

wwPDB NMR Structure Validation Summary Report (i)

Jun 5, 2023 – 03:00 PM JST

PDB ID : 7FGT BMRB ID : 36433

Title: Discovery of DS15060524; Gene targeting chimera (GeneTAC) for the treat-

ment of Friedreich's Ataxia (FRDA)

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Deposited on : 2021-07-28

This is a wwPDB NMR Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

wwPDB-RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

 $\begin{array}{ccc} wwPDB\text{-ShiftChecker} &:& v1.2\\ BMRB \ Restraints \ Analysis &:& v1.2 \end{array}$

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

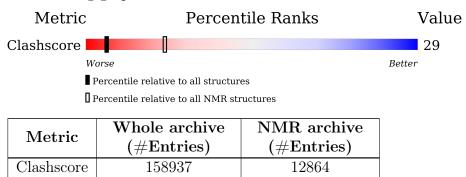
Validation Pipeline (wwPDB-VP) : 2.33

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 28%.

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.



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

Mol	Chain	Length	Quality of chain					
1	A	9	33%	67%				
2	В	9	33%	67%				



2 Ensemble composition and analysis (i)

This entry contains 11 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.



3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 692 atoms, of which 263 are hydrogens and 0 are deuteriums.

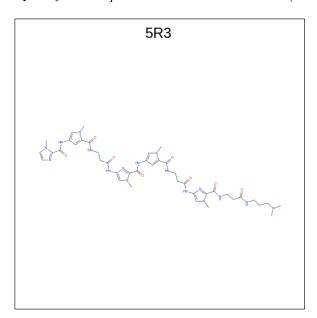
• Molecule 1 is a DNA chain called DNA (5'-D(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues		Atoms					
1	Λ	0	Total	С	Н	N	О	Р	0
1	A	A 9	290	90	101	45	46	8	U

• Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*TP*CP*TP*TP*CP*TP*T)-3').

Mol	Chain	Residues		Atoms						
9	D	0	Total	С	Н	N	О	Р	0	
2	2 B	B 9	281	87	107	21	58	8	U	

• Molecule 3 is $\{N\}-[3-[3-(dimethylamino)propylamino]-3-oxidanylidene-propyl]-1-methyl-4-[3-[[1-methyl-4-[(1-methyl-imidazol-2-yl)carbonylamino]pyrrol-2-yl]carbonylamino]propanoylamino]imidazol-2-yl]carbonylamino]pyrrol-2-yl$



Mol	Chain	Residues	Atoms					
2	2 1	1	Total	С	Н	N	О	
)	A		121	41	55	17	8	



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: DNA (5'-D(*AP*AP*GP*AP*AP*GP*AP*AP*G)-3')

Chain A: 33% 67%

A1 A2 G3 A4 A5 G6 A7 A8

• Molecule 2: DNA (5'-D(*CP*TP*TP*CP*TP*TP*CP*TP*T)-3')

Chain B: 33% 67%

C10 T11 T12 C13 T14 T15 C16 T17

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

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: DNA (5'-D(*AP*AP*GP*AP*AP*GP*AP*AP*G)-3')

Chain A: 22% 78%

A1 A2 G3 G6 G6 A7 A7

• Molecule 2: DNA (5'-D(*CP*TP*TP*CP*TP*TP*CP*TP*T)-3')

Chain B: 22% 78%

C10 T111 T12 C13 T14 T15 C16 T15



Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: na.

Of the 100 calculated structures, 11 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
CNS	refinement	1.3
CNS	structure calculation	1.3

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	164
Number of shifts mapped to atoms	164
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	28%



6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5R3

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	189	101	101	6±3
2	В	174	107	107	12±2
3	A	66	55	0	10±3
All	All	4719	2893	2288	202

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 29.

5 of 44 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	${f Models}$	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
3:A:101:5R3:C63	2:B:15:DT:H5'	0.67	2.20	10	11
2:B:14:DT:H2"	2:B:15:DT:C6	0.65	2.26	4	11
3:A:101:5R3:CM3	2:B:16:DC:H1'	0.63	2.22	10	1
1:A:4:DA:H4'	3:A:101:5R3:C65	0.60	2.26	3	4
2:B:15:DT:H2"	2:B:16:DC:H6	0.58	1.56	1	11



6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

There are no protein molecules in this entry.

6.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mal	Type	Chain	Pog	Link	Bond lengths Counts RMSZ #Z>2			
10101	туре	Chain	lites	Lilik	Counts	RMSZ	#Z>2	
3	5R3	A	101	-	59,70,70	2.47 ± 0.02	20±1 (33±0%)	

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard



deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mal	Type	Chain	Pog	Link	Bond angles Counts RMSZ #Z>2			
IVIOI	Туре	Chain	rtes	Link	Counts	RMSZ	#Z>2	
3	5R3	A	101	-	61,97,97	1.96 ± 0.04	16±1 (25±1%)	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5R3	A	101	-	-	$0\pm0,35,61,61$	$0\pm0,5,5,5$

5 of 21 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Iol Chain I		Trens	Atoms	\mathbf{Z}	Observed(Å)	$Ideal(\mathring{A})$	Models	
IVIOI	Chain	Res	Type	Atoms	L	Observed(A)	Ideal(A)	Worst	Total
3	A	101	5R3	C16-N16	7.36	1.50	1.33	3	11
3	A	101	5R3	C32-C42	5.76	1.44	1.39	4	11
3	A	101	5R3	C74-N84	5.45	1.45	1.33	4	11
3	A	101	5R3	C72-N82	5.00	1.44	1.33	4	11
3	A	101	5R3	C75-N85	4.95	1.44	1.33	3	11

5 of 19 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol Chain	hain Dag Trun	Dec Trme	Atoms Z	7	Observed(0)	$\mathrm{Ideal}(^{o})$	Models		
MIOI	Chain	Res	Type	Atoms		$\operatorname{Observed}(^{o})$	ideai()	Worst	Total
3	A	101	5R3	C25-C75-N85	5.84	121.40	115.60	10	11
3	A	101	5R3	C21-C71-N81	5.57	119.73	113.69	10	11
3	A	101	5R3	C45-N94-C94	5.17	118.99	128.25	5	11
3	A	101	5R3	C43-N92-C92	4.70	119.83	128.25	10	11
3	A	101	5R3	C54-C44-C34	4.40	108.20	106.05	5	11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In



addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

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 (i)

The completeness of assignment taking into account all chemical shift lists is 28% for the well-defined parts and 28% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: $shift_table_for_BMRB_210825.txt$

7.1.1 Bookkeeping (i)

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	164
Number of shifts mapped to atoms	164
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 28%, i.e. 97 atoms were assigned a chemical shift out of a possible 351. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}{ m H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Sugar	57/216 (26%)	57/126 (45%)	0/90 (0%)	0/0 (%)
Base	40/135 (30%)	40/81 (49%)	0/33~(0%)	0/21 (0%)
Overall	97/351 (28%)	97/207~(47%)	0/123~(0%)	0/21~(0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.



7.1.5 Random Coil Index (RCI) plots (i)

No $random\ coil\ index(RCI)$ plot could be generated from the current chemical shift list. RCI is only applicable to proteins



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	241
Intra-residue ($ i-j =0$)	79
Sequential ($ i-j =1$)	71
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range (i-j ≥5)	39
Inter-chain	52
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	188
Number of unmapped restraints	0
Number of restraints per residue	23.8
Number of long range restraints per residue ¹	2.2

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 (i)

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 (i)

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)	13.4	0.2
0.2-0.5 (Medium)	5.7	0.45
>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.

Bins $(^{\circ})$	Average number of violations per model	$\mathbf{Max} \ (^{\circ})$
1.0-10.0 (Small)	9.5	4.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None



9 Distance violation analysis (i)

9.1 Summary of distance violations (i)

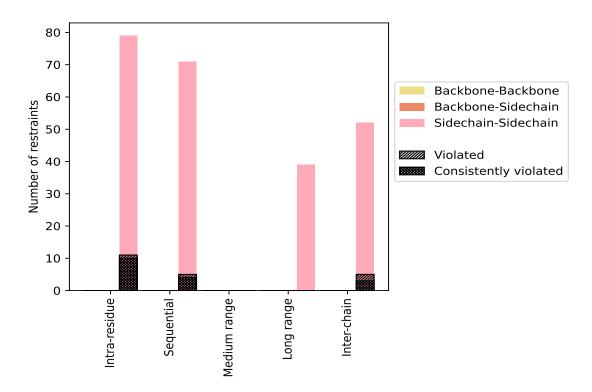
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Donton into topo o	Commit	$\%^{1}$	Vio	olated ⁵	3	Consis	tently	$\overline{ m Violated^4}$
Restraints type	Count	70	Count	$\%^2$	$ \%^1$	Count	$\%^2$	$\%^1$
Intra-residue (i-j =0)	79	32.8	11	13.9	4.6	10	12.7	4.1
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	79	32.8	11	13.9	4.6	10	12.7	4.1
Sequential (i-j =1)	71	29.5	5	7.0	2.1	4	5.6	1.7
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	71	29.5	5	7.0	2.1	4	5.6	1.7
Medium range ($ i-j >1 \& i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \ge 5$)	39	16.2	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	39	16.2	0	0.0	0.0	0	0.0	0.0
Inter-chain	52	21.6	5	9.6	2.1	3	5.8	1.2
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	52	21.6	5	9.6	2.1	3	5.8	1.2
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	241	100.0	21	8.7	8.7	17	7.1	7.1
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	241	100.0	21	8.7	8.7	17	7.1	7.1

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)

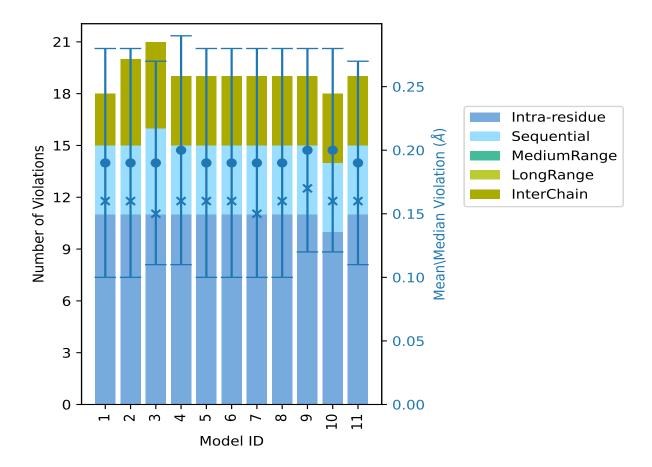
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

MadalID		Nun	nber o	f viola	ations	5	M (8)	M (Å)	SD^6 (Å)	Madian (Å)
Model ID	IR^1	SQ^2	MR^3	LR^4	IC^5	Total	Mean (Å)	Max (Å)	\mathbf{SD}^6 (Å)	Median (Å)
1	11	4	0	0	3	18	0.19	0.44	0.09	0.16
2	11	4	0	0	5	20	0.19	0.44	0.09	0.16
3	11	5	0	0	5	21	0.19	0.44	0.08	0.15
4	11	4	0	0	4	19	0.2	0.45	0.09	0.16
5	11	4	0	0	4	19	0.19	0.44	0.09	0.16
6	11	4	0	0	4	19	0.19	0.44	0.09	0.16
7	11	4	0	0	4	19	0.19	0.44	0.09	0.15
8	11	4	0	0	4	19	0.19	0.44	0.09	0.16
9	11	4	0	0	4	19	0.2	0.45	0.08	0.17
10	10	4	0	0	4	18	0.2	0.44	0.08	0.16
11	11	4	0	0	4	19	0.19	0.44	0.08	0.16



 $^1{\rm Intra-residue}$ restraints, $^2{\rm Sequential}$ restraints, $^3{\rm Medium}$ range restraints, $^4{\rm Long}$ range restraints, $^5{\rm Inter-chain}$ restraints, $^6{\rm Standard}$ deviation

9.2.1 Bar graph: Distance Violation statistics for each model (i)



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

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 220(IR:68, SQ:66, MR:0, LR:39, IC:47) 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	1	0	0	0	1	1	9.1	
0	0	0	0	1	1	2	18.2	
0	0	0	0	0	0	3	27.3	

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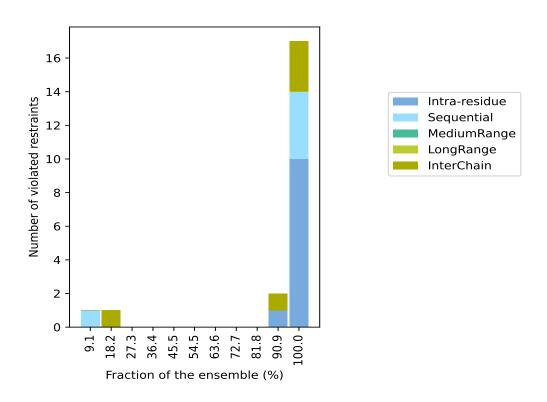


Continued	trom	mmoningala	maaa
COMBINE	THOTH.	memous	DULUE.

Nu	ımber	of vio	lated	Fractio	n of the ensemble		
IR^1	SQ^2	MR^3	LR^4	IC^5	Total	Count ⁶	%
0	0	0	0	0	0	4	36.4
0	0	0	0	0	0	5	45.5
0	0	0	0	0	0	6	54.5
0	0	0	0	0	0	7	63.6
0	0	0	0	0	0	8	72.7
0	0	0	0	0	0	9	81.8
1	0	0	0	1	2	10	90.9
10	4	0	0	3	17	11	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)



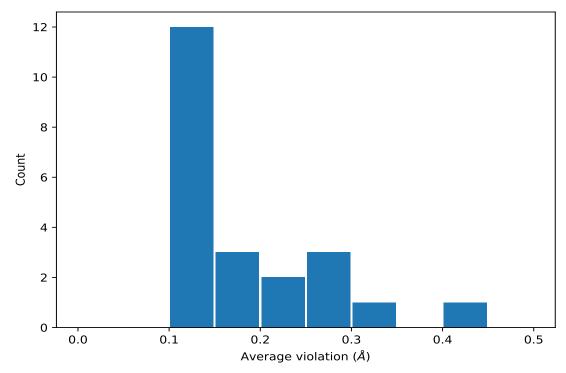
9.4 Most violated distance restraints in the ensemble (i)

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	\mathbf{Models}^1	Mean (Å)	${ m SD}^1 \ (m \AA)$	Median (Å)
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	11	0.44	0.0	0.44
(2,202)	2:B:13:DC:H2"	2:B:13:DC:H6	11	0.35	0.0	0.35
(2,185)	1:A:1:DA:H2"	1:A:1:DA:H8	11	0.27	0.0	0.27
(2,121)	2:B:15:DT:H5"	2:B:15:DT:H6	11	0.26	0.01	0.26
(2,2)	2:B:13:DC:H1'	2:B:13:DC:H6	11	0.26	0.0	0.26
(2,205)	2:B:15:DT:H1'	2:B:16:DC:H6	11	0.2	0.0	0.2
(2,117)	2:B:15:DT:H1'	3:A:101:5R3:HN4	11	0.2	0.01	0.2
(2,203)	2:B:14:DT:H2'	2:B:15:DT:H6	11	0.19	0.01	0.19
(2,71)	2:B:10:DC:H2"	2:B:11:DT:H6	11	0.17	0.0	0.17
(2,66)	1:A:9:DG:H2"	1:A:9:DG:H8	11	0.16	0.01	0.16

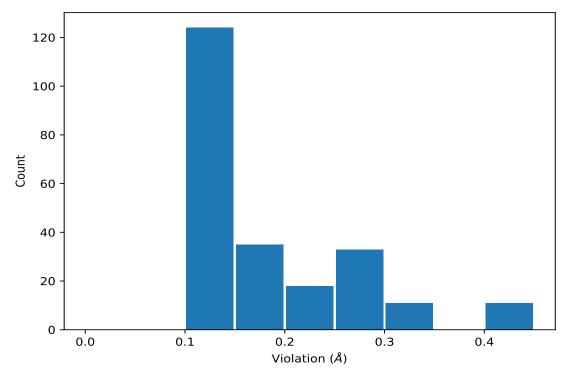
¹Number of violated models, ²Standard deviation



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)
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	4	0.45
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	9	0.45
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	1	0.44
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	2	0.44
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	3	0.44
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	5	0.44
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	6	0.44
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	7	0.44
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	8	0.44
(2,195)	1:A:8:DA:H2"	1:A:8:DA:H8	10	0.44



10 Dihedral-angle violation analysis (i)

10.1 Summary of dihedral-angle violations (i)

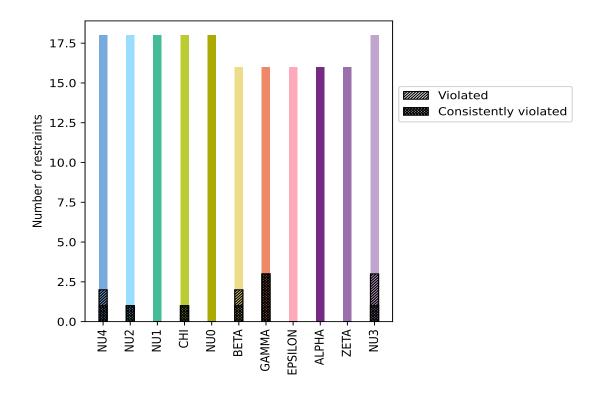
The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

A 1 - 4	Compt	$\%^{1}$	Vic	lated ⁵	3	Consis	$\overline{ m Violated}^4$	
Angle type	Count	70	Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
NU4	18	9.6	2	11.1	1.1	1	5.6	0.5
NU2	18	9.6	1	5.6	0.5	1	5.6	0.5
NU1	18	9.6	0	0.0	0.0	0	0.0	0.0
CHI	18	9.6	1	5.6	0.5	1	5.6	0.5
NU0	18	9.6	0	0.0	0.0	0	0.0	0.0
BETA	16	8.5	2	12.5	1.1	1	6.2	0.5
GAMMA	16	8.5	3	18.8	1.6	3	18.8	1.6
EPSILON	16	8.5	0	0.0	0.0	0	0.0	0.0
ALPHA	16	8.5	0	0.0	0.0	0	0.0	0.0
ZETA	16	8.5	0	0.0	0.0	0	0.0	0.0
NU3	18	9.6	3	16.7	1.6	1	5.6	0.5
Total	188	100.0	12	6.4	6.4	8	4.3	4.3

 $^{^1}$ 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

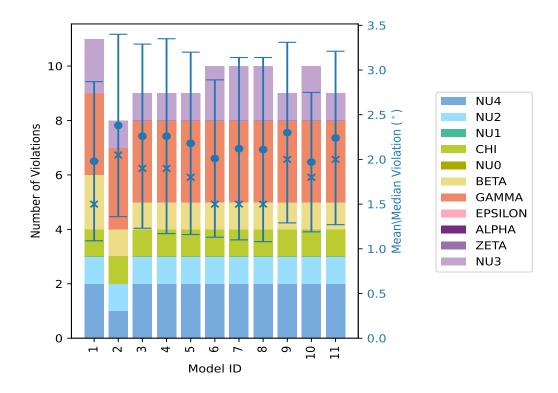
10.2 Dihedral-angle violation statistics for each model (i)

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							nber of viol						Mean (°)	Max (°)	SD (°)
cdci ib	NU4	NU2	NU1	CHI	NU0	BETA	GAMMA	EPSILON	ALPHA	ZETA	NU3	Total	1.12011 ()	()	22 ()
1	2	1	0	1	0	2	3	0	0	0	2	11	1.98	3.7	0.89
2	1	1	0	1	0	1	3	0	0	0	1	8	2.38	3.7	1.02
3	2	1	0	1	0	1	3	0	0	0	1	9	2.26	3.7	1.03
4	2	1	0	1	0	1	3	0	0	0	1	9	2.26	4.0	1.09
5	2	1	0	1	0	1	3	0	0	0	1	9	2.18	3.6	1.02
6	2	1	0	1	0	1	3	0	0	0	2	10	2.01	3.6	0.88
7	2	1	0	1	0	1	3	0	0	0	2	10	2.12	3.9	1.02
8	2	1	0	1	0	1	3	0	0	0	2	10	2.11	3.9	1.03
9	2	1	0	1	0	1	3	0	0	0	1	9	2.3	3.8	1.01
10	2	1	0	1	0	1	3	0	0	0	2	10	1.97	3.6	0.78
11	2	1	0	1	0	1	3	0	0	0	1	9	2.24	3.6	0.97



10.2.1 Bar graph: Dihedral violation statistics for each model (i)



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

10.3 Dihedral-angle violation statistics for the ensemble (i)

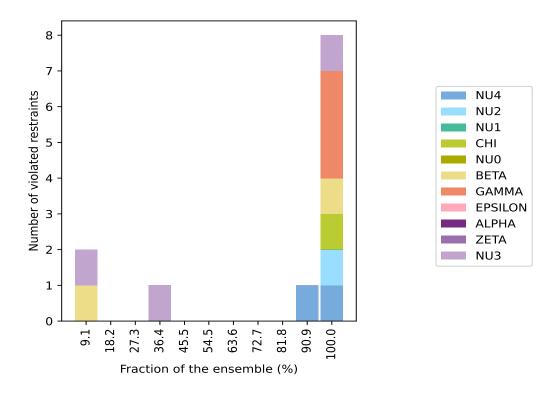
Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

	Number of violated restraints											Fraction	n of the e
NU4	NU2	NU1	CHI	NU0	BETA	GAMMA	EPSILON	ALPHA	ZETA	NU3	Total	Count ¹	%
0	0	0	0	0	1	0	0	0	0	1	2	1	9.
0	0	0	0	0	0	0	0	0	0	0	0	2	18
0	0	0	0	0	0	0	0	0	0	0	0	3	27
0	0	0	0	0	0	0	0	0	0	1	1	4	36
0	0	0	0	0	0	0	0	0	0	0	0	5	45
0	0	0	0	0	0	0	0	0	0	0	0	6	54
0	0	0	0	0	0	0	0	0	0	0	0	7	63
0	0	0	0	0	0	0	0	0	0	0	0	8	72
0	0	0	0	0	0	0	0	0	0	0	0	9	81
1	0	0	0	0	0	0	0	0	0	0	1	10	90
1	1	0	1	0	1	3	0	0	0	1	8	11	100

¹ Number of models with violations



10.3.1 Bar graph: Dihedral-angle Violation statistics for the ensemble (i)

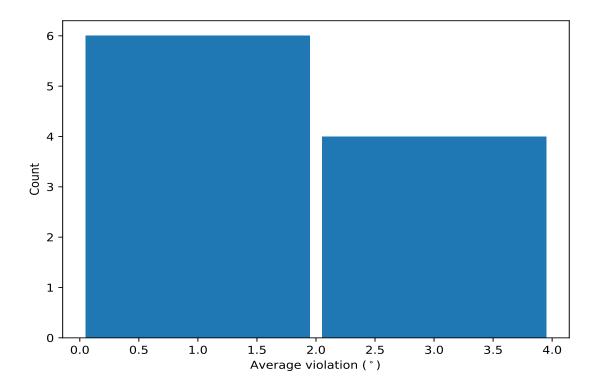


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram: Distribution of mean dihedral-angle 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





10.4.2 Table: Most violated dihedral-angle 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	\mathbf{Models}^1	Mean	\mathbf{SD}^2	Median
(1,86)	1:A:1:DA:O4'	1:A:1:DA:C1'	1:A:1:DA:N9	1:A:1:DA:C4	11	3.64	0.06	3.6
(1,119)	2:B:15:DT:O5'	2:B:15:DT:C5'	2:B:15:DT:C4'	2:B:15:DT:C3'	11	3.46	0.48	3.6
(1,157)	2:B:14:DT:C1'	2:B:14:DT:C2'	2:B:14:DT:C3'	2:B:14:DT:C4'	11	3.38	0.17	3.4
(1,158)	2:B:14:DT:C2'	2:B:14:DT:C3'	2:B:14:DT:C4'	2:B:14:DT:O4'	11	2.24	0.06	2.2
(1,55)	1:A:3:DG:C3'	1:A:3:DG:C4'	1:A:3:DG:O4'	1:A:3:DG:C1'	11	1.75	0.19	1.8
(1,99)	2:B:11:DT:O5'	2:B:11:DT:C5'	2:B:11:DT:C4'	2:B:11:DT:C3'	11	1.51	0.18	1.5
(1,114)	2:B:14:DT:O5'	2:B:14:DT:C5'	2:B:14:DT:C4'	2:B:14:DT:C3'	11	1.46	0.11	1.5
(1,4)	1:A:2:DA:P	1:A:2:DA:O5'	1:A:2:DA:C5'	1:A:2:DA:C4'	11	1.21	0.11	1.2
(1,179)	2:B:18:DT:C3'	2:B:18:DT:C4'	2:B:18:DT:O4'	2:B:18:DT:C1'	10	1.12	0.04	1.1
(1,59)	1:A:4:DA:C2'	1:A:4:DA:C3'	1:A:4:DA:C4'	1:A:4:DA:O4'	4	1.35	0.15	1.4

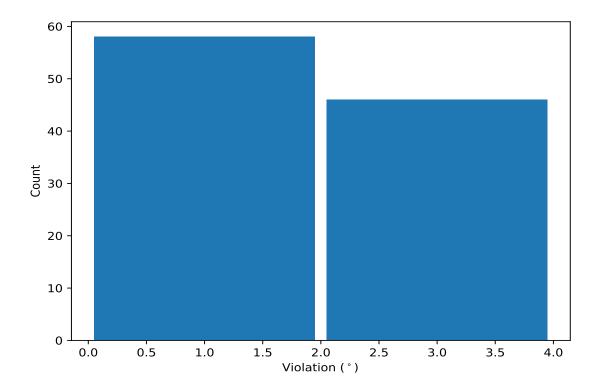
¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

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 provides the list of violations for 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,119)	2:B:15:DT:O5'	2:B:15:DT:C5'	2:B:15:DT:C4'	2:B:15:DT:C3'	4	4.0
(1,119)	2:B:15:DT:O5'	2:B:15:DT:C5'	2:B:15:DT:C4'	2:B:15:DT:C3'	7	3.9
(1,119)	2:B:15:DT:O5'	2:B:15:DT:C5'	2:B:15:DT:C4'	2:B:15:DT:C3'	8	3.9
(1,86)	1:A:1:DA:O4'	1:A:1:DA:C1'	1:A:1:DA:N9	1:A:1:DA:C4	9	3.8
(1,86)	1:A:1:DA:O4'	1:A:1:DA:C1'	1:A:1:DA:N9	1:A:1:DA:C4	1	3.7
(1,86)	1:A:1:DA:O4'	1:A:1:DA:C1'	1:A:1:DA:N9	1:A:1:DA:C4	3	3.7
(1,119)	2:B:15:DT:O5'	2:B:15:DT:C5'	2:B:15:DT:C4'	2:B:15:DT:C3'	2	3.7
(1,86)	1:A:1:DA:O4'	1:A:1:DA:C1'	1:A:1:DA:N9	1:A:1:DA:C4	2	3.6
(1,86)	1:A:1:DA:O4'	1:A:1:DA:C1'	1:A:1:DA:N9	1:A:1:DA:C4	4	3.6
(1,86)	1:A:1:DA:O4'	1:A:1:DA:C1'	1:A:1:DA:N9	1:A:1:DA:C4	5	3.6

