wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	6K3J
BMRB ID	:	36193
Title	:	Solution structure of APOBEC3G-CD2 with ssDNA, Product A
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Deposited on	:	2019-05-19

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 (i)) were used in the production of this report:

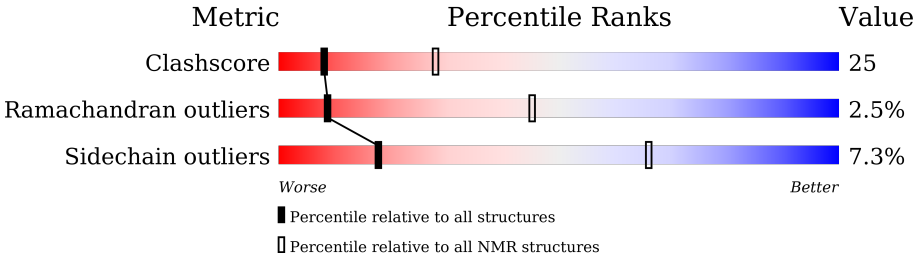
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 78%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	188	63% 35% .
2	B	10	10% 80% 10%

2 Ensemble composition and analysis (i)

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:197-A:384 (188)	1.24	1

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3332 atoms, of which 1576 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA dC->dU-editing enzyme APOBEC-3G.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	188	3020	985	1463	275	283	14	0

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*TP*CP*UP*(IUR)P*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms							Trace
			Total	C	H	I	N	O	P	
2	B	10	311	97	113	1	30	61	9	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	1	1	1

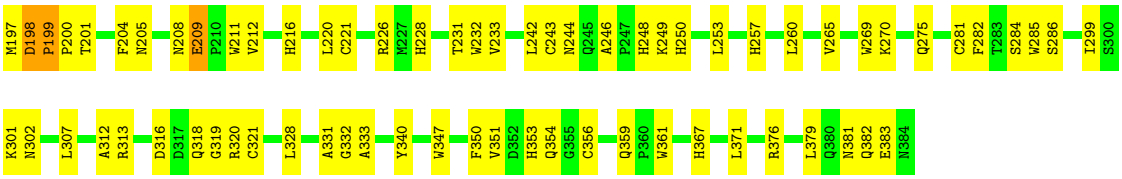
4 Residue-property plots (i)

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 dC->dU-editing enzyme APOBEC-3G

Chain A: 63% 35% •



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

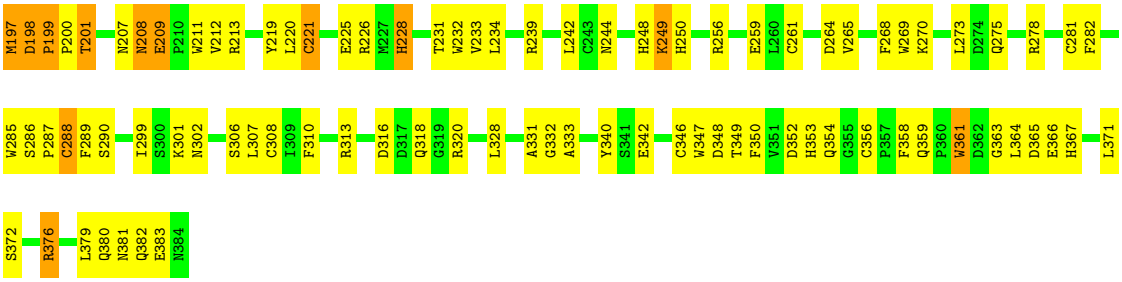
Chain B: 10% 80% 10%

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

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

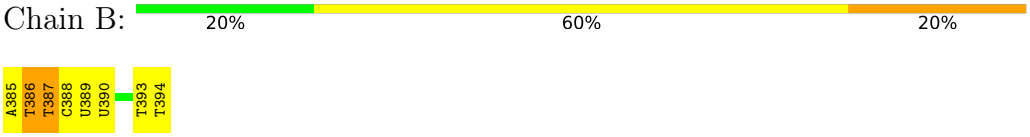
• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 53% 40% 6%



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

Chain B:



5 Refinement protocol and experimental data overview (i)

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

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
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2221
Number of shifts mapped to atoms	2221
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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: ZN, 5IU

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	1.02±0.00	0±0/1604 (0.0± 0.0%)	0.92±0.00	0±0/2171 (0.0± 0.0%)
2	B	1.25±0.02	1±0/197 (0.4± 0.2%)	1.50±0.03	7±1/299 (2.4± 0.2%)
All	All	1.05	17/36020 (0.0%)	1.01	145/49400 (0.3%)

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
2	B	386	DT	C5-C7	5.50	1.53	1.50	16	16
2	B	387	DT	C5-C7	5.01	1.53	1.50	7	1

5 of 9 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	386	DT	C6-C5-C7	-6.03	119.28	122.90	13	20
2	B	387	DT	C6-C5-C7	-5.99	119.30	122.90	19	20
2	B	393	DT	C6-C5-C7	-5.79	119.42	122.90	17	20
2	B	394	DT	C6-C5-C7	-5.79	119.43	122.90	15	20
2	B	387	DT	C4-C5-C6	5.47	121.28	118.00	6	20

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	1557	1463	1452	80±8
2	B	198	113	113	15±5
All	All	35120	31520	31300	1642

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 25.

5 of 671 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:253:LEU:HD22	1:A:253:LEU:H	0.93	1.24	5	1
1:A:281:CYS:SG	1:A:309:ILE:HG23	0.86	2.09	6	6
1:A:299:ILE:HD12	1:A:331:ALA:O	0.84	1.73	12	14
1:A:208:ASN:O	1:A:212:VAL:HG13	0.83	1.73	14	3
1:A:209:GLU:O	1:A:212:VAL:HG13	0.81	1.75	15	3

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	186/188 (99%)	172±1 (92±1%)	10±2 (5±1%)	5±1 (2±0%)	9	45
All	All	3720/3760 (99%)	3430 (92%)	198 (5%)	92 (2%)	9	45

5 of 13 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	199	PRO	20
1	A	200	PRO	20
1	A	382	GLN	17
1	A	320	ARG	13
1	A	212	VAL	9

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	169/169 (100%)	157±3 (93±2%)	12±3 (7±2%)	18	66
All	All	3380/3380 (100%)	3132 (93%)	248 (7%)	18	66

5 of 52 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	198	ASP	20
1	A	286	SER	18
1	A	221	CYS	17
1	A	197	MET	15
1	A	361	TRP	15

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	5IU	B	390	2	18,21,22	0.42±0.04	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
2	5IU	B	390	2	26,30,33	0.47±0.03	0±0 (0±0%)

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
2	5IU	B	390	2	-	0±0,7,21,22	0±0,2,2,2

There are no bond-length outliers.

There are no bond-angle outliers.

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 78% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *data_A3G_PrC.str*

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	2221
Number of shifts mapped to atoms	2221
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	17

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	175	-0.28 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	165	0.69 ± 0.09	Should be checked
$^{13}C'$	160	-0.10 ± 0.09	None needed (< 0.5 ppm)
^{15}N	171	-0.21 ± 0.34	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 78%, i.e. 2177 atoms were assigned a chemical shift out of a possible 2784. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	864/934 (93%)	358/378 (95%)	335/376 (89%)	171/180 (95%)
Sidechain	1049/1352 (78%)	743/869 (86%)	295/420 (70%)	11/63 (17%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	205/328 (62%)	115/162 (71%)	84/143 (59%)	6/23 (26%)
Sugar	50/108 (46%)	50/63 (79%)	0/45 (0%)	0/0 (—%)
Base	9/62 (15%)	9/35 (26%)	0/18 (0%)	0/9 (0%)
Overall	2177/2784 (78%)	1275/1507 (85%)	714/1002 (71%)	188/275 (68%)

7.1.4 Statistically unusual chemical shifts (i)

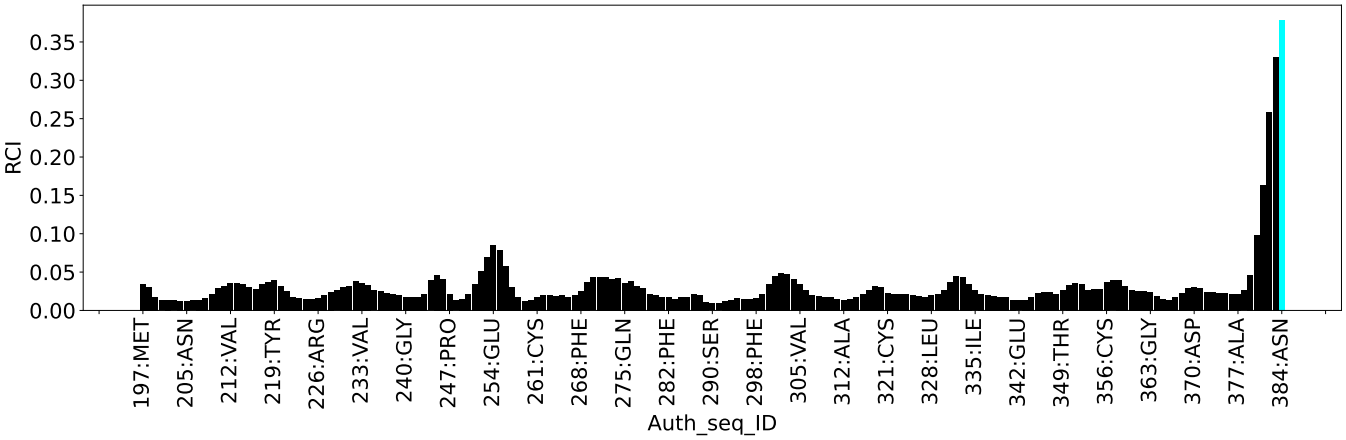
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	206	PHE	CD2	122.14	125.53 – 137.61	-7.8
1	A	340	TYR	CE2	127.67	111.68 – 124.17	7.8
1	A	206	PHE	CD1	122.14	125.33 – 137.83	-7.5
1	A	310	PHE	CD2	122.67	125.53 – 137.61	-7.4
1	A	340	TYR	CE1	127.67	111.24 – 124.66	7.2
1	A	310	PHE	CD1	122.67	125.33 – 137.83	-7.1
1	A	314	ILE	CG2	26.07	10.93 – 24.12	6.5
1	A	247	PRO	CD	43.58	45.11 – 55.58	-6.5
1	A	249	LYS	CD	22.29	23.50 – 34.42	-6.1
1	A	325	LEU	CG	33.09	21.37 – 32.19	5.8
1	A	222	TYR	CE2	125.05	111.68 – 124.17	5.7
1	A	355	GLY	H	11.65	5.23 – 11.42	5.4
1	A	219	TYR	CD1	125.40	125.84 – 139.60	-5.3
1	A	222	TYR	CE1	125.05	111.24 – 124.66	5.3
1	A	358	PHE	CD2	125.21	125.53 – 137.61	-5.3
1	A	358	PHE	CD1	125.21	125.33 – 137.83	-5.1
1	A	294	GLU	CG	30.13	30.20 – 42.01	-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:


RCI
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
197:MET
205:ASN
212:VAL
219:TYR
226:ARG
233:VAL
240:GLY
247:PRO
254:GLU
261:CYS
268:PHE
275:GLN
282:PHE
290:SER
298:PHE
305:VAL
312:ALA
321:CYS
328:LEU
335:ILE
342:GLU
349:THR
356:CYS
363:GLY
370:ASP
377:ALA
384:ASN
Auth_seq_ID

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	2702
Intra-residue (|i-j|=0)	1298
Sequential (|i-j|=1)	571
Medium range (|i-j|>1 and |i-j|<5)	358
Long range (|i-j|≥5)	432
Inter-chain	43
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	13.6
Number of long range restraints per residue[1]	2.2

[1]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 (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)	49.4	0.2
0.2-0.5 (Medium)	16.4	0.5
>0.5 (Large)	25.6	4.5

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 (i)

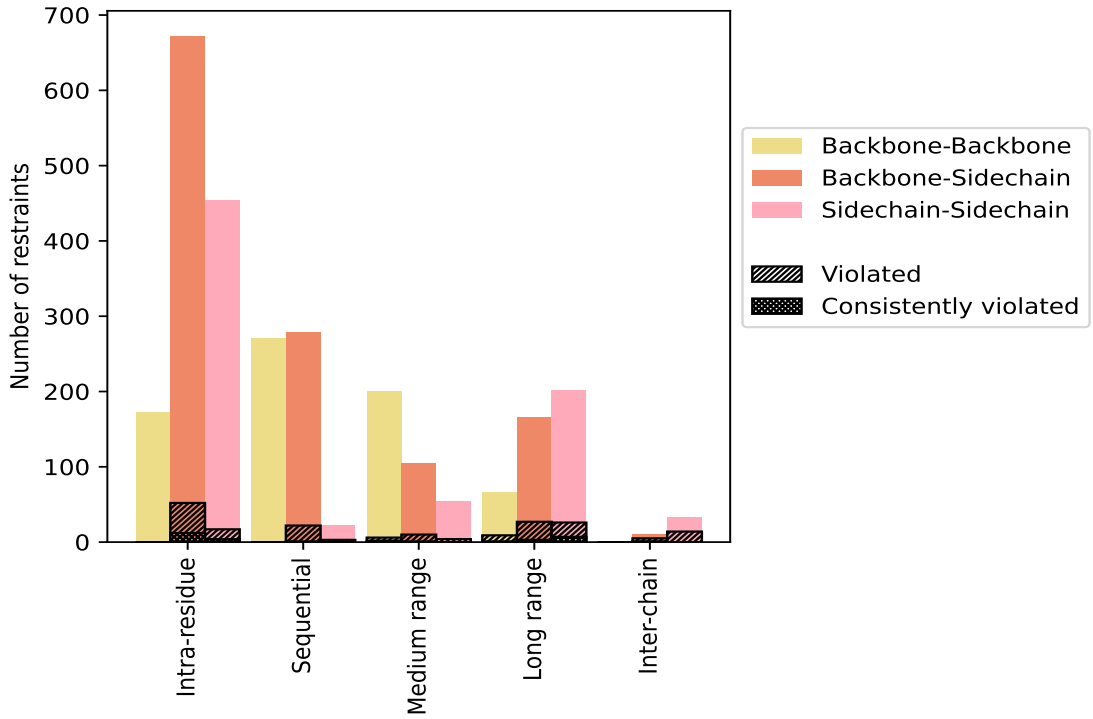
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1298	48.0	69	5.3	2.6	16	1.2	0.6
Backbone-Backbone	172	6.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	672	24.9	52	7.7	1.9	12	1.8	0.4
Sidechain-Sidechain	454	16.8	17	3.7	0.6	4	0.9	0.1
Sequential (|i-j|=1)	571	21.1	25	4.4	0.9	1	0.2	0.0
Backbone-Backbone	271	10.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	278	10.3	22	7.9	0.8	1	0.4	0.0
Sidechain-Sidechain	22	0.8	3	13.6	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	358	13.2	20	5.6	0.7	3	0.8	0.1
Backbone-Backbone	200	7.4	6	3.0	0.2	2	1.0	0.1
Backbone-Sidechain	104	3.8	10	9.6	0.4	1	1.0	0.0
Sidechain-Sidechain	54	2.0	4	7.4	0.1	0	0.0	0.0
Long range (|i-j|≥5)	432	16.0	62	14.4	2.3	11	2.5	0.4
Backbone-Backbone	66	2.4	9	13.6	0.3	1	1.5	0.0
Backbone-Sidechain	165	6.1	27	16.4	1.0	3	1.8	0.1
Sidechain-Sidechain	201	7.4	26	12.9	1.0	7	3.5	0.3
Inter-chain	43	1.6	19	44.2	0.7	1	2.3	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	10	0.4	5	50.0	0.2	1	10.0	0.0
Sidechain-Sidechain	33	1.2	14	42.4	0.5	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	2702	100.0	195	7.2	7.2	32	1.2	1.2
Backbone-Backbone	709	26.2	15	2.1	0.6	3	0.4	0.1
Backbone-Sidechain	1229	45.5	116	9.4	4.3	18	1.5	0.7
Sidechain-Sidechain	764	28.3	64	8.4	2.4	11	1.4	0.4

[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	38	10	9	32	8	97	0.38	3.63	0.47	0.18
2	36	8	7	33	4	88	0.45	2.38	0.48	0.2
3	41	11	9	32	5	98	0.43	2.89	0.52	0.19
4	36	10	8	33	5	92	0.4	2.65	0.43	0.19
5	36	10	9	30	6	91	0.42	2.28	0.45	0.18
6	37	11	11	34	4	97	0.41	4.5	0.55	0.2
7	38	13	9	30	5	95	0.41	2.6	0.47	0.17
8	35	15	8	31	6	95	0.46	2.68	0.53	0.19
9	36	10	9	33	6	94	0.43	3.05	0.54	0.18
10	34	8	7	32	6	87	0.48	2.55	0.52	0.19
11	36	11	8	30	6	91	0.42	2.65	0.49	0.19

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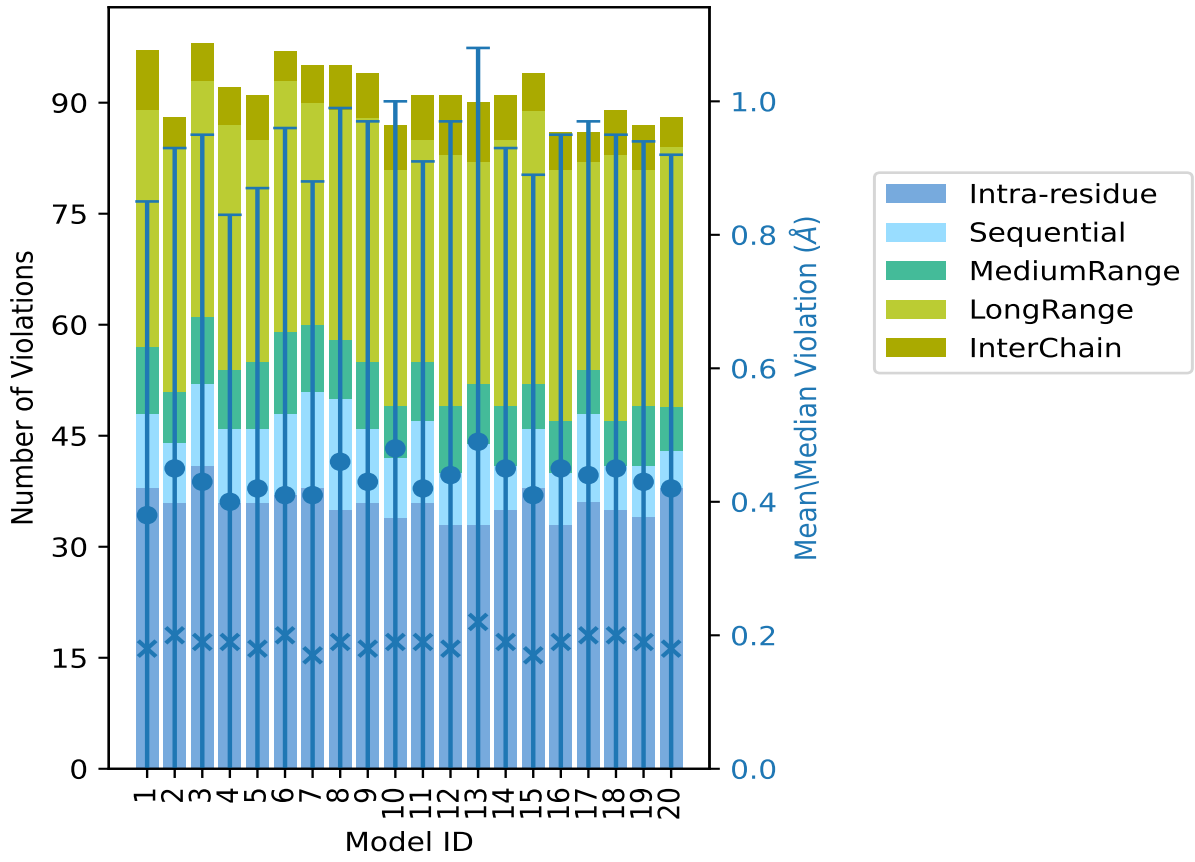
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	33	7	9	34	8	91	0.44	3.42	0.53	0.18
13	33	11	8	30	8	90	0.49	2.64	0.59	0.22
14	35	6	8	36	6	91	0.45	2.63	0.48	0.19
15	38	8	6	37	5	94	0.41	2.75	0.48	0.17
16	33	7	7	34	5	86	0.45	2.71	0.5	0.19
17	36	12	6	28	4	86	0.44	3.06	0.53	0.2
18	35	6	6	36	6	89	0.45	2.42	0.5	0.2
19	34	7	8	32	6	87	0.43	2.6	0.51	0.19
20	38	5	6	35	4	88	0.42	2.72	0.5	0.18

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]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

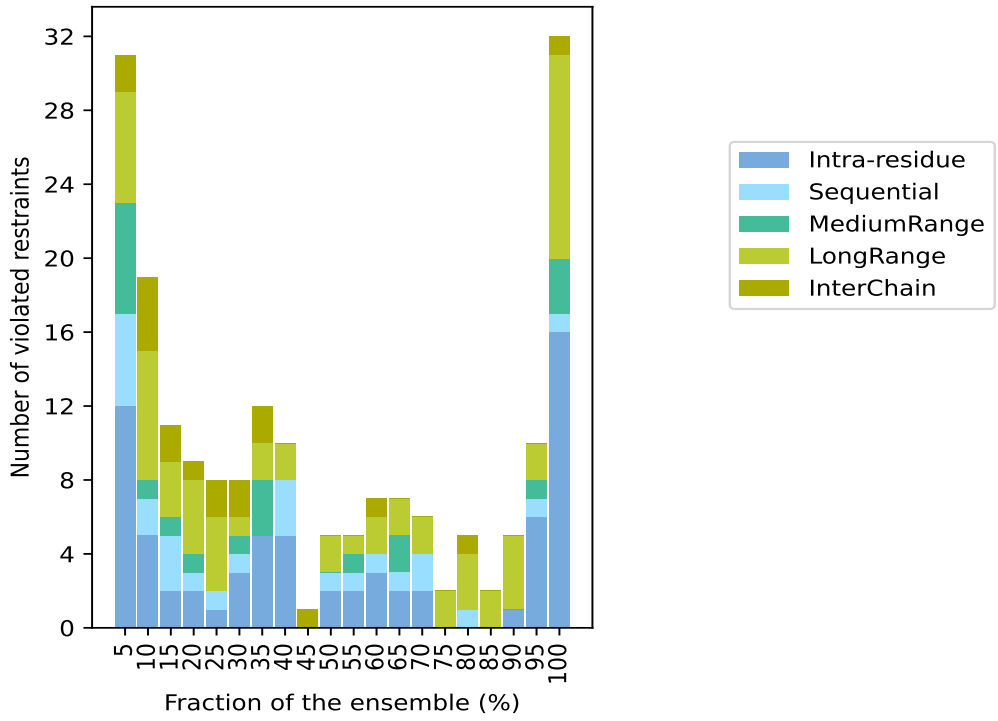
9.3 Distance violation statistics for the ensemble (i)

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, 2507(IR:1229, SQ:546, MR:338, LR:370, IC:24) 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]	%
12	5	6	6	2	31	1	5.0
5	2	1	7	4	19	2	10.0
2	3	1	3	2	11	3	15.0
2	1	1	4	1	9	4	20.0
1	1	0	4	2	8	5	25.0
3	1	1	1	2	8	6	30.0
5	0	3	2	2	12	7	35.0
5	3	0	2	0	10	8	40.0
0	0	0	0	1	1	9	45.0
2	1	0	2	0	5	10	50.0
2	1	1	1	0	5	11	55.0
3	1	0	2	1	7	12	60.0
2	1	2	2	0	7	13	65.0
2	2	0	2	0	6	14	70.0
0	0	0	2	0	2	15	75.0
0	1	0	3	1	5	16	80.0
0	0	0	2	0	2	17	85.0
1	0	0	4	0	5	18	90.0
6	1	1	2	0	10	19	95.0
16	1	3	11	1	32	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

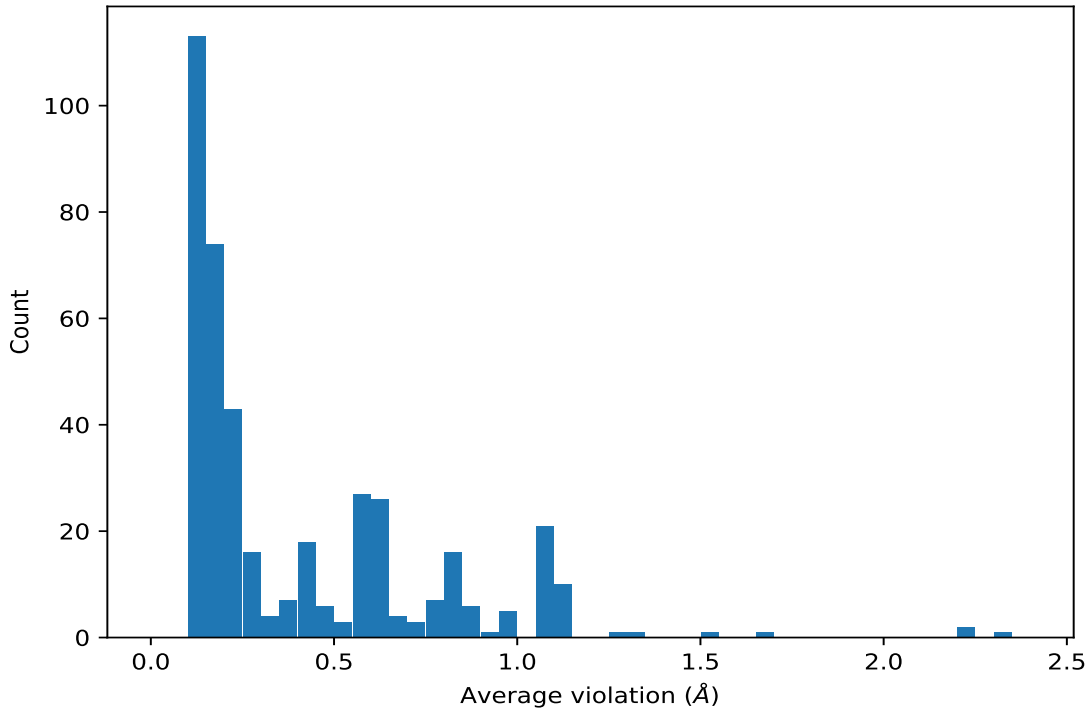
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,611)	1:A:245:GLN:H	1:A:256:ARG:H	20	2.34	0.53	2.6
(1,2670)	2:B:386:DT:H5'	1:A:366:GLU:HA	20	2.22	0.9	2.13
(1,2670)	2:B:386:DT:H5"	1:A:366:GLU:HA	20	2.22	0.9	2.13
(1,567)	1:A:241:PHE:HZ	1:A:247:PRO:HA	20	1.34	0.03	1.35
(1,620)	1:A:246:ALA:HB1	1:A:252:PHE:HB2	20	1.1	0.23	1.19
(1,620)	1:A:246:ALA:HB1	1:A:252:PHE:HB3	20	1.1	0.23	1.19
(1,620)	1:A:246:ALA:HB2	1:A:252:PHE:HB2	20	1.1	0.23	1.19
(1,620)	1:A:246:ALA:HB2	1:A:252:PHE:HB3	20	1.1	0.23	1.19
(1,620)	1:A:246:ALA:HB3	1:A:252:PHE:HB2	20	1.1	0.23	1.19
(1,620)	1:A:246:ALA:HB3	1:A:252:PHE:HB3	20	1.1	0.23	1.19
(1,857)	1:A:263:LEU:HD11	1:A:298:PHE:H	20	1.09	0.18	1.08
(1,857)	1:A:263:LEU:HD12	1:A:298:PHE:H	20	1.09	0.18	1.08
(1,857)	1:A:263:LEU:HD13	1:A:298:PHE:H	20	1.09	0.18	1.08
(1,857)	1:A:263:LEU:HD21	1:A:298:PHE:H	20	1.09	0.18	1.08
(1,857)	1:A:263:LEU:HD22	1:A:298:PHE:H	20	1.09	0.18	1.08
(1,857)	1:A:263:LEU:HD23	1:A:298:PHE:H	20	1.09	0.18	1.08

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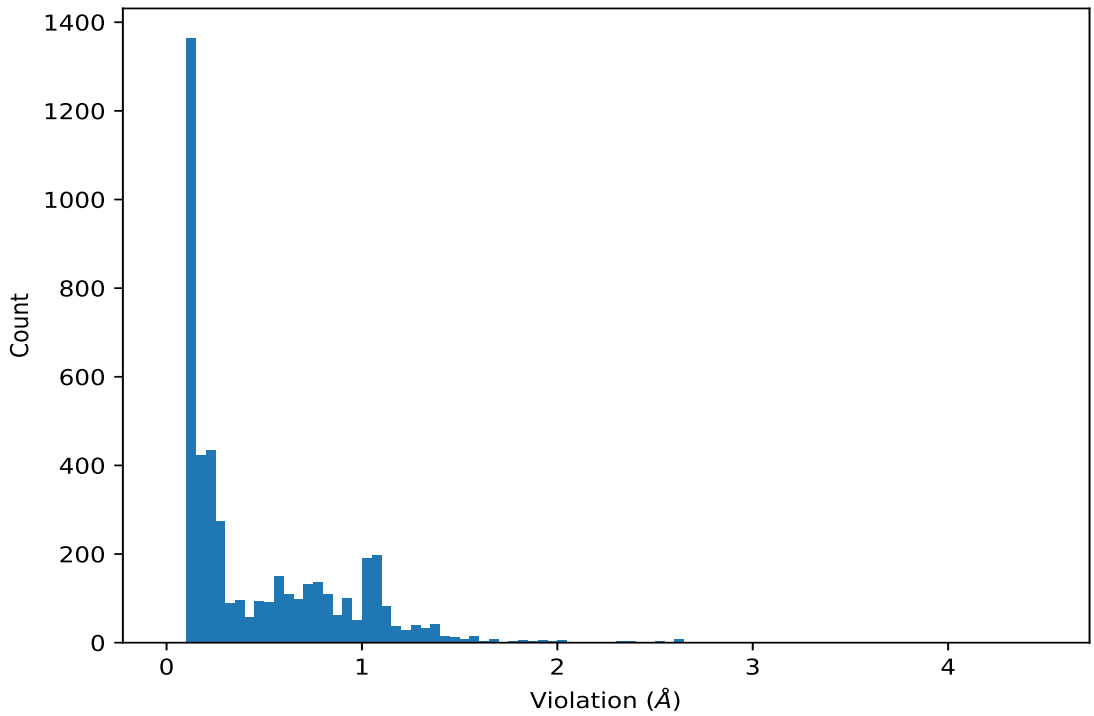
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,182)	1:A:211:TRP:HE1	1:A:284:SER:HB2	20	1.07	0.03	1.08
(1,182)	1:A:211:TRP:HE1	1:A:284:SER:HB3	20	1.07	0.03	1.08
(1,662)	1:A:249:LYS:HD2	1:A:254:GLU:HG2	20	1.06	0.05	1.06
(1,662)	1:A:249:LYS:HD2	1:A:254:GLU:HG3	20	1.06	0.05	1.06
(1,662)	1:A:249:LYS:HD3	1:A:254:GLU:HG2	20	1.06	0.05	1.06
(1,662)	1:A:249:LYS:HD3	1:A:254:GLU:HG3	20	1.06	0.05	1.06
(1,1648)	1:A:313:ARG:HD2	1:A:337:ILE:HD11	20	1.06	0.05	1.06
(1,1648)	1:A:313:ARG:HD2	1:A:337:ILE:HD12	20	1.06	0.05	1.06
(1,1648)	1:A:313:ARG:HD2	1:A:337:ILE:HD13	20	1.06	0.05	1.06
(1,1648)	1:A:313:ARG:HD3	1:A:337:ILE:HD11	20	1.06	0.05	1.06
(1,1648)	1:A:313:ARG:HD3	1:A:337:ILE:HD12	20	1.06	0.05	1.06
(1,1648)	1:A:313:ARG:HD3	1:A:337:ILE:HD13	20	1.06	0.05	1.06
(1,2628)	2:B:387:DT:H6	2:B:387:DT:H5'	20	0.81	0.24	0.84
(1,2628)	2:B:387:DT:H6	2:B:387:DT:H5"	20	0.81	0.24	0.84
(1,1437)	1:A:301:LYS:HG2	1:A:309:ILE:HD11	20	0.77	0.2	0.81

[1]Number of violated models, [2]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 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)
(1,2670)	2:B:386:DT:H5'	1:A:366:GLU:HA	6	4.5
(1,2670)	2:B:386:DT:H5"	1:A:366:GLU:HA	6	4.5
(1,2670)	2:B:386:DT:H5'	1:A:366:GLU:HA	1	3.63
(1,2670)	2:B:386:DT:H5"	1:A:366:GLU:HA	1	3.63
(1,2670)	2:B:386:DT:H5'	1:A:366:GLU:HA	12	3.42
(1,2670)	2:B:386:DT:H5"	1:A:366:GLU:HA	12	3.42
(1,611)	1:A:245:GLN:H	1:A:256:ARG:H	17	3.06
(1,2670)	2:B:386:DT:H5'	1:A:366:GLU:HA	9	3.05
(1,2670)	2:B:386:DT:H5"	1:A:366:GLU:HA	9	3.05
(1,611)	1:A:245:GLN:H	1:A:256:ARG:H	3	2.89
(1,2670)	2:B:386:DT:H5'	1:A:366:GLU:HA	15	2.75
(1,2670)	2:B:386:DT:H5"	1:A:366:GLU:HA	15	2.75
(1,611)	1:A:245:GLN:H	1:A:256:ARG:H	20	2.72
(1,611)	1:A:245:GLN:H	1:A:256:ARG:H	16	2.71
(1,611)	1:A:245:GLN:H	1:A:256:ARG:H	8	2.68

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found