



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:36 PM UTC

PDB ID : 6HPI / pdb_00006hpi
BMRB ID : 26780
Title : NMR structure of the pro-inflammatory cytokine interleukin-36alpha
Authors : Ohlenschlaeger, O.; Imhof, D.
Deposited on : 2018-09-21

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

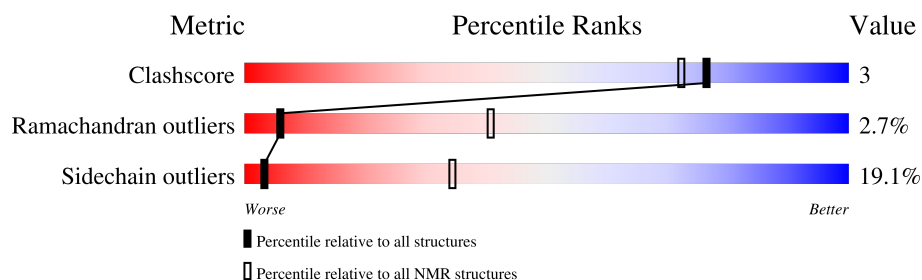
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	158	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:9-A:143, A:148-A:158 (146)	0.61	1

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

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

The models can be grouped into 3 clusters and 10 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2487 atoms, of which 1248 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interleukin-36 alpha.

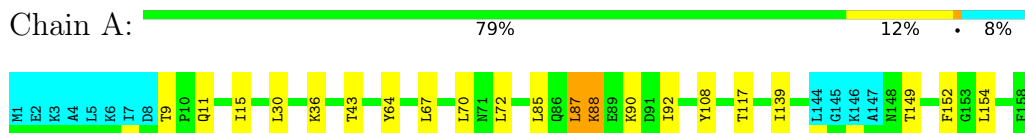
Mol	Chain	Residues	Atoms						Trace
1	A	158	Total	C	H	N	O	S	0
			2487	788	1248	210	232	9	

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: Interleukin-36 alpha

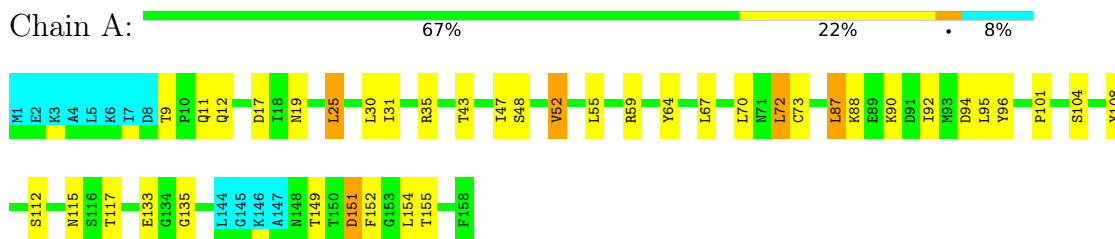


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

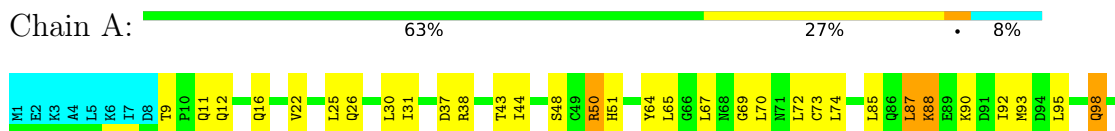
4.2.1 Score per residue for model 1 (medoid)

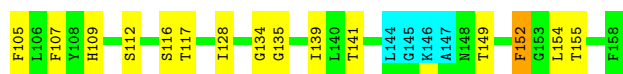
- Molecule 1: Interleukin-36 alpha



4.2.2 Score per residue for model 2

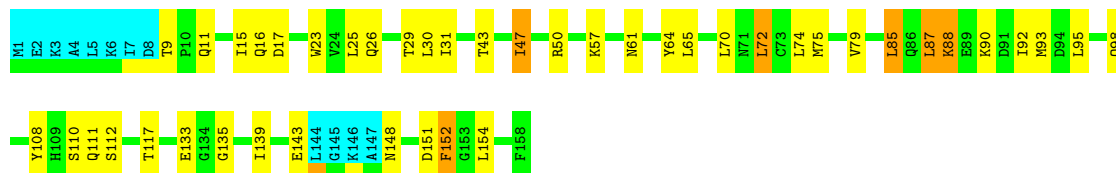
- Molecule 1: Interleukin-36 alpha





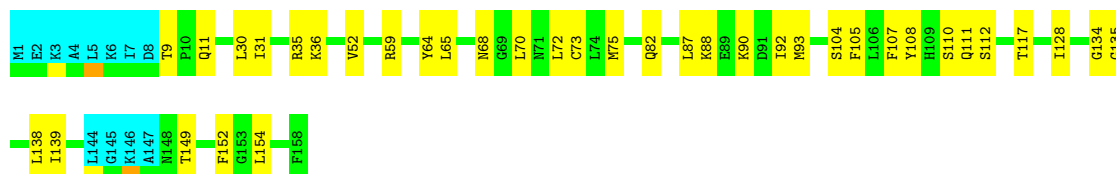
4.2.3 Score per residue for model 3

- Molecule 1: Interleukin-36 alpha



4.2.4 Score per residue for model 4

- Molecule 1: Interleukin-36 alpha



4.2.5 Score per residue for model 5

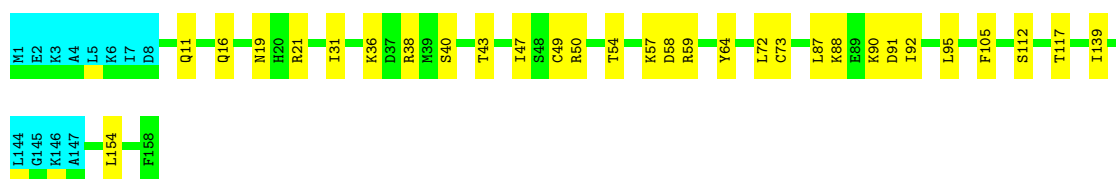
- Molecule 1: Interleukin-36 alpha



4.2.6 Score per residue for model 6

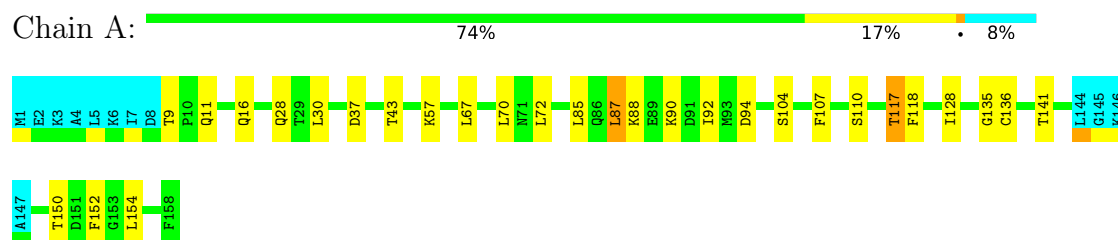
- Molecule 1: Interleukin-36 alpha





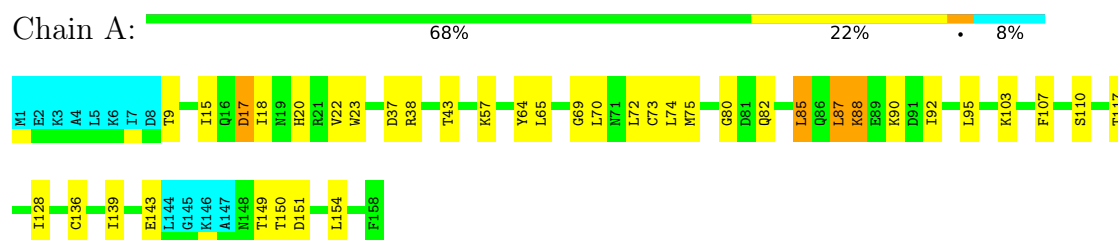
4.2.7 Score per residue for model 7

- Molecule 1: Interleukin-36 alpha



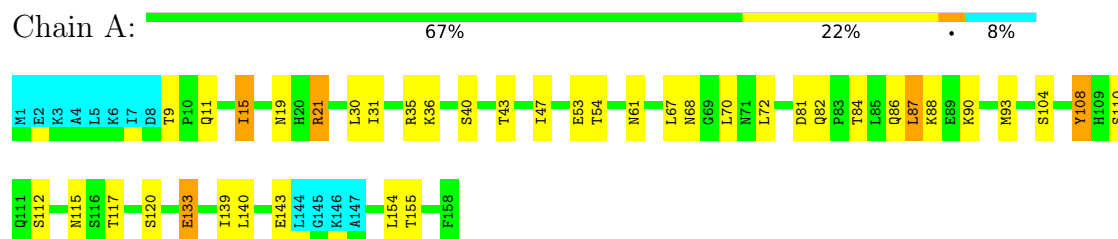
4.2.8 Score per residue for model 8

- Molecule 1: Interleukin-36 alpha



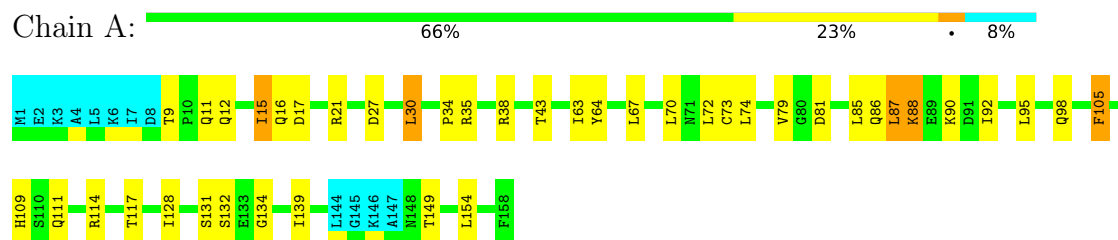
4.2.9 Score per residue for model 9

- Molecule 1: Interleukin-36 alpha



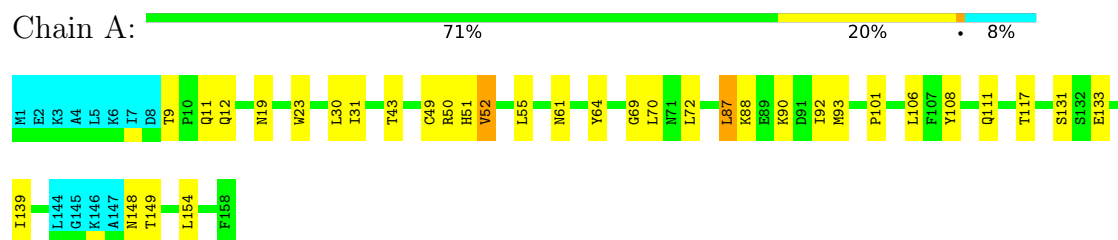
4.2.10 Score per residue for model 10

- Molecule 1: Interleukin-36 alpha



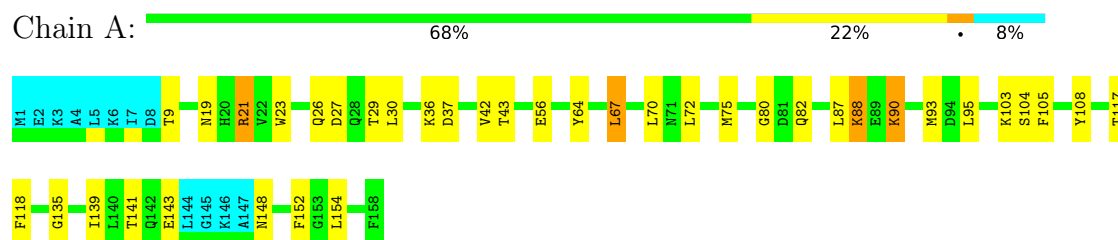
4.2.11 Score per residue for model 11

- Molecule 1: Interleukin-36 alpha



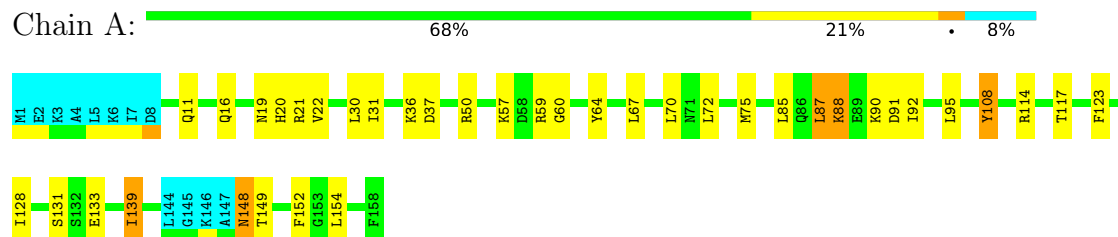
4.2.12 Score per residue for model 12

- Molecule 1: Interleukin-36 alpha



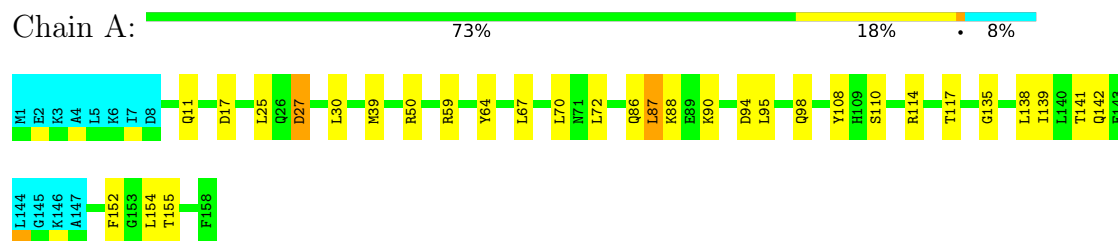
4.2.13 Score per residue for model 13

- Molecule 1: Interleukin-36 alpha



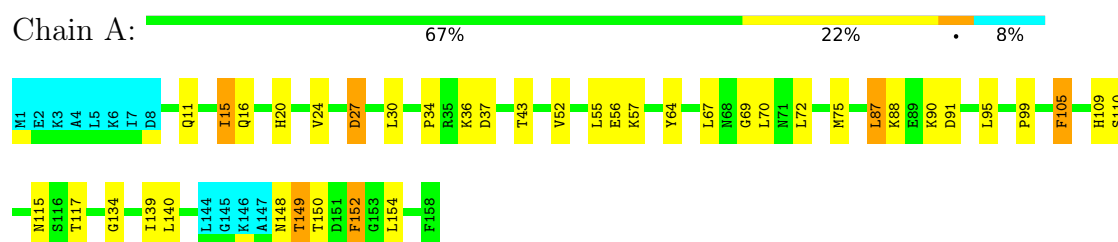
4.2.14 Score per residue for model 14

- Molecule 1: Interleukin-36 alpha



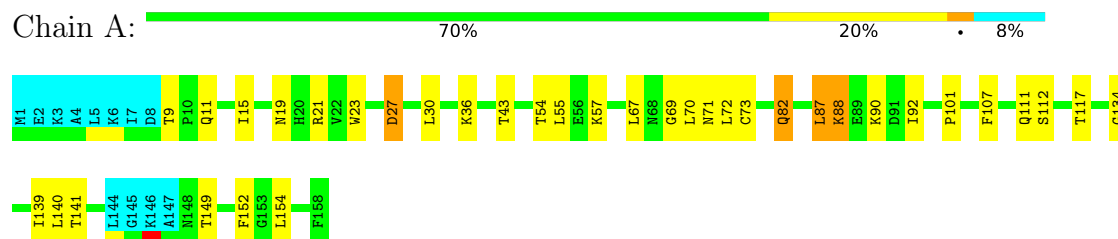
4.2.15 Score per residue for model 15

- Molecule 1: Interleukin-36 alpha



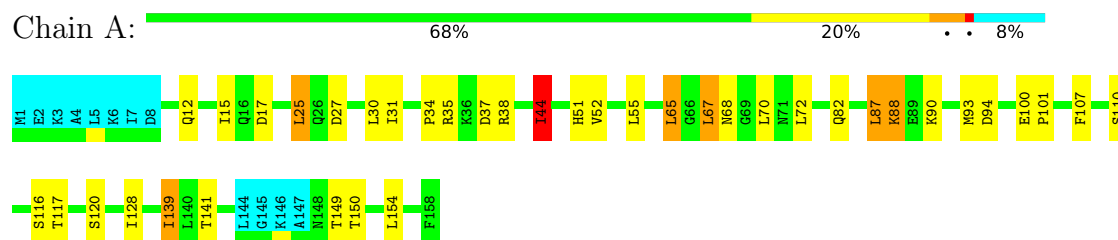
4.2.16 Score per residue for model 16

- Molecule 1: Interleukin-36 alpha



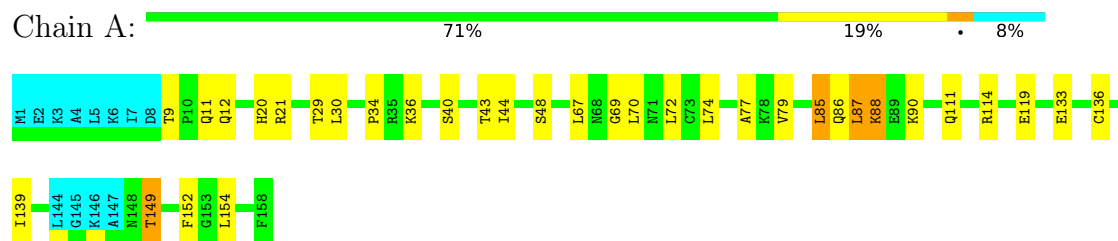
4.2.17 Score per residue for model 17

- Molecule 1: Interleukin-36 alpha



4.2.18 Score per residue for model 18

- Molecule 1: Interleukin-36 alpha



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
OPALp	refinement	
CYANA	structure calculation	

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	1819
Number of shifts mapped to atoms	1819
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.67±0.02	0±0/1174 (0.0± 0.0%)	1.38±0.04	3±2/1594 (0.2± 0.1%)
All	All	0.67	0/23480 (0.0%)	1.38	65/31880 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.9
All	All	0	19

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	148	ASN	CA-C-N	7.12	135.13	121.54	11	1
1	A	148	ASN	C-N-CA	7.12	135.13	121.54	11	1
1	A	142	GLN	N-CA-C	-6.85	104.56	113.12	14	1
1	A	151	ASP	CA-CB-CG	6.80	119.40	112.60	1	3
1	A	152	PHE	CA-C-N	6.74	128.74	120.51	3	1
1	A	152	PHE	C-N-CA	6.74	128.74	120.51	3	1
1	A	105	PHE	CA-CB-CG	6.61	120.41	113.80	2	7
1	A	82	GLN	N-CA-C	6.54	115.66	108.14	4	1
1	A	22	VAL	N-CA-C	-6.38	103.00	110.21	13	2
1	A	149	THR	CB-CA-C	6.10	120.36	109.38	15	1
1	A	79	VAL	CA-C-N	6.04	133.25	121.41	10	1
1	A	79	VAL	C-N-CA	6.04	133.25	121.41	10	1
1	A	59	ARG	N-CA-C	-6.03	105.00	112.72	14	1
1	A	115	ASN	CA-CB-CG	5.98	118.58	112.60	15	1
1	A	158	PHE	CA-CB-CG	5.91	119.71	113.80	20	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	57	LYS	CA-C-N	5.84	128.11	120.28	8	3
1	A	57	LYS	C-N-CA	5.84	128.11	120.28	8	3
1	A	109	HIS	CA-CB-CG	5.74	119.54	113.80	19	2
1	A	123	PHE	CA-CB-CG	5.65	119.45	113.80	5	1
1	A	56	GLU	CA-C-N	5.65	132.33	121.54	15	1
1	A	56	GLU	C-N-CA	5.65	132.33	121.54	15	1
1	A	16	GLN	CA-C-N	5.55	132.14	121.54	10	2
1	A	16	GLN	C-N-CA	5.55	132.14	121.54	10	2
1	A	151	ASP	N-CA-C	5.55	118.07	107.75	8	1
1	A	44	ILE	CA-CB-CG1	5.55	119.83	110.40	17	1
1	A	94	ASP	CA-C-N	5.55	127.72	120.28	17	2
1	A	94	ASP	C-N-CA	5.55	127.72	120.28	17	2
1	A	25	LEU	N-CA-C	-5.55	101.16	109.15	1	2
1	A	82	GLN	N-CA-CB	-5.53	104.33	111.35	4	1
1	A	17	ASP	CA-C-N	5.47	127.46	120.56	8	1
1	A	17	ASP	C-N-CA	5.47	127.46	120.56	8	1
1	A	109	HIS	CB-CG-CD2	-5.37	124.22	131.20	10	2
1	A	139	ILE	CA-CB-CG1	5.34	119.48	110.40	17	1
1	A	52	VAL	CA-C-N	5.25	128.05	120.38	11	1
1	A	52	VAL	C-N-CA	5.25	128.05	120.38	11	1
1	A	20	HIS	CB-CG-CD2	-5.25	124.38	131.20	19	1
1	A	150	THR	CA-C-N	5.24	130.13	122.85	8	1
1	A	150	THR	C-N-CA	5.24	130.13	122.85	8	1
1	A	81	ASP	N-CA-C	5.17	119.72	113.41	10	1
1	A	37	ASP	N-CA-C	-5.17	106.10	112.72	2	1
1	A	21	ARG	CD-NE-CZ	5.09	131.52	124.40	12	1
1	A	18	ILE	N-CA-C	5.08	115.29	110.42	8	1
1	A	82	GLN	CA-C-N	5.04	124.95	119.76	16	1
1	A	82	GLN	C-N-CA	5.04	124.95	119.76	16	1
1	A	98	GLN	OE1-CD-NE2	-5.03	117.57	122.60	2	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	59	ARG	Sidechain	4
1	A	50	ARG	Sidechain	4
1	A	35	ARG	Sidechain	2
1	A	96	TYR	Sidechain	2
1	A	114	ARG	Sidechain	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	107	PHE	Sidechain	1
1	A	21	ARG	Sidechain	1
1	A	118	PHE	Sidechain	1
1	A	27	ASP	Sidechain	1
1	A	108	TYR	Sidechain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1149	1144	1144	7±2
All	All	22980	22880	22880	139

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:HD11	1:A:67:LEU:HD21	0.78	1.53	7	1
1:A:74:LEU:HA	1:A:87:LEU:HD22	0.73	1.60	3	1
1:A:74:LEU:HA	1:A:87:LEU:HD12	0.70	1.63	8	4
1:A:85:LEU:HD22	1:A:87:LEU:HD11	0.68	1.65	20	3
1:A:30:LEU:HD11	1:A:67:LEU:HD11	0.68	1.65	16	7
1:A:85:LEU:HD11	1:A:128:ILE:HG23	0.68	1.65	10	3
1:A:30:LEU:HD21	1:A:67:LEU:HD11	0.65	1.67	18	4
1:A:30:LEU:HD12	1:A:87:LEU:HG	0.65	1.68	16	2
1:A:30:LEU:HD12	1:A:87:LEU:HD13	0.65	1.68	17	5
1:A:85:LEU:CD2	1:A:87:LEU:HD11	0.63	2.23	8	2
1:A:44:ILE:HG22	1:A:65:LEU:HD22	0.62	1.71	17	1
1:A:73:CYS:SG	1:A:92:ILE:HG23	0.62	2.35	5	8
1:A:85:LEU:HD11	1:A:128:ILE:HG22	0.61	1.72	8	2
1:A:107:PHE:CD2	1:A:128:ILE:HD11	0.59	2.33	2	2
1:A:30:LEU:CD1	1:A:67:LEU:HD21	0.59	2.28	7	1
1:A:87:LEU:HD12	1:A:87:LEU:H	0.58	1.57	15	7
1:A:87:LEU:N	1:A:87:LEU:HD13	0.58	2.14	19	6
1:A:64:TYR:CD1	1:A:92:ILE:HG22	0.57	2.33	5	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LEU:HD21	1:A:101:PRO:HB2	0.56	1.77	11	3
1:A:64:TYR:CD1	1:A:95:LEU:HD12	0.56	2.36	15	6
1:A:25:LEU:HD13	1:A:72:LEU:CD2	0.55	2.31	1	1
1:A:67:LEU:HD21	1:A:87:LEU:HD22	0.54	1.78	12	1
1:A:30:LEU:HD12	1:A:87:LEU:HD22	0.54	1.77	9	3
1:A:23:TRP:O	1:A:42:VAL:HG21	0.54	2.03	12	1
1:A:30:LEU:HD12	1:A:87:LEU:HD12	0.53	1.79	3	1
1:A:64:TYR:CD1	1:A:92:ILE:HG23	0.53	2.39	13	1
1:A:55:LEU:HD21	1:A:101:PRO:CB	0.53	2.34	11	4
1:A:74:LEU:HD23	1:A:87:LEU:HD21	0.53	1.80	2	2
1:A:60:GLY:HA3	1:A:108:TYR:CE1	0.52	2.40	19	2
1:A:139:ILE:HD11	1:A:148:ASN:HD21	0.51	1.64	13	1
1:A:49:CYS:SG	1:A:106:LEU:HD22	0.50	2.47	11	1
1:A:85:LEU:CD2	1:A:87:LEU:HD21	0.49	2.37	3	1
1:A:149:THR:HG21	1:A:152:PHE:CE2	0.48	2.44	20	3
1:A:64:TYR:CE1	1:A:95:LEU:HD12	0.47	2.44	10	4
1:A:107:PHE:CE2	1:A:128:ILE:HD11	0.47	2.43	5	3
1:A:52:VAL:HA	1:A:55:LEU:HD23	0.47	1.87	11	4
1:A:87:LEU:H	1:A:87:LEU:HD22	0.47	1.70	8	3
1:A:16:GLN:HE21	1:A:22:VAL:HG22	0.46	1.70	2	1
1:A:15:ILE:HD12	1:A:23:TRP:CH2	0.46	2.46	3	1
1:A:23:TRP:CD2	1:A:138:LEU:HD11	0.45	2.46	19	2
1:A:30:LEU:HD11	1:A:67:LEU:CD1	0.45	2.40	16	2
1:A:30:LEU:HD21	1:A:67:LEU:CD1	0.45	2.40	18	1
1:A:64:TYR:CG	1:A:92:ILE:HG22	0.45	2.46	4	1
1:A:47:ILE:HD12	1:A:92:ILE:CG2	0.45	2.42	3	1
1:A:30:LEU:HD13	1:A:138:LEU:HD12	0.44	1.89	14	2
1:A:85:LEU:HD11	1:A:128:ILE:CG2	0.44	2.42	7	1
1:A:85:LEU:HD23	1:A:87:LEU:HD11	0.43	1.90	8	1
1:A:25:LEU:HD22	1:A:72:LEU:CD2	0.43	2.43	3	1
1:A:85:LEU:HD22	1:A:87:LEU:HD12	0.43	1.90	7	1
1:A:87:LEU:N	1:A:87:LEU:HD23	0.43	2.29	3	1
1:A:44:ILE:CG2	1:A:65:LEU:HD11	0.42	2.45	2	1
1:A:90:LYS:HE2	1:A:90:LYS:HA	0.42	1.91	12	1
1:A:15:ILE:HD12	1:A:23:TRP:CZ3	0.42	2.50	8	1
1:A:16:GLN:CB	1:A:22:VAL:HG22	0.41	2.45	20	1
1:A:45:ALA:CB	1:A:92:ILE:HD11	0.41	2.45	5	1
1:A:64:TYR:CE1	1:A:92:ILE:HG22	0.41	2.50	5	1
1:A:24:VAL:C	1:A:30:LEU:HD23	0.41	2.41	15	1
1:A:21:ARG:HB2	1:A:23:TRP:CH2	0.41	2.51	16	1
1:A:117:THR:C	1:A:118:PHE:CD2	0.41	2.99	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ALA:CB	1:A:86:GLN:HE21	0.41	2.29	18	1
1:A:85:LEU:HD22	1:A:87:LEU:HD21	0.40	1.93	3	1
1:A:47:ILE:HG13	1:A:92:ILE:HD12	0.40	1.90	5	1
1:A:30:LEU:CD1	1:A:87:LEU:HD22	0.40	2.46	10	1
1:A:108:TYR:CD1	1:A:108:TYR:C	0.40	3.00	9	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	145/158 (92%)	121±3 (84±2%)	20±3 (14±2%)	4±2 (3±1%)	6	41
All	All	2900/3160 (92%)	2428 (84%)	394 (14%)	78 (3%)	6	41

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	88	LYS	17
1	A	135	GLY	9
1	A	69	GLY	8
1	A	134	GLY	7
1	A	27	ASP	5
1	A	133	GLU	4
1	A	34	PRO	4
1	A	17	ASP	3
1	A	79	VAL	3
1	A	15	ILE	3
1	A	38	ARG	2
1	A	152	PHE	2
1	A	80	GLY	2
1	A	131	SER	2
1	A	149	THR	2
1	A	143	GLU	1
1	A	35	ARG	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	57	LYS	1
1	A	99	PRO	1
1	A	100	GLU	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	131/140 (94%)	106±4 (81±3%)	25±4 (19±3%)	3	34
All	All	2620/2800 (94%)	2119 (81%)	501 (19%)	3	34

All 92 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	72	LEU	20
1	A	90	LYS	20
1	A	154	LEU	20
1	A	70	LEU	19
1	A	87	LEU	19
1	A	117	THR	19
1	A	139	ILE	18
1	A	11	GLN	17
1	A	43	THR	16
1	A	88	LYS	15
1	A	9	THR	14
1	A	152	PHE	12
1	A	36	LYS	11
1	A	31	ILE	10
1	A	149	THR	10
1	A	93	MET	9
1	A	108	TYR	8
1	A	110	SER	8
1	A	12	GLN	7
1	A	19	ASN	7
1	A	112	SER	7
1	A	75	MET	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	47	ILE	6
1	A	104	SER	6
1	A	111	GLN	6
1	A	15	ILE	6
1	A	21	ARG	6
1	A	37	ASP	6
1	A	82	GLN	6
1	A	67	LEU	5
1	A	50	ARG	5
1	A	98	GLN	5
1	A	141	THR	5
1	A	68	ASN	5
1	A	17	ASP	4
1	A	155	THR	4
1	A	25	LEU	4
1	A	26	GLN	4
1	A	57	LYS	4
1	A	65	LEU	4
1	A	16	GLN	4
1	A	91	ASP	4
1	A	20	HIS	4
1	A	143	GLU	4
1	A	86	GLN	4
1	A	140	LEU	4
1	A	48	SER	3
1	A	94	ASP	3
1	A	51	HIS	3
1	A	29	THR	3
1	A	61	ASN	3
1	A	85	LEU	3
1	A	133	GLU	3
1	A	58	ASP	3
1	A	38	ARG	3
1	A	40	SER	3
1	A	54	THR	3
1	A	92	ILE	3
1	A	136	CYS	3
1	A	150	THR	3
1	A	114	ARG	3
1	A	148	ASN	3
1	A	27	ASP	3
1	A	52	VAL	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	115	ASN	2
1	A	116	SER	2
1	A	107	PHE	2
1	A	103	LYS	2
1	A	120	SER	2
1	A	35	ARG	2
1	A	63	ILE	2
1	A	105	PHE	2
1	A	132	SER	2
1	A	39	MET	2
1	A	71	ASN	2
1	A	44	ILE	2
1	A	151	ASP	1
1	A	109	HIS	1
1	A	59	ARG	1
1	A	49	CYS	1
1	A	28	GLN	1
1	A	53	GLU	1
1	A	81	ASP	1
1	A	84	THR	1
1	A	30	LEU	1
1	A	131	SER	1
1	A	23	TRP	1
1	A	64	TYR	1
1	A	56	GLU	1
1	A	123	PHE	1
1	A	119	GLU	1
1	A	106	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no 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 83% for the well-defined parts and 84% 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	1819
Number of shifts mapped to atoms	1819
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	19

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	158	0.23 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	147	-0.03 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	142	0.19 ± 0.11	None needed (< 0.5 ppm)
^{15}N	143	-0.27 ± 0.39	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 83%, i.e. 1657 atoms were assigned a chemical shift out of a possible 1996. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	694/722 (96%)	287/293 (98%)	276/292 (95%)	131/137 (96%)
Sidechain	961/1132 (85%)	648/738 (88%)	313/353 (89%)	0/41 (0%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	2/142 (1%)	1/71 (1%)	0/66 (0%)	1/5 (20%)
Overall	1657/1996 (83%)	936/1102 (85%)	589/711 (83%)	132/183 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1819 atoms were assigned a chemical shift out of a possible 2164. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	754/783 (96%)	311/318 (98%)	300/316 (95%)	143/149 (96%)
Sidechain	1063/1239 (86%)	718/808 (89%)	345/387 (89%)	0/44 (0%)
Aromatic	2/142 (1%)	1/71 (1%)	0/66 (0%)	1/5 (20%)
Overall	1819/2164 (84%)	1030/1197 (86%)	645/769 (84%)	144/198 (73%)

7.1.4 Statistically unusual chemical shifts ⓘ

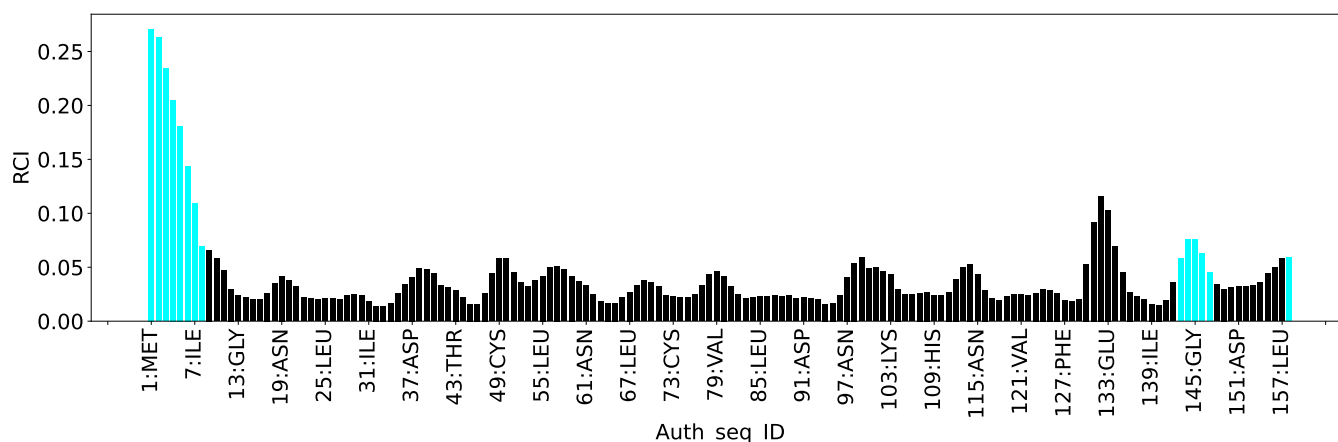
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	116	SER	HB2	6.32	2.61 – 5.13	9.7
1	A	116	SER	HB3	6.32	2.49 – 5.20	9.1
1	A	83	PRO	HG2	-0.31	0.41 – 3.45	-7.4
1	A	142	GLN	HG2	0.42	1.01 – 3.62	-7.3
1	A	17	ASP	CB	29.60	32.98 – 48.76	-7.1
1	A	100	GLU	CG	27.92	30.20 – 42.01	-6.9
1	A	83	PRO	HG3	-0.07	0.33 – 3.48	-6.3
1	A	16	GLN	CG	27.20	28.36 – 39.21	-6.1
1	A	103	LYS	HD3	2.87	0.54 – 2.65	6.0
1	A	95	LEU	HB3	-0.51	-0.26 – 3.31	-5.7
1	A	62	PRO	HD2	1.73	1.93 – 5.38	-5.6
1	A	35	ARG	HG2	3.02	0.26 – 2.87	5.6
1	A	83	PRO	HB2	0.20	0.37 – 3.78	-5.5
1	A	119	GLU	HG2	1.14	1.24 – 3.30	-5.5
1	A	34	PRO	CA	55.15	55.85 – 70.84	-5.5
1	A	83	PRO	HB3	0.09	0.25 – 3.76	-5.5
1	A	35	ARG	HG3	3.02	0.15 – 2.94	5.3
1	A	59	ARG	HB3	0.38	0.43 – 3.11	-5.2
1	A	62	PRO	HD3	1.73	1.76 – 5.48	-5.1

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	5086
Intra-residue ($ i-j =0$)	258
Sequential ($ i-j =1$)	1443
Medium range ($ i-j >1$ and $ i-j <5$)	833
Long range ($ i-j \geq 5$)	2480
Inter-chain	0
Hydrogen bond restraints	72
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	32.2
Number of long range restraints per residue ¹	16.1

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)	2.4	0.12
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

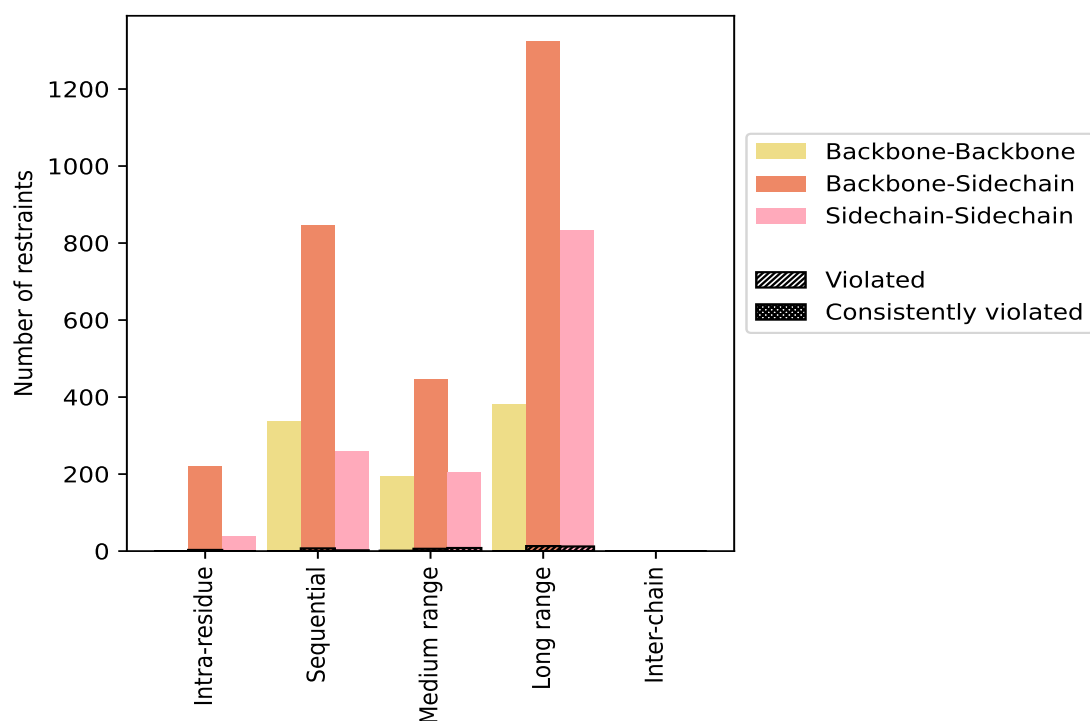
9.1 Summary of distance violations

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 ($i-j =0$)	258	5.1	3	1.2	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	219	4.3	3	1.4	0.1	0	0.0	0.0
Sidechain-Sidechain	39	0.8	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	1443	28.4	9	0.6	0.2	0	0.0	0.0
Backbone-Backbone	336	6.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	847	16.7	7	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	260	5.1	2	0.8	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	833	16.4	14	1.7	0.3	0	0.0	0.0
Backbone-Backbone	194	3.8	1	0.5	0.0	0	0.0	0.0
Backbone-Sidechain	435	8.6	5	1.1	0.1	0	0.0	0.0
Sidechain-Sidechain	204	4.0	8	3.9	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	2480	48.8	25	1.0	0.5	0	0.0	0.0
Backbone-Backbone	382	7.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1264	24.9	13	1.0	0.3	0	0.0	0.0
Sidechain-Sidechain	834	16.4	12	1.4	0.2	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	72	1.4	1	1.4	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	5086	100.0	52	1.0	1.0	0	0.0	0.0
Backbone-Backbone	912	17.9	1	0.1	0.0	0	0.0	0.0
Backbone-Sidechain	2837	55.8	29	1.0	0.6	0	0.0	0.0
Sidechain-Sidechain	1337	26.3	22	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 [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfide 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	0	0	4	0	4	0.1	0.1	0.0	0.1
2	0	0	1	3	0	4	0.1	0.11	0.0	0.1
3	0	1	1	2	0	4	0.11	0.11	0.0	0.11
4	0	2	1	4	0	7	0.11	0.11	0.0	0.11
5	0	0	1	4	0	5	0.11	0.11	0.0	0.11
6	0	0	0	1	0	1	0.1	0.1	0.0	0.1
7	0	0	0	2	0	2	0.1	0.1	0.0	0.1
8	0	1	2	3	0	6	0.1	0.12	0.01	0.1
9	0	1	2	4	0	7	0.11	0.11	0.0	0.11
10	0	2	2	2	0	6	0.1	0.11	0.0	0.1

Continued on next page...

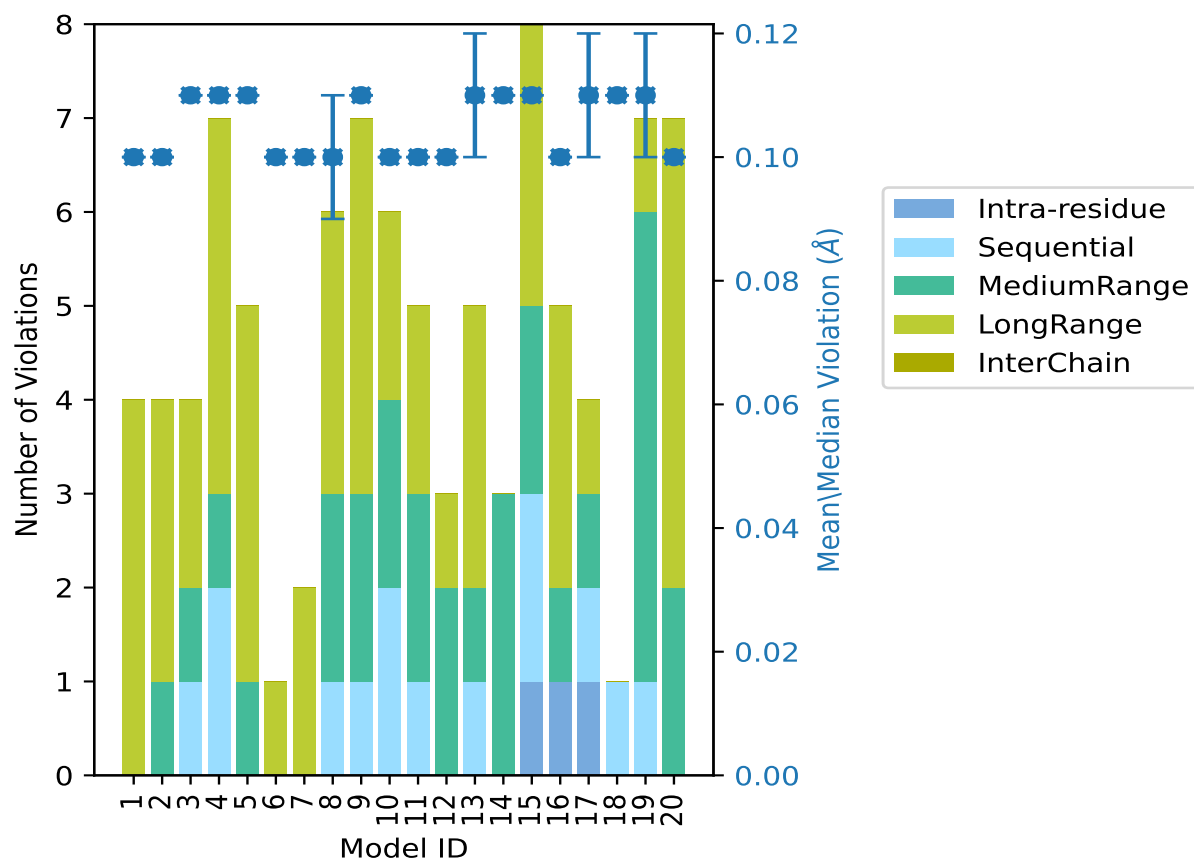
Continued from previous page...

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	2	2	0	5	0.1	0.11	0.0	0.1
12	0	0	2	1	0	3	0.1	0.1	0.0	0.1
13	0	1	1	3	0	5	0.11	0.12	0.01	0.11
14	0	0	3	0	0	3	0.11	0.11	0.0	0.11
15	1	2	2	3	0	8	0.11	0.11	0.0	0.11
16	1	0	1	3	0	5	0.1	0.11	0.0	0.1
17	1	1	1	1	0	4	0.11	0.12	0.01	0.11
18	0	1	0	0	0	1	0.11	0.11	0.0	0.11
19	0	1	5	1	0	7	0.11	0.12	0.01	0.11
20	0	0	2	5	0	7	0.1	0.11	0.0	0.1

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

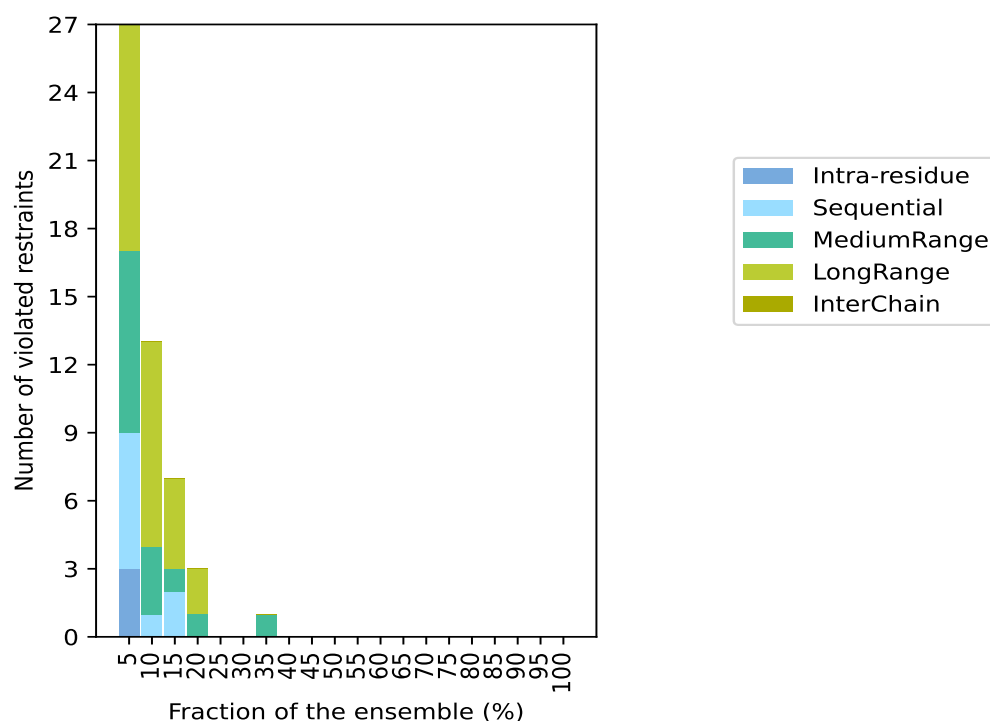
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 4963(IR:255, SQ:1434, MR:819, LR:2455, IC:0) restraints are 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	%
3	6	8	10	0	27	1	5.0
0	1	3	9	0	13	2	10.0
0	2	1	4	0	7	3	15.0
0	0	1	2	0	3	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	1	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	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	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

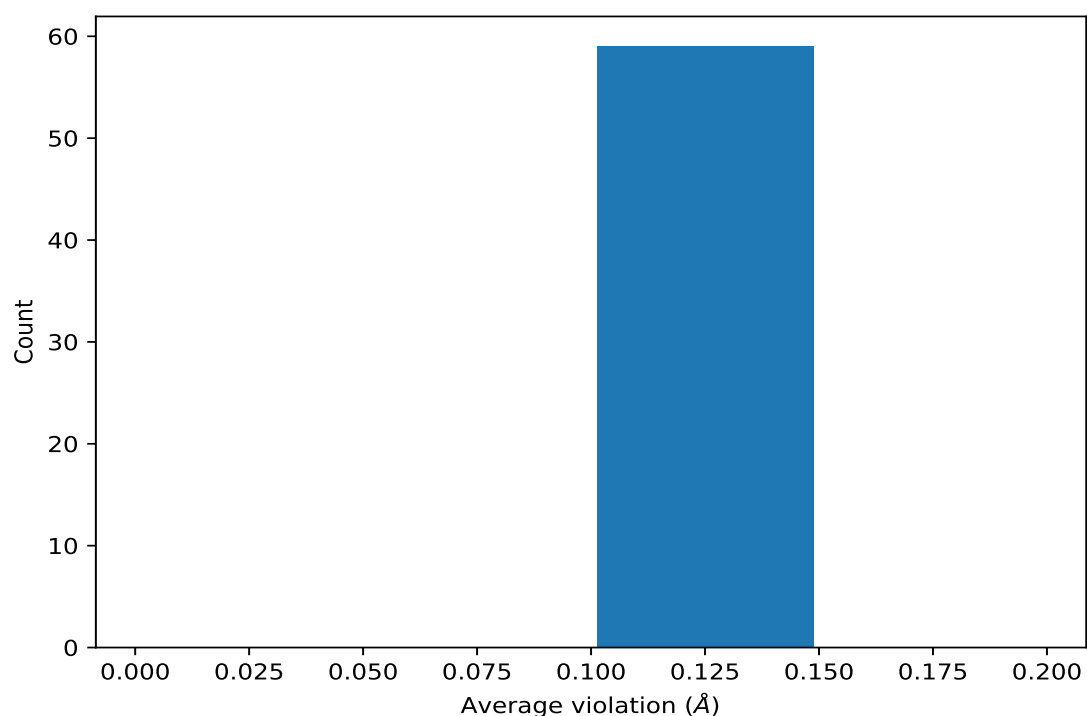
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD2	7	0.11	0.01	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD3	7	0.11	0.01	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG21	4	0.11	0.0	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG22	4	0.11	0.0	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG23	4	0.11	0.0	0.11
(2,1058)	1:21:A:ARG:HG2	1:149:A:THR:HA	4	0.1	0.0	0.11
(2,1058)	1:21:A:ARG:HG3	1:149:A:THR:HA	4	0.1	0.0	0.11
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE2	4	0.1	0.0	0.1
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE3	4	0.1	0.0	0.1
(1,858)	1:87:A:LEU:H	1:88:A:LYS:HD2	3	0.11	0.0	0.11
(1,858)	1:87:A:LEU:H	1:88:A:LYS:HD3	3	0.11	0.0	0.11
(2,568)	1:98:A:GLN:H	1:100:A:GLU:HG2	3	0.11	0.01	0.11
(2,568)	1:98:A:GLN:H	1:100:A:GLU:HG3	3	0.11	0.01	0.11
(2,1038)	1:20:A:HIS:HA	1:21:A:ARG:HD2	3	0.11	0.0	0.11
(2,1038)	1:20:A:HIS:HA	1:21:A:ARG:HD3	3	0.11	0.0	0.11
(1,202)	1:21:A:ARG:HB2	1:132:A:SER:H	3	0.11	0.01	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,202)	1:21:A:ARG:HB3	1:132:A:SER:H	3	0.11	0.01	0.1
(2,1627)	1:70:A:LEU:HD11	1:88:A:LYS:HA	3	0.1	0.0	0.1
(2,1627)	1:70:A:LEU:HD12	1:88:A:LYS:HA	3	0.1	0.0	0.1
(2,1627)	1:70:A:LEU:HD13	1:88:A:LYS:HA	3	0.1	0.0	0.1
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB1	3	0.1	0.0	0.1
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB2	3	0.1	0.0	0.1
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB3	3	0.1	0.0	0.1
(2,1506)	1:54:A:THR:HG21	1:102:A:VAL:HA	3	0.1	0.0	0.1
(2,1506)	1:54:A:THR:HG22	1:102:A:VAL:HA	3	0.1	0.0	0.1
(2,1506)	1:54:A:THR:HG23	1:102:A:VAL:HA	3	0.1	0.0	0.1
(1,1586)	1:16:A:GLN:HG2	1:22:A:VAL:HB	2	0.11	0.0	0.11
(1,1586)	1:16:A:GLN:HG3	1:22:A:VAL:HB	2	0.11	0.0	0.11
(1,1784)	1:33:A:VAL:HB	1:39:A:MET:HE1	2	0.11	0.0	0.11
(1,1784)	1:33:A:VAL:HB	1:39:A:MET:HE2	2	0.11	0.0	0.11
(1,1784)	1:33:A:VAL:HB	1:39:A:MET:HE3	2	0.11	0.0	0.11
(2,794)	1:5:A:LEU:HG	1:6:A:LYS:HE2	2	0.11	0.0	0.11
(2,794)	1:5:A:LEU:HG	1:6:A:LYS:HE3	2	0.11	0.0	0.11
(1,136)	1:15:A:ILE:HA	1:154:A:LEU:HD11	2	0.11	0.0	0.11
(1,136)	1:15:A:ILE:HA	1:154:A:LEU:HD12	2	0.11	0.0	0.11
(1,136)	1:15:A:ILE:HA	1:154:A:LEU:HD13	2	0.11	0.0	0.11
(1,272)	1:25:A:LEU:HB2	1:29:A:THR:H	2	0.11	0.0	0.11
(1,272)	1:25:A:LEU:HB3	1:29:A:THR:H	2	0.11	0.0	0.11
(1,1551)	1:15:A:ILE:HA	1:154:A:LEU:HD11	2	0.11	0.0	0.11
(1,1551)	1:15:A:ILE:HA	1:154:A:LEU:HD12	2	0.11	0.0	0.11
(1,1551)	1:15:A:ILE:HA	1:154:A:LEU:HD13	2	0.11	0.0	0.11
(1,1593)	1:18:A:ILE:HB	1:21:A:ARG:HB2	2	0.11	0.0	0.11
(1,1593)	1:18:A:ILE:HB	1:21:A:ARG:HB3	2	0.11	0.0	0.11
(2,960)	1:15:A:ILE:HB	1:149:A:THR:HG21	2	0.11	0.0	0.11
(2,960)	1:15:A:ILE:HB	1:149:A:THR:HG22	2	0.11	0.0	0.11
(2,960)	1:15:A:ILE:HB	1:149:A:THR:HG23	2	0.11	0.0	0.11
(2,1013)	1:18:A:ILE:HD11	1:149:A:THR:HA	2	0.11	0.0	0.11
(2,1013)	1:18:A:ILE:HD12	1:149:A:THR:HA	2	0.11	0.0	0.11
(2,1013)	1:18:A:ILE:HD13	1:149:A:THR:HA	2	0.11	0.0	0.11
(2,2038)	1:129:A:ALA:HB1	1:144:A:LEU:HG	2	0.11	0.0	0.11
(2,2038)	1:129:A:ALA:HB2	1:144:A:LEU:HG	2	0.11	0.0	0.11
(2,2038)	1:129:A:ALA:HB3	1:144:A:LEU:HG	2	0.11	0.0	0.11
(2,2046)	1:130:A:VAL:HA	1:149:A:THR:HG21	2	0.11	0.0	0.11
(2,2046)	1:130:A:VAL:HA	1:149:A:THR:HG22	2	0.11	0.0	0.11
(2,2046)	1:130:A:VAL:HA	1:149:A:THR:HG23	2	0.11	0.0	0.11
(1,2658)	1:130:A:VAL:HB	1:132:A:SER:HB2	2	0.1	0.0	0.1
(1,2658)	1:130:A:VAL:HB	1:132:A:SER:HB3	2	0.1	0.0	0.1
(2,858)	1:10:A:PRO:HG2	1:92:A:ILE:HB	2	0.1	0.0	0.1

Continued on next page...

Continued from previous page...

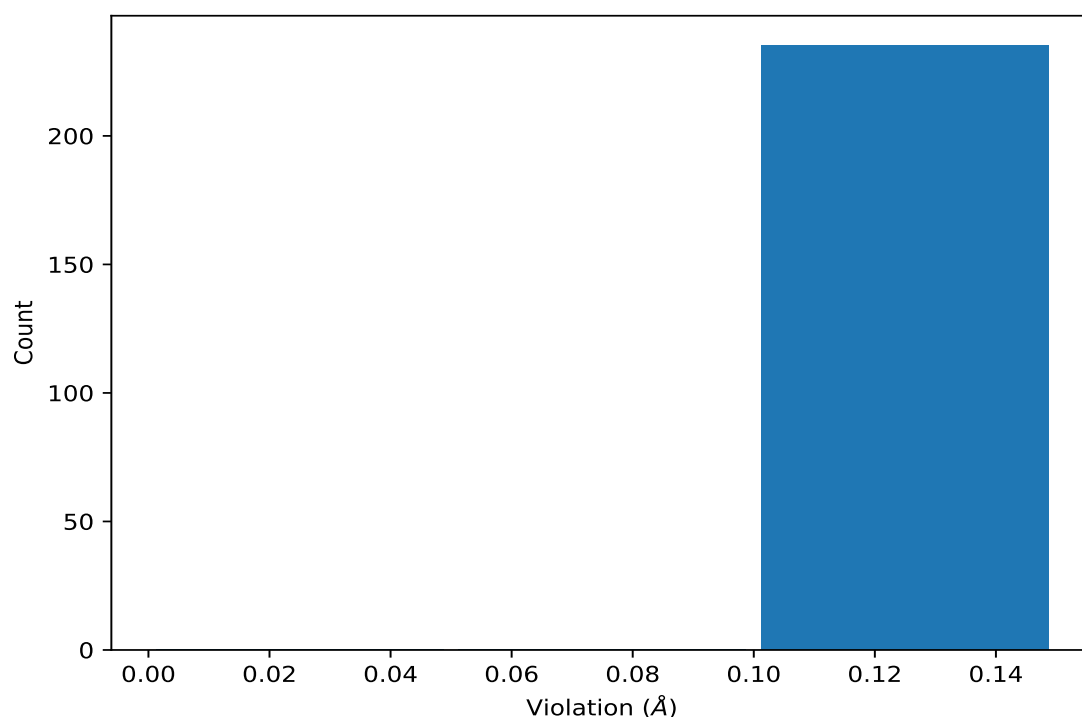
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,858)	1:10:A:PRO:HG3	1:92:A:ILE:HB	2	0.1	0.0	0.1

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 [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2137)	1:144:A:LEU:HD21	1:146:A:LYS:HA	8	0.12
(2,2137)	1:144:A:LEU:HD22	1:146:A:LYS:HA	8	0.12
(2,2137)	1:144:A:LEU:HD23	1:146:A:LYS:HA	8	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2129)	1:144:A:LEU:HB2	1:146:A:LYS:HD2	19	0.12
(2,2129)	1:144:A:LEU:HB2	1:146:A:LYS:HD3	19	0.12
(2,2129)	1:144:A:LEU:HB3	1:146:A:LYS:HD2	19	0.12
(2,2129)	1:144:A:LEU:HB3	1:146:A:LYS:HD3	19	0.12
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD2	19	0.12
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD3	19	0.12
(2,825)	1:7:A:ILE:HB	1:9:A:THR:HG21	19	0.12
(2,825)	1:7:A:ILE:HB	1:9:A:THR:HG22	19	0.12
(2,825)	1:7:A:ILE:HB	1:9:A:THR:HG23	19	0.12
(2,568)	1:98:A:GLN:H	1:100:A:GLU:HG2	17	0.12
(2,568)	1:98:A:GLN:H	1:100:A:GLU:HG3	17	0.12
(1,202)	1:21:A:ARG:HB2	1:132:A:SER:H	13	0.12
(1,202)	1:21:A:ARG:HB3	1:132:A:SER:H	13	0.12
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE2	14	0.11
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE3	14	0.11
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB1	16	0.11
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB2	16	0.11
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB3	16	0.11
(2,2046)	1:130:A:VAL:HA	1:149:A:THR:HG21	13	0.11
(2,2046)	1:130:A:VAL:HA	1:149:A:THR:HG22	13	0.11
(2,2046)	1:130:A:VAL:HA	1:149:A:THR:HG23	13	0.11
(2,2038)	1:129:A:ALA:HB1	1:144:A:LEU:HG	13	0.11
(2,2038)	1:129:A:ALA:HB2	1:144:A:LEU:HG	13	0.11
(2,2038)	1:129:A:ALA:HB3	1:144:A:LEU:HG	13	0.11
(2,1763)	1:79:A:VAL:HG11	1:139:A:ILE:HB	17	0.11
(2,1763)	1:79:A:VAL:HG12	1:139:A:ILE:HB	17	0.11
(2,1763)	1:79:A:VAL:HG13	1:139:A:ILE:HB	17	0.11
(2,1627)	1:70:A:LEU:HD11	1:88:A:LYS:HA	4	0.11
(2,1627)	1:70:A:LEU:HD12	1:88:A:LYS:HA	4	0.11
(2,1627)	1:70:A:LEU:HD13	1:88:A:LYS:HA	4	0.11
(2,1338)	1:44:A:ILE:HA	1:92:A:ILE:HG21	3	0.11
(2,1338)	1:44:A:ILE:HA	1:92:A:ILE:HG22	3	0.11
(2,1338)	1:44:A:ILE:HA	1:92:A:ILE:HG23	3	0.11
(2,1258)	1:33:A:VAL:HG11	1:36:A:LYS:HE2	19	0.11
(2,1258)	1:33:A:VAL:HG11	1:36:A:LYS:HE3	19	0.11
(2,1258)	1:33:A:VAL:HG12	1:36:A:LYS:HE2	19	0.11
(2,1258)	1:33:A:VAL:HG12	1:36:A:LYS:HE3	19	0.11
(2,1258)	1:33:A:VAL:HG13	1:36:A:LYS:HE2	19	0.11
(2,1258)	1:33:A:VAL:HG13	1:36:A:LYS:HE3	19	0.11
(2,1058)	1:21:A:ARG:HG2	1:149:A:THR:HA	9	0.11
(2,1058)	1:21:A:ARG:HG3	1:149:A:THR:HA	9	0.11
(2,1058)	1:21:A:ARG:HG2	1:149:A:THR:HA	15	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1058)	1:21:A:ARG:HG3	1:149:A:THR:HA	15	0.11
(2,1038)	1:20:A:HIS:HA	1:21:A:ARG:HD2	8	0.11
(2,1038)	1:20:A:HIS:HA	1:21:A:ARG:HD3	8	0.11
(2,1038)	1:20:A:HIS:HA	1:21:A:ARG:HD2	15	0.11
(2,1038)	1:20:A:HIS:HA	1:21:A:ARG:HD3	15	0.11
(2,1038)	1:20:A:HIS:HA	1:21:A:ARG:HD2	18	0.11
(2,1038)	1:20:A:HIS:HA	1:21:A:ARG:HD3	18	0.11
(2,1013)	1:18:A:ILE:HD11	1:149:A:THR:HA	20	0.11
(2,1013)	1:18:A:ILE:HD12	1:149:A:THR:HA	20	0.11
(2,1013)	1:18:A:ILE:HD13	1:149:A:THR:HA	20	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD2	3	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD3	3	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD2	9	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD3	9	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD2	11	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD3	11	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD2	14	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD3	14	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD2	16	0.11
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD3	16	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG21	9	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG22	9	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG23	9	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG21	10	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG22	10	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG23	10	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG21	15	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG22	15	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG23	15	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG21	19	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG22	19	0.11
(2,1005)	1:18:A:ILE:HA	1:149:A:THR:HG23	19	0.11
(2,960)	1:15:A:ILE:HB	1:149:A:THR:HG21	5	0.11
(2,960)	1:15:A:ILE:HB	1:149:A:THR:HG22	5	0.11
(2,960)	1:15:A:ILE:HB	1:149:A:THR:HG23	5	0.11
(2,794)	1:5:A:LEU:HG	1:6:A:LYS:HE2	3	0.11
(2,794)	1:5:A:LEU:HG	1:6:A:LYS:HE3	3	0.11
(2,794)	1:5:A:LEU:HG	1:6:A:LYS:HE2	4	0.11
(2,794)	1:5:A:LEU:HG	1:6:A:LYS:HE3	4	0.11
(2,568)	1:98:A:GLN:H	1:100:A:GLU:HG2	2	0.11
(2,568)	1:98:A:GLN:H	1:100:A:GLU:HG3	2	0.11
(1,2318)	1:88:A:LYS:HE2	1:89:A:GLU:HG2	9	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2318)	1:88:A:LYS:HE2	1:89:A:GLU:HG3	9	0.11
(1,2318)	1:88:A:LYS:HE3	1:89:A:GLU:HG2	9	0.11
(1,2318)	1:88:A:LYS:HE3	1:89:A:GLU:HG3	9	0.11
(1,1942)	1:50:A:ARG:HD2	1:96:A:TYR:HB2	5	0.11
(1,1942)	1:50:A:ARG:HD2	1:96:A:TYR:HB3	5	0.11
(1,1942)	1:50:A:ARG:HD3	1:96:A:TYR:HB2	5	0.11
(1,1942)	1:50:A:ARG:HD3	1:96:A:TYR:HB3	5	0.11
(1,1784)	1:33:A:VAL:HB	1:39:A:MET:HE1	3	0.11
(1,1784)	1:33:A:VAL:HB	1:39:A:MET:HE2	3	0.11
(1,1784)	1:33:A:VAL:HB	1:39:A:MET:HE3	3	0.11
(1,1784)	1:33:A:VAL:HB	1:39:A:MET:HE1	5	0.11
(1,1784)	1:33:A:VAL:HB	1:39:A:MET:HE2	5	0.11
(1,1784)	1:33:A:VAL:HB	1:39:A:MET:HE3	5	0.11
(1,1593)	1:18:A:ILE:HB	1:21:A:ARG:HB2	15	0.11
(1,1593)	1:18:A:ILE:HB	1:21:A:ARG:HB3	15	0.11
(1,1586)	1:16:A:GLN:HG2	1:22:A:VAL:HB	4	0.11
(1,1586)	1:16:A:GLN:HG3	1:22:A:VAL:HB	4	0.11
(1,1586)	1:16:A:GLN:HG2	1:22:A:VAL:HB	20	0.11
(1,1586)	1:16:A:GLN:HG3	1:22:A:VAL:HB	20	0.11
(1,1551)	1:15:A:ILE:HA	1:154:A:LEU:HD11	4	0.11
(1,1551)	1:15:A:ILE:HA	1:154:A:LEU:HD12	4	0.11
(1,1551)	1:15:A:ILE:HA	1:154:A:LEU:HD13	4	0.11
(1,858)	1:87:A:LEU:H	1:88:A:LYS:HD2	4	0.11
(1,858)	1:87:A:LEU:H	1:88:A:LYS:HD3	4	0.11
(1,858)	1:87:A:LEU:H	1:88:A:LYS:HD2	10	0.11
(1,858)	1:87:A:LEU:H	1:88:A:LYS:HD3	10	0.11
(1,858)	1:87:A:LEU:H	1:88:A:LYS:HD2	17	0.11
(1,858)	1:87:A:LEU:H	1:88:A:LYS:HD3	17	0.11
(1,544)	1:57:A:LYS:H	1:57:A:LYS:HG2	15	0.11
(1,544)	1:57:A:LYS:H	1:57:A:LYS:HG3	15	0.11
(1,272)	1:25:A:LEU:HB2	1:29:A:THR:H	14	0.11
(1,272)	1:25:A:LEU:HB3	1:29:A:THR:H	14	0.11
(1,136)	1:15:A:ILE:HA	1:154:A:LEU:HD11	4	0.11
(1,136)	1:15:A:ILE:HA	1:154:A:LEU:HD12	4	0.11
(1,136)	1:15:A:ILE:HA	1:154:A:LEU:HD13	4	0.11
(3,52)	1:79:A:VAL:N	1:82:A:GLN:O	10	0.1
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE2	4	0.1
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE3	4	0.1
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE2	19	0.1
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE3	19	0.1
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE2	20	0.1
(2,2128)	1:144:A:LEU:HG	1:146:A:LYS:HE3	20	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB1	15	0.1
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB2	15	0.1
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB3	15	0.1
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB1	20	0.1
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB2	20	0.1
(2,2074)	1:133:A:GLU:HA	1:147:A:ALA:HB3	20	0.1
(2,2046)	1:130:A:VAL:HA	1:149:A:THR:HG21	20	0.1
(2,2046)	1:130:A:VAL:HA	1:149:A:THR:HG22	20	0.1
(2,2046)	1:130:A:VAL:HA	1:149:A:THR:HG23	20	0.1
(2,2038)	1:129:A:ALA:HB1	1:144:A:LEU:HG	8	0.1
(2,2038)	1:129:A:ALA:HB2	1:144:A:LEU:HG	8	0.1
(2,2038)	1:129:A:ALA:HB3	1:144:A:LEU:HG	8	0.1
(2,1946)	1:119:A:GLU:HB3	1:140:A:LEU:HD21	7	0.1
(2,1946)	1:119:A:GLU:HB3	1:140:A:LEU:HD22	7	0.1
(2,1946)	1:119:A:GLU:HB3	1:140:A:LEU:HD23	7	0.1
(2,1769)	1:79:A:VAL:HG21	1:139:A:ILE:HB	16	0.1
(2,1769)	1:79:A:VAL:HG22	1:139:A:ILE:HB	16	0.1
(2,1769)	1:79:A:VAL:HG23	1:139:A:ILE:HB	16	0.1
(2,1627)	1:70:A:LEU:HD11	1:88:A:LYS:HA	7	0.1
(2,1627)	1:70:A:LEU:HD12	1:88:A:LYS:HA	7	0.1
(2,1627)	1:70:A:LEU:HD13	1:88:A:LYS:HA	7	0.1
(2,1627)	1:70:A:LEU:HD11	1:88:A:LYS:HA	20	0.1
(2,1627)	1:70:A:LEU:HD12	1:88:A:LYS:HA	20	0.1
(2,1627)	1:70:A:LEU:HD13	1:88:A:LYS:HA	20	0.1
(2,1506)	1:54:A:THR:HG21	1:102:A:VAL:HA	1	0.1
(2,1506)	1:54:A:THR:HG22	1:102:A:VAL:HA	1	0.1
(2,1506)	1:54:A:THR:HG23	1:102:A:VAL:HA	1	0.1
(2,1506)	1:54:A:THR:HG21	1:102:A:VAL:HA	2	0.1
(2,1506)	1:54:A:THR:HG22	1:102:A:VAL:HA	2	0.1
(2,1506)	1:54:A:THR:HG23	1:102:A:VAL:HA	2	0.1
(2,1506)	1:54:A:THR:HG21	1:102:A:VAL:HA	16	0.1
(2,1506)	1:54:A:THR:HG22	1:102:A:VAL:HA	16	0.1
(2,1506)	1:54:A:THR:HG23	1:102:A:VAL:HA	16	0.1
(2,1299)	1:39:A:MET:HG2	1:41:A:PRO:HG2	20	0.1
(2,1299)	1:39:A:MET:HG2	1:41:A:PRO:HG3	20	0.1
(2,1299)	1:39:A:MET:HG3	1:41:A:PRO:HG2	20	0.1
(2,1299)	1:39:A:MET:HG3	1:41:A:PRO:HG3	20	0.1
(2,1293)	1:39:A:MET:HE1	1:41:A:PRO:HA	9	0.1
(2,1293)	1:39:A:MET:HE2	1:41:A:PRO:HA	9	0.1
(2,1293)	1:39:A:MET:HE3	1:41:A:PRO:HA	9	0.1
(2,1272)	1:35:A:ARG:HA	1:36:A:LYS:HE2	11	0.1
(2,1272)	1:35:A:ARG:HA	1:36:A:LYS:HE3	11	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1058)	1:21:A:ARG:HG2	1:149:A:THR:HA	1	0.1
(2,1058)	1:21:A:ARG:HG3	1:149:A:THR:HA	1	0.1
(2,1058)	1:21:A:ARG:HG2	1:149:A:THR:HA	5	0.1
(2,1058)	1:21:A:ARG:HG3	1:149:A:THR:HA	5	0.1
(2,1013)	1:18:A:ILE:HD11	1:149:A:THR:HA	6	0.1
(2,1013)	1:18:A:ILE:HD12	1:149:A:THR:HA	6	0.1
(2,1013)	1:18:A:ILE:HD13	1:149:A:THR:HA	6	0.1
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD2	12	0.1
(2,1007)	1:18:A:ILE:HB	1:21:A:ARG:HD3	12	0.1
(2,960)	1:15:A:ILE:HB	1:149:A:THR:HG21	9	0.1
(2,960)	1:15:A:ILE:HB	1:149:A:THR:HG22	9	0.1
(2,960)	1:15:A:ILE:HB	1:149:A:THR:HG23	9	0.1
(2,858)	1:10:A:PRO:HG2	1:92:A:ILE:HB	9	0.1
(2,858)	1:10:A:PRO:HG3	1:92:A:ILE:HB	9	0.1
(2,858)	1:10:A:PRO:HG2	1:92:A:ILE:HB	12	0.1
(2,858)	1:10:A:PRO:HG3	1:92:A:ILE:HB	12	0.1
(2,568)	1:98:A:GLN:H	1:100:A:GLU:HG2	5	0.1
(2,568)	1:98:A:GLN:H	1:100:A:GLU:HG3	5	0.1
(1,2735)	1:141:A:THR:HG21	1:143:A:GLU:HA	12	0.1
(1,2735)	1:141:A:THR:HG22	1:143:A:GLU:HA	12	0.1
(1,2735)	1:141:A:THR:HG23	1:143:A:GLU:HA	12	0.1
(1,2666)	1:131:A:SER:HA	1:139:A:ILE:HD11	2	0.1
(1,2666)	1:131:A:SER:HA	1:139:A:ILE:HD12	2	0.1
(1,2666)	1:131:A:SER:HA	1:139:A:ILE:HD13	2	0.1
(1,2658)	1:130:A:VAL:HB	1:132:A:SER:HB2	10	0.1
(1,2658)	1:130:A:VAL:HB	1:132:A:SER:HB3	10	0.1
(1,2658)	1:130:A:VAL:HB	1:132:A:SER:HB2	11	0.1
(1,2658)	1:130:A:VAL:HB	1:132:A:SER:HB3	11	0.1
(1,2559)	1:120:A:SER:HB2	1:140:A:LEU:HD21	1	0.1
(1,2559)	1:120:A:SER:HB2	1:140:A:LEU:HD22	1	0.1
(1,2559)	1:120:A:SER:HB2	1:140:A:LEU:HD23	1	0.1
(1,1972)	1:53:A:GLU:HG2	1:54:A:THR:HA	13	0.1
(1,1972)	1:53:A:GLU:HG3	1:54:A:THR:HA	13	0.1
(1,1920)	1:49:A:CYS:HB2	1:50:A:ARG:HA	19	0.1
(1,1680)	1:24:A:VAL:HB	1:31:A:ILE:HG12	11	0.1
(1,1680)	1:24:A:VAL:HB	1:31:A:ILE:HG13	11	0.1
(1,1593)	1:18:A:ILE:HB	1:21:A:ARG:HB2	13	0.1
(1,1593)	1:18:A:ILE:HB	1:21:A:ARG:HB3	13	0.1
(1,1551)	1:15:A:ILE:HA	1:154:A:LEU:HD11	8	0.1
(1,1551)	1:15:A:ILE:HA	1:154:A:LEU:HD12	8	0.1
(1,1551)	1:15:A:ILE:HA	1:154:A:LEU:HD13	8	0.1
(1,1138)	1:120:A:SER:HB2	1:140:A:LEU:HD21	1	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1138)	1:120:A:SER:HB2	1:140:A:LEU:HD22	1	0.1
(1,1138)	1:120:A:SER:HB2	1:140:A:LEU:HD23	1	0.1
(1,870)	1:88:A:LYS:HB2	1:89:A:GLU:H	10	0.1
(1,870)	1:88:A:LYS:HB3	1:89:A:GLU:H	10	0.1
(1,538)	1:56:A:GLU:HA	1:59:A:ARG:H	15	0.1
(1,510)	1:55:A:LEU:H	1:101:A:PRO:HB2	10	0.1
(1,510)	1:55:A:LEU:H	1:101:A:PRO:HB3	10	0.1
(1,272)	1:25:A:LEU:HB2	1:29:A:THR:H	8	0.1
(1,272)	1:25:A:LEU:HB3	1:29:A:THR:H	8	0.1
(1,202)	1:21:A:ARG:HB2	1:132:A:SER:H	2	0.1
(1,202)	1:21:A:ARG:HB3	1:132:A:SER:H	2	0.1
(1,202)	1:21:A:ARG:HB2	1:132:A:SER:H	11	0.1
(1,202)	1:21:A:ARG:HB3	1:132:A:SER:H	11	0.1
(1,136)	1:15:A:ILE:HA	1:154:A:LEU:HD11	8	0.1
(1,136)	1:15:A:ILE:HA	1:154:A:LEU:HD12	8	0.1
(1,136)	1:15:A:ILE:HA	1:154:A:LEU:HD13	8	0.1
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HD2	16	0.1
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HD3	16	0.1
(1,8)	1:3:A:LYS:HD2	1:4:A:ALA:H	15	0.1
(1,8)	1:3:A:LYS:HD3	1:4:A:ALA:H	15	0.1
(1,5)	1:3:A:LYS:H	1:3:A:LYS:HD2	17	0.1
(1,5)	1:3:A:LYS:H	1:3:A:LYS:HD3	17	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found