



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:10 PM UTC

PDB ID : 6B3N / pdb_00006b3n
BMRB ID : 30348
Title : Solution structure of the N-terminal domain of the effector NleG5-1 from Escherichia coli O157:H7 str. Sakai
Authors : Valleau, D.; Houlston, S.; Lemak, A.; Anderson, W.F.; Arrowsmith, C.; Savchenko, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2017-09-22

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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

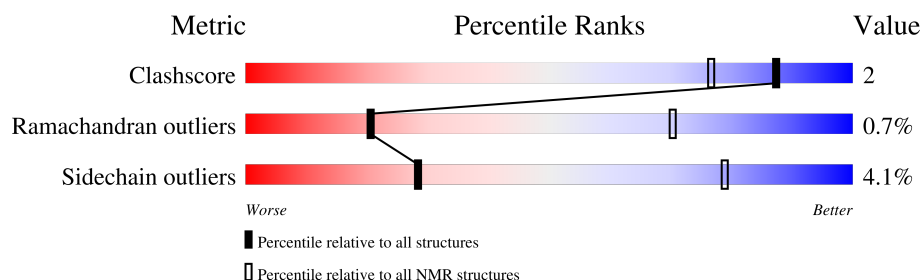
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	137	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 19 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:2-A:49, A:55-A:62, A:66-A:84 (75)	0.74	19
2	A:90-A:100 (11)	0.53	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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1585 atoms, of which 795 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NleG5-1.

Mol	Chain	Residues	Atoms						Trace
1	A	100	Total	C	H	N	O	S	0
			1585	494	795	138	154	4	

There are 21 discrepancies between the modelled and reference sequences:

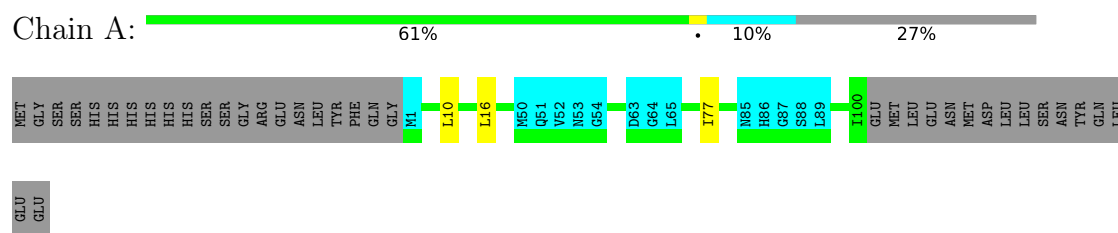
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q8X4X3
A	-19	GLY	-	expression tag	UNP Q8X4X3
A	-18	SER	-	expression tag	UNP Q8X4X3
A	-17	SER	-	expression tag	UNP Q8X4X3
A	-16	HIS	-	expression tag	UNP Q8X4X3
A	-15	HIS	-	expression tag	UNP Q8X4X3
A	-14	HIS	-	expression tag	UNP Q8X4X3
A	-13	HIS	-	expression tag	UNP Q8X4X3
A	-12	HIS	-	expression tag	UNP Q8X4X3
A	-11	HIS	-	expression tag	UNP Q8X4X3
A	-10	SER	-	expression tag	UNP Q8X4X3
A	-9	SER	-	expression tag	UNP Q8X4X3
A	-8	GLY	-	expression tag	UNP Q8X4X3
A	-7	ARG	-	expression tag	UNP Q8X4X3
A	-6	GLU	-	expression tag	UNP Q8X4X3
A	-5	ASN	-	expression tag	UNP Q8X4X3
A	-4	LEU	-	expression tag	UNP Q8X4X3
A	-3	TYR	-	expression tag	UNP Q8X4X3
A	-2	PHE	-	expression tag	UNP Q8X4X3
A	-1	GLN	-	expression tag	UNP Q8X4X3
A	0	GLY	-	expression tag	UNP Q8X4X3

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

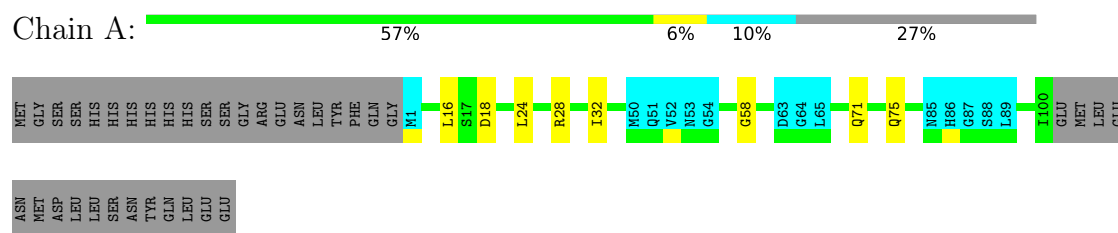
- Molecule 1: NleG5-1



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 19. Colouring as in section 4.1 above.

- Molecule 1: NleG5-1



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 lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1253
Number of shifts mapped to atoms	1119
Number of unparsed shifts	0
Number of shifts with mapping errors	134
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality

6.1 Standard geometry

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	1.32±0.02	0±1/700 (0.1± 0.1%)	0.97±0.02	0±0/949 (0.0± 0.0%)
All	All	1.32	9/14000 (0.1%)	0.97	0/18980 (0.0%)

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	0.1±0.2
All	All	0	1

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	19	ILE	CA-CB	5.91	1.58	1.54	6	4
1	A	47	ILE	CA-CB	5.61	1.59	1.53	3	1
1	A	77	ILE	CA-CB	5.38	1.60	1.54	8	4

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	39	ARG	Sidechain	1

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	690	701	701	3±1
All	All	13800	14020	14020	57

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 2.

5 of 36 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ARG:HG2	1:A:44:MET:SD	0.61	2.35	8	4
1:A:37:GLN:HB3	1:A:44:MET:SD	0.57	2.37	20	1
1:A:57:MET:HE1	1:A:91:SER:HA	0.55	1.78	6	1
1:A:57:MET:SD	1:A:81:GLU:HB2	0.54	2.42	10	1
1:A:40:LEU:HD11	1:A:80:ILE:HD11	0.52	1.80	5	2

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	85/137 (62%)	76±3 (90±3%)	8±3 (10±4%)	1±1 (1±1%)	20	70
All	All	1700/2740 (62%)	1523 (90%)	165 (10%)	12 (1%)	20	70

5 of 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	58	GLY	4
1	A	7	PRO	3
1	A	18	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	3	VAL	1
1	A	49	PRO	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	80/125 (64%)	77±2 (96±2%)	3±2 (4±2%)	28	79
All	All	1600/2500 (64%)	1534 (96%)	66 (4%)	28	79

5 of 23 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	16	LEU	11
1	A	77	ILE	11
1	A	10	LEU	10
1	A	42	GLU	5
1	A	78	GLU	3

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 82% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *ECS1996_cshifts*

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	1253
Number of shifts mapped to atoms	1119
Number of unparsed shifts	0
Number of shifts with mapping errors	134
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 134) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	GLU	HA	4.092	0.04	1
1	A	101	GLU	HB2	2.076	0.04	2
1	A	101	GLU	HB3	2.076	0.04	2
1	A	101	GLU	C	178.107	0.40	1
1	A	101	GLU	CA	59.021	0.40	1
1	A	101	GLU	CB	29.529	0.40	1
1	A	102	MET	H	8.023	0.04	1
1	A	102	MET	HA	4.402	0.04	1
1	A	102	MET	HB2	2.553	0.04	2
1	A	102	MET	HB3	2.689	0.04	2
1	A	102	MET	HG2	2.161	0.04	2
1	A	102	MET	HG3	2.075	0.04	2
1	A	102	MET	C	177.243	0.40	1
1	A	102	MET	CA	56.523	0.40	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	102	MET	CB	32.073	0.40	1
1	A	102	MET	CG	32.779	0.40	1
1	A	102	MET	N	117.553	0.40	1
1	A	103	LEU	H	7.894	0.04	1
1	A	103	LEU	HA	4.264	0.04	1
1	A	103	LEU	HB2	1.582	0.04	2
1	A	103	LEU	HB3	1.582	0.04	2
1	A	103	LEU	C	178.386	0.40	1
1	A	103	LEU	CA	56.337	0.40	1
1	A	103	LEU	CB	42.421	0.40	1
1	A	103	LEU	N	121.207	0.40	1
1	A	104	GLU	H	8.296	0.04	1
1	A	104	GLU	HA	4.456	0.04	1
1	A	104	GLU	HB2	1.933	0.04	2
1	A	104	GLU	HB3	1.933	0.04	2
1	A	104	GLU	HG2	2.067	0.04	2
1	A	104	GLU	HG3	2.067	0.04	2
1	A	104	GLU	C	175.934	0.40	1
1	A	104	GLU	CA	55.759	0.40	1
1	A	104	GLU	CB	33.545	0.40	1
1	A	104	GLU	CG	33.545	0.40	1
1	A	104	GLU	N	119.568	0.40	1
1	A	105	ASN	H	8.322	0.04	1
1	A	105	ASN	HA	4.598	0.04	1
1	A	105	ASN	HB2	2.738	0.04	2
1	A	105	ASN	HB3	2.605	0.04	2
1	A	105	ASN	CA	54.592	0.40	1
1	A	105	ASN	CB	40.893	0.40	1
1	A	105	ASN	N	120.735	0.40	1
1	A	106	MET	HA	4.2	0.04	1
1	A	106	MET	C	176.676	0.40	1
1	A	106	MET	CA	57.271	0.40	1
1	A	107	ASP	H	8.145	0.04	1
1	A	107	ASP	HA	4.648	0.04	1
1	A	107	ASP	HB2	2.938	0.04	2
1	A	107	ASP	HB3	2.775	0.04	2
1	A	107	ASP	C	175.274	0.40	1
1	A	107	ASP	CA	53.394	0.40	1
1	A	107	ASP	CB	38.432	0.40	1
1	A	107	ASP	N	118.045	0.40	1
1	A	108	LEU	H	8.07	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	LEU	HA	4.306	0.04	1
1	A	108	LEU	HB2	1.613	0.04	2
1	A	108	LEU	HB3	1.613	0.04	2
1	A	108	LEU	C	177.941	0.40	1
1	A	108	LEU	CA	55.593	0.40	1
1	A	108	LEU	CB	42.383	0.40	1
1	A	108	LEU	N	119.313	0.40	1
1	A	109	LEU	H	8.084	0.04	1
1	A	109	LEU	HA	4.312	0.04	1
1	A	109	LEU	HB2	1.758	0.04	2
1	A	109	LEU	HB3	1.605	0.04	2
1	A	109	LEU	HD11	0.891	0.04	2
1	A	109	LEU	HD12	0.891	0.04	2
1	A	109	LEU	HD13	0.891	0.04	2
1	A	109	LEU	HG	1.596	0.04	1
1	A	109	LEU	C	178.051	0.40	1
1	A	109	LEU	CA	56.023	0.40	1
1	A	109	LEU	CB	42.052	0.40	1
1	A	109	LEU	CD1	25.271	0.40	2
1	A	109	LEU	CG	27.252	0.40	1
1	A	109	LEU	N	120.754	0.40	1
1	A	110	SER	H	8.143	0.04	1
1	A	110	SER	HA	4.343	0.04	1
1	A	110	SER	HB2	3.855	0.04	2
1	A	110	SER	HB3	3.855	0.04	2
1	A	110	SER	CA	59.177	0.40	1
1	A	110	SER	CB	63.4	0.40	1
1	A	110	SER	N	115.464	0.40	1
1	A	112	TYR	HA	4.535	0.04	1
1	A	112	TYR	HB2	3.048	0.04	2
1	A	112	TYR	HB3	3.004	0.04	2
1	A	112	TYR	C	175.228	0.40	1
1	A	112	TYR	CA	57.623	0.40	1
1	A	112	TYR	CB	39.681	0.40	1
1	A	113	GLN	H	8.198	0.04	1
1	A	113	GLN	HA	4.24	0.04	1
1	A	113	GLN	HB2	2.029	0.04	2
1	A	113	GLN	HB3	1.901	0.04	2
1	A	113	GLN	HG2	2.301	0.04	2
1	A	113	GLN	HG3	2.301	0.04	2
1	A	113	GLN	C	175.57	0.40	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	GLN	CA	55.698	0.40	1
1	A	113	GLN	CB	29.357	0.40	1
1	A	113	GLN	CG	33.75	0.40	1
1	A	113	GLN	N	122.609	0.40	1
1	A	114	LEU	H	8.058	0.04	1
1	A	114	LEU	HA	4.282	0.04	1
1	A	114	LEU	HB2	1.632	0.04	2
1	A	114	LEU	HB3	1.632	0.04	2
1	A	114	LEU	HD11	0.921	0.04	2
1	A	114	LEU	HD12	0.921	0.04	2
1	A	114	LEU	HD13	0.921	0.04	2
1	A	114	LEU	HD21	0.869	0.04	2
1	A	114	LEU	HD22	0.869	0.04	2
1	A	114	LEU	HD23	0.869	0.04	2
1	A	114	LEU	C	177.417	0.40	1
1	A	114	LEU	CA	55.286	0.40	1
1	A	114	LEU	CB	42.513	0.40	1
1	A	114	LEU	CD1	24.943	0.40	2
1	A	114	LEU	CD2	23.469	0.40	2
1	A	114	LEU	N	123.072	0.40	1
1	A	115	GLU	H	8.333	0.04	1
1	A	115	GLU	HA	4.284	0.04	1
1	A	115	GLU	HB2	2.084	0.04	2
1	A	115	GLU	HB3	1.965	0.04	2
1	A	115	GLU	C	179.159	0.40	1
1	A	115	GLU	CA	56.901	0.40	1
1	A	115	GLU	CB	29.878	0.40	1
1	A	115	GLU	N	121.837	0.40	1
1	A	116	GLU	H	8.34	0.04	1
1	A	116	GLU	HA	4.849	0.04	1
1	A	116	GLU	HB2	2.062	0.04	2
1	A	116	GLU	HB3	1.936	0.04	2
1	A	116	GLU	HG2	2.621	0.04	2
1	A	116	GLU	HG3	2.55	0.04	2
1	A	116	GLU	CA	52.966	0.40	1
1	A	116	GLU	CB	32.681	0.40	1
1	A	116	GLU	CG	31.971	0.40	1
1	A	116	GLU	N	118.901	0.40	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	109	-0.17 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	97	0.17 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	95	-0.21 ± 0.10	None needed (< 0.5 ppm)
^{15}N	97	0.13 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1009 atoms were assigned a chemical shift out of a possible 1228. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	393/425 (92%)	162/172 (94%)	157/172 (91%)	74/81 (91%)
Sidechain	592/749 (79%)	404/488 (83%)	188/230 (82%)	0/31 (0%)
Aromatic	24/54 (44%)	16/26 (62%)	8/27 (30%)	0/1 (0%)
Overall	1009/1228 (82%)	582/686 (85%)	353/429 (82%)	74/113 (65%)

7.1.4 Statistically unusual chemical shifts [i](#)

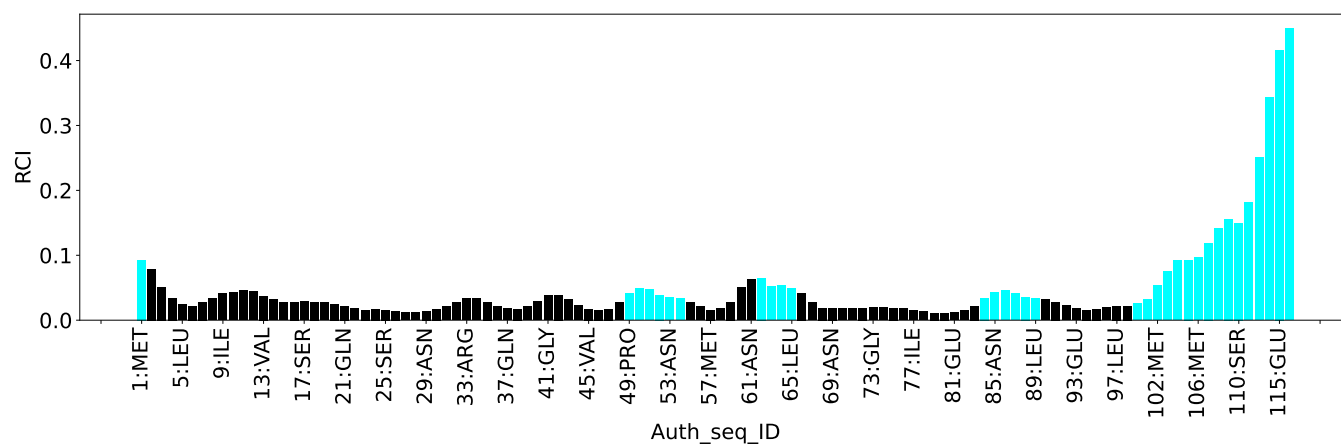
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	58	GLY	HA2	5.80	2.15 – 5.77	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	1784
Intra-residue ($ i-j =0$)	486
Sequential ($ i-j =1$)	438
Medium range ($ i-j >1$ and $ i-j <5$)	357
Long range ($ i-j \geq 5$)	503
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	13.0
Number of long range restraints per residue ¹	3.7

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)	12.1	0.2
0.2-0.5 (Medium)	2.9	0.45
>0.5 (Large)	0.1	0.52

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 ⓘ

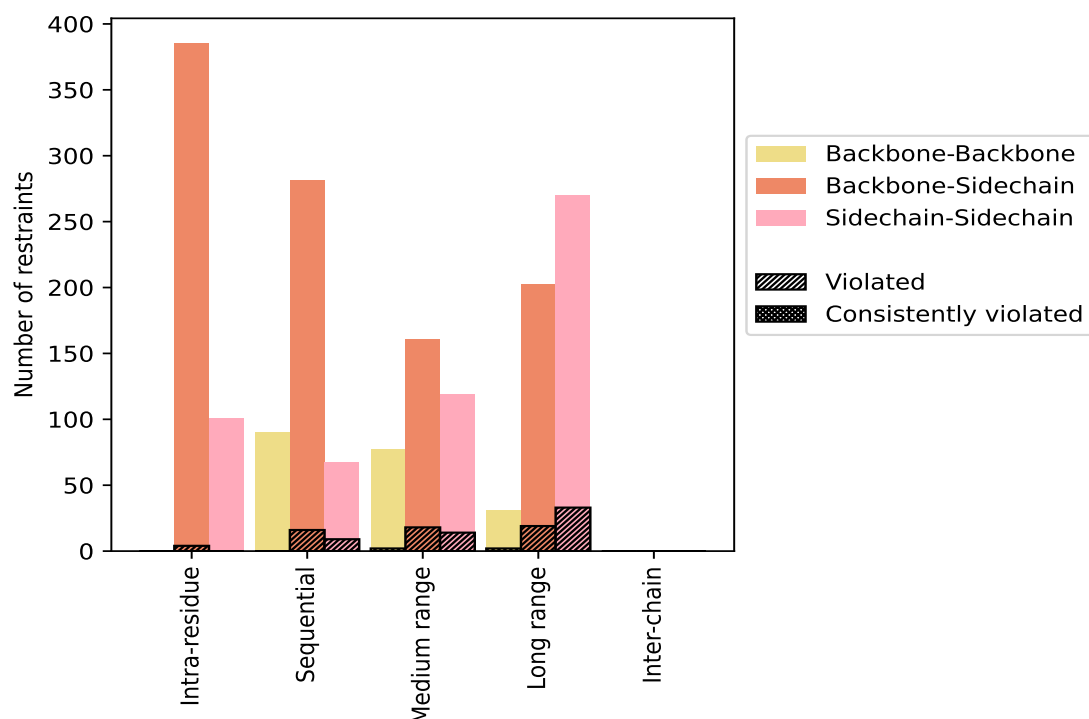
9.1 Summary of distance violations ⓘ

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)	486	27.2	4	0.8	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	385	21.6	4	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	101	5.7	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	438	24.6	25	5.7	1.4	0	0.0	0.0
Backbone-Backbone	90	5.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	281	15.8	16	5.7	0.9	0	0.0	0.0
Sidechain-Sidechain	67	3.8	9	13.4	0.5	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	357	20.0	34	9.5	1.9	0	0.0	0.0
Backbone-Backbone	77	4.3	2	2.6	0.1	0	0.0	0.0
Backbone-Sidechain	161	9.0	18	11.2	1.0	0	0.0	0.0
Sidechain-Sidechain	119	6.7	14	11.8	0.8	0	0.0	0.0
Long range (i-j ≥5)	503	28.2	54	10.7	3.0	0	0.0	0.0
Backbone-Backbone	31	1.7	2	6.5	0.1	0	0.0	0.0
Backbone-Sidechain	202	11.3	19	9.4	1.1	0	0.0	0.0
Sidechain-Sidechain	270	15.1	33	12.2	1.8	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1784	100.0	117	6.6	6.6	0	0.0	0.0
Backbone-Backbone	198	11.1	4	2.0	0.2	0	0.0	0.0
Backbone-Sidechain	1029	57.7	57	5.5	3.2	0	0.0	0.0
Sidechain-Sidechain	557	31.2	56	10.1	3.1	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	3	10	0	15	0.14	0.2	0.04	0.13
2	1	5	4	7	0	17	0.17	0.35	0.08	0.14
3	1	3	5	7	0	16	0.18	0.45	0.08	0.17
4	1	2	3	8	0	14	0.18	0.52	0.1	0.15
5	0	5	8	8	0	21	0.16	0.45	0.07	0.14
6	1	2	2	8	0	13	0.15	0.26	0.04	0.14
7	0	3	7	5	0	15	0.17	0.3	0.05	0.15
8	1	2	4	8	0	15	0.17	0.36	0.06	0.16
9	1	2	5	12	0	20	0.14	0.19	0.03	0.13
10	2	7	4	12	0	25	0.15	0.31	0.05	0.13

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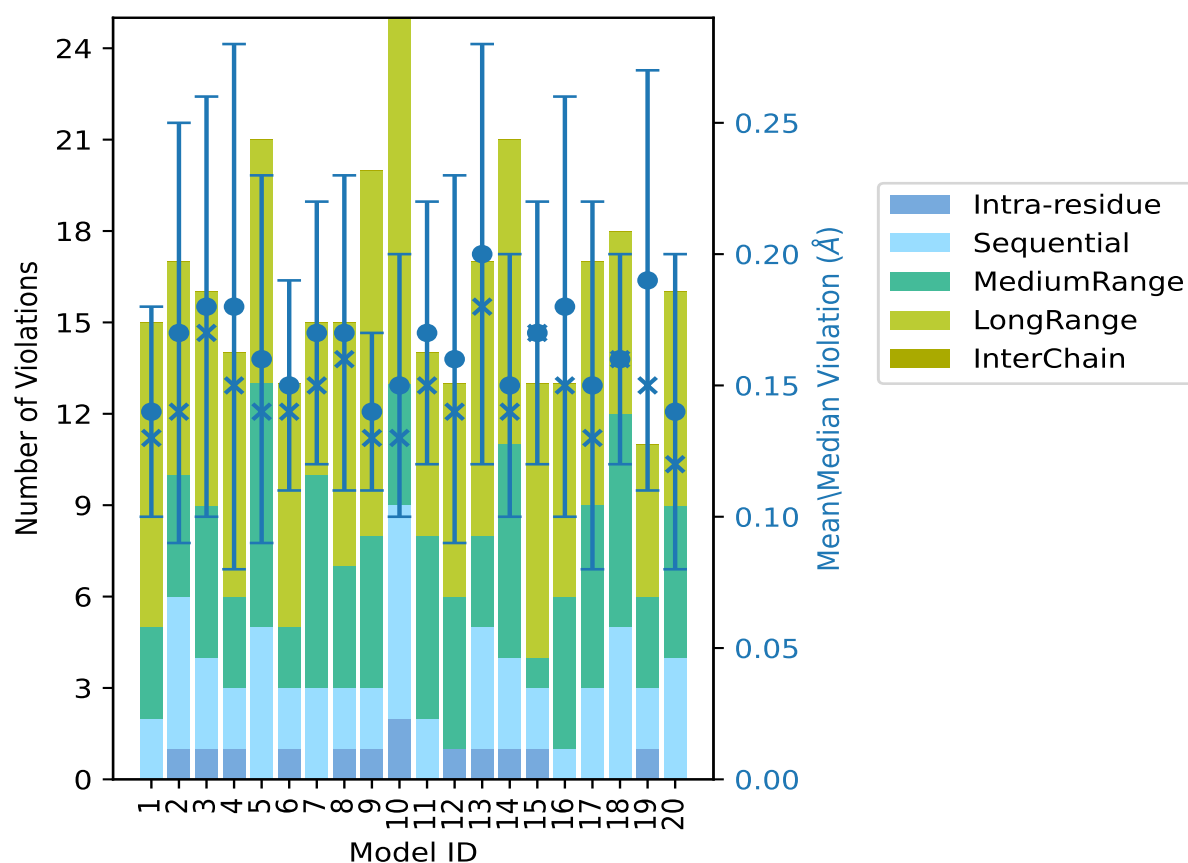
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	2	6	6	0	14	0.17	0.24	0.05	0.15
12	1	0	5	7	0	13	0.16	0.35	0.07	0.14
13	1	4	3	9	0	17	0.2	0.35	0.08	0.18
14	1	3	7	10	0	21	0.15	0.28	0.05	0.14
15	1	2	1	9	0	13	0.17	0.26	0.05	0.17
16	0	1	5	7	0	13	0.18	0.39	0.08	0.15
17	0	3	6	8	0	17	0.15	0.41	0.07	0.13
18	0	5	7	6	0	18	0.16	0.27	0.04	0.16
19	1	2	3	5	0	11	0.19	0.37	0.08	0.15
20	0	4	5	7	0	16	0.14	0.33	0.06	0.12

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 ⓘ

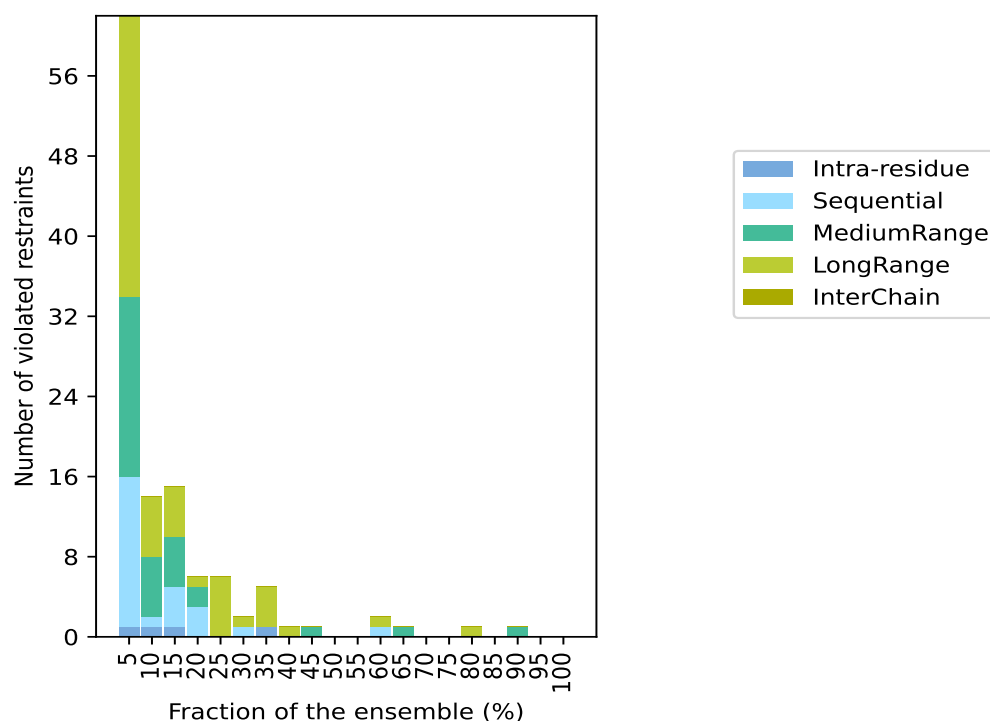
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1667(IR:482, SQ:413, MR:323, LR:449, IC:0) restraints are 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	%
1	15	18	28	0	62	1	5.0
1	1	6	6	0	14	2	10.0
1	4	5	5	0	15	3	15.0
0	3	2	1	0	6	4	20.0
0	0	0	6	0	6	5	25.0
0	1	0	1	0	2	6	30.0
1	0	0	4	0	5	7	35.0
0	0	0	1	0	1	8	40.0
0	0	1	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	1	0	1	0	2	12	60.0
0	0	1	0	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	1	0	1	16	80.0
0	0	0	0	0	0	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

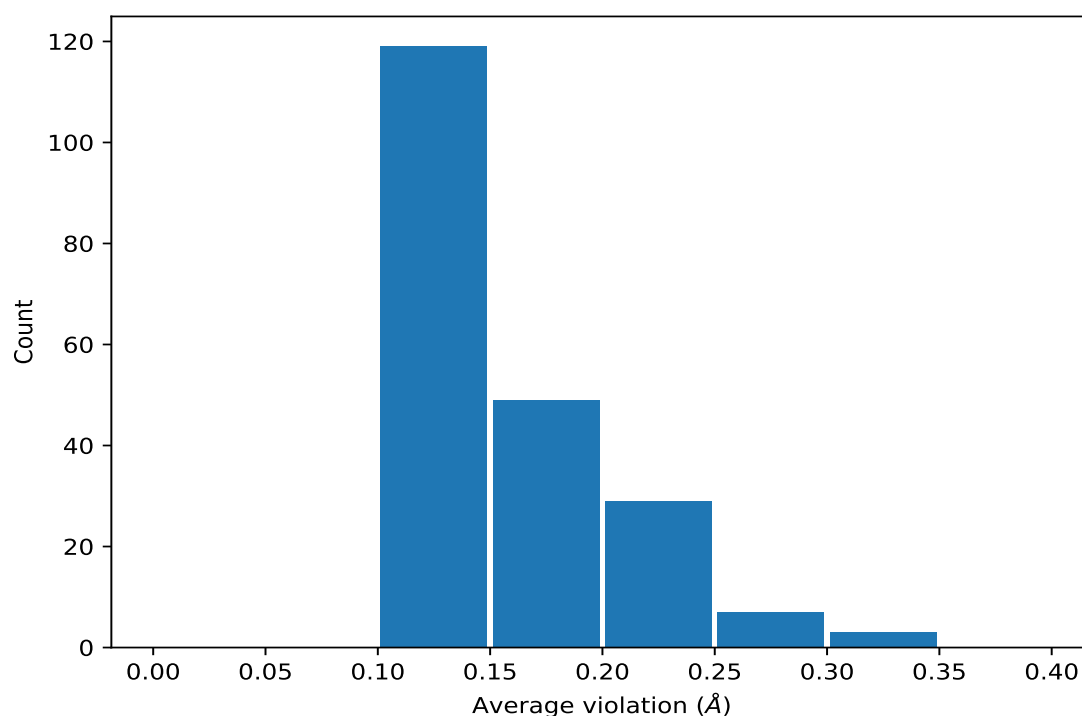
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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)
(1,1184)	1:6:A:THR:HG21	1:9:A:ILE:HD11	18	0.18	0.04	0.18
(1,1184)	1:6:A:THR:HG21	1:9:A:ILE:HD12	18	0.18	0.04	0.18
(1,1184)	1:6:A:THR:HG21	1:9:A:ILE:HD13	18	0.18	0.04	0.18
(1,1184)	1:6:A:THR:HG22	1:9:A:ILE:HD11	18	0.18	0.04	0.18
(1,1184)	1:6:A:THR:HG22	1:9:A:ILE:HD12	18	0.18	0.04	0.18
(1,1184)	1:6:A:THR:HG22	1:9:A:ILE:HD13	18	0.18	0.04	0.18
(1,1184)	1:6:A:THR:HG23	1:9:A:ILE:HD11	18	0.18	0.04	0.18
(1,1184)	1:6:A:THR:HG23	1:9:A:ILE:HD12	18	0.18	0.04	0.18
(1,1184)	1:6:A:THR:HG23	1:9:A:ILE:HD13	18	0.18	0.04	0.18
(1,1042)	1:60:A:LEU:HB3	1:77:A:ILE:HD11	16	0.16	0.03	0.15
(1,1042)	1:60:A:LEU:HB3	1:77:A:ILE:HD12	16	0.16	0.03	0.15
(1,1042)	1:60:A:LEU:HB3	1:77:A:ILE:HD13	16	0.16	0.03	0.15
(1,759)	1:6:A:THR:HG21	1:9:A:ILE:H	13	0.15	0.04	0.15
(1,759)	1:6:A:THR:HG22	1:9:A:ILE:H	13	0.15	0.04	0.15
(1,759)	1:6:A:THR:HG23	1:9:A:ILE:H	13	0.15	0.04	0.15
(1,1469)	1:30:A:GLN:HG2	1:31:A:THR:H	12	0.35	0.09	0.34

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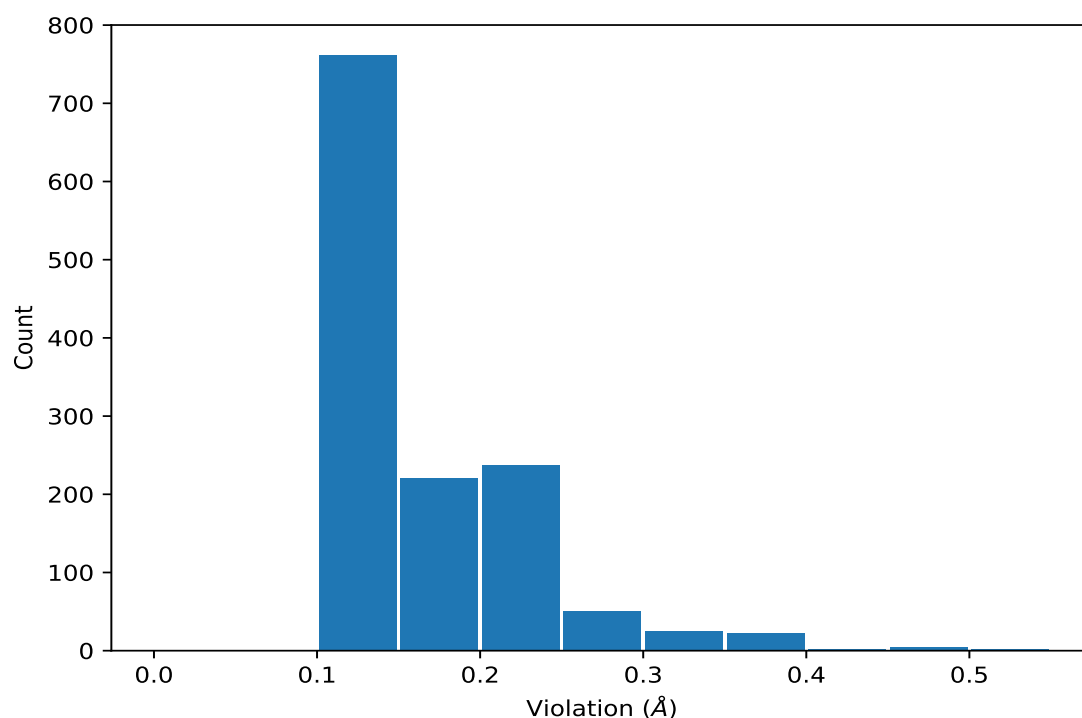
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1469)	1:30:A:GLN:HG3	1:31:A:THR:H	12	0.35	0.09	0.34
(1,479)	1:8:A:TYR:HD1	1:19:A:ILE:HG13	12	0.14	0.03	0.14
(1,479)	1:8:A:TYR:HD2	1:19:A:ILE:HG13	12	0.14	0.03	0.14
(1,422)	1:62:A:GLN:HA	1:66:A:SER:H	9	0.15	0.03	0.15
(1,1661)	1:65:A:LEU:HD11	1:70:A:ILE:H	8	0.16	0.04	0.15
(1,1661)	1:65:A:LEU:HD12	1:70:A:ILE:H	8	0.16	0.04	0.15
(1,1661)	1:65:A:LEU:HD13	1:70:A:ILE:H	8	0.16	0.04	0.15
(1,1661)	1:65:A:LEU:HD21	1:70:A:ILE:H	8	0.16	0.04	0.15
(1,1661)	1:65:A:LEU:HD22	1:70:A:ILE:H	8	0.16	0.04	0.15
(1,1661)	1:65:A:LEU:HD23	1:70:A:ILE:H	8	0.16	0.04	0.15
(1,1654)	1:65:A:LEU:H	1:65:A:LEU:HD11	7	0.22	0.01	0.22
(1,1654)	1:65:A:LEU:H	1:65:A:LEU:HD12	7	0.22	0.01	0.22
(1,1654)	1:65:A:LEU:H	1:65:A:LEU:HD13	7	0.22	0.01	0.22
(1,1654)	1:65:A:LEU:H	1:65:A:LEU:HD21	7	0.22	0.01	0.22
(1,1654)	1:65:A:LEU:H	1:65:A:LEU:HD22	7	0.22	0.01	0.22
(1,1654)	1:65:A:LEU:H	1:65:A:LEU:HD23	7	0.22	0.01	0.22
(1,1663)	1:65:A:LEU:HD11	1:70:A:ILE:HG12	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD11	1:70:A:ILE:HG13	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD12	1:70:A:ILE:HG12	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD12	1:70:A:ILE:HG13	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD13	1:70:A:ILE:HG12	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD13	1:70:A:ILE:HG13	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD21	1:70:A:ILE:HG12	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD21	1:70:A:ILE:HG13	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD22	1:70:A:ILE:HG12	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD22	1:70:A:ILE:HG13	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD23	1:70:A:ILE:HG12	7	0.16	0.04	0.14
(1,1663)	1:65:A:LEU:HD23	1:70:A:ILE:HG13	7	0.16	0.04	0.14
(1,1234)	1:8:A:TYR:HE1	1:19:A:ILE:HG12	7	0.16	0.03	0.15

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 provides the 10 worst performing restraints, sorted by the violation 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)
(1,1469)	1:30:A:GLN:HG2	1:31:A:THR:H	4	0.52
(1,1469)	1:30:A:GLN:HG3	1:31:A:THR:H	4	0.52
(1,1469)	1:30:A:GLN:HG2	1:31:A:THR:H	3	0.45
(1,1469)	1:30:A:GLN:HG3	1:31:A:THR:H	3	0.45
(1,1469)	1:30:A:GLN:HG2	1:31:A:THR:H	5	0.45
(1,1469)	1:30:A:GLN:HG3	1:31:A:THR:H	5	0.45
(1,1469)	1:30:A:GLN:HG2	1:31:A:THR:H	17	0.41
(1,1469)	1:30:A:GLN:HG3	1:31:A:THR:H	17	0.41
(1,1469)	1:30:A:GLN:HG2	1:31:A:THR:H	16	0.39
(1,1469)	1:30:A:GLN:HG3	1:31:A:THR:H	16	0.39
(1,1394)	1:17:A:SER:HB2	1:18:A:ASP:H	19	0.37
(1,1394)	1:17:A:SER:HB3	1:18:A:ASP:H	19	0.37
(1,1550)	1:43:A:LEU:HD11	1:72:A:ILE:HD11	8	0.36
(1,1550)	1:43:A:LEU:HD11	1:72:A:ILE:HD12	8	0.36
(1,1550)	1:43:A:LEU:HD11	1:72:A:ILE:HD13	8	0.36
(1,1550)	1:43:A:LEU:HD12	1:72:A:ILE:HD11	8	0.36
(1,1550)	1:43:A:LEU:HD12	1:72:A:ILE:HD12	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:43:A:LEU:HD12	1:72:A:ILE:HD13	8	0.36
(1,1550)	1:43:A:LEU:HD13	1:72:A:ILE:HD11	8	0.36
(1,1550)	1:43:A:LEU:HD13	1:72:A:ILE:HD12	8	0.36
(1,1550)	1:43:A:LEU:HD13	1:72:A:ILE:HD13	8	0.36
(1,1550)	1:43:A:LEU:HD21	1:72:A:ILE:HD11	8	0.36
(1,1550)	1:43:A:LEU:HD21	1:72:A:ILE:HD12	8	0.36
(1,1550)	1:43:A:LEU:HD21	1:72:A:ILE:HD13	8	0.36
(1,1550)	1:43:A:LEU:HD22	1:72:A:ILE:HD11	8	0.36
(1,1550)	1:43:A:LEU:HD22	1:72:A:ILE:HD12	8	0.36
(1,1550)	1:43:A:LEU:HD22	1:72:A:ILE:HD13	8	0.36
(1,1550)	1:43:A:LEU:HD23	1:72:A:ILE:HD11	8	0.36
(1,1550)	1:43:A:LEU:HD23	1:72:A:ILE:HD12	8	0.36
(1,1550)	1:43:A:LEU:HD23	1:72:A:ILE:HD13	8	0.36
(1,1191)	1:57:A:MET:HE1	1:89:A:LEU:HD21	2	0.35
(1,1191)	1:57:A:MET:HE1	1:89:A:LEU:HD22	2	0.35
(1,1191)	1:57:A:MET:HE1	1:89:A:LEU:HD23	2	0.35
(1,1191)	1:57:A:MET:HE2	1:89:A:LEU:HD21	2	0.35
(1,1191)	1:57:A:MET:HE2	1:89:A:LEU:HD22	2	0.35
(1,1191)	1:57:A:MET:HE2	1:89:A:LEU:HD23	2	0.35
(1,1191)	1:57:A:MET:HE3	1:89:A:LEU:HD21	2	0.35
(1,1191)	1:57:A:MET:HE3	1:89:A:LEU:HD22	2	0.35
(1,1191)	1:57:A:MET:HE3	1:89:A:LEU:HD23	2	0.35
(1,862)	1:87:A:GLY:HA2	1:88:A:SER:HB2	13	0.35
(1,862)	1:87:A:GLY:HA2	1:88:A:SER:HB3	13	0.35
(1,394)	1:43:A:LEU:H	1:43:A:LEU:HG	12	0.35

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found