



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 5, 2023 – 07:15 PM EDT

PDB ID : 2M8A  
BMRB ID : 19226  
Title : 2'F-ANA/2'F-RNA alternated sequences  
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Deposited on : 2013-05-14

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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)  
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) : 2.33



## 2 Ensemble composition and analysis

This entry contains 10 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

There is only 1 type of molecule in this entry. The entry contains 752 atoms, of which 244 are hydrogens and 0 are deuteriums.

- Molecule 1 is DNA/RNA hybrid called 2'F-RNA/2'F-ANA chimeric duplex.

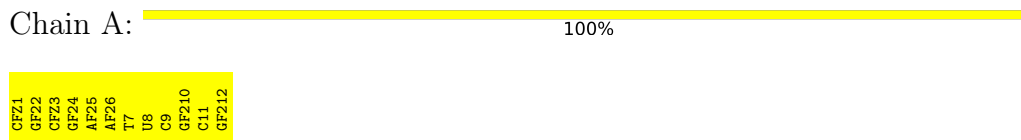
Mol	Chain	Residues	Atoms							Trace
			Total	C	F	H	N	O	P	
1	A	12	376	115	12	122	46	70	11	0
1	B	12	376	115	12	122	46	70	11	0

## 4 Residue-property plots

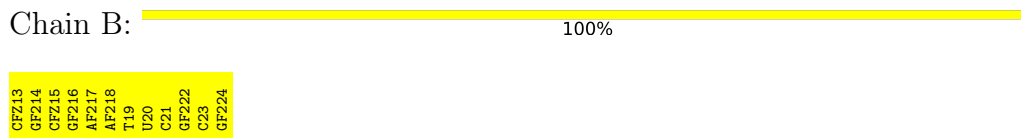
### 4.1 Average score per residue in the NMR ensemble

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: 2'F-RNA/2'F-ANA chimeric duplex



- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

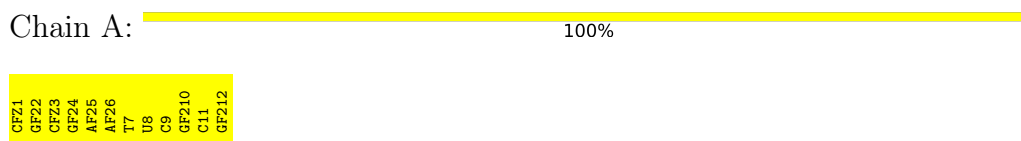


### 4.2 Scores per residue for each member of the ensemble

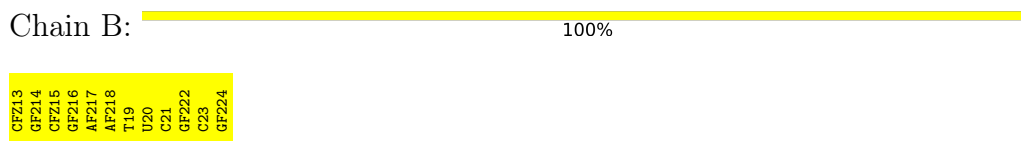
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex




- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex



### 4.2.2 Score per residue for model 2

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain A:  100%

GFZ1  
GF22  
CFZ3  
GF24  
AF25  
AF26  
T7  
U8  
C9  
GF210  
C11  
GF212

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain B:  100%

GFZ13  
GF214  
GF215  
GF216  
AF217  
AF218  
T19  
U20  
C21  
GF222  
C23  
GF224

### 4.2.3 Score per residue for model 3

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain A:  100%

GFZ1  
GF22  
CFZ3  
GF24  
AF25  
AF26  
T7  
U8  
C9  
GF210  
C11  
GF212

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain B:  100%

GFZ13  
GF214  
GF215  
GF216  
AF217  
AF218  
T19  
U20  
C21  
GF222  
C23  
GF224

### 4.2.4 Score per residue for model 4

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain A:  100%

GFZ1  
GF22  
CFZ3  
GF24  
AF25  
AF26  
T7  
U8  
C9  
GF210  
C11  
GF212

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain B:  100%

GFZ13  
GFZ14  
GFZ15  
GFZ16  
GFZ17  
AF218  
T19  
U20  
C21  
GF222  
C23  
GF224


#### 4.2.5 Score per residue for model 5

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain A:  100%

GFZ1  
GF22  
GFZ3  
GF24  
AF25  
AF26  
T7  
U8  
C9  
GF210  
C11  
GF212


- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain B:  100%

GFZ13  
GFZ14  
GFZ15  
GFZ16  
GFZ17  
AF218  
T19  
U20  
C21  
GF222  
C23  
GF224


#### 4.2.6 Score per residue for model 6

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain A:  100%

GFZ1  
GF22  
GFZ3  
GF24  
AF25  
AF26  
T7  
U8  
C9  
GF210  
C11  
GF212


- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain B:  100%

GFZ13  
GFZ14  
GFZ15  
GFZ16  
GFZ17  
AF218  
T19  
U20  
C21  
GF222  
C23  
GF224


#### 4.2.7 Score per residue for model 7

- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain A:  100%

GFZ1  
GF22  
GFZ3  
GF24  
AF25  
AF26  
T7  
U8  
C9  
GF210  
C11  
GF212


- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain B:  100%

GFZ13  
GF214  
GF215  
GF216  
GF217  
AF218  
T19  
U20  
C21  
GF222  
C23  
GF224


#### 4.2.8 Score per residue for model 8

- Molecule 1: 2'-F-RNA/2'-F-ANA chimeric duplex

Chain A:  100%

GFZ1  
GF22  
GF23  
GF24  
AF25  
AF26  
T7  
U8  
C9  
GF210  
C11  
GF212


- Molecule 1: 2'-F-RNA/2'-F-ANA chimeric duplex

Chain B:  100%

GFZ13  
GF214  
GF215  
GF216  
GF217  
AF218  
T19  
U20  
C21  
GF222  
C23  
GF224


#### 4.2.9 Score per residue for model 9

- Molecule 1: 2'-F-RNA/2'-F-ANA chimeric duplex

Chain A:  100%

GFZ1  
GF22  
GF23  
GF24  
AF25  
AF26  
T7  
U8  
C9  
GF210  
C11  
GF212

- Molecule 1: 2'-F-RNA/2'-F-ANA chimeric duplex

Chain B:  100%

GFZ13  
GF214  
GF215  
GF216  
GF217  
AF218  
T19  
U20  
C21  
GF222  
C23  
GF224

#### 4.2.10 Score per residue for model 10

- Molecule 1: 2'-F-RNA/2'-F-ANA chimeric duplex

Chain A:  100%

GFZ1  
GF22  
GF23  
GF24  
AF25  
AF26  
T7  
U8  
C9  
GF210  
C11  
GF212



- Molecule 1: 2'F-RNA/2'F-ANA chimeric duplex

Chain B:

100%

GFZ13  
GFZ14  
GFZ15  
GFZ16  
AF217  
AF218  
T19  
U20  
C21  
GF222  
C23  
GF224

## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 10 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
Amber	geometry optimization	
Amber	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	98
Number of shifts mapped to atoms	98
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

## 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: TAF, AF2, CFZ, UFT, CFL, GF2

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
All	All	5080	2440	2420	-

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 -.

There are no clashes.

### 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](#)

24 non-standard protein/DNA/RNA residues are 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.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	TAF	B	19	1	20,22,23	0.68±0.03	0±0 (0±0%)
1	GF2	B	22	1	18,25,26	0.98±0.09	1±0 (6±2%)
1	CFZ	A	1	1	18,18,22	0.57±0.02	0±0 (0±0%)
1	UFT	B	20	1	18,21,22	0.66±0.03	0±0 (0±0%)
1	TAF	A	7	1	20,22,23	0.65±0.03	0±0 (0±0%)
1	GF2	A	12	1	18,25,26	1.01±0.02	1±0 (5±0%)
1	CFL	B	23	1	18,21,22	0.66±0.02	0±0 (0±0%)
1	CFL	A	11	1	18,21,22	0.65±0.02	0±0 (0±0%)
1	GF2	B	14	1	18,25,26	0.98±0.02	1±0 (5±0%)
1	AF2	A	5	1	18,24,25	0.83±0.04	1±0 (5±1%)
1	GF2	A	10	1	18,25,26	0.94±0.02	1±0 (6±1%)
1	CFZ	B	15	1	18,21,22	0.72±0.03	0±0 (0±0%)
1	UFT	A	8	1	18,21,22	0.63±0.02	0±0 (0±0%)
1	GF2	A	4	1	18,25,26	0.98±0.02	1±0 (5±0%)
1	AF2	B	18	1	18,24,25	0.82±0.03	1±0 (4±2%)
1	CFZ	A	3	1	18,21,22	0.72±0.03	0±0 (0±0%)
1	CFL	B	21	1	18,21,22	0.65±0.03	0±0 (0±0%)
1	AF2	A	6	1	18,24,25	0.87±0.02	1±0 (5±0%)
1	GF2	B	16	1	18,25,26	0.98±0.02	1±0 (5±1%)
1	GF2	B	24	1	18,25,26	0.98±0.01	1±0 (5±0%)
1	AF2	B	17	1	18,24,25	0.84±0.02	1±0 (5±1%)
1	CFZ	B	13	1	18,18,22	0.55±0.02	0±0 (0±0%)
1	GF2	A	2	1	18,25,26	0.98±0.01	1±0 (5±0%)
1	CFL	A	9	1	18,21,22	0.64±0.02	0±0 (0±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.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	TAF	B	19	1	27,32,35	1.38±0.10	4±1 (15±4%)
1	GF2	B	22	1	19,37,40	1.94±0.11	5±1 (24±4%)
1	CFZ	A	1	1	26,26,33	1.81±0.06	5±1 (17±2%)
1	UFT	B	20	1	26,30,33	1.64±0.11	4±1 (16±4%)
1	TAF	A	7	1	27,32,35	1.29±0.07	3±1 (10±3%)
1	GF2	A	12	1	19,37,40	2.23±0.21	4±0 (21±1%)
1	CFL	B	23	1	26,30,33	1.59±0.10	4±0 (16±1%)
1	CFL	A	11	1	26,30,33	1.50±0.10	4±0 (14±1%)
1	GF2	B	14	1	19,37,40	1.91±0.08	5±1 (27±3%)
1	AF2	A	5	1	18,35,38	1.81±0.09	4±1 (21±4%)
1	GF2	A	10	1	19,37,40	1.92±0.04	4±0 (23±2%)
1	CFZ	B	15	1	26,30,33	1.33±0.03	3±1 (12±2%)
1	UFT	A	8	1	26,30,33	1.66±0.07	4±1 (15±4%)
1	GF2	A	4	1	19,37,40	1.97±0.05	5±0 (26±1%)
1	AF2	B	18	1	18,35,38	1.81±0.03	4±1 (21±3%)
1	CFZ	A	3	1	26,30,33	1.33±0.07	4±1 (15±4%)
1	CFL	B	21	1	26,30,33	1.03±0.07	2±1 (6±2%)
1	AF2	A	6	1	18,35,38	1.91±0.06	4±0 (21±1%)
1	GF2	B	16	1	19,37,40	1.97±0.08	5±1 (24±3%)
1	GF2	B	24	1	19,37,40	2.16±0.18	4±0 (22±2%)
1	AF2	B	17	1	18,35,38	1.84±0.04	4±1 (20±3%)
1	CFZ	B	13	1	26,26,33	1.84±0.03	5±1 (19±2%)
1	GF2	A	2	1	19,37,40	1.87±0.05	5±1 (25±2%)
1	CFL	A	9	1	26,30,33	1.02±0.03	2±0 (6±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
1	CFZ	A	1	1	-	0±0,6,22,26	0±0,2,2,2
1	AF2	A	5	1	-	0±0,3,25,26	0±0,3,3,3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GF2	B	24	1	-	0±0,3,25,26	0±0,3,3,3
1	AF2	B	17	1	-	0±0,3,25,26	0±0,3,3,3
1	GF2	A	12	1	-	0±0,3,25,26	0±0,3,3,3
1	CFL	B	21	1	-	0±0,7,25,26	0±0,2,2,2
1	CFZ	B	15	1	-	0±0,7,25,26	0±0,2,2,2
1	UFT	A	8	1	-	0±0,7,25,26	0±0,2,2,2
1	GF2	B	14	1	-	0±0,3,25,26	0±0,3,3,3
1	AF2	A	6	1	-	0±0,3,25,26	0±0,3,3,3
1	TAF	A	7	1	-	0±0,7,25,26	0±0,2,2,2
1	CFL	A	11	1	-	0±0,7,25,26	0±0,2,2,2
1	CFZ	B	13	1	-	0±0,6,22,26	0±0,2,2,2
1	GF2	B	22	1	-	0±0,3,25,26	0±0,3,3,3
1	CFL	A	9	1	-	0±0,7,25,26	0±0,2,2,2
1	GF2	A	2	1	-	0±0,3,25,26	0±0,3,3,3
1	UFT	B	20	1	-	0±0,7,25,26	0±0,2,2,2
1	CFZ	A	3	1	-	0±0,7,25,26	0±0,2,2,2
1	TAF	B	19	1	-	0±0,7,25,26	0±0,2,2,2
1	GF2	A	10	1	-	0±0,3,25,26	0±0,3,3,3
1	AF2	B	18	1	-	0±0,3,25,26	0±0,3,3,3
1	GF2	B	16	1	-	0±0,3,25,26	0±0,3,3,3
1	GF2	A	4	1	-	0±0,3,25,26	0±0,3,3,3
1	CFL	B	23	1	-	0±0,7,25,26	0±0,2,2,2

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	B	16	GF2	C8-N7	2.56	1.30	1.35	2	9
1	B	22	GF2	C2'-C1'	2.53	1.49	1.53	10	1
1	B	14	GF2	C8-N7	2.51	1.30	1.35	7	10
1	A	2	GF2	C8-N7	2.49	1.30	1.35	3	10
1	A	4	GF2	C8-N7	2.49	1.30	1.35	9	10
1	B	22	GF2	C8-N7	2.43	1.30	1.35	10	10
1	B	18	AF2	C8-N7	2.40	1.30	1.34	6	8
1	A	12	GF2	C8-N7	2.38	1.31	1.35	2	8
1	B	24	GF2	C8-N7	2.29	1.31	1.35	4	10
1	A	5	AF2	C8-N7	2.27	1.30	1.34	2	9
1	A	10	GF2	C8-N7	2.26	1.31	1.35	7	10
1	B	17	AF2	C8-N7	2.24	1.30	1.34	5	9
1	A	6	AF2	C8-N7	2.18	1.30	1.34	5	10
1	A	12	GF2	C5-C4	2.06	1.37	1.43	6	2
1	A	10	GF2	C5-C4	2.05	1.37	1.43	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	22	GF2	C5-C4	2.01	1.38	1.43	8	1

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	12	GF2	C3'-C2'-C1'	9.06	92.16	103.13	6	9
1	B	24	GF2	C3'-C2'-C1'	8.56	92.77	103.13	6	10
1	B	23	CFL	C3'-C2'-C1'	6.34	95.45	103.13	5	10
1	B	13	CFZ	F2'-C2'-C3'	6.23	122.27	109.22	10	10
1	B	20	UFT	F2'-C2'-C1'	6.16	121.92	109.08	4	10
1	A	1	CFZ	F2'-C2'-C3'	6.06	121.91	109.22	5	10
1	B	16	GF2	F-C2'-C3'	5.81	121.39	109.22	4	10
1	A	11	CFL	C3'-C2'-C1'	5.71	96.22	103.13	9	10
1	A	4	GF2	F-C2'-C3'	5.67	121.08	109.22	10	10
1	A	6	AF2	F-C2'-C3'	5.57	120.89	109.22	1	10
1	B	18	AF2	F-C2'-C3'	5.18	120.07	109.22	8	10
1	A	8	UFT	F2'-C2'-C3'	5.16	120.03	109.22	3	10
1	B	14	GF2	F-C2'-C3'	5.16	120.02	109.22	10	10
1	A	2	GF2	F-C2'-C3'	5.05	119.80	109.22	10	10
1	A	5	AF2	F-C2'-C3'	4.96	119.61	109.22	8	10
1	B	22	GF2	F-C2'-C1'	4.85	98.96	109.08	6	10
1	B	17	AF2	F-C2'-C3'	4.82	119.32	109.22	3	10
1	A	10	GF2	F-C2'-C1'	4.65	99.38	109.08	6	10
1	B	20	UFT	F2'-C2'-C3'	4.63	118.92	109.22	2	7
1	A	1	CFZ	F2'-C2'-C1'	4.59	99.50	109.08	9	10
1	A	8	UFT	F2'-C2'-C1'	4.57	99.55	109.08	5	10
1	A	12	GF2	O6-C6-N1	4.50	115.33	120.65	4	10
1	A	3	CFZ	F2'-C2'-C3'	4.49	118.61	109.22	7	10
1	B	15	CFZ	F2'-C2'-C3'	4.48	118.60	109.22	7	10
1	B	13	CFZ	F2'-C2'-C1'	4.42	99.86	109.08	4	10
1	B	24	GF2	O6-C6-N1	4.34	115.53	120.65	6	10
1	B	22	GF2	F-C2'-C3'	4.31	118.24	109.22	7	9
1	B	18	AF2	F-C2'-C1'	4.27	100.18	109.08	6	10
1	A	10	GF2	F-C2'-C3'	4.21	118.03	109.22	10	10
1	A	5	AF2	F-C2'-C1'	4.19	100.34	109.08	4	10
1	B	16	GF2	F-C2'-C1'	4.07	100.60	109.08	6	10
1	B	17	AF2	F-C2'-C1'	4.03	100.69	109.08	5	10
1	A	4	GF2	F-C2'-C1'	4.01	100.72	109.08	6	10
1	B	16	GF2	O6-C6-N1	3.97	115.96	120.65	9	9
1	B	14	GF2	F-C2'-C1'	3.90	100.96	109.08	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	2	GF2	F-C2'-C1'	3.87	101.01	109.08	10	10
1	A	12	GF2	O6-C6-C5	3.76	131.71	124.37	4	10
1	A	6	AF2	F-C2'-C1'	3.71	101.35	109.08	5	10
1	B	19	TAF	C6-C5-C4	3.68	121.11	118.03	4	10
1	B	22	GF2	O6-C6-N1	3.65	116.34	120.65	3	10
1	A	10	GF2	O6-C6-N1	3.62	116.38	120.65	7	10
1	B	24	GF2	O6-C6-C5	3.60	131.41	124.37	5	10
1	B	19	TAF	O4'-C1'-N1	3.59	116.57	108.36	3	4
1	B	14	GF2	C2'-C3'-C4'	3.53	97.84	102.40	8	2
1	A	1	CFZ	O4'-C1'-N1	3.48	116.33	108.36	9	10
1	A	4	GF2	O6-C6-N1	3.48	116.54	120.65	9	10
1	B	20	UFT	O4'-C1'-C2'	3.47	102.21	105.79	3	3
1	B	14	GF2	O3'-C3'-C4'	3.39	120.85	111.05	8	9
1	B	23	CFL	O5'-C5'-C4'	3.34	120.37	108.99	8	10
1	A	2	GF2	O6-C6-N1	3.33	116.71	120.65	9	10
1	A	4	GF2	O3'-C3'-C4'	3.32	120.66	111.05	8	10
1	B	16	GF2	O6-C6-C5	3.29	130.81	124.37	9	9
1	A	3	CFZ	C2'-C3'-C4'	3.29	98.16	102.40	4	6
1	B	17	AF2	C5-C6-N6	3.26	125.30	120.35	4	10
1	A	11	CFL	O5'-C5'-C4'	3.23	119.97	108.99	4	8
1	B	19	TAF	C5M-C5-C6	3.23	118.54	122.85	6	10
1	A	10	GF2	O6-C6-C5	3.17	130.57	124.37	1	10
1	B	22	GF2	O6-C6-C5	3.17	130.56	124.37	5	10
1	B	13	CFZ	O4'-C1'-N1	3.16	115.58	108.36	5	10
1	B	23	CFL	F-C2'-C1'	3.15	115.64	109.08	3	10
1	B	20	UFT	C3'-C2'-C1'	3.12	99.36	103.13	4	1
1	A	7	TAF	C6-C5-C4	3.11	120.63	118.03	1	10
1	B	14	GF2	O6-C6-N1	3.05	117.05	120.65	5	10
1	B	20	UFT	C2'-C1'-N1	3.04	109.56	114.20	2	3
1	A	5	AF2	C5-C6-N6	3.04	124.97	120.35	10	8
1	B	16	GF2	O3'-C3'-C4'	3.03	119.82	111.05	10	8
1	B	20	UFT	O3'-C3'-C4'	3.03	102.30	111.05	5	8
1	A	4	GF2	O6-C6-C5	2.99	130.22	124.37	5	10
1	A	7	TAF	C5M-C5-C6	2.98	118.87	122.85	4	10
1	A	5	AF2	O3'-C3'-C4'	2.95	119.58	111.05	4	8
1	A	2	GF2	O6-C6-C5	2.95	130.13	124.37	9	10
1	A	9	CFL	O2-C2-N3	2.93	117.57	122.33	8	10
1	A	8	UFT	C4'-O4'-C1'	2.90	103.07	109.47	4	8
1	A	11	CFL	F-C2'-C1'	2.87	115.06	109.08	9	10
1	B	14	GF2	O6-C6-C5	2.86	129.96	124.37	6	10
1	B	24	GF2	F-C2'-C1'	2.86	115.04	109.08	9	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	21	CFL	O5'-C5'-C4'	2.85	118.67	108.99	8	5
1	B	21	CFL	O2-C2-N3	2.82	117.75	122.33	4	10
1	B	15	CFZ	O3'-C3'-C4'	2.81	119.17	111.05	4	2
1	B	15	CFZ	F2'-C2'-C1'	2.76	103.32	109.08	5	5
1	A	3	CFZ	O3'-C3'-C4'	2.75	119.01	111.05	2	5
1	A	6	AF2	O3'-C3'-C4'	2.71	118.89	111.05	2	6
1	B	23	CFL	F-C2'-C3'	2.71	114.90	109.22	6	3
1	A	2	GF2	O3'-C3'-C4'	2.68	118.79	111.05	2	8
1	B	23	CFL	O2-C2-N3	2.67	117.99	122.33	4	10
1	B	22	GF2	O3'-C3'-C4'	2.65	103.39	111.05	10	2
1	A	11	CFL	O2-C2-N3	2.65	118.03	122.33	9	10
1	A	12	GF2	O4'-C1'-C2'	2.65	103.06	105.79	2	2
1	B	13	CFZ	O3'-C3'-C4'	2.65	118.70	111.05	10	3
1	B	17	AF2	O3'-C3'-C4'	2.62	118.62	111.05	8	5
1	A	1	CFZ	C4'-O4'-C1'	2.61	103.71	109.47	9	9
1	A	12	GF2	F-C2'-C1'	2.61	114.52	109.08	5	10
1	A	9	CFL	O5'-C5'-C4'	2.58	117.75	108.99	8	6
1	A	8	UFT	C2'-C1'-N1	2.55	110.31	114.20	10	5
1	A	6	AF2	C5-C6-N6	2.53	124.20	120.35	2	7
1	B	18	AF2	O4'-C4'-C3'	2.53	100.10	105.11	9	8
1	B	19	TAF	C2'-C1'-N1	2.53	110.33	114.20	3	6
1	A	7	TAF	C2'-C3'-C4'	2.53	105.67	102.40	2	1
1	B	22	GF2	C2'-C3'-C4'	2.52	105.66	102.40	8	3
1	A	7	TAF	F2'-C2'-C1'	2.47	114.22	109.08	8	2
1	B	21	CFL	C2'-C1'-N1	2.47	117.97	114.20	4	1
1	B	19	TAF	C3'-C2'-C1'	2.46	106.11	103.13	10	3
1	B	15	CFZ	C2'-C3'-C4'	2.46	99.23	102.40	10	1
1	A	10	GF2	O3'-C3'-C4'	2.45	118.14	111.05	1	5
1	B	13	CFZ	C4'-O4'-C1'	2.43	104.10	109.47	5	8
1	A	3	CFZ	O2-C2-N3	2.43	118.38	122.33	10	10
1	A	3	CFZ	F2'-C2'-C1'	2.43	104.02	109.08	7	6
1	B	22	GF2	O4'-C1'-C2'	2.43	103.29	105.79	10	1
1	A	6	AF2	O4'-C4'-C3'	2.41	100.34	105.11	9	4
1	A	2	GF2	C2'-C3'-C4'	2.40	99.30	102.40	3	1
1	A	8	UFT	C2'-C3'-C4'	2.40	105.50	102.40	8	1
1	A	8	UFT	O3'-C3'-C4'	2.38	117.92	111.05	10	5
1	B	15	CFZ	O2-C2-N3	2.36	118.49	122.33	6	10
1	B	20	UFT	O4'-C1'-N1	2.34	113.71	108.36	7	5
1	B	20	UFT	C4'-O4'-C1'	2.33	104.34	109.47	7	5
1	A	1	CFZ	O3'-C3'-C4'	2.32	117.76	111.05	7	3
1	B	20	UFT	C2'-C3'-C4'	2.31	99.41	102.40	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	18	AF2	O3'-C3'-C4'	2.31	117.72	111.05	8	6
1	B	24	GF2	C2'-C3'-C4'	2.29	105.36	102.40	4	1
1	B	13	CFZ	C5-C4-N4	2.28	116.98	120.57	4	1
1	B	22	GF2	C3'-C2'-C1'	2.27	100.38	103.13	8	1
1	A	3	CFZ	C2'-C1'-N1	2.25	110.76	114.20	8	3
1	B	14	GF2	C3'-C2'-C1'	2.25	105.86	103.13	8	1
1	B	24	GF2	O4'-C1'-C2'	2.25	103.47	105.79	7	3
1	A	5	AF2	C4-C5-N7	2.24	111.73	109.40	4	1
1	A	5	AF2	C3'-C2'-C1'	2.24	105.84	103.13	4	1
1	B	19	TAF	F2'-C2'-C1'	2.24	113.74	109.08	3	1
1	B	18	AF2	C2'-C3'-C4'	2.22	99.54	102.40	3	1
1	B	13	CFZ	O4'-C4'-C3'	2.21	100.74	105.11	9	7
1	A	1	CFZ	O4'-C4'-C3'	2.20	100.77	105.11	3	3
1	A	3	CFZ	C3'-C2'-C1'	2.19	105.78	103.13	9	1
1	A	8	UFT	O4'-C1'-N1	2.17	113.32	108.36	4	2
1	B	19	TAF	C5-C6-N1	2.16	121.11	123.34	5	7
1	A	6	AF2	C4-C5-N7	2.16	111.65	109.40	4	1
1	B	15	CFZ	C2'-C1'-N1	2.14	110.92	114.20	7	4
1	B	17	AF2	N6-C6-N1	2.14	114.12	118.57	1	2
1	B	13	CFZ	N4-C4-N3	2.13	121.70	117.97	4	1
1	B	19	TAF	O3'-C3'-C4'	2.13	117.19	111.05	10	1
1	A	7	TAF	C5-C6-N1	2.11	121.16	123.34	5	4
1	A	6	AF2	C2'-C3'-C4'	2.11	99.67	102.40	4	1
1	A	1	CFZ	O4'-C4'-C5'	2.10	113.76	109.21	10	1
1	B	15	CFZ	O4'-C1'-C2'	2.10	107.96	105.79	9	1
1	A	4	GF2	C3'-C2'-C1'	2.09	105.66	103.13	2	1
1	B	19	TAF	C5M-C5-C4	2.06	121.03	118.77	6	1
1	B	18	AF2	C5-C6-N6	2.06	123.48	120.35	5	4
1	A	5	AF2	N6-C6-N1	2.04	114.34	118.57	10	1
1	B	22	GF2	O5'-C5'-C4'	2.02	115.86	108.99	3	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates i

There are no monosaccharides 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 i

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% 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 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	98
Number of shifts mapped to atoms	98
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 —%, i.e. 0 atoms were assigned a chemical shift out of a possible 0. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is —%, i.e. 0 atoms were assigned a chemical shift out of a possible 0. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
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#### 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

### 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	282
Intra-residue ( $ i-j =0$ )	161
Sequential ( $ i-j =1$ )	94
Medium range ( $ i-j >1$ and $ i-j <5$ )	0
Long range ( $ i-j \geq 5$ )	0
Inter-chain	27
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.8
Number of long range restraints per residue <sup>1</sup>	0.0

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

### 8.2 Residual restraint violations

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

#### 8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	26.4	0.2
0.2-0.5 (Medium)	7.6	0.45
>0.5 (Large)	5.1	32.16

### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis [i](#)

### 9.1 Summary of distance violations [i](#)

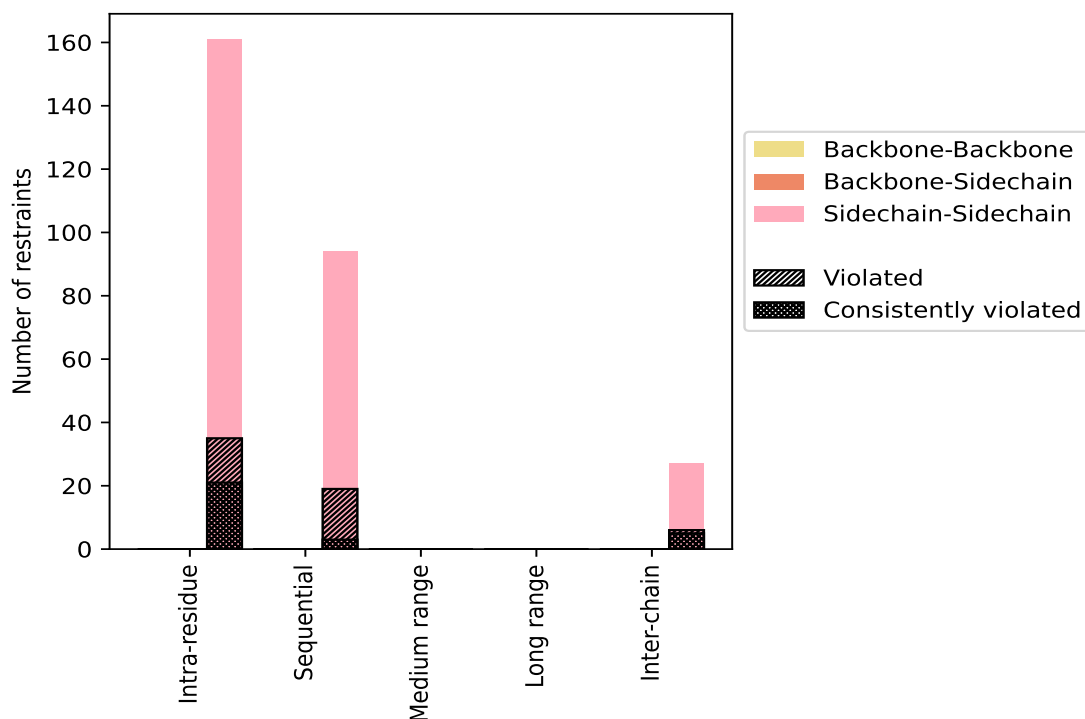
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>161</b>	<b>57.1</b>	<b>35</b>	<b>21.7</b>	<b>12.4</b>	<b>21</b>	<b>13.0</b>	<b>7.4</b>
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	161	57.1	35	21.7	12.4	21	13.0	7.4
<b>Sequential (<math> i-j =1</math>)</b>	<b>94</b>	<b>33.3</b>	<b>19</b>	<b>20.2</b>	<b>6.7</b>	<b>3</b>	<b>3.2</b>	<b>1.1</b>
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	94	33.3	19	20.2	6.7	3	3.2	1.1
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Inter-chain</b>	<b>27</b>	<b>9.6</b>	<b>6</b>	<b>22.2</b>	<b>2.1</b>	<b>5</b>	<b>18.5</b>	<b>1.8</b>
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	27	9.6	6	22.2	2.1	5	18.5	1.8
<b>Hydrogen bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>282</b>	<b>100.0</b>	<b>60</b>	<b>21.3</b>	<b>21.3</b>	<b>29</b>	<b>10.3</b>	<b>10.3</b>
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	282	100.0	60	21.3	21.3	29	10.3	10.3

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 disulfid bonds are counted in their appropriate category on the x-axis

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

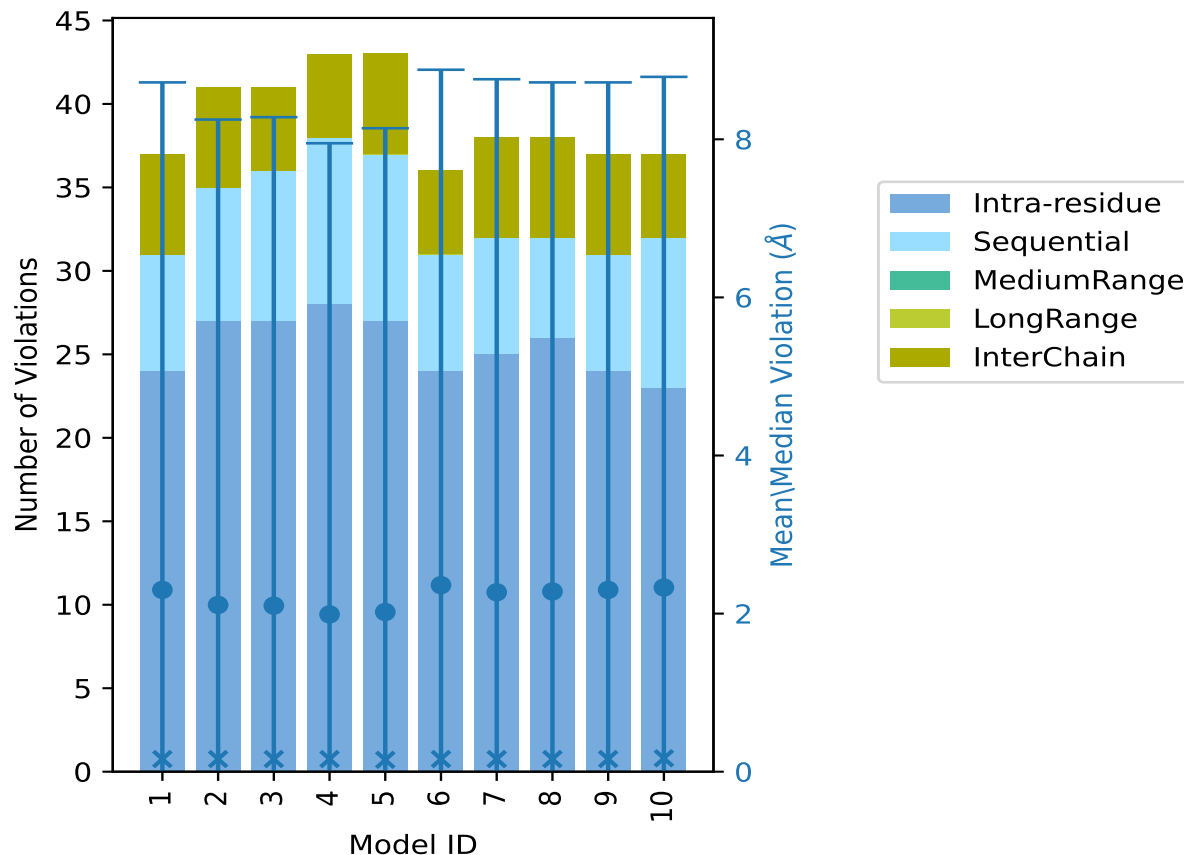
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	24	7	0	0	6	37	2.3	31.2	6.42	0.16
2	27	8	0	0	6	41	2.11	31.08	6.14	0.16
3	27	9	0	0	5	41	2.1	31.38	6.18	0.16
4	28	10	0	0	5	43	1.99	31.42	5.96	0.16
5	27	10	0	0	6	43	2.02	32.06	6.12	0.15
6	24	7	0	0	5	36	2.36	31.7	6.52	0.16
7	25	7	0	0	6	38	2.27	32.16	6.49	0.16
8	26	6	0	0	6	38	2.28	32.02	6.44	0.16
9	24	7	0	0	6	37	2.3	31.02	6.42	0.16
10	23	9	0	0	5	37	2.33	31.21	6.46	0.17

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>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, 222(IR:126, SQ:75, MR:0, LR:0, IC:21) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
7	7	0	0	0	14	1	10.0
2	4	0	0	0	6	2	20.0
1	1	0	0	0	2	3	30.0
0	0	0	0	0	0	4	40.0

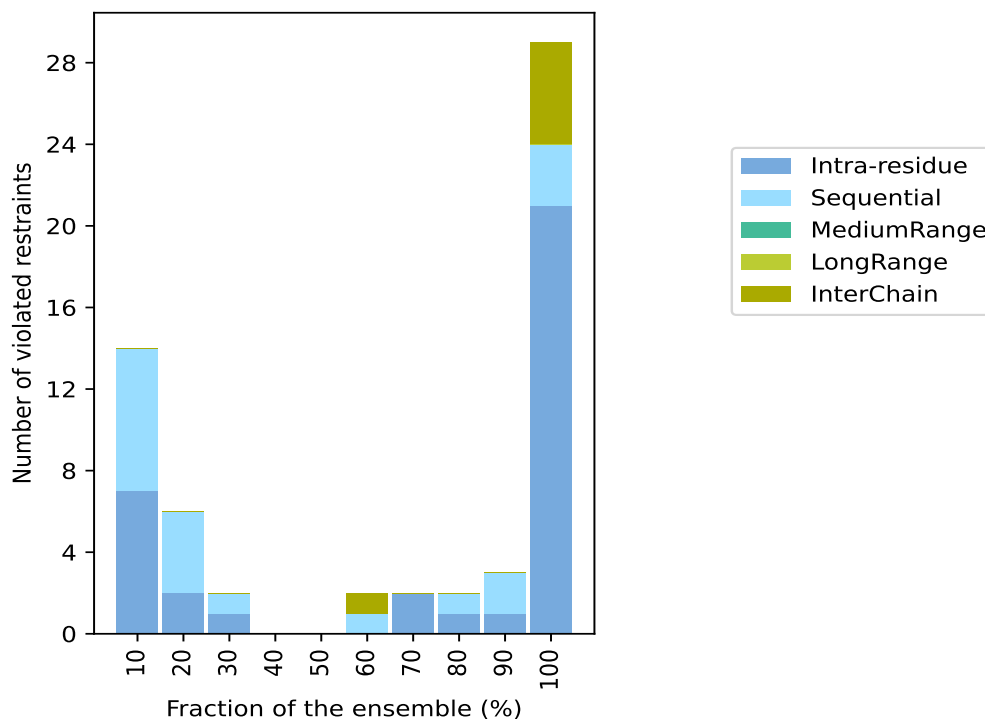
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	0	0	0	5	50.0
0	1	0	0	1	2	6	60.0
2	0	0	0	0	2	7	70.0
1	1	0	0	0	2	8	80.0
1	2	0	0	0	3	9	90.0
21	3	0	0	5	29	10	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

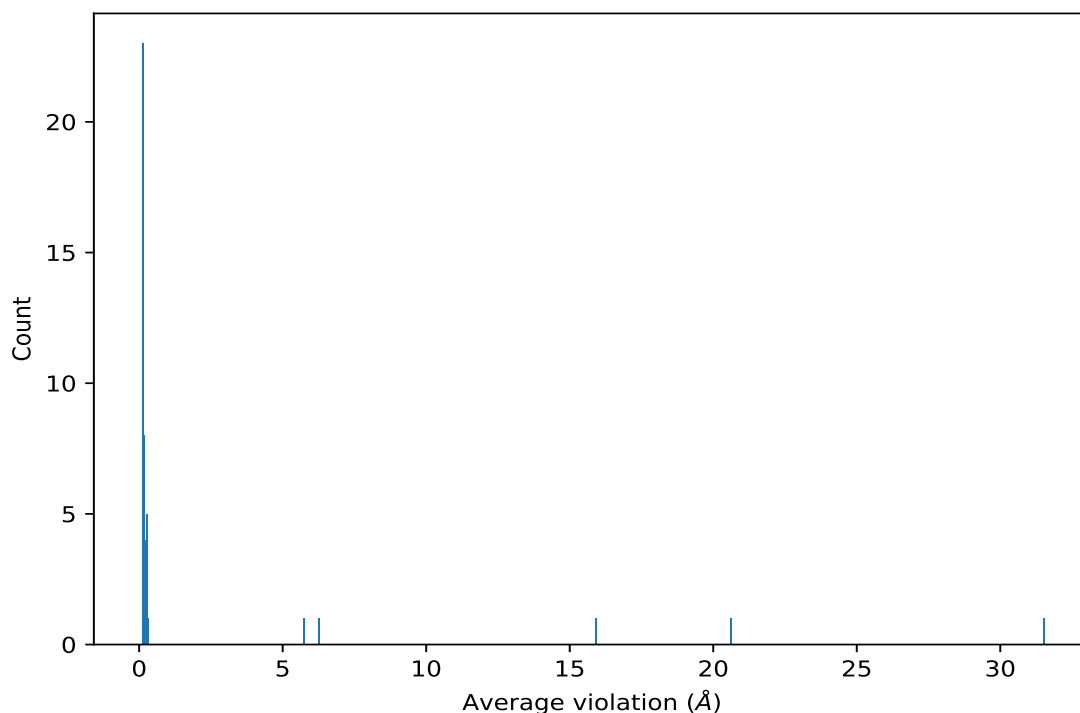
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	10	31.52	0.41	31.4
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	10	20.6	0.27	20.7
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	10	15.91	0.27	15.91
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	10	6.3	0.07	6.3
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	10	5.7	0.13	5.69
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	10	0.28	0.03	0.3
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	10	0.28	0.03	0.26
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	10	0.27	0.04	0.26
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	10	0.26	0.02	0.26
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	10	0.23	0.01	0.23
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	10	0.23	0.01	0.22
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	10	0.22	0.02	0.23
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	10	0.2	0.02	0.2
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	10	0.17	0.09	0.14
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	10	0.17	0.01	0.17
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	10	0.16	0.0	0.16

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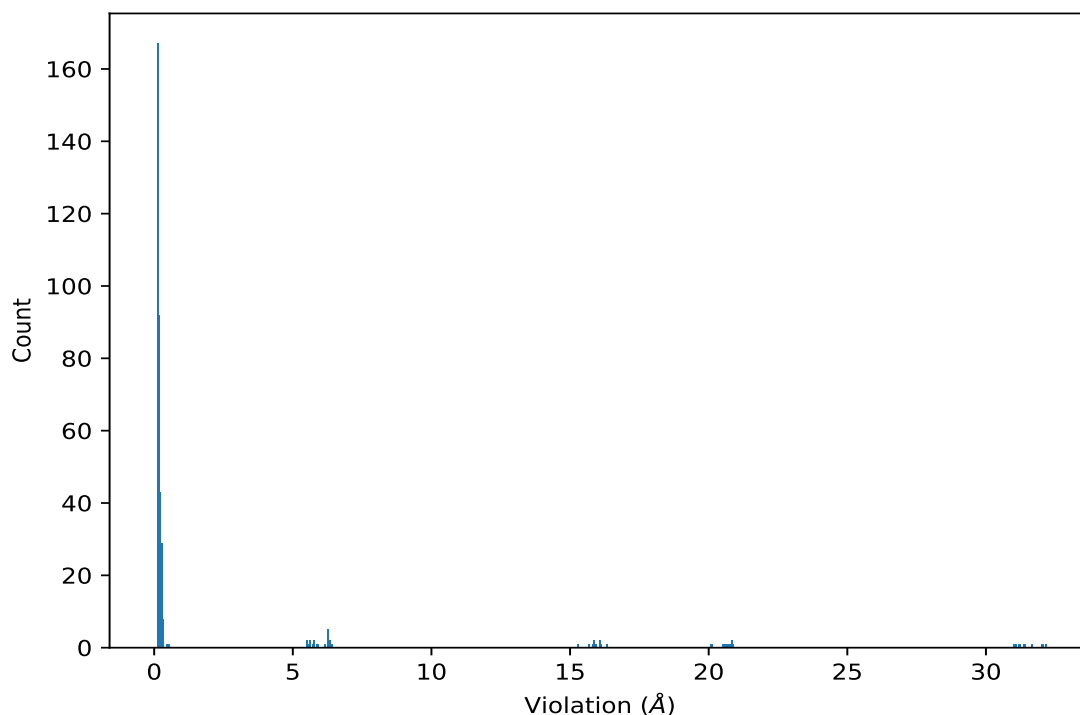
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	10	0.16	0.01	0.16
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	10	0.16	0.01	0.16
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	10	0.16	0.01	0.16
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	10	0.16	0.01	0.16
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	10	0.15	0.0	0.15
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	10	0.15	0.01	0.15
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	10	0.15	0.01	0.15
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	10	0.15	0.0	0.15
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	10	0.15	0.01	0.15
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	10	0.14	0.01	0.15
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	10	0.14	0.01	0.14
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	10	0.14	0.02	0.14
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	10	0.14	0.01	0.14
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	9	0.14	0.01	0.15
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	9	0.14	0.02	0.14
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	9	0.14	0.02	0.13
(2,9)	1:B:15:CFZ:F2'	1:B:16:GF2:H8	8	0.16	0.03	0.15
(1,98)	1:A:6:AF2:H2	1:A:6:AF2:H2'	8	0.13	0.02	0.13
(1,167)	1:A:3:CFZ:H4'	1:A:3:CFZ:H6	7	0.14	0.02	0.14
(1,246)	1:B:19:TAF:F2'	1:B:19:TAF:H3'	7	0.13	0.02	0.12
(1,96)	1:A:5:AF2:H2	1:B:21:CFL:H1'	6	0.15	0.02	0.15
(1,134)	1:A:6:AF2:H8	1:A:7:TAF:H6	6	0.13	0.01	0.13
(1,66)	1:B:20:UFT:H2'	1:B:20:UFT:H6	3	0.25	0.03	0.26
(2,8)	1:B:16:GF2:F	1:B:17:AF2:H8	3	0.12	0.01	0.11
(1,70)	1:B:24:GF2:H2'	1:B:24:GF2:H8	2	0.32	0.22	0.32
(1,88)	1:B:20:UFT:H2'	1:B:21:CFL:H6	2	0.15	0.02	0.15
(1,108)	1:B:18:AF2:H2	1:B:18:AF2:H2'	2	0.13	0.01	0.13
(1,125)	1:A:11:CFL:H5	1:A:10:GF2:H2'	2	0.12	0.02	0.12
(2,3)	1:A:4:GF2:F	1:A:5:AF2:H8	2	0.12	0.0	0.12
(1,105)	1:B:17:AF2:H2	1:B:18:AF2:H2	2	0.12	0.0	0.12

<sup>1</sup>Number of violated models, <sup>2</sup>Standard 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)
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	7	32.16
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	5	32.06
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	8	32.02
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	6	31.7
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	4	31.42
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	3	31.38
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	10	31.21
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	1	31.2
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	2	31.08
(1,57)	1:B:23:CFL:H2'	1:A:11:CFL:H6	9	31.02
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	7	20.9
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	5	20.82
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	10	20.81
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	2	20.76
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	9	20.73
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	3	20.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	1	20.59
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	8	20.5
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	4	20.12
(1,79)	1:B:21:CFL:H2'	1:A:10:GF2:H8	6	20.09
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	10	16.33
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	3	16.15
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	9	16.09
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	2	16.08
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	7	15.95
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	1	15.87
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	5	15.87
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	8	15.82
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	6	15.66
(1,55)	1:B:21:CFL:H2'	1:A:9:CFL:H6	4	15.29
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	6	6.44
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	8	6.36
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	3	6.34
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	10	6.33
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	2	6.3
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	5	6.3
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	9	6.29
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	1	6.28
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	7	6.25
(1,77)	1:B:19:TAF:H2'	1:A:8:UFT:H6	4	6.16
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	6	5.9
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	8	5.88
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	4	5.77
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	2	5.76
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	1	5.74
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	5	5.64
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	7	5.62
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	3	5.57
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	9	5.55
(1,53)	1:B:19:TAF:H2'	1:A:7:TAF:H6	10	5.53
(1,70)	1:B:24:GF2:H2'	1:B:24:GF2:H8	4	0.54
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	10	0.45
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	4	0.34
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	5	0.33
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	10	0.33
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	2	0.33
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	8	0.32
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	7	0.31
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	8	0.31
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	10	0.3
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	1	0.3
(1,66)	1:B:20:UFT:H2'	1:B:20:UFT:H6	5	0.29
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	2	0.29
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	9	0.29
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	5	0.29
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	9	0.29
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	1	0.28
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	3	0.28
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	6	0.27
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	1	0.27
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	4	0.27
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	7	0.27
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	2	0.26
(1,66)	1:B:20:UFT:H2'	1:B:20:UFT:H6	3	0.26
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	3	0.26
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	4	0.26
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	8	0.26
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	9	0.26
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	6	0.26
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	4	0.26
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	6	0.26
(1,156)	1:B:23:CFL:H3'	1:B:23:CFL:H6	7	0.25
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	5	0.25
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	8	0.25
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	10	0.25
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	9	0.25
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	6	0.25
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	10	0.25
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	8	0.24
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	9	0.24
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	9	0.24
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	3	0.24
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	2	0.24
(1,114)	1:A:1:CFZ:H5	1:A:1:CFZ:H1'	3	0.24
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	1	0.23
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	5	0.23
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	10	0.23
(1,58)	1:A:12:GF2:H2'	1:A:12:GF2:H8	2	0.23
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	2	0.23
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	6	0.23
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	7	0.23
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	8	0.23
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	2	0.23
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	3	0.23
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	5	0.23
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	6	0.23
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	9	0.23
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	7	0.23
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	2	0.23
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	6	0.22
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	7	0.22
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	4	0.22
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	5	0.22
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	10	0.22
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	1	0.22
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	4	0.22
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	7	0.22
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	8	0.22
(1,211)	1:A:9:CFL:F	1:A:9:CFL:H1'	10	0.22
(1,149)	1:A:11:CFL:H3'	1:A:11:CFL:H6	2	0.22
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	8	0.22
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	9	0.22
(1,66)	1:B:20:UFT:H2'	1:B:20:UFT:H6	4	0.21
(1,222)	1:B:21:CFL:F	1:B:21:CFL:H1'	3	0.21
(1,116)	1:B:13:CFZ:H5	1:B:13:CFZ:H1'	1	0.21
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	3	0.2
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	2	0.2
(1,198)	1:B:19:TAF:H4'	1:B:19:TAF:H1'	3	0.2
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	1	0.2
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	6	0.2
(2,9)	1:B:15:CFZ:F2'	1:B:16:GF2:H8	4	0.19
(2,9)	1:B:15:CFZ:F2'	1:B:16:GF2:H8	8	0.19
(1,90)	1:B:22:GF2:H2'	1:B:23:CFL:H6	10	0.19
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	5	0.19
(2,9)	1:B:15:CFZ:F2'	1:B:16:GF2:H8	9	0.18
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	10	0.18
(1,95)	1:A:5:AF2:H2	1:A:6:AF2:H2'	4	0.18
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	1	0.18
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	8	0.18
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	3	0.18
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	4	0.18
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	7	0.18
(1,96)	1:A:5:AF2:H2	1:B:21:CFL:H1'	2	0.17
(1,96)	1:A:5:AF2:H2	1:B:21:CFL:H1'	8	0.17
(1,88)	1:B:20:UFT:H2'	1:B:21:CFL:H6	4	0.17
(1,246)	1:B:19:TAF:F2'	1:B:19:TAF:H3'	10	0.17
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	3	0.17
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	4	0.17
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	5	0.17
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	10	0.17
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	1	0.17
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	10	0.17
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	3	0.17
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	7	0.17
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	10	0.17
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	8	0.17
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	7	0.17
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	8	0.17
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	9	0.17
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	10	0.17
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	4	0.17
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	10	0.17
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	1	0.17
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	2	0.17
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	4	0.17
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	5	0.17
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	3	0.17
(1,200)	1:B:21:CFL:H4'	1:B:21:CFL:H1'	5	0.17
(1,167)	1:A:3:CFZ:H4'	1:A:3:CFZ:H6	8	0.17
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	2	0.17
(1,129)	1:B:23:CFL:H5	1:B:22:GF2:H2'	2	0.17
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	2	0.17
(2,9)	1:B:15:CFZ:F2'	1:B:16:GF2:H8	3	0.16
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	2	0.16
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	6	0.16
(1,98)	1:A:6:AF2:H2	1:A:6:AF2:H2'	2	0.16
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	3	0.16
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	8	0.16
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	2	0.16
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	6	0.16
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	10	0.16
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	2	0.16
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	7	0.16
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	8	0.16
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	9	0.16
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	6	0.16
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	8	0.16
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	4	0.16
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	5	0.16
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	6	0.16
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	9	0.16
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	5	0.16
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	7	0.16
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	1	0.16
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	2	0.16
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	3	0.16
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	4	0.16
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	5	0.16
(1,210)	1:A:8:UFT:F2'	1:A:8:UFT:H1'	6	0.16
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	2	0.16
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	8	0.16
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	1	0.16
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	3	0.16
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	9	0.16
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	7	0.16
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	9	0.16
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	2	0.16
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	1	0.16
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	2	0.16
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	6	0.16
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	7	0.16
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	8	0.16
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	9	0.16
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	10	0.16
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	1	0.16
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	7	0.16
(1,167)	1:A:3:CFZ:H4'	1:A:3:CFZ:H6	3	0.16
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	5	0.16
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	4	0.16
(1,110)	1:B:18:AF2:H2	1:B:19:TAF:H2'	10	0.16
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	3	0.15
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:A:6:AF2:H2	1:A:6:AF2:H2'	1	0.15
(1,98)	1:A:6:AF2:H2	1:A:6:AF2:H2'	8	0.15
(1,96)	1:A:5:AF2:H2	1:B:21:CFL:H1'	1	0.15
(1,45)	1:B:22:GF2:H1'	1:B:23:CFL:H6	10	0.15
(1,246)	1:B:19:TAF:F2'	1:B:19:TAF:H3'	4	0.15
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	4	0.15
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	8	0.15
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	2	0.15
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	7	0.15
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	10	0.15
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	1	0.15
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	3	0.15
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	4	0.15
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	5	0.15
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	7	0.15
(1,218)	1:B:17:AF2:F	1:B:17:AF2:H1'	9	0.15
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	1	0.15
(1,217)	1:B:16:GF2:F	1:B:16:GF2:H1'	6	0.15
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	2	0.15
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	3	0.15
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	4	0.15
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	7	0.15
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	3	0.15
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	4	0.15
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	7	0.15
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	9	0.15
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	10	0.15
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	2	0.15
(1,214)	1:B:13:CFZ:F2'	1:B:13:CFZ:H1'	8	0.15
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	1	0.15
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	4	0.15
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	1	0.15
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	2	0.15
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	4	0.15
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	6	0.15
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	7	0.15
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	8	0.15
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	9	0.15
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	10	0.15
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	1	0.15
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	5	0.15
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	10	0.15
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	5	0.15
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	6	0.15
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	7	0.15
(1,206)	1:A:3:CFZ:F2'	1:A:3:CFZ:H1'	8	0.15
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	3	0.15
(1,205)	1:A:4:GF2:F	1:A:4:GF2:H1'	6	0.15
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	4	0.15
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	4	0.15
(1,203)	1:A:1:CFZ:F2'	1:A:1:CFZ:H1'	5	0.15
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	4	0.15
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	5	0.15
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	9	0.15
(1,147)	1:A:7:TAF:H3'	1:A:7:TAF:H6	4	0.15
(1,134)	1:A:6:AF2:H8	1:A:7:TAF:H6	8	0.15
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	1	0.15
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	9	0.15
(2,9)	1:B:15:CFZ:F2'	1:B:16:GF2:H8	5	0.14
(2,9)	1:B:15:CFZ:F2'	1:B:16:GF2:H8	10	0.14
(2,8)	1:B:16:GF2:F	1:B:17:AF2:H8	4	0.14
(1,98)	1:A:6:AF2:H2	1:A:6:AF2:H2'	4	0.14
(1,96)	1:A:5:AF2:H2	1:B:21:CFL:H1'	7	0.14
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	1	0.14
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	5	0.14
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	6	0.14
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	7	0.14
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	1	0.14
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	3	0.14
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	4	0.14
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	5	0.14
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	9	0.14
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	9	0.14
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	1	0.14
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	2	0.14
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	5	0.14
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	8	0.14
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	2	0.14
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	3	0.14
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	6	0.14
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	9	0.14
(1,212)	1:A:10:GF2:F	1:A:10:GF2:H1'	10	0.14
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:A:6:AF2:F	1:A:6:AF2:H1'	5	0.14
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	3	0.14
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	4	0.14
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	9	0.14
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	1	0.14
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	3	0.14
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	6	0.14
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	7	0.14
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	8	0.14
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	9	0.14
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	10	0.14
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	2	0.14
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	6	0.14
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	8	0.14
(1,167)	1:A:3:CFZ:H4'	1:A:3:CFZ:H6	6	0.14
(1,167)	1:A:3:CFZ:H4'	1:A:3:CFZ:H6	7	0.14
(1,134)	1:A:6:AF2:H8	1:A:7:TAF:H6	5	0.14
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	1	0.14
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	9	0.14
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	3	0.14
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	10	0.14
(1,125)	1:A:11:CFL:H5	1:A:10:GF2:H2'	2	0.14
(1,108)	1:B:18:AF2:H2	1:B:18:AF2:H2'	8	0.14
(2,9)	1:B:15:CFZ:F2'	1:B:16:GF2:H8	7	0.13
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	4	0.13
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	7	0.13
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	8	0.13
(1,96)	1:A:5:AF2:H2	1:B:21:CFL:H1'	9	0.13
(1,88)	1:B:20:UFT:H2'	1:B:21:CFL:H6	3	0.13
(1,246)	1:B:19:TAF:F2'	1:B:19:TAF:H3'	3	0.13
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	2	0.13
(1,223)	1:B:22:GF2:F	1:B:22:GF2:H1'	9	0.13
(1,219)	1:B:18:AF2:F	1:B:18:AF2:H1'	6	0.13
(1,216)	1:B:15:CFZ:F2'	1:B:15:CFZ:H1'	5	0.13
(1,215)	1:B:14:GF2:F	1:B:14:GF2:H1'	6	0.13
(1,207)	1:A:5:AF2:F	1:A:5:AF2:H1'	6	0.13
(1,204)	1:A:2:GF2:F	1:A:2:GF2:H1'	5	0.13
(1,167)	1:A:3:CFZ:H4'	1:A:3:CFZ:H6	1	0.13
(1,134)	1:A:6:AF2:H8	1:A:7:TAF:H6	1	0.13
(1,134)	1:A:6:AF2:H8	1:A:7:TAF:H6	6	0.13
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	3	0.13
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	7	0.13
(1,121)	1:B:21:CFL:H5	1:B:20:UFT:H6	3	0.13
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	1	0.12
(2,4)	1:A:3:CFZ:F2'	1:A:4:GF2:H8	5	0.12
(2,3)	1:A:4:GF2:F	1:A:5:AF2:H8	9	0.12
(2,3)	1:A:4:GF2:F	1:A:5:AF2:H8	10	0.12
(2,11)	1:B:23:CFL:F	1:B:24:GF2:H8	6	0.12
(1,98)	1:A:6:AF2:H2	1:A:6:AF2:H2'	7	0.12
(1,246)	1:B:19:TAF:F2'	1:B:19:TAF:H3'	5	0.12
(1,246)	1:B:19:TAF:F2'	1:B:19:TAF:H3'	9	0.12
(1,167)	1:A:3:CFZ:H4'	1:A:3:CFZ:H6	5	0.12
(1,134)	1:A:6:AF2:H8	1:A:7:TAF:H6	4	0.12
(1,134)	1:A:6:AF2:H8	1:A:7:TAF:H6	7	0.12
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	6	0.12
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	8	0.12
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	5	0.12
(1,126)	1:A:11:CFL:H5	1:A:10:GF2:H1'	6	0.12
(1,122)	1:B:21:CFL:H5	1:B:20:UFT:H2'	5	0.12
(1,108)	1:B:18:AF2:H2	1:B:18:AF2:H2'	2	0.12
(1,105)	1:B:17:AF2:H2	1:B:18:AF2:H2	4	0.12
(2,9)	1:B:15:CFZ:F2'	1:B:16:GF2:H8	2	0.11
(2,8)	1:B:16:GF2:F	1:B:17:AF2:H8	1	0.11
(2,8)	1:B:16:GF2:F	1:B:17:AF2:H8	5	0.11
(1,98)	1:A:6:AF2:H2	1:A:6:AF2:H2'	5	0.11
(1,98)	1:A:6:AF2:H2	1:A:6:AF2:H2'	6	0.11
(1,98)	1:A:6:AF2:H2	1:A:6:AF2:H2'	9	0.11
(1,96)	1:A:5:AF2:H2	1:B:21:CFL:H1'	5	0.11
(1,70)	1:B:24:GF2:H2'	1:B:24:GF2:H8	3	0.11
(1,68)	1:B:22:GF2:H2'	1:B:22:GF2:H8	10	0.11
(1,26)	1:A:2:GF2:H1'	1:A:3:CFZ:H6	5	0.11
(1,246)	1:B:19:TAF:F2'	1:B:19:TAF:H3'	2	0.11
(1,246)	1:B:19:TAF:F2'	1:B:19:TAF:H3'	7	0.11
(1,176)	1:B:15:CFZ:H4'	1:B:15:CFZ:H6	3	0.11
(1,167)	1:A:3:CFZ:H4'	1:A:3:CFZ:H6	2	0.11
(1,155)	1:B:21:CFL:H3'	1:B:21:CFL:H6	4	0.11
(1,148)	1:A:9:CFL:H3'	1:A:9:CFL:H6	8	0.11
(1,130)	1:B:23:CFL:H5	1:B:22:GF2:H1'	4	0.11
(1,125)	1:A:11:CFL:H5	1:A:10:GF2:H2'	10	0.11
(1,105)	1:B:17:AF2:H2	1:B:18:AF2:H2	3	0.11

## 10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value