A:111:ASN:ND2	0.42	2.29	13	1
1:A:16:GLU:O	1:A:20:GLN:HG2	0.42	2.14	8	1
1:A:39:GLU:HG2	1:A:81:VAL:HG12	0.42	1.91	20	1
1:A:109:ILE:O	1:A:113:MET:HG2	0.42	2.15	7	1
1:A:98:ARG:HG3	1:A:101:MET:H	0.42	1.75	12	1
1:A:20:GLN:NE2	1:A:44:TRP:HH2	0.42	2.13	2	1
1:A:32:LEU:O	1:A:38:ALA:HB2	0.41	2.15	1	1
1:A:71:GLU:O	1:A:77:ALA:HB1	0.41	2.15	3	1
1:A:19:LEU:HD12	1:A:25:LEU:HD21	0.41	1.90	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD12	1:A:78:LEU:N	0.41	2.30	1	1
1:A:98:ARG:O	1:A:101:MET:HG3	0.41	2.15	10	1
1:A:109:ILE:CG2	1:A:110:PHE:N	0.41	2.82	3	1
1:A:43:PHE:O	1:A:46:ALA:HB3	0.41	2.15	8	1
1:A:39:GLU:HB3	1:A:79:SER:HB3	0.41	1.93	1	1
1:A:96:GLU:HG3	1:A:96:GLU:O	0.41	2.16	1	1
1:A:69:TYR:HA	1:A:73:LEU:HB2	0.41	1.92	5	2
1:A:53:ILE:HD13	1:A:60:GLN:HB3	0.41	1.92	10	1
1:A:83:ILE:HG12	1:A:84:ASP:N	0.41	2.28	12	1
1:A:46:ALA:HB1	1:A:68:ILE:HG12	0.41	1.93	19	1
1:A:107:LEU:O	1:A:110:PHE:HB3	0.41	2.15	3	1
1:A:47:CYS:SG	1:A:103:ARG:HA	0.41	2.55	4	1
1:A:34:LYS:HE2	1:A:34:LYS:HA	0.41	1.91	7	1
1:A:59:GLN:O	1:A:63:GLN:HG2	0.41	2.16	15	1
1:A:47:CYS:SG	1:A:106:GLN:HG2	0.41	2.56	17	1
1:A:38:ALA:O	1:A:42:THR:HG22	0.40	2.16	1	1
1:A:78:LEU:N	1:A:78:LEU:HD12	0.40	2.31	3	1
1:A:89:LEU:HD23	1:A:89:LEU:N	0.40	2.30	5	1
1:A:102:PHE:N	1:A:102:PHE:CD1	0.40	2.89	9	1
1:A:89:LEU:HD22	1:A:89:LEU:H	0.40	1.75	10	1
1:A:88:TRP:CG	1:A:89:LEU:H	0.40	2.34	14	1
1:A:44:TRP:HA	1:A:47:CYS:SG	0.40	2.56	2	1
1:A:98:ARG:O	1:A:101:MET:HB2	0.40	2.17	3	1
1:A:17:ARG:HD3	1:A:17:ARG:C	0.40	2.42	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	123/154 (80%)	107±3 (87±2%)	13±3 (10±2%)	3±1 (2±1%)	7	47
All	All	2460/3080 (80%)	2149 (87%)	257 (10%)	54 (2%)	7	47

All 20 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	125	PRO	8
1	A	83	ILE	7
1	A	55	ALA	5
1	A	81	VAL	5
1	A	101	MET	5
1	A	75	SER	5
1	A	82	ASN	3
1	A	85	ARG	3
1	A	54	PRO	2
1	A	33	LYS	1
1	A	76	GLN	1
1	A	84	ASP	1
1	A	37	SER	1
1	A	38	ALA	1
1	A	126	LEU	1
1	A	88	TRP	1
1	A	71	GLU	1
1	A	90	GLY	1
1	A	100	ASP	1
1	A	116	ASP	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/133 (81%)	104±2 (96±2%)	4±2 (4±2%)	32	82
All	All	2160/2660 (81%)	2084 (96%)	76 (4%)	32	82

All 29 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	25	LEU	13
1	A	35	GLU	7
1	A	101	MET	7
1	A	109	ILE	5
1	A	39	GLU	3
1	A	81	VAL	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	20	GLN	3
1	A	89	LEU	3
1	A	83	ILE	3
1	A	98	ARG	3
1	A	129	GLU	2
1	A	64	GLU	2
1	A	76	GLN	2
1	A	91	GLU	2
1	A	33	LYS	2
1	A	34	LYS	2
1	A	106	GLN	2
1	A	48	GLU	1
1	A	63	GLN	1
1	A	59	GLN	1
1	A	88	TRP	1
1	A	52	GLN	1
1	A	40	ASN	1
1	A	103	ARG	1
1	A	92	GLU	1
1	A	112	LEU	1
1	A	49	ARG	1
1	A	71	GLU	1
1	A	108	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 82% 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	1729
Number of shifts mapped to atoms	1575
Number of unparsed shifts	0
Number of shifts with mapping errors	154
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 154 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	GLY	H	7.944	0.010	1
1	A	137	GLY	HA2	4.005	0.010	2
1	A	137	GLY	HA3	3.886	0.010	2
1	A	137	GLY	C	169.46	0.100	1
1	A	137	GLY	N	109.747	0.050	1
1	A	138	ARG	H	8.402	0.010	1
1	A	138	ARG	HA	4.695	0.010	1
1	A	138	ARG	HB2	1.646	0.010	2
1	A	138	ARG	HB3	1.79	0.010	2
1	A	138	ARG	HG2	1.611	0.010	1
1	A	138	ARG	HG3	1.611	0.010	1
1	A	138	ARG	C	168.099	0.100	1
1	A	138	ARG	CA	53.78	0.100	1
1	A	138	ARG	CB	31.456	0.100	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	ARG	N	121.283	0.050	1
1	A	139	PRO	HA	4.344	0.010	1
1	A	139	PRO	HB2	1.787	0.010	2
1	A	139	PRO	HB3	2.269	0.010	2
1	A	139	PRO	HD2	3.609	0.010	2
1	A	139	PRO	HD3	3.848	0.010	2
1	A	139	PRO	C	171.393	0.100	1
1	A	139	PRO	CB	32.406	0.100	1
1	A	139	PRO	CD	50.86	0.100	1
1	A	140	LEU	H	8.461	0.010	1
1	A	140	LEU	HA	4.359	0.010	1
1	A	140	LEU	HB2	1.616	0.010	2
1	A	140	LEU	HB3	1.777	0.010	2
1	A	140	LEU	HD11	0.954	0.010	2
1	A	140	LEU	HD12	0.954	0.010	2
1	A	140	LEU	HD13	0.954	0.010	2
1	A	140	LEU	HD21	0.903	0.010	2
1	A	140	LEU	HD22	0.903	0.010	2
1	A	140	LEU	HD23	0.903	0.010	2
1	A	140	LEU	C	171.73	0.100	1
1	A	140	LEU	CA	55.156	0.100	1
1	A	140	LEU	CB	43.124	0.100	1
1	A	140	LEU	N	124.095	0.050	1
1	A	141	ARG	H	8.538	0.010	1
1	A	141	ARG	HA	4.488	0.010	1
1	A	141	ARG	HB2	1.786	0.010	2
1	A	141	ARG	HB3	1.918	0.010	2
1	A	141	ARG	HD2	3.198	0.010	1
1	A	141	ARG	HD3	3.198	0.010	1
1	A	141	ARG	HG2	1.657	0.010	1
1	A	141	ARG	HG3	1.657	0.010	1
1	A	141	ARG	C	170.926	0.100	1
1	A	141	ARG	CA	55.017	0.100	1
1	A	141	ARG	CB	31.822	0.100	1
1	A	141	ARG	N	122.155	0.050	1
1	A	142	GLU	H	8.992	0.010	1
1	A	142	GLU	HA	4.289	0.010	1
1	A	142	GLU	HB2	1.94	0.010	1
1	A	142	GLU	HB3	1.94	0.010	1
1	A	142	GLU	HG2	2.281	0.010	1
1	A	142	GLU	HG3	2.281	0.010	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	142	GLU	C	169.492	0.100	1
1	A	142	GLU	CA	55.698	0.100	1
1	A	142	GLU	CB	28.9	0.100	1
1	A	142	GLU	N	124.071	0.050	1
1	A	143	PRO	HA	4.238	0.010	1
1	A	143	PRO	HB2	1.682	0.010	1
1	A	143	PRO	HB3	1.682	0.010	1
1	A	143	PRO	HD2	3.387	0.010	2
1	A	143	PRO	HD3	3.451	0.010	2
1	A	143	PRO	HG2	0.863	0.010	2
1	A	143	PRO	HG3	1.506	0.010	2
1	A	143	PRO	C	171.979	0.100	1
1	A	143	PRO	CA	64.093	0.100	1
1	A	143	PRO	CB	31.737	0.100	1
1	A	143	PRO	CG	27.012	0.100	1
1	A	144	GLY	H	8.7	0.010	1
1	A	144	GLY	HA2	3.97	0.010	2
1	A	144	GLY	HA3	3.87	0.010	2
1	A	144	GLY	C	169.313	0.100	1
1	A	144	GLY	N	109.63	0.050	1
1	A	145	SER	H	8.038	0.010	1
1	A	145	SER	HA	4.439	0.010	1
1	A	145	SER	HB2	3.864	0.010	2
1	A	145	SER	HB3	3.907	0.010	2
1	A	145	SER	C	169.577	0.100	1
1	A	145	SER	CA	58.878	0.100	1
1	A	145	SER	N	115.269	0.050	1
1	A	146	SER	H	8.389	0.010	1
1	A	146	SER	HA	4.279	0.010	1
1	A	146	SER	C	169.197	0.100	1
1	A	146	SER	N	117.901	0.050	1
1	A	147	ARG	H	8.332	0.010	1
1	A	147	ARG	HA	4.335	0.010	1
1	A	147	ARG	HB2	1.742	0.010	2
1	A	147	ARG	HB3	1.871	0.010	2
1	A	147	ARG	HD2	3.184	0.010	1
1	A	147	ARG	HD3	3.184	0.010	1
1	A	147	ARG	HG2	1.617	0.010	1
1	A	147	ARG	HG3	1.617	0.010	1
1	A	147	ARG	C	170.948	0.100	1
1	A	147	ARG	CA	56.357	0.100	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	ARG	CB	30.82	0.100	1
1	A	147	ARG	CG	27.448	0.100	1
1	A	147	ARG	N	122.479	0.050	1
1	A	148	LEU	H	8.274	0.010	1
1	A	148	LEU	HA	4.313	0.010	1
1	A	148	LEU	HB2	1.582	0.010	1
1	A	148	LEU	HB3	1.582	0.010	1
1	A	148	LEU	HD11	0.9	0.010	2
1	A	148	LEU	HD12	0.9	0.010	2
1	A	148	LEU	HD13	0.9	0.010	2
1	A	148	LEU	HD21	0.863	0.010	2
1	A	148	LEU	HD22	0.863	0.010	2
1	A	148	LEU	HD23	0.863	0.010	2
1	A	148	LEU	C	172.531	0.100	1
1	A	148	LEU	CA	55.639	0.100	1
1	A	148	LEU	CB	42.745	0.100	1
1	A	148	LEU	N	123.226	0.050	1
1	A	149	GLY	H	8.464	0.010	1
1	A	149	GLY	HA2	3.928	0.010	1
1	A	149	GLY	HA3	3.928	0.010	1
1	A	149	GLY	C	168.512	0.100	1
1	A	149	GLY	CA	45.364	0.100	1
1	A	149	GLY	N	109.99	0.050	1
1	A	150	SER	H	8.174	0.010	1
1	A	150	SER	HA	4.777	0.010	1
1	A	150	SER	HB2	3.798	0.010	2
1	A	150	SER	HB3	3.858	0.010	2
1	A	150	SER	C	167.909	0.100	1
1	A	150	SER	CA	56.579	0.100	1
1	A	150	SER	N	116.657	0.050	1
1	A	151	PRO	HA	4.437	0.010	1
1	A	151	PRO	HB2	1.969	0.010	2
1	A	151	PRO	HB3	2.281	0.010	2
1	A	151	PRO	C	171.31	0.100	1
1	A	151	PRO	CA	63.906	0.100	1
1	A	151	PRO	CB	32.366	0.100	1
1	A	152	ASP	H	8.285	0.010	1
1	A	152	ASP	HA	4.562	0.010	1
1	A	152	ASP	HB2	2.564	0.010	2
1	A	152	ASP	HB3	2.681	0.010	2
1	A	152	ASP	C	170.413	0.100	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	152	ASP	CB	41.324	0.100	1
1	A	152	ASP	N	119.487	0.050	1
1	A	153	ALA	H	8.105	0.010	1
1	A	153	ALA	HA	4.387	0.010	1
1	A	153	ALA	HB1	1.407	0.010	1
1	A	153	ALA	HB2	1.407	0.010	1
1	A	153	ALA	HB3	1.407	0.010	1
1	A	153	ALA	C	171.639	0.100	1
1	A	153	ALA	CA	52.77	0.100	1
1	A	153	ALA	CB	19.626	0.100	1
1	A	153	ALA	N	124.488	0.050	1
1	A	154	THR	H	7.79	0.010	1
1	A	154	THR	HA	4.119	0.010	1
1	A	154	THR	HB	4.201	0.010	1
1	A	154	THR	C	174.024	0.100	1
1	A	154	THR	CB	71.093	0.100	1
1	A	154	THR	N	118.814	0.050	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	134	-0.71 ± 0.11	Should be checked
$^{13}\text{C}_\beta$	126	0.07 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	150	4.97 ± 0.05	Should be applied
^{15}N	142	0.45 ± 0.47	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 1472 atoms were assigned a chemical shift out of a possible 1756. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	594/605 (98%)	242/242 (100%)	235/246 (96%)	117/117 (100%)
Sidechain	739/969 (76%)	532/626 (85%)	201/298 (67%)	6/45 (13%)
Aromatic	139/182 (76%)	80/89 (90%)	56/90 (62%)	3/3 (100%)
Overall	1472/1756 (84%)	854/957 (89%)	492/634 (78%)	126/165 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1575 atoms were assigned a chemical shift out of a possible 1919. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	644/668 (96%)	263/267 (99%)	254/272 (93%)	127/129 (98%)
Sidechain	792/1069 (74%)	574/691 (83%)	212/332 (64%)	6/46 (13%)
Aromatic	139/182 (76%)	80/89 (90%)	56/90 (62%)	3/3 (100%)
Overall	1575/1919 (82%)	917/1047 (88%)	522/694 (75%)	136/178 (76%)

7.1.4 Statistically unusual chemical shifts ⓘ

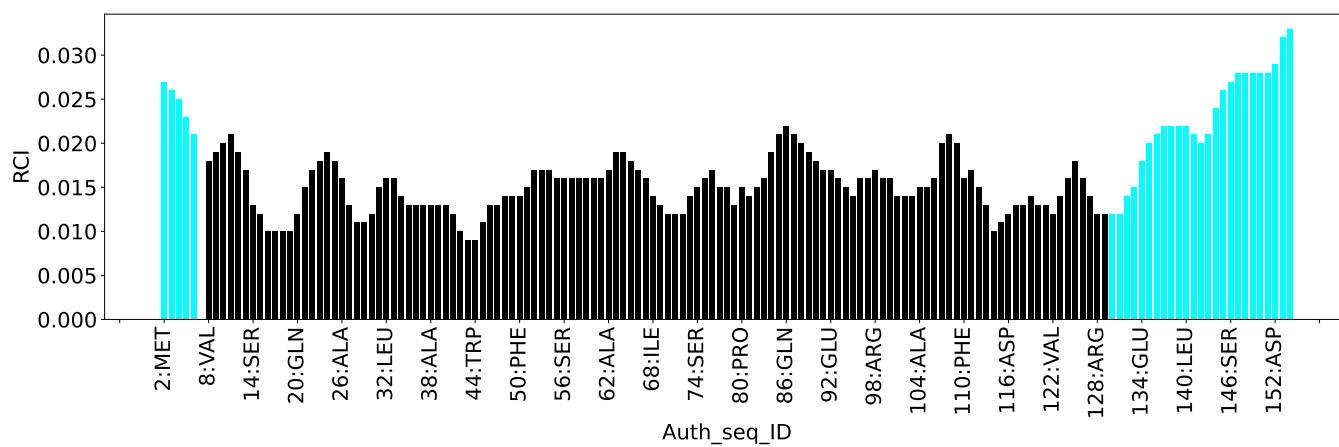
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	19	LEU	HD21	-1.03	-0.65 – 2.13	-6.3
1	A	19	LEU	HD22	-1.03	-0.65 – 2.13	-6.3
1	A	19	LEU	HD23	-1.03	-0.65 – 2.13	-6.3
1	A	24	GLY	HA2	1.73	2.15 – 5.77	-6.2
1	A	71	GLU	HG2	1.02	1.24 – 3.30	-6.0
1	A	96	GLU	C	166.91	167.55 – 186.36	-5.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2025
Intra-residue ($ i-j =0$)	1
Sequential ($ i-j =1$)	637
Medium range ($ i-j >1$ and $ i-j <5$)	611
Long range ($ i-j \geq 5$)	709
Inter-chain	0
Hydrogen bond restraints	67
Disulfide bond restraints	0
Total dihedral-angle restraints	14
Number of unmapped restraints	50
Number of restraints per residue	13.2
Number of long range restraints per residue ¹	4.6

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	7.4	0.2
0.2-0.5 (Medium)	2.2	0.5
>0.5 (Large)	1.4	1.26

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.3	3.24
10.0-20.0 (Medium)	0.1	14.17
>20.0 (Large)	None	None

9 Distance violation analysis

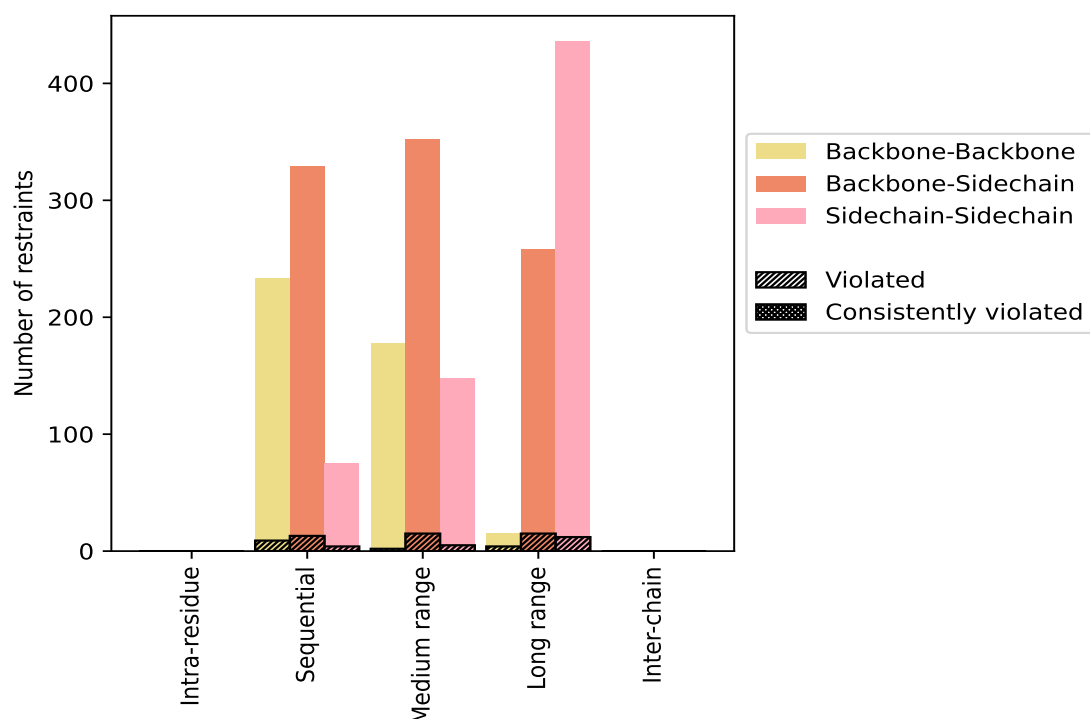
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1	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	1	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
Sequential ($i-j =1$)	637	31.5	26	4.1	1.3	0	0.0	0.0
Backbone-Backbone	233	11.5	9	3.9	0.4	0	0.0	0.0
Backbone-Sidechain	329	16.2	13	4.0	0.6	0	0.0	0.0
Sidechain-Sidechain	75	3.7	4	5.3	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	611	30.2	21	3.4	1.0	0	0.0	0.0
Backbone-Backbone	178	8.8	2	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	285	14.1	14	4.9	0.7	0	0.0	0.0
Sidechain-Sidechain	148	7.3	5	3.4	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	709	35.0	31	4.4	1.5	0	0.0	0.0
Backbone-Backbone	15	0.7	4	26.7	0.2	0	0.0	0.0
Backbone-Sidechain	258	12.7	15	5.8	0.7	0	0.0	0.0
Sidechain-Sidechain	436	21.5	12	2.8	0.6	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	67	3.3	1	1.5	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2025	100.0	79	3.9	3.9	0	0.0	0.0
Backbone-Backbone	426	21.0	15	3.5	0.7	0	0.0	0.0
Backbone-Sidechain	940	46.4	43	4.6	2.1	0	0.0	0.0
Sidechain-Sidechain	659	32.5	21	3.2	1.0	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	2	5	4	0	11	0.22	0.53	0.14	0.16
2	0	4	3	6	0	13	0.23	0.76	0.17	0.15
3	0	5	6	4	0	15	0.26	1.26	0.29	0.15
4	0	3	4	7	0	14	0.26	0.69	0.18	0.16
5	0	4	3	4	0	11	0.2	0.7	0.17	0.14
6	0	1	4	5	0	10	0.22	0.55	0.14	0.15
7	0	3	4	5	0	12	0.23	0.99	0.24	0.16
8	0	3	3	7	0	13	0.28	0.79	0.19	0.19
9	0	3	6	5	0	14	0.22	0.59	0.13	0.16
10	0	4	6	6	0	16	0.17	0.45	0.09	0.12

Continued on next page...

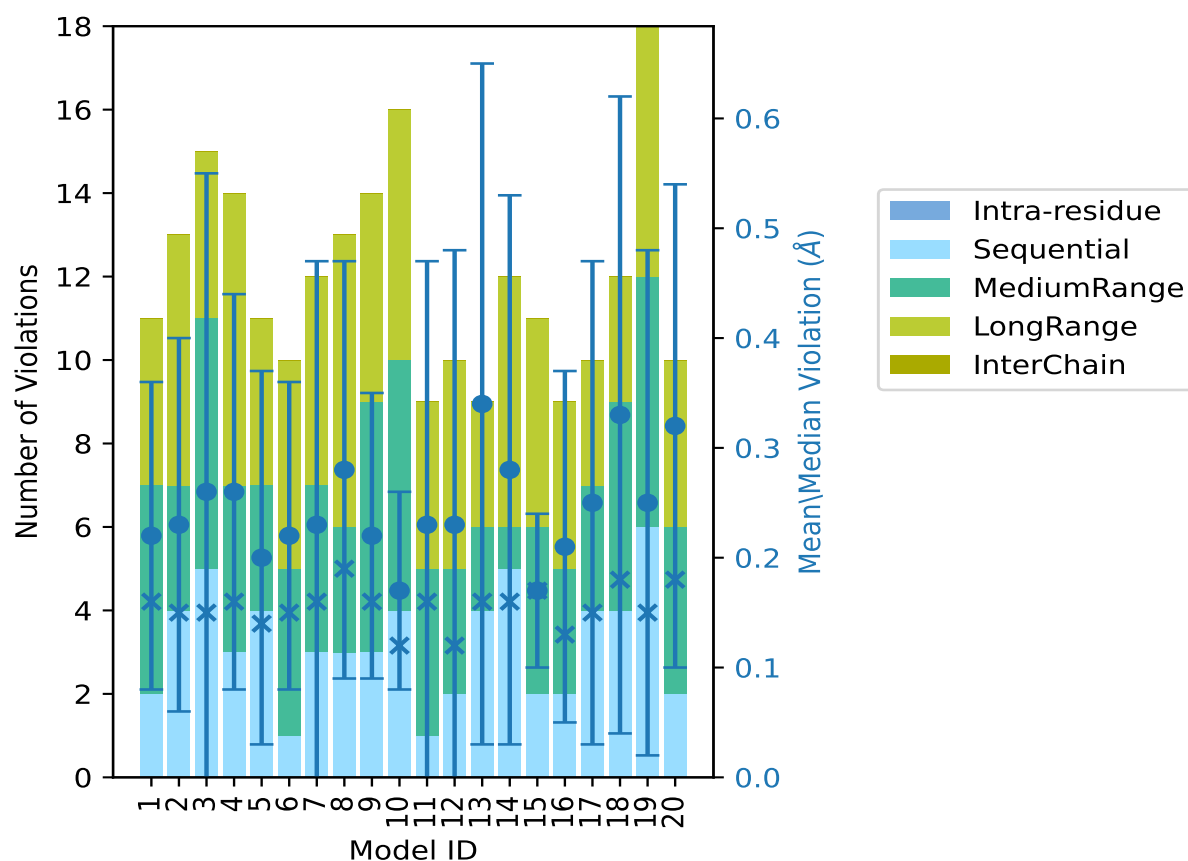
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	4	4	0	9	0.23	0.9	0.24	0.16
12	0	2	3	5	0	10	0.23	0.94	0.25	0.12
13	0	4	2	3	0	9	0.34	0.98	0.31	0.16
14	0	5	1	6	0	12	0.28	0.95	0.25	0.16
15	0	2	4	5	0	11	0.17	0.35	0.07	0.17
16	0	2	3	4	0	9	0.21	0.57	0.16	0.13
17	0	4	3	3	0	10	0.25	0.85	0.22	0.15
18	0	4	5	3	0	12	0.33	0.92	0.29	0.18
19	0	6	6	6	0	18	0.25	1.07	0.23	0.15
20	0	2	4	4	0	10	0.32	0.66	0.22	0.18

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

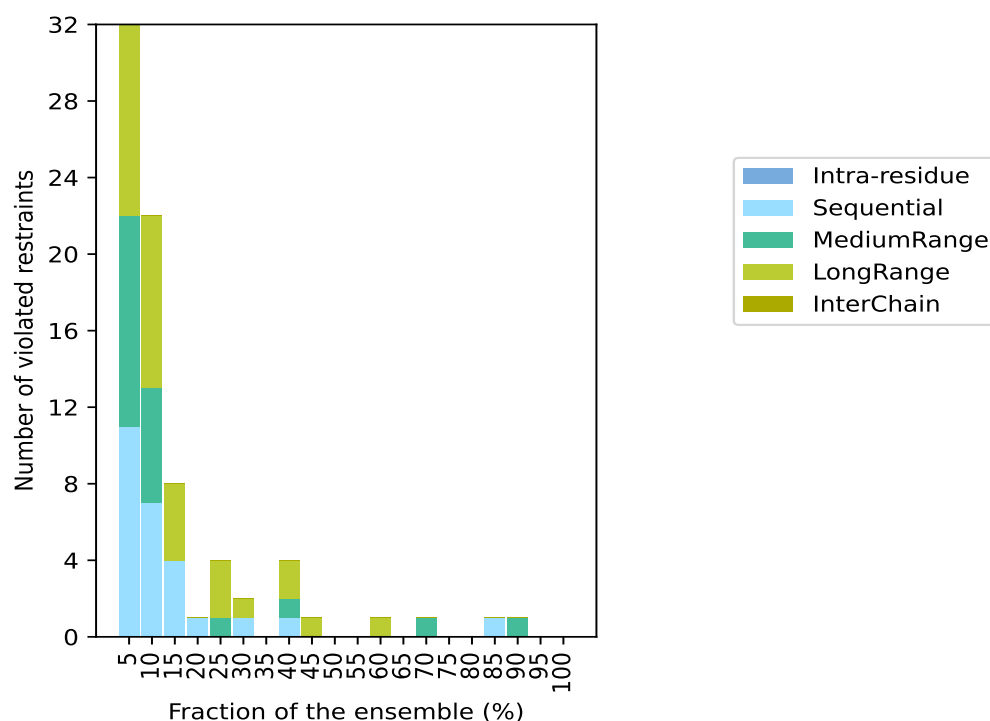
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1880(IR:1, SQ:611, MR:590, LR:678, IC:0) restraints are not 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	%
0	11	11	10	0	32	1	5.0
0	7	6	9	0	22	2	10.0
0	4	0	4	0	8	3	15.0
0	1	0	0	0	1	4	20.0
0	0	1	3	0	4	5	25.0
0	1	0	1	0	2	6	30.0
0	0	0	0	0	0	7	35.0
0	1	1	2	0	4	8	40.0
0	0	0	1	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	1	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	1	0	0	0	1	17	85.0
0	0	1	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

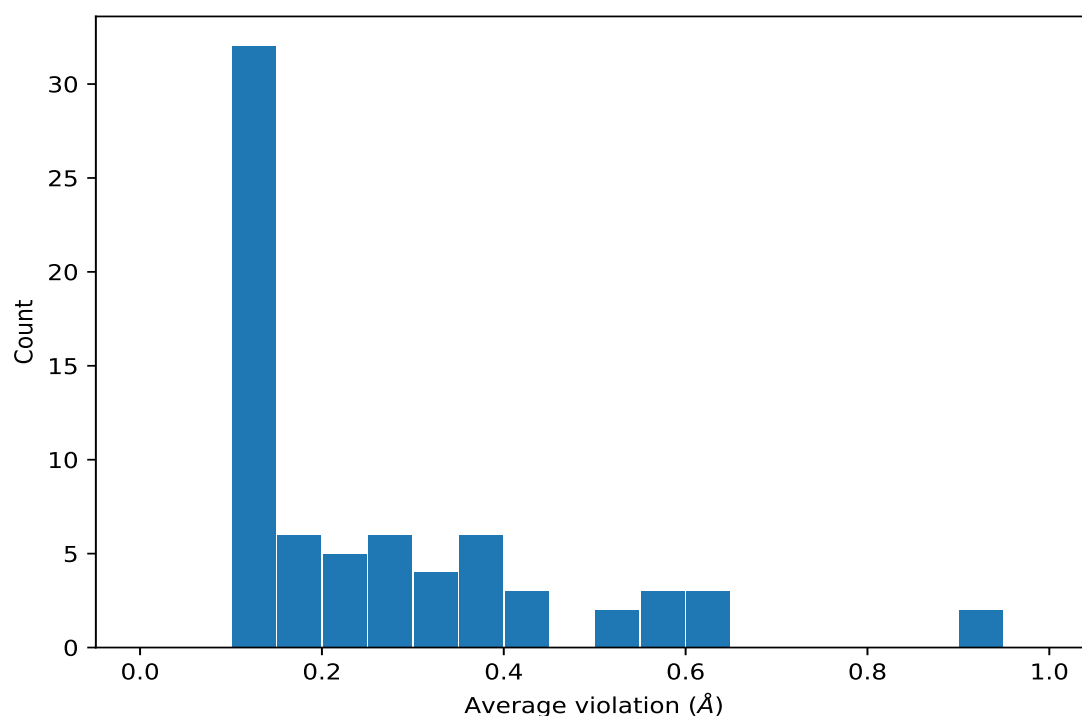
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	18	0.16	0.03	0.17
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	17	0.16	0.03	0.16
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	14	0.16	0.05	0.15
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	12	0.38	0.25	0.38
(1,849)	1:27:A:TYR:H	1:31:A:PHE:HE1	12	0.38	0.25	0.38
(1,849)	1:27:A:TYR:H	1:31:A:PHE:HE2	12	0.38	0.25	0.38
(1,1653)	1:79:A:SER:H	1:73:A:LEU:H	9	0.38	0.22	0.36
(1,1653)	1:79:A:SER:H	1:36:A:PHE:HE2	9	0.38	0.22	0.36
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE1	8	0.95	0.16	0.94
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE2	8	0.95	0.16	0.94
(1,612)	1:15:A:PHE:HD2	1:113:A:MET:HB3	8	0.39	0.19	0.47
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD11	8	0.15	0.05	0.13
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD12	8	0.15	0.05	0.13
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD13	8	0.15	0.05	0.13
(1,1590)	1:74:A:SER:H	1:71:A:GLU:HA	8	0.13	0.02	0.12
(1,930)	1:32:A:LEU:HD12	1:31:A:PHE:HB2	6	0.44	0.25	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,930)	1:32:A:LEU:HD13	1:31:A:PHE:HB2	6	0.44	0.25	0.42
(1,930)	1:32:A:LEU:HD11	1:31:A:PHE:HB2	6	0.44	0.25	0.42
(1,1701)	1:81:A:VAL:H	1:73:A:LEU:HG	6	0.35	0.05	0.34
(1,816)	1:25:A:LEU:HD23	1:42:A:THR:HA	5	0.58	0.21	0.6
(1,816)	1:25:A:LEU:HD22	1:42:A:THR:HA	5	0.58	0.21	0.6
(1,816)	1:25:A:LEU:HD21	1:42:A:THR:HA	5	0.58	0.21	0.6
(1,1643)	1:79:A:SER:HB3	1:36:A:PHE:HE2	5	0.28	0.09	0.26
(1,1643)	1:79:A:SER:HB2	1:72:A:PHE:HE1	5	0.28	0.09	0.26
(1,309)	1:118:A:TYR:H	1:113:A:MET:HB2	5	0.13	0.03	0.11
(1,328)	1:119:A:ALA:H	1:116:A:ASP:H	5	0.12	0.02	0.12
(1,969)	1:36:A:PHE:H	1:37:A:SER:HB3	4	0.14	0.03	0.13
(1,1864)	1:92:A:GLU:HG3	1:89:A:LEU:HD22	3	0.64	0.31	0.7
(1,1864)	1:92:A:GLU:HG3	1:93:A:VAL:HG23	3	0.64	0.31	0.7
(1,1864)	1:92:A:GLU:HG2	1:93:A:VAL:HG23	3	0.64	0.31	0.7
(1,195)	1:110:A:PHE:H	1:109:A:ILE:HB	3	0.29	0.12	0.27
(1,550)	1:135:A:ALA:H	1:134:A:GLU:H	3	0.21	0.06	0.17
(1,1715)	1:83:A:ILE:HB	1:108:A:GLN:HB3	3	0.16	0.04	0.16
(1,626)	1:15:A:PHE:H	1:14:A:SER:HB2	3	0.13	0.04	0.1
(1,381)	1:122:A:VAL:HA	1:11:A:TRP:HZ3	3	0.13	0.01	0.13
(1,1634)	1:78:A:LEU:H	1:71:A:GLU:HA	3	0.12	0.01	0.12
(1,160)	1:11:A:TRP:HE1	1:23:A:LEU:HG	3	0.11	0.01	0.11
(1,1642)	1:79:A:SER:HB2	1:72:A:PHE:HD1	2	0.5	0.02	0.5
(1,1642)	1:79:A:SER:HB3	1:36:A:PHE:HZ	2	0.5	0.02	0.5
(1,539)	1:133:A:ALA:H	1:134:A:GLU:HG3	2	0.35	0.23	0.35
(1,539)	1:133:A:ALA:H	1:129:A:GLU:HB2	2	0.35	0.23	0.35
(1,1396)	1:65:A:ALA:H	1:66:A:ARG:HB3	2	0.32	0.08	0.32
(1,1211)	1:5:A:GLU:H	1:4:A:GLU:HB2	2	0.25	0.07	0.25
(1,1649)	1:47:A:CYS:HA	1:68:A:ILE:HG21	2	0.25	0.01	0.25
(1,1649)	1:47:A:CYS:HA	1:68:A:ILE:HG22	2	0.25	0.01	0.25
(1,1210)	1:5:A:GLU:H	1:4:A:GLU:HB3	2	0.24	0.08	0.24
(1,1660)	1:79:A:SER:H	1:78:A:LEU:H	2	0.22	0.02	0.22
(1,885)	1:29:A:THR:H	1:18:A:LEU:HD13	2	0.22	0.1	0.22
(1,885)	1:29:A:THR:H	1:32:A:LEU:HD22	2	0.22	0.1	0.22
(1,544)	1:133:A:ALA:H	1:134:A:GLU:H	2	0.17	0.03	0.17
(1,18)	1:100:A:ASP:H	1:98:A:ARG:HG2	2	0.16	0.01	0.16
(1,1309)	1:59:A:GLN:H	1:58:A:THR:H	2	0.14	0.01	0.14
(1,1265)	1:55:A:ALA:HA	1:98:A:ARG:HA	2	0.12	0.02	0.12
(1,1288)	1:57:A:ASP:H	1:60:A:GLN:HB2	2	0.12	0.02	0.12
(1,846)	1:27:A:TYR:HE1	1:126:A:LEU:HB2	2	0.12	0.02	0.12
(1,846)	1:27:A:TYR:HE1	1:126:A:LEU:HB3	2	0.12	0.02	0.12
(1,846)	1:27:A:TYR:HE2	1:126:A:LEU:HB2	2	0.12	0.02	0.12
(1,846)	1:27:A:TYR:HE2	1:126:A:LEU:HB3	2	0.12	0.02	0.12

Continued on next page...

Continued from previous page...

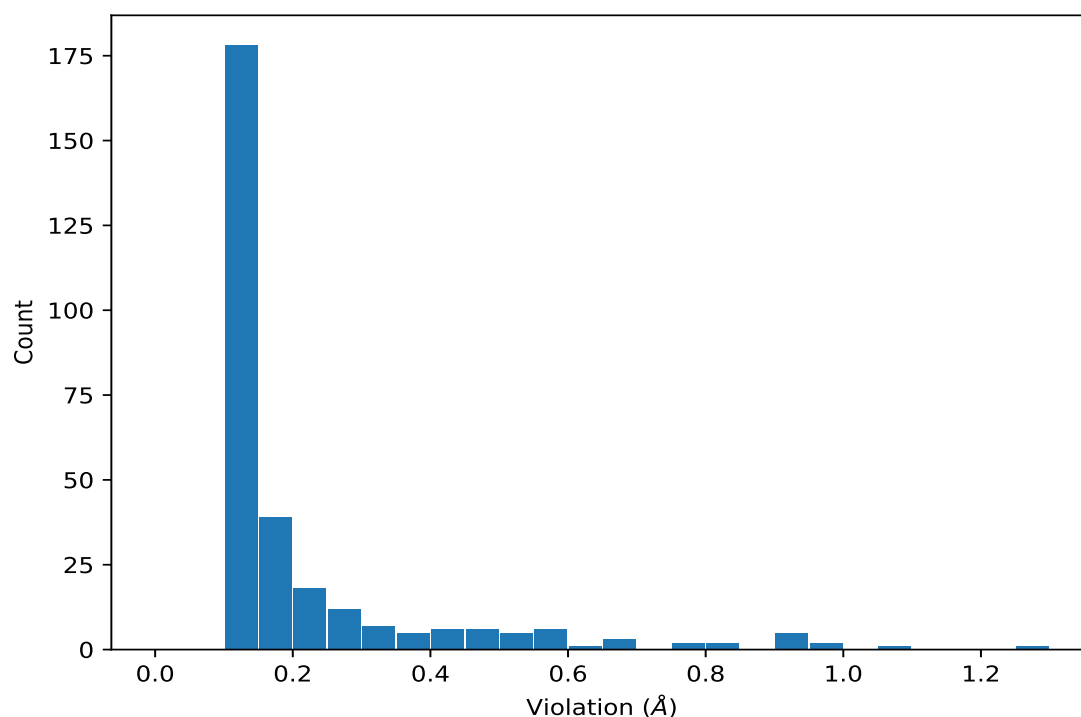
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,39)	1:102:A:PHE:HD1	1:89:A:LEU:HD11	2	0.12	0.01	0.12
(1,39)	1:102:A:PHE:HD1	1:89:A:LEU:HD12	2	0.12	0.01	0.12
(1,39)	1:102:A:PHE:HD1	1:89:A:LEU:HD13	2	0.12	0.01	0.12
(1,39)	1:102:A:PHE:HD2	1:89:A:LEU:HD11	2	0.12	0.01	0.12
(1,39)	1:102:A:PHE:HD2	1:89:A:LEU:HD12	2	0.12	0.01	0.12
(1,39)	1:102:A:PHE:HD2	1:89:A:LEU:HD13	2	0.12	0.01	0.12
(1,554)	1:136:A:GLU:H	1:135:A:ALA:H	2	0.12	0.0	0.12
(1,16)	1:100:A:ASP:H	1:97:A:PRO:HB2	2	0.11	0.0	0.11
(1,52)	1:102:A:PHE:H	1:98:A:ARG:HG2	2	0.11	0.01	0.11
(1,991)	1:38:A:ALA:H	1:32:A:LEU:HB2	2	0.11	0.0	0.11
(1,1855)	1:91:A:GLU:H	1:69:A:TYR:HE1	2	0.11	0.0	0.11
(1,1855)	1:91:A:GLU:H	1:69:A:TYR:HE2	2	0.11	0.0	0.11
(1,1106)	1:44:A:TRP:HE1	1:107:A:LEU:HG	2	0.11	0.0	0.11
(1,1779)	1:88:A:TRP:HE1	1:105:A:GLN:HA	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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)
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE1	3	1.26
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE1	19	1.07
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE1	7	0.99
(1,1864)	1:92:A:GLU:HG3	1:89:A:LEU:HD22	13	0.98
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE2	14	0.95
(1,816)	1:25:A:LEU:HD22	1:42:A:THR:HA	12	0.94
(1,930)	1:32:A:LEU:HD13	1:31:A:PHE:HB2	18	0.92
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE1	18	0.92
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE2	11	0.9
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE2	17	0.85
(1,1653)	1:79:A:SER:H	1:36:A:PHE:HE2	13	0.82
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	8	0.79
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	2	0.76
(1,1864)	1:92:A:GLU:HG2	1:93:A:VAL:HG23	5	0.7
(1,612)	1:15:A:PHE:HD2	1:113:A:MET:HB3	4	0.69
(1,907)	1:30:A:GLU:H	1:28:A:PHE:HE2	20	0.66
(1,816)	1:25:A:LEU:HD22	1:42:A:THR:HA	14	0.64
(1,816)	1:25:A:LEU:HD21	1:42:A:THR:HA	20	0.6
(1,1653)	1:79:A:SER:H	1:36:A:PHE:HE2	20	0.59
(1,849)	1:27:A:TYR:H	1:31:A:PHE:HE2	9	0.59
(1,539)	1:133:A:ALA:H	1:134:A:GLU:HG3	18	0.58
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	16	0.57
(1,1644)	1:79:A:SER:HB3	1:36:A:PHE:HD2	6	0.55
(1,612)	1:15:A:PHE:HD2	1:113:A:MET:HB3	1	0.53
(1,1642)	1:79:A:SER:HB3	1:36:A:PHE:HZ	20	0.52
(1,1653)	1:79:A:SER:H	1:73:A:LEU:H	4	0.51
(1,612)	1:15:A:PHE:HD2	1:113:A:MET:HB3	19	0.51
(1,930)	1:32:A:LEU:HD11	1:31:A:PHE:HB2	19	0.5
(1,1642)	1:79:A:SER:HB2	1:72:A:PHE:HD1	4	0.49
(1,612)	1:15:A:PHE:HD2	1:113:A:MET:HB3	8	0.48
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	1	0.47
(1,612)	1:15:A:PHE:HD2	1:113:A:MET:HB3	3	0.46
(1,849)	1:27:A:TYR:H	1:31:A:PHE:HE2	10	0.45
(1,195)	1:110:A:PHE:H	1:109:A:ILE:HB	3	0.45
(1,1653)	1:79:A:SER:H	1:73:A:LEU:H	8	0.44
(1,930)	1:32:A:LEU:HD13	1:31:A:PHE:HB2	14	0.43
(1,1701)	1:81:A:VAL:H	1:73:A:LEU:HG	16	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:81:A:VAL:H	1:73:A:LEU:HG	8	0.41
(1,1396)	1:65:A:ALA:H	1:66:A:ARG:HB3	9	0.41
(1,930)	1:32:A:LEU:HD11	1:31:A:PHE:HB2	17	0.4
(1,1643)	1:79:A:SER:HB3	1:36:A:PHE:HE2	6	0.39
(1,1643)	1:79:A:SER:HB3	1:36:A:PHE:HE2	4	0.38
(1,816)	1:25:A:LEU:HD23	1:42:A:THR:HA	2	0.37
(1,1701)	1:81:A:VAL:H	1:73:A:LEU:HG	9	0.36
(1,1653)	1:79:A:SER:H	1:73:A:LEU:H	7	0.36
(1,816)	1:25:A:LEU:HD23	1:42:A:THR:HA	15	0.35
(1,1701)	1:81:A:VAL:H	1:73:A:LEU:HG	12	0.33
(1,1211)	1:5:A:GLU:H	1:4:A:GLU:HB2	13	0.32
(1,1210)	1:5:A:GLU:H	1:4:A:GLU:HB3	4	0.32
(1,885)	1:29:A:THR:H	1:32:A:LEU:HD22	19	0.32
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	5	0.32
(1,324)	1:119:A:ALA:HB1	1:123:A:LYS:HE3	10	0.31
(1,550)	1:135:A:ALA:H	1:134:A:GLU:H	2	0.3
(1,1701)	1:81:A:VAL:H	1:73:A:LEU:HG	2	0.29
(1,1701)	1:81:A:VAL:H	1:73:A:LEU:HG	17	0.29
(1,1653)	1:79:A:SER:H	1:73:A:LEU:H	6	0.29
(1,195)	1:110:A:PHE:H	1:109:A:ILE:HB	14	0.27
(1,1649)	1:47:A:CYS:HA	1:68:A:ILE:HG21	8	0.26
(1,1643)	1:79:A:SER:HB2	1:72:A:PHE:HE1	18	0.26
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	10	0.26
(1,1660)	1:79:A:SER:H	1:78:A:LEU:H	13	0.25
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD11	9	0.25
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD12	9	0.25
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD13	9	0.25
(1,1864)	1:92:A:GLU:HG3	1:93:A:VAL:HG23	4	0.24
(1,1649)	1:47:A:CYS:HA	1:68:A:ILE:HG22	15	0.24
(1,1396)	1:65:A:ALA:H	1:66:A:ARG:HB3	19	0.24
(1,1643)	1:79:A:SER:HB2	1:72:A:PHE:HE1	14	0.23
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	1	0.23
(1,1715)	1:83:A:ILE:HB	1:108:A:GLN:HB3	11	0.22
(1,930)	1:32:A:LEU:HD12	1:31:A:PHE:HB2	3	0.22
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	8	0.21
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	12	0.21
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD11	18	0.21
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD12	18	0.21
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD13	18	0.21
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	20	0.2
(1,1823)	1:89:A:LEU:H	1:90:A:GLY:H	19	0.2
(1,1660)	1:79:A:SER:H	1:78:A:LEU:H	10	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	3	0.2
(1,612)	1:15:A:PHE:HD2	1:113:A:MET:HB3	15	0.2
(1,544)	1:133:A:ALA:H	1:134:A:GLU:H	10	0.2
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	1	0.19
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	3	0.19
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	19	0.19
(1,1239)	1:53:A:ILE:HD11	1:64:A:GLU:HB2	8	0.19
(1,1239)	1:53:A:ILE:HD12	1:64:A:GLU:HB2	8	0.19
(1,1239)	1:53:A:ILE:HD13	1:64:A:GLU:HB2	8	0.19
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	1	0.19
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	2	0.19
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	11	0.19
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	18	0.19
(1,626)	1:15:A:PHE:H	1:14:A:SER:HB2	19	0.19
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	8	0.18
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	9	0.18
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	15	0.18
(1,1211)	1:5:A:GLU:H	1:4:A:GLU:HB2	14	0.18
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	8	0.18
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	9	0.18
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	15	0.18
(1,309)	1:118:A:TYR:H	1:113:A:MET:HB2	6	0.18
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	7	0.17
(1,1653)	1:79:A:SER:H	1:73:A:LEU:H	9	0.17
(1,1142)	1:45:A:LYS:HD3	1:42:A:THR:HA	3	0.17
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	15	0.17
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	20	0.17
(1,969)	1:36:A:PHE:H	1:37:A:SER:HB3	11	0.17
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	4	0.17
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	16	0.17
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	17	0.17
(1,550)	1:135:A:ALA:H	1:134:A:GLU:H	7	0.17
(1,328)	1:119:A:ALA:H	1:116:A:ASP:H	18	0.17
(1,307)	1:118:A:TYR:H	1:113:A:MET:HA	7	0.17
(1,18)	1:100:A:ASP:H	1:98:A:ARG:HG2	18	0.17
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	2	0.16
(1,1715)	1:83:A:ILE:HB	1:108:A:GLN:HB3	1	0.16
(1,1590)	1:74:A:SER:H	1:71:A:GLU:HA	11	0.16
(1,1210)	1:5:A:GLU:H	1:4:A:GLU:HB3	13	0.16
(1,930)	1:32:A:LEU:HD12	1:31:A:PHE:HB2	7	0.16
(1,550)	1:135:A:ALA:H	1:134:A:GLU:H	6	0.16
(1,195)	1:110:A:PHE:H	1:109:A:ILE:HB	5	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	4	0.15
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	17	0.15
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	18	0.15
(1,1710)	1:82:A:ASN:H	1:81:A:VAL:HB	5	0.15
(1,1653)	1:79:A:SER:H	1:73:A:LEU:H	2	0.15
(1,1606)	1:76:A:GLN:H	1:74:A:SER:HB3	3	0.15
(1,1590)	1:74:A:SER:H	1:71:A:GLU:HA	9	0.15
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	16	0.15
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	17	0.15
(1,1029)	1:40:A:ASN:H	1:39:A:GLU:HB3	1	0.15
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD11	7	0.15
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD12	7	0.15
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD13	7	0.15
(1,969)	1:36:A:PHE:H	1:37:A:SER:HB3	3	0.15
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	13	0.15
(1,661)	1:17:A:ARG:HA	1:16:A:GLU:HG2	8	0.15
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	5	0.15
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	19	0.15
(1,612)	1:15:A:PHE:HD2	1:113:A:MET:HB3	9	0.15
(1,300)	1:117:A:SER:H	1:120:A:ARG:HB3	15	0.15
(1,18)	1:100:A:ASP:H	1:98:A:ARG:HG2	19	0.15
(2,64)	1:127:A:TYR:O	1:131:A:LEU:H	20	0.14
(1,1775)	1:88:A:TRP:HD1	1:85:A:ARG:HB2	9	0.14
(1,1643)	1:79:A:SER:HB2	1:72:A:PHE:HE1	5	0.14
(1,1634)	1:78:A:LEU:H	1:71:A:GLU:HA	13	0.14
(1,1630)	1:77:A:ALA:H	1:76:A:GLN:H	3	0.14
(1,1590)	1:74:A:SER:H	1:71:A:GLU:HA	1	0.14
(1,1309)	1:59:A:GLN:H	1:58:A:THR:H	9	0.14
(1,1288)	1:57:A:ASP:H	1:60:A:GLN:HB2	11	0.14
(1,1265)	1:55:A:ALA:HA	1:98:A:ARG:HA	2	0.14
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	19	0.14
(1,846)	1:27:A:TYR:HE1	1:126:A:LEU:HB2	7	0.14
(1,846)	1:27:A:TYR:HE1	1:126:A:LEU:HB3	7	0.14
(1,846)	1:27:A:TYR:HE2	1:126:A:LEU:HB2	7	0.14
(1,846)	1:27:A:TYR:HE2	1:126:A:LEU:HB3	7	0.14
(1,662)	1:17:A:ARG:H	1:16:A:GLU:HB3	17	0.14
(1,544)	1:133:A:ALA:H	1:134:A:GLU:H	12	0.14
(1,381)	1:122:A:VAL:HA	1:11:A:TRP:HZ3	4	0.14
(1,309)	1:118:A:TYR:H	1:113:A:MET:HB2	2	0.14
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	14	0.13
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	16	0.13
(1,1590)	1:74:A:SER:H	1:71:A:GLU:HA	8	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:59:A:GLN:H	1:58:A:THR:H	10	0.13
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	4	0.13
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD11	14	0.13
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD12	14	0.13
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD13	14	0.13
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD11	17	0.13
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD12	17	0.13
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD13	17	0.13
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	6	0.13
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	13	0.13
(1,612)	1:15:A:PHE:HD2	1:113:A:MET:HB3	7	0.13
(1,481)	1:129:A:GLU:H	1:126:A:LEU:HG	18	0.13
(1,381)	1:122:A:VAL:HA	1:11:A:TRP:HZ3	10	0.13
(1,160)	1:11:A:TRP:HE1	1:23:A:LEU:HG	15	0.13
(1,39)	1:102:A:PHE:HD1	1:89:A:LEU:HD11	10	0.13
(1,39)	1:102:A:PHE:HD1	1:89:A:LEU:HD12	10	0.13
(1,39)	1:102:A:PHE:HD1	1:89:A:LEU:HD13	10	0.13
(1,39)	1:102:A:PHE:HD2	1:89:A:LEU:HD11	10	0.13
(1,39)	1:102:A:PHE:HD2	1:89:A:LEU:HD12	10	0.13
(1,39)	1:102:A:PHE:HD2	1:89:A:LEU:HD13	10	0.13
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	10	0.12
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	12	0.12
(1,1867)	1:92:A:GLU:H	1:93:A:VAL:HA	13	0.12
(1,1634)	1:78:A:LEU:H	1:71:A:GLU:HA	19	0.12
(1,1590)	1:74:A:SER:H	1:71:A:GLU:HA	7	0.12
(1,1590)	1:74:A:SER:H	1:71:A:GLU:HA	12	0.12
(1,1487)	1:70:A:GLN:HG3	1:69:A:TYR:HE1	2	0.12
(1,1487)	1:70:A:GLN:HG3	1:69:A:TYR:HE2	2	0.12
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	6	0.12
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	7	0.12
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	9	0.12
(1,1020)	1:40:A:ASN:HD21	1:32:A:LEU:HG	5	0.12
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	19	0.12
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	10	0.12
(1,554)	1:136:A:GLU:H	1:135:A:ALA:H	18	0.12
(1,554)	1:136:A:GLU:H	1:135:A:ALA:H	20	0.12
(1,539)	1:133:A:ALA:H	1:129:A:GLU:HB2	12	0.12
(1,469)	1:128:A:ARG:HA	1:131:A:LEU:HB3	3	0.12
(1,328)	1:119:A:ALA:H	1:116:A:ASP:H	3	0.12
(1,328)	1:119:A:ALA:H	1:116:A:ASP:H	9	0.12
(1,52)	1:102:A:PHE:H	1:98:A:ARG:HG2	16	0.12
(1,1855)	1:91:A:GLU:H	1:69:A:TYR:HE1	12	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1855)	1:91:A:GLU:H	1:69:A:TYR:HE2	12	0.11
(1,1855)	1:91:A:GLU:H	1:69:A:TYR:HE1	14	0.11
(1,1855)	1:91:A:GLU:H	1:69:A:TYR:HE2	14	0.11
(1,1779)	1:88:A:TRP:HE1	1:105:A:GLN:HA	11	0.11
(1,1716)	1:83:A:ILE:HD11	1:105:A:GLN:HA	19	0.11
(1,1716)	1:83:A:ILE:HD12	1:105:A:GLN:HA	19	0.11
(1,1716)	1:83:A:ILE:HD13	1:105:A:GLN:HA	19	0.11
(1,1715)	1:83:A:ILE:HB	1:108:A:GLN:HB3	14	0.11
(1,1685)	1:81:A:VAL:HG11	1:109:A:ILE:HG12	15	0.11
(1,1685)	1:81:A:VAL:HG12	1:109:A:ILE:HG12	15	0.11
(1,1685)	1:81:A:VAL:HG13	1:109:A:ILE:HG12	15	0.11
(1,1634)	1:78:A:LEU:H	1:71:A:GLU:HA	10	0.11
(1,1590)	1:74:A:SER:H	1:71:A:GLU:HA	5	0.11
(1,1288)	1:57:A:ASP:H	1:60:A:GLN:HB2	10	0.11
(1,1287)	1:57:A:ASP:H	1:56:A:SER:H	8	0.11
(1,1267)	1:55:A:ALA:HA	1:99:A:PRO:HB2	14	0.11
(1,1265)	1:55:A:ALA:HA	1:98:A:ARG:HA	16	0.11
(1,1251)	1:53:A:ILE:H	1:52:A:GLN:HB3	15	0.11
(1,1114)	1:44:A:TRP:HE1	1:48:A:GLU:HB3	4	0.11
(1,1106)	1:44:A:TRP:HE1	1:107:A:LEU:HG	12	0.11
(1,1068)	1:41:A:VAL:H	1:44:A:TRP:HE3	2	0.11
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD11	4	0.11
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD12	4	0.11
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD13	4	0.11
(1,1001)	1:39:A:GLU:HB3	1:72:A:PHE:HA	17	0.11
(1,991)	1:38:A:ALA:H	1:32:A:LEU:HB2	11	0.11
(1,991)	1:38:A:ALA:H	1:32:A:LEU:HB2	20	0.11
(1,969)	1:36:A:PHE:H	1:37:A:SER:HB3	17	0.11
(1,969)	1:36:A:PHE:H	1:37:A:SER:HB3	19	0.11
(1,885)	1:29:A:THR:H	1:18:A:LEU:HD13	1	0.11
(1,883)	1:29:A:THR:HG21	1:26:A:ALA:HB1	1	0.11
(1,883)	1:29:A:THR:HG21	1:26:A:ALA:HB2	1	0.11
(1,883)	1:29:A:THR:HG21	1:26:A:ALA:HB3	1	0.11
(1,883)	1:29:A:THR:HG22	1:26:A:ALA:HB1	1	0.11
(1,883)	1:29:A:THR:HG22	1:26:A:ALA:HB2	1	0.11
(1,883)	1:29:A:THR:HG22	1:26:A:ALA:HB3	1	0.11
(1,883)	1:29:A:THR:HG23	1:26:A:ALA:HB1	1	0.11
(1,883)	1:29:A:THR:HG23	1:26:A:ALA:HB2	1	0.11
(1,883)	1:29:A:THR:HG23	1:26:A:ALA:HB3	1	0.11
(1,849)	1:27:A:TYR:H	1:11:A:TRP:HZ3	3	0.11
(1,849)	1:27:A:TYR:H	1:31:A:PHE:HE1	4	0.11
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	6	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	7	0.11
(1,660)	1:16:A:GLU:H	1:19:A:LEU:HG	20	0.11
(1,381)	1:122:A:VAL:HA	1:11:A:TRP:HZ3	11	0.11
(1,328)	1:119:A:ALA:H	1:116:A:ASP:H	6	0.11
(1,309)	1:118:A:TYR:H	1:113:A:MET:HB2	10	0.11
(1,309)	1:118:A:TYR:H	1:113:A:MET:HB2	18	0.11
(1,160)	1:11:A:TRP:HE1	1:23:A:LEU:HG	8	0.11
(1,39)	1:102:A:PHE:HD1	1:89:A:LEU:HD11	9	0.11
(1,39)	1:102:A:PHE:HD1	1:89:A:LEU:HD12	9	0.11
(1,39)	1:102:A:PHE:HD1	1:89:A:LEU:HD13	9	0.11
(1,39)	1:102:A:PHE:HD2	1:89:A:LEU:HD11	9	0.11
(1,39)	1:102:A:PHE:HD2	1:89:A:LEU:HD12	9	0.11
(1,39)	1:102:A:PHE:HD2	1:89:A:LEU:HD13	9	0.11
(1,16)	1:100:A:ASP:H	1:97:A:PRO:HB2	5	0.11
(1,16)	1:100:A:ASP:H	1:97:A:PRO:HB2	6	0.11
(1,1856)	1:91:A:GLU:H	1:88:A:TRP:HH2	19	0.1
(1,1825)	1:9:A:ALA:HA	1:127:A:TYR:HE1	19	0.1
(1,1825)	1:9:A:ALA:HA	1:127:A:TYR:HE2	19	0.1
(1,1779)	1:88:A:TRP:HE1	1:105:A:GLN:HA	10	0.1
(1,1653)	1:79:A:SER:H	1:73:A:LEU:H	5	0.1
(1,1590)	1:74:A:SER:H	1:71:A:GLU:HA	15	0.1
(1,1106)	1:44:A:TRP:HE1	1:107:A:LEU:HG	16	0.1
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD11	3	0.1
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD12	3	0.1
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD13	3	0.1
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD11	19	0.1
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD12	19	0.1
(1,1007)	1:39:A:GLU:H	1:32:A:LEU:HD13	19	0.1
(1,846)	1:27:A:TYR:HE1	1:126:A:LEU:HB2	3	0.1
(1,846)	1:27:A:TYR:HE1	1:126:A:LEU:HB3	3	0.1
(1,846)	1:27:A:TYR:HE2	1:126:A:LEU:HB2	3	0.1
(1,846)	1:27:A:TYR:HE2	1:126:A:LEU:HB3	3	0.1
(1,744)	1:20:A:GLN:H	1:19:A:LEU:HB2	14	0.1
(1,682)	1:18:A:LEU:HD21	1:19:A:LEU:HD11	16	0.1
(1,682)	1:18:A:LEU:HD21	1:19:A:LEU:HD12	16	0.1
(1,682)	1:18:A:LEU:HD21	1:19:A:LEU:HD13	16	0.1
(1,682)	1:18:A:LEU:HD22	1:19:A:LEU:HD11	16	0.1
(1,682)	1:18:A:LEU:HD22	1:19:A:LEU:HD12	16	0.1
(1,682)	1:18:A:LEU:HD22	1:19:A:LEU:HD13	16	0.1
(1,682)	1:18:A:LEU:HD23	1:19:A:LEU:HD11	16	0.1
(1,682)	1:18:A:LEU:HD23	1:19:A:LEU:HD12	16	0.1
(1,682)	1:18:A:LEU:HD23	1:19:A:LEU:HD13	16	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:15:A:PHE:H	1:14:A:SER:HB2	2	0.1
(1,626)	1:15:A:PHE:H	1:14:A:SER:HB2	5	0.1
(1,374)	1:121:A:PHE:H	1:123:A:LYS:HB3	10	0.1
(1,328)	1:119:A:ALA:H	1:116:A:ASP:H	1	0.1
(1,309)	1:118:A:TYR:H	1:113:A:MET:HB2	12	0.1
(1,160)	1:11:A:TRP:HE1	1:23:A:LEU:HG	10	0.1
(1,52)	1:102:A:PHE:H	1:98:A:ARG:HG2	2	0.1
(1,51)	1:102:A:PHE:H	1:68:A:ILE:HD11	4	0.1
(1,51)	1:102:A:PHE:H	1:68:A:ILE:HD12	4	0.1
(1,51)	1:102:A:PHE:H	1:68:A:ILE:HD13	4	0.1

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

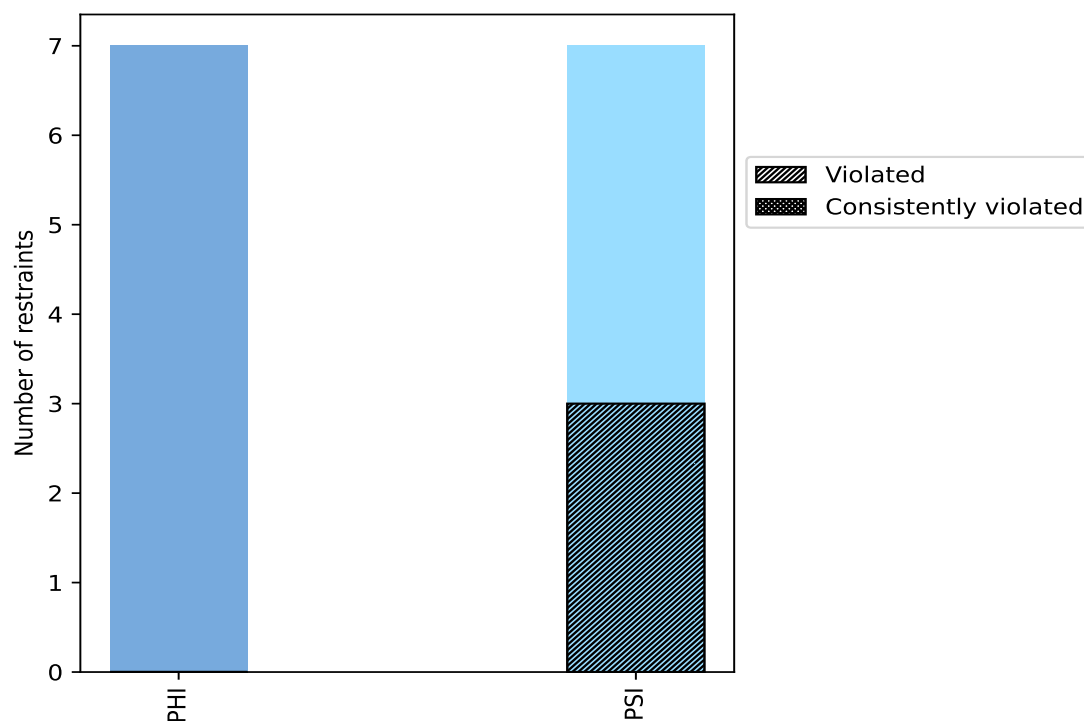
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	7	50.0	0	0.0	0.0	0	0.0	0.0
PSI	7	50.0	3	42.9	21.4	0	0.0	0.0
Total	14	100.0	3	21.4	21.4	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



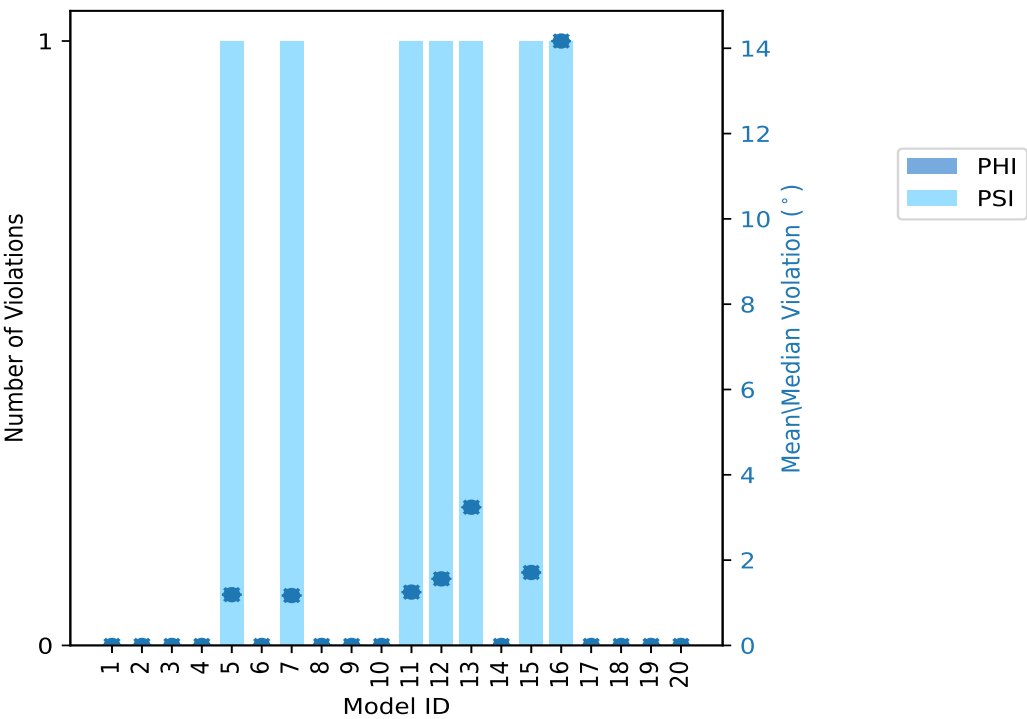
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
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	0	0	0	0.0	0.0	0.0	0.0
5	0	1	1	1.19	1.19	0.0	1.19
6	0	0	0	0.0	0.0	0.0	0.0
7	0	1	1	1.17	1.17	0.0	1.17
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	1	1	1.25	1.25	0.0	1.25
12	0	1	1	1.56	1.56	0.0	1.56
13	0	1	1	3.24	3.24	0.0	3.24
14	0	0	0	0.0	0.0	0.0	0.0
15	0	1	1	1.71	1.71	0.0	1.71
16	0	1	1	14.17	14.17	0.0	14.17
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

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	
PHI	PSI	Total	Count ¹	%
0	0	0	1	5.0
0	2	2	2	10.0
0	1	1	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	0	0	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

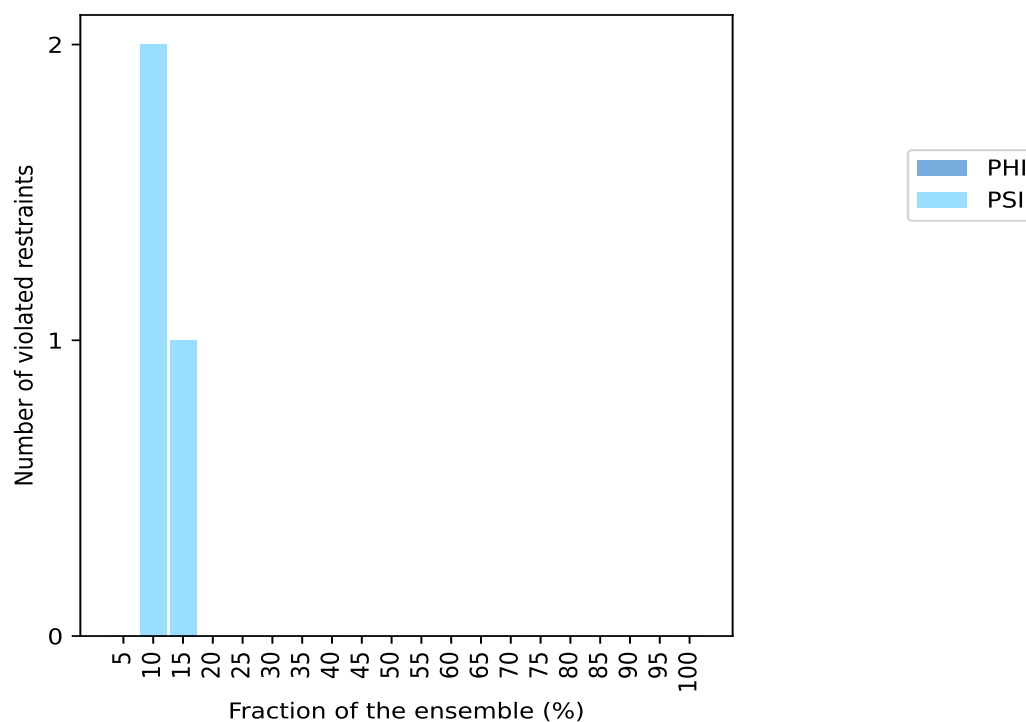
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	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 ⓘ

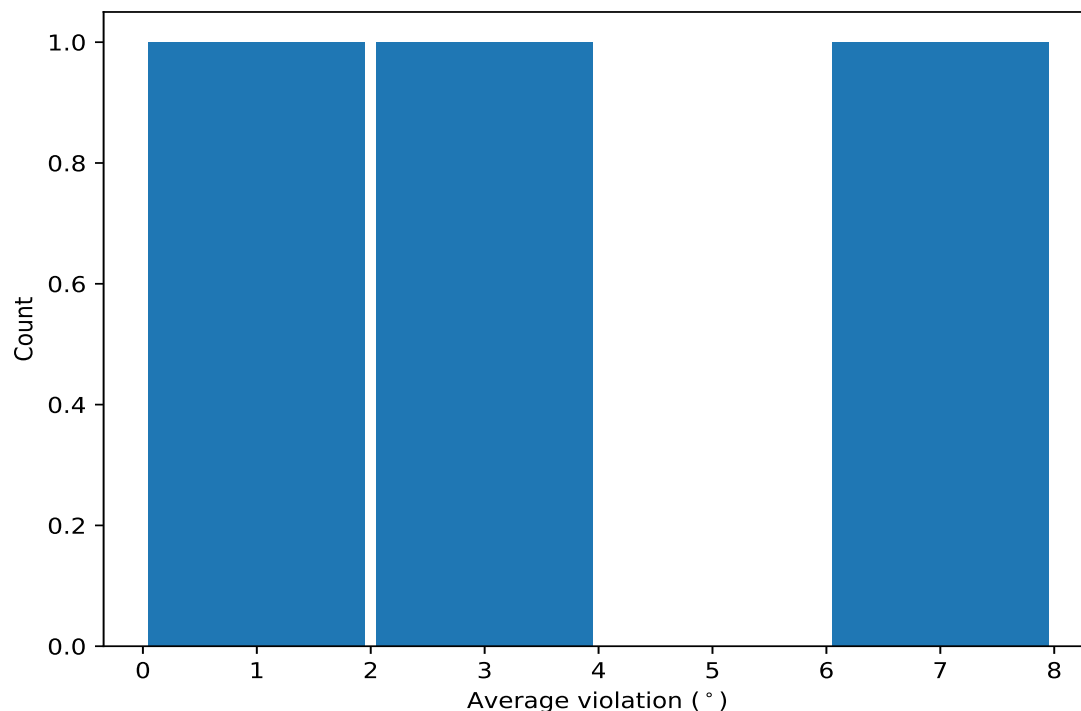


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 [i](#)

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

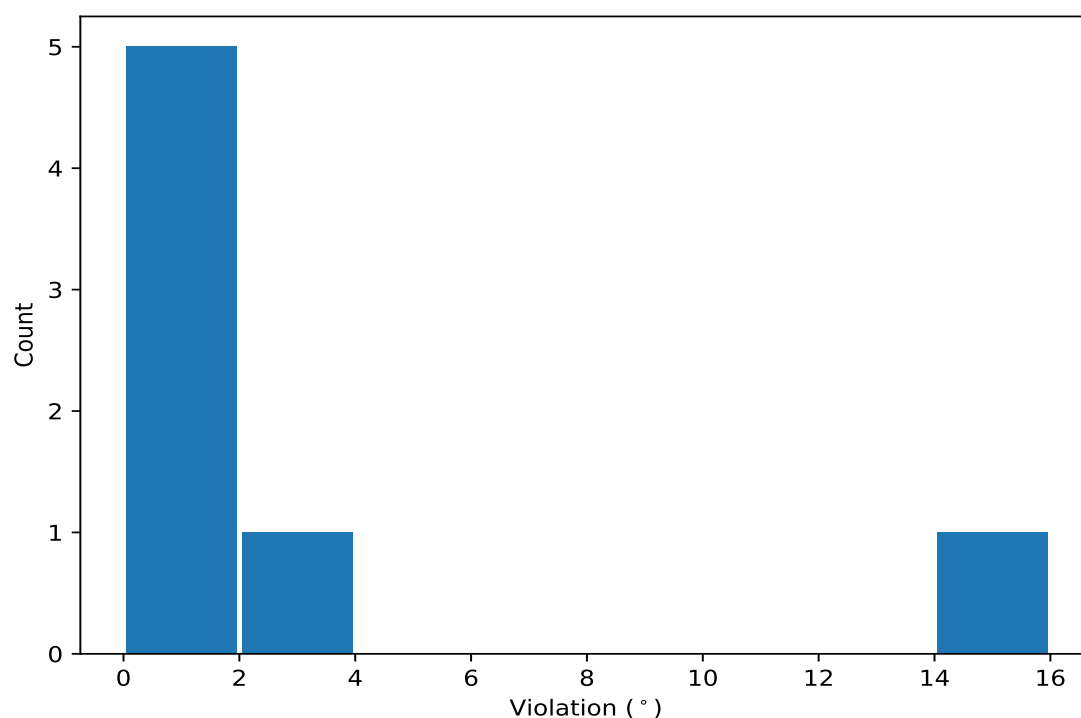
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,1)	1:8:A:VAL:N	1:8:A:VAL:CA	1:8:A:VAL:C	1:9:A:ALA:N	3	2.05	0.87	1.71
(1,9)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:GLU:N	2	7.67	6.5	7.67
(1,3)	1:9:A:ALA:N	1:9:A:ALA:CA	1:9:A:ALA:C	1:10:A:SER:N	2	1.4	0.16	1.4

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,9)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:GLU:N	16	14.17
(1,1)	1:8:A:VAL:N	1:8:A:VAL:CA	1:8:A:VAL:C	1:9:A:ALA:N	13	3.24
(1,1)	1:8:A:VAL:N	1:8:A:VAL:CA	1:8:A:VAL:C	1:9:A:ALA:N	15	1.71
(1,3)	1:9:A:ALA:N	1:9:A:ALA:CA	1:9:A:ALA:C	1:10:A:SER:N	12	1.56
(1,3)	1:9:A:ALA:N	1:9:A:ALA:CA	1:9:A:ALA:C	1:10:A:SER:N	11	1.25
(1,1)	1:8:A:VAL:N	1:8:A:VAL:CA	1:8:A:VAL:C	1:9:A:ALA:N	5	1.19
(1,9)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:GLU:N	7	1.17