Full wwPDB NMR Structure Validation Report (i)

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BMRB ID	:	30361
Title	:	Solution structure of de novo macrocycle design11_ss
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This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (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:

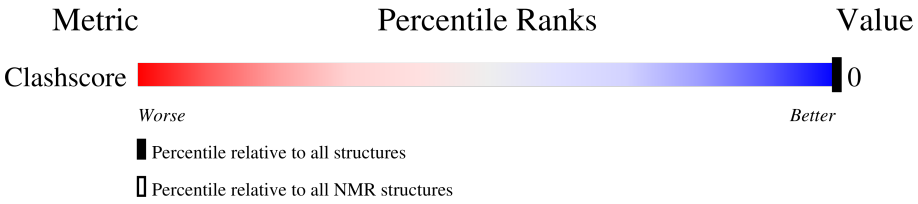
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 52%.

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

Molprobity failed to run

2 Ensemble composition and analysis (i)

This entry contains 20 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 is only 1 type of molecule in this entry. The entry contains 152 atoms, of which 71 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein (with D amino acids) called (DAL)Q(DPR)(DCY)(DLY)DS(DTY)(DCY)P(DSN).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	11	152	49	71	13	17	2	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.

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

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.2 Score per residue for model 2

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.3 Score per residue for model 3

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.4 Score per residue for model 4

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.5 Score per residue for model 5

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.6 Score per residue for model 6

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.7 Score per residue for model 7

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.8 Score per residue for model 8

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.9 Score per residue for model 9

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.10 Score per residue for model 10

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.11 Score per residue for model 11

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.12 Score per residue for model 12

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.13 Score per residue for model 13

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.14 Score per residue for model 14

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.15 Score per residue for model 15

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.16 Score per residue for model 16

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.17 Score per residue for model 17

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.18 Score per residue for model 18

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.19 Score per residue for model 19

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.20 Score per residue for model 20

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

5 Refinement protocol and experimental data overview

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

Of the 200 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
GROMACS	refinement	2016.1
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	51
Number of shifts mapped to atoms	51
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	52%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, DSN, DPR, DCY, DTY, DLY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.54±0.03	0±0/28 (0.0± 0.0%)	1.93±0.42	1±1/33 (2.0± 2.8%)
All	All	0.54	0/560 (0.0%)	1.97	13/660 (2.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	6	ASP	CB-CG-OD1	15.46	132.21	118.30	19	2
1	A	6	ASP	CB-CG-OD2	8.37	125.83	118.30	5	6
1	A	10	PRO	N-CA-CB	6.41	111.00	103.30	7	1
1	A	10	PRO	CA-N-CD	-5.13	104.32	111.50	7	1
1	A	2	GLN	CB-CA-C	5.12	120.63	110.40	15	1
1	A	7	SER	N-CA-CB	5.09	118.13	110.50	11	1
1	A	6	ASP	OD1-CG-OD2	-5.06	113.68	123.30	19	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	1620	1420	1289	-

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

6.3.1 Protein backbone

There are no protein molecules in this entry.

6.3.2 Protein sidechains

There are no protein molecules in this entry.

6.3.3 RNA

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 52% for the well-defined parts and 52% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *11cpp_bmrb.txt*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	51
Number of shifts mapped to atoms	51
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

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 52%, i.e. 23 atoms were assigned a chemical shift out of a possible 44. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	7/18 (39%)	7/7 (100%)	0/8 (0%)	0/3 (0%)
Sidechain	16/26 (62%)	16/16 (100%)	0/9 (0%)	0/1 (0%)
Overall	23/44 (52%)	23/23 (100%)	0/17 (0%)	0/4 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 23 atoms were assigned a chemical shift out of a possible 44. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	7/18 (39%)	7/7 (100%)	0/8 (0%)	0/3 (0%)
Sidechain	16/26 (62%)	16/16 (100%)	0/9 (0%)	0/1 (0%)
Overall	23/44 (52%)	23/23 (100%)	0/17 (0%)	0/4 (0%)

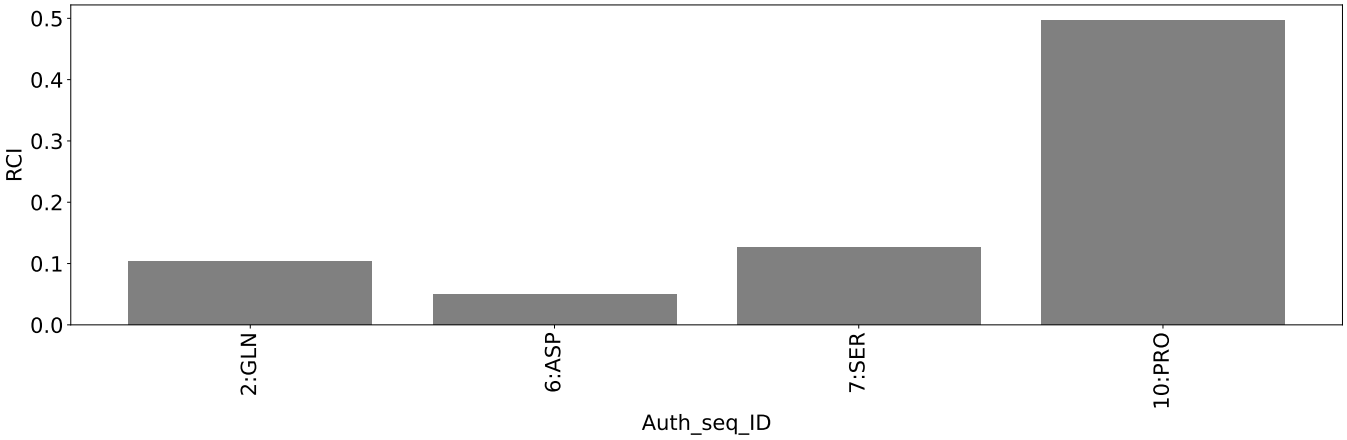
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	86
Intra-residue (|i-j|=0)	38
Sequential (|i-j|=1)	25
Medium range (|i-j|>1 and |i-j|<5)	6
Long range (|i-j|≥5)	17
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	4
Number of restraints per residue	7.8
Number of long range restraints per residue[1]	1.5

[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

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)	1.9	0.2
0.2-0.5 (Medium)	3.2	0.49
>0.5 (Large)	1.9	0.94

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)

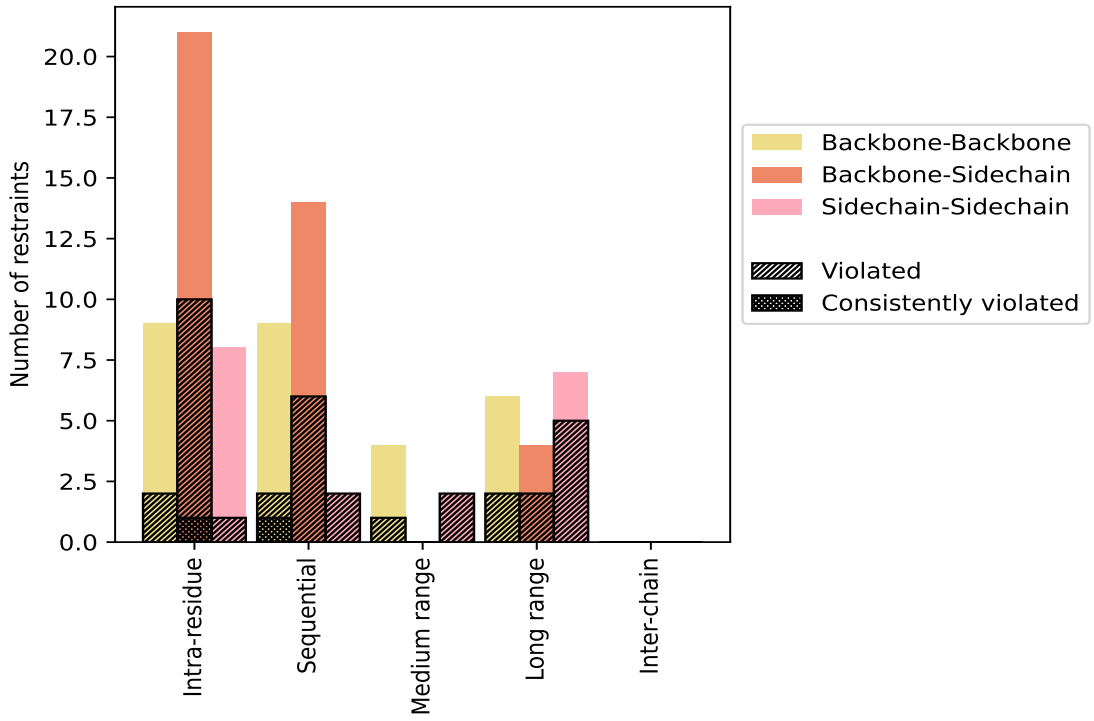
9.1 Summary of distance violations (i)

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)	38	44.2	13	34.2	15.1	1	2.6	1.2
Backbone-Backbone	9	10.5	2	22.2	2.3	0	0.0	0.0
Backbone-Sidechain	21	24.4	10	47.6	11.6	1	4.8	1.2
Sidechain-Sidechain	8	9.3	1	12.5	1.2	0	0.0	0.0
Sequential (|i-j|=1)	25	29.1	10	40.0	11.6	1	4.0	1.2
Backbone-Backbone	9	10.5	2	22.2	2.3	1	11.1	1.2
Backbone-Sidechain	14	16.3	6	42.9	7.0	0	0.0	0.0
Sidechain-Sidechain	2	2.3	2	100.0	2.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	6	7.0	3	50.0	3.5	0	0.0	0.0
Backbone-Backbone	4	4.7	1	25.0	1.2	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	2	2.3	2	100.0	2.3	0	0.0	0.0
Long range (|i-j|≥5)	17	19.8	9	52.9	10.5	0	0.0	0.0
Backbone-Backbone	6	7.0	2	33.3	2.3	0	0.0	0.0
Backbone-Sidechain	4	4.7	2	50.0	2.3	0	0.0	0.0
Sidechain-Sidechain	7	8.1	5	71.4	5.8	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	86	100.0	35	40.7	40.7	2	2.3	2.3
Backbone-Backbone	28	32.6	7	25.0	8.1	1	3.6	1.2
Backbone-Sidechain	39	45.3	18	46.2	20.9	1	2.6	1.2
Sidechain-Sidechain	19	22.1	10	52.6	11.6	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



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

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	4	1	2	0	0	7	0.37	0.63	0.15	0.38
2	1	2	0	2	0	5	0.41	0.63	0.11	0.37
3	2	3	1	0	0	6	0.25	0.41	0.1	0.22
4	3	2	1	2	0	8	0.46	0.94	0.27	0.45
5	3	3	0	4	0	10	0.31	0.56	0.15	0.26
6	3	1	1	4	0	9	0.34	0.59	0.15	0.35
7	4	1	0	4	0	9	0.3	0.72	0.23	0.16
8	3	1	0	0	0	4	0.41	0.75	0.24	0.36
9	3	2	0	2	0	7	0.35	0.6	0.15	0.28
10	2	4	0	2	0	8	0.42	0.66	0.17	0.39
11	1	2	0	1	0	4	0.34	0.54	0.16	0.34

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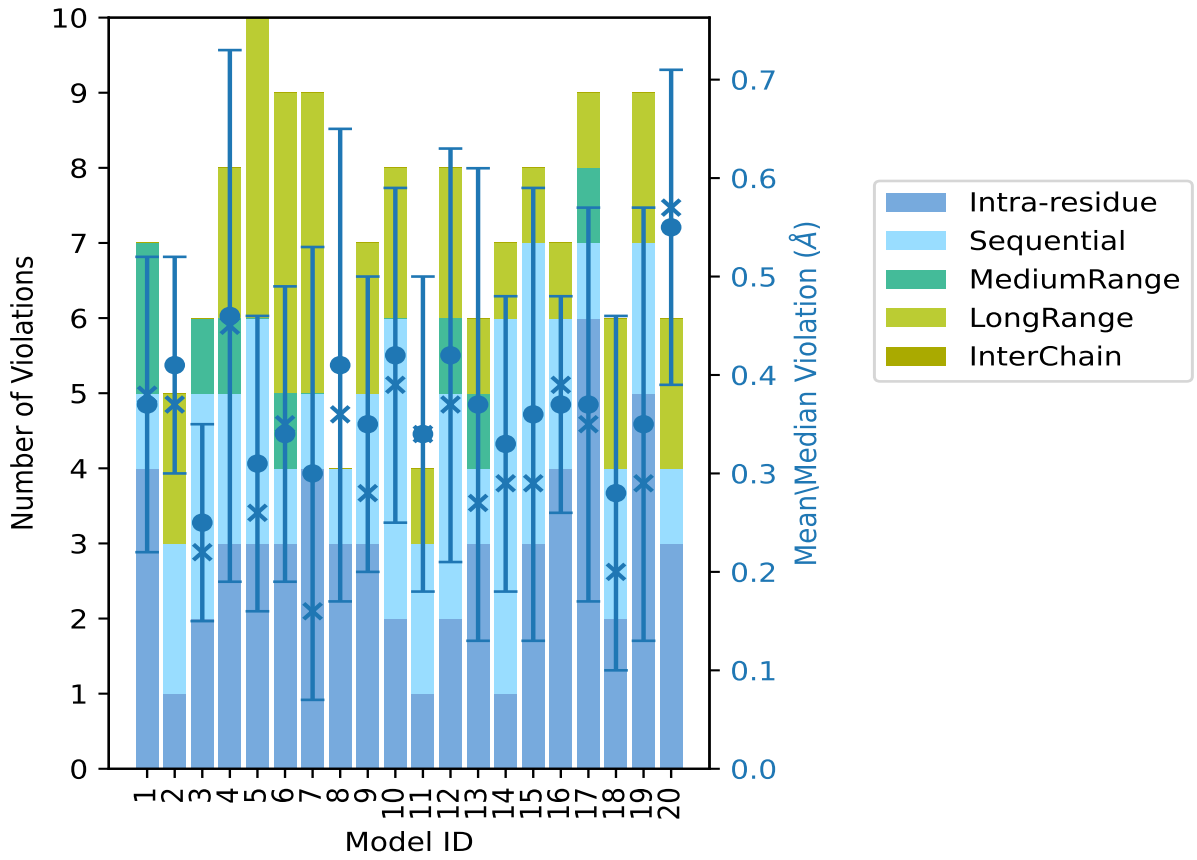
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	3	1	2	0	8	0.42	0.79	0.21	0.37
13	3	1	1	1	0	6	0.37	0.8	0.24	0.27
14	1	5	0	1	0	7	0.33	0.55	0.15	0.29
15	3	4	0	1	0	8	0.36	0.85	0.23	0.29
16	4	2	0	1	0	7	0.37	0.57	0.11	0.39
17	6	1	1	1	0	9	0.37	0.73	0.2	0.35
18	2	2	0	2	0	6	0.28	0.6	0.18	0.2
19	5	2	0	2	0	9	0.35	0.81	0.22	0.29
20	3	1	0	2	0	6	0.55	0.73	0.16	0.57

[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



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

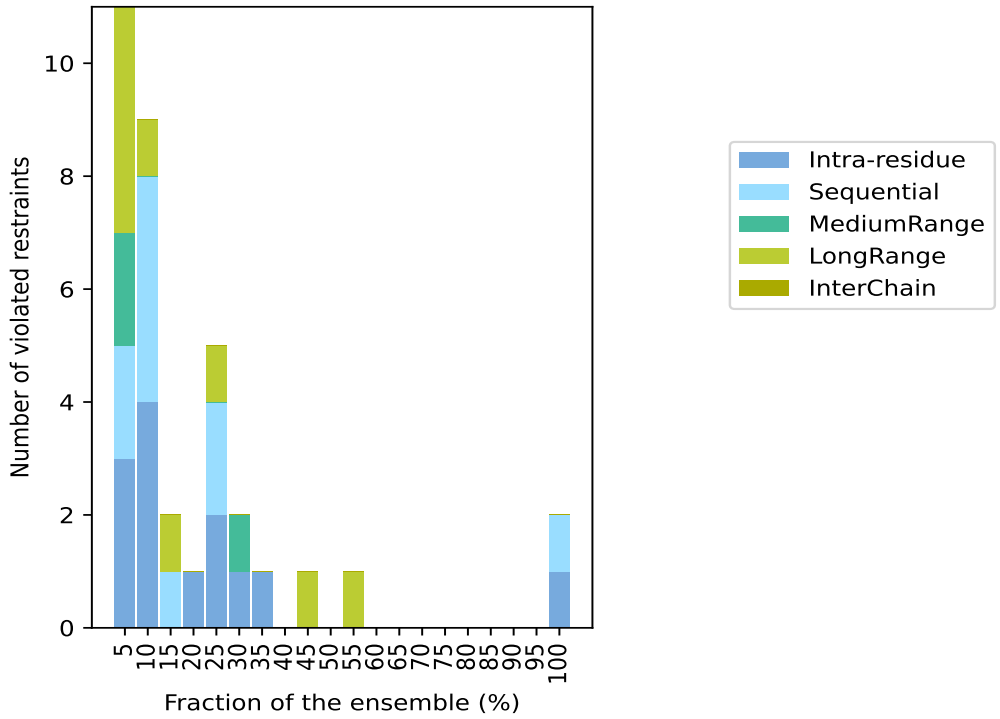
9.3 Distance violation statistics for the ensemble (i)

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, 51(IR:25, SQ:15, MR:3, LR:8, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
3	2	2	4	0	11	1	5.0
4	4	0	1	0	9	2	10.0
0	1	0	1	0	2	3	15.0
1	0	0	0	0	1	4	20.0
2	2	0	1	0	5	5	25.0
1	0	1	0	0	2	6	30.0
1	0	0	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	1	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	1	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
1	1	0	0	0	2	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

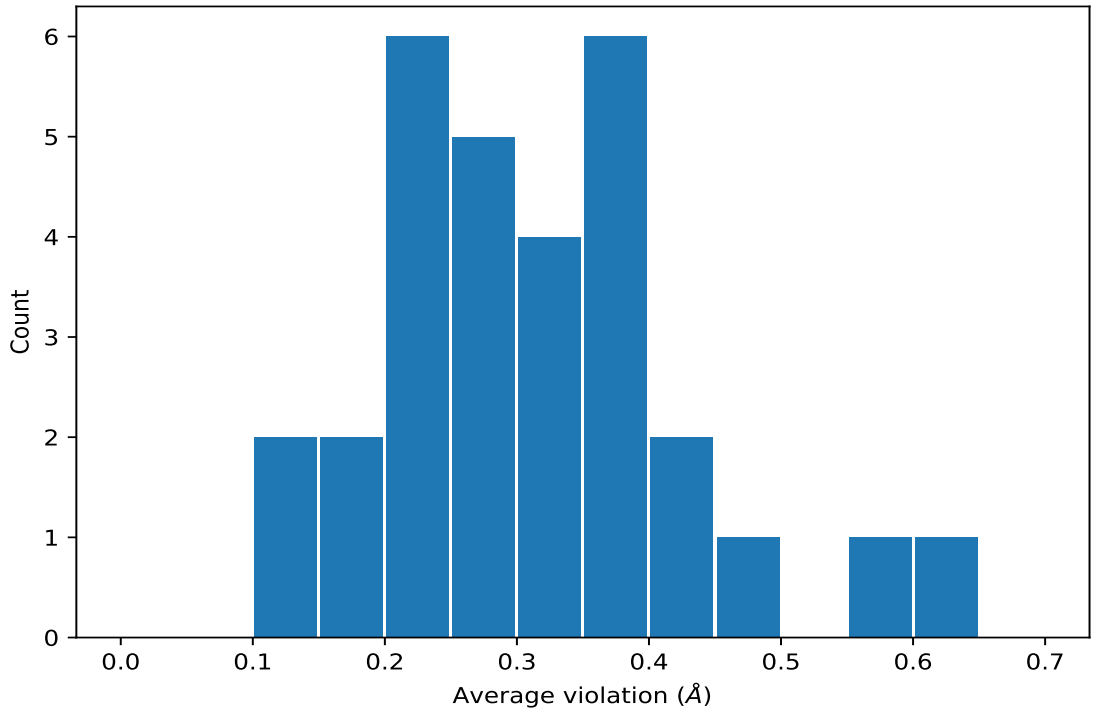
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	20	0.63	0.12	0.6
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	20	0.46	0.15	0.44
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	11	0.26	0.14	0.21
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	11	0.26	0.14	0.21
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	11	0.26	0.14	0.21
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	9	0.37	0.14	0.33
(1,67)	1:A:8:DTY:HA	1:A:8:DTY:HD1	7	0.34	0.12	0.36
(1,14)	1:A:8:DTY:HA	1:A:4:DCY:H	6	0.3	0.14	0.24
(1,50)	1:A:4:DCY:HB3	1:A:4:DCY:H	6	0.2	0.09	0.18
(1,46)	1:A:3:DPR:HD3	1:A:8:DTY:HD1	5	0.56	0.25	0.56
(1,52)	1:A:5:DLY:HB3	1:A:5:DLY:H	5	0.39	0.04	0.39
(1,59)	1:A:7:SER:HA	1:A:8:DTY:HD1	5	0.36	0.18	0.37
(1,45)	1:A:3:DPR:HD3	1:A:2:GLN:HA	5	0.27	0.08	0.26
(1,57)	1:A:6:ASP:HB2	1:A:6:ASP:H	5	0.21	0.1	0.17
(1,41)	1:A:3:DPR:HB3	1:A:3:DPR:HA	4	0.13	0.01	0.13
(1,47)	1:A:3:DPR:HD3	1:A:8:DTY:HE1	3	0.42	0.23	0.26

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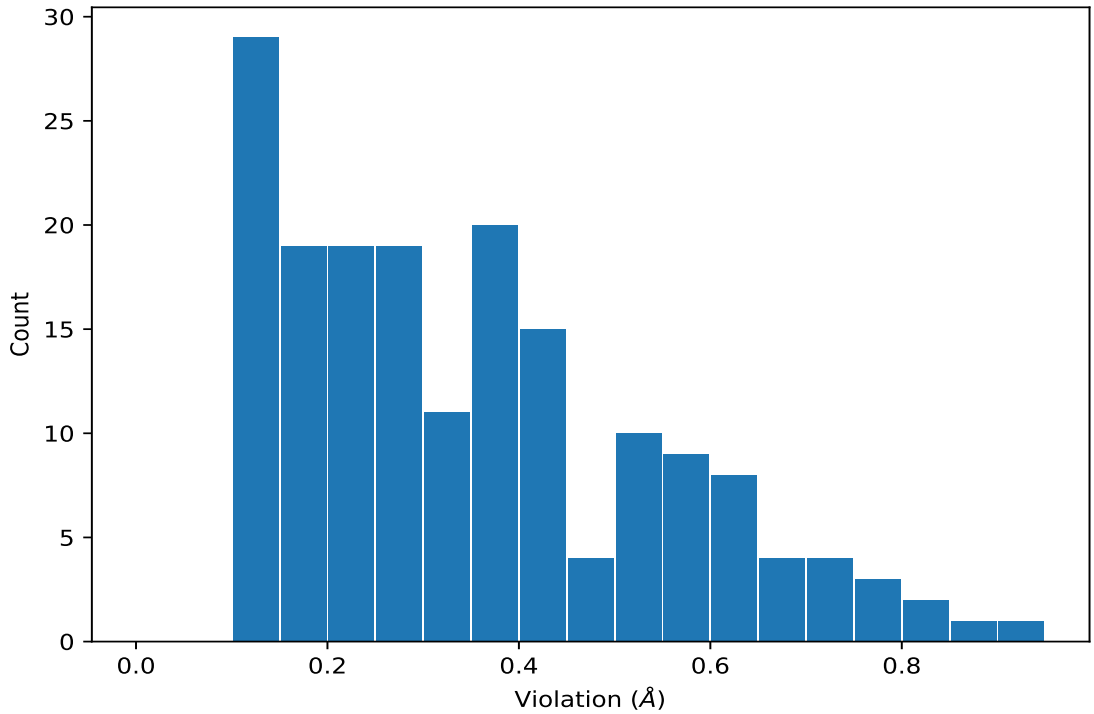
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,61)	1:A:7:SER:HB2	1:A:8:DTY:HE1	3	0.32	0.15	0.26
(1,61)	1:A:7:SER:HB3	1:A:8:DTY:HE1	3	0.32	0.15	0.26
(1,36)	1:A:2:GLN:HG2	1:A:2:GLN:H	2	0.42	0.11	0.42
(1,60)	1:A:7:SER:HB2	1:A:8:DTY:HD1	2	0.37	0.03	0.37
(1,60)	1:A:7:SER:HB3	1:A:8:DTY:HD1	2	0.37	0.03	0.37
(1,83)	1:A:10:PRO:HD2	1:A:9:DCY:HA	2	0.36	0.19	0.36
(1,39)	1:A:2:GLN:HG3	1:A:11:DSN:HA	2	0.26	0.03	0.26
(1,29)	1:A:1:DAL:HB1	1:A:2:GLN:H	2	0.24	0.12	0.24
(1,29)	1:A:1:DAL:HB2	1:A:2:GLN:H	2	0.24	0.12	0.24
(1,29)	1:A:1:DAL:HB3	1:A:2:GLN:H	2	0.24	0.12	0.24
(1,6)	1:A:4:DCY:HA	1:A:5:DLY:H	2	0.23	0.07	0.23
(1,51)	1:A:4:DCY:HB2	1:A:4:DCY:H	2	0.18	0.04	0.18
(1,2)	1:A:2:GLN:HA	1:A:2:GLN:H	2	0.16	0.01	0.16
(1,32)	1:A:2:GLN:HE22	1:A:2:GLN:HE21	2	0.12	0.0	0.12

[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 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)
(1,46)	1:A:3:DPR:HD3	1:A:8:DTY:HD1	4	0.94
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	15	0.85
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	19	0.81
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	13	0.8
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	12	0.79
(1,47)	1:A:3:DPR:HD3	1:A:8:DTY:HE1	4	0.75
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	8	0.75
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	17	0.73
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	20	0.73
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	20	0.72
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	7	0.72
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	7	0.67
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	10	0.66
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	10	0.66
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	10	0.66
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	1	0.63
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	2	0.63
(1,59)	1:A:7:SER:HA	1:A:8:DTY:HD1	12	0.61
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	17	0.61
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	20	0.61
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	10	0.61
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	9	0.6
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	18	0.6
(1,46)	1:A:3:DPR:HD3	1:A:8:DTY:HD1	10	0.59
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	4	0.59
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	6	0.59
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	16	0.57
(1,46)	1:A:3:DPR:HD3	1:A:8:DTY:HD1	5	0.56
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	13	0.56
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	15	0.56
(1,83)	1:A:10:PRO:HD2	1:A:9:DCY:HA	14	0.55
(1,14)	1:A:8:DTY:HA	1:A:4:DCY:H	12	0.55
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	11	0.54
(1,79)	1:A:9:DCY:HB2	1:A:4:DCY:HB3	20	0.53
(1,46)	1:A:3:DPR:HD3	1:A:8:DTY:HD1	6	0.53
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	8	0.53
(1,61)	1:A:7:SER:HB2	1:A:8:DTY:HE1	19	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:A:7:SER:HB3	1:A:8:DTY:HE1	19	0.52
(1,36)	1:A:2:GLN:HG2	1:A:2:GLN:H	17	0.52
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	14	0.52
(1,59)	1:A:7:SER:HA	1:A:8:DTY:HD1	9	0.51
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	5	0.51
(1,67)	1:A:8:DTY:HA	1:A:8:DTY:HD1	19	0.49
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	1	0.47
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	4	0.46
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	6	0.45
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	10	0.44
(1,14)	1:A:8:DTY:HA	1:A:4:DCY:H	4	0.44
(1,52)	1:A:5:DLY:HB3	1:A:5:DLY:H	19	0.43
(1,37)	1:A:2:GLN:HG2	1:A:11:DSN:HA	5	0.43
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	9	0.43
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	11	0.43
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	16	0.43
(1,52)	1:A:5:DLY:HB3	1:A:5:DLY:H	17	0.42
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	18	0.42
(1,67)	1:A:8:DTY:HA	1:A:8:DTY:HD1	1	0.41
(1,67)	1:A:8:DTY:HA	1:A:8:DTY:HD1	16	0.41
(1,45)	1:A:3:DPR:HD3	1:A:2:GLN:HA	15	0.41
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	3	0.41
(1,60)	1:A:7:SER:HB2	1:A:8:DTY:HD1	5	0.4
(1,60)	1:A:7:SER:HB3	1:A:8:DTY:HD1	5	0.4
(1,52)	1:A:5:DLY:HB3	1:A:5:DLY:H	16	0.39
(1,15)	1:A:8:DTY:HA	1:A:9:DCY:H	12	0.39
(1,52)	1:A:5:DLY:HB3	1:A:5:DLY:H	1	0.38
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	2	0.38
(1,59)	1:A:7:SER:HA	1:A:8:DTY:HD1	2	0.37
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	14	0.37
(1,67)	1:A:8:DTY:HA	1:A:8:DTY:HD1	20	0.36
(1,50)	1:A:4:DCY:HB3	1:A:4:DCY:H	7	0.36
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	2	0.36
(1,29)	1:A:1:DAL:HB1	1:A:2:GLN:H	15	0.36
(1,29)	1:A:1:DAL:HB2	1:A:2:GLN:H	15	0.36
(1,29)	1:A:1:DAL:HB3	1:A:2:GLN:H	15	0.36
(1,73)	1:A:8:DTY:HB2	1:A:10:PRO:HD3	1	0.35
(1,67)	1:A:8:DTY:HA	1:A:8:DTY:HD1	17	0.35
(1,57)	1:A:6:ASP:HB2	1:A:6:ASP:H	6	0.35
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	3	0.35
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	6	0.35
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	12	0.35
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	12	0.35
(1,60)	1:A:7:SER:HB2	1:A:8:DTY:HD1	10	0.34
(1,60)	1:A:7:SER:HB3	1:A:8:DTY:HD1	10	0.34
(1,52)	1:A:5:DLY:HB3	1:A:5:DLY:H	20	0.33
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	12	0.33
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	2	0.32
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	2	0.32
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	2	0.32
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	13	0.32
(1,36)	1:A:2:GLN:HG2	1:A:2:GLN:H	5	0.31
(1,6)	1:A:4:DCY:HA	1:A:5:DLY:H	10	0.3
(1,57)	1:A:6:ASP:HB2	1:A:6:ASP:H	16	0.3
(1,45)	1:A:3:DPR:HD3	1:A:2:GLN:HA	16	0.29
(1,39)	1:A:2:GLN:HG3	1:A:11:DSN:HA	14	0.29
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	19	0.29
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	9	0.28
(1,55)	1:A:5:DLY:HG3	1:A:6:ASP:H	14	0.27
(1,61)	1:A:7:SER:HB2	1:A:8:DTY:HE1	10	0.26
(1,61)	1:A:7:SER:HB3	1:A:8:DTY:HE1	10	0.26
(1,47)	1:A:3:DPR:HD3	1:A:8:DTY:HE1	6	0.26
(1,45)	1:A:3:DPR:HD3	1:A:2:GLN:HA	3	0.26
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	9	0.26
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	9	0.26
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	9	0.26
(1,14)	1:A:8:DTY:HA	1:A:4:DCY:H	17	0.26
(1,50)	1:A:4:DCY:HB3	1:A:4:DCY:H	1	0.25
(1,47)	1:A:3:DPR:HD3	1:A:8:DTY:HE1	19	0.25
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	11	0.25
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	11	0.25
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	11	0.25
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	7	0.25
(1,39)	1:A:2:GLN:HG3	1:A:11:DSN:HA	6	0.23
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	18	0.23
(1,51)	1:A:4:DCY:HB2	1:A:4:DCY:H	13	0.22
(1,50)	1:A:4:DCY:HB3	1:A:4:DCY:H	15	0.22
(1,45)	1:A:3:DPR:HD3	1:A:2:GLN:HA	4	0.22
(1,34)	1:A:2:GLN:HG3	1:A:2:GLN:H	9	0.22
(1,27)	1:A:8:DTY:HA	1:A:3:DPR:HA	5	0.22
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	15	0.21
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	15	0.21
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:A:8:DTY:HA	1:A:4:DCY:H	6	0.21
(1,67)	1:A:8:DTY:HA	1:A:8:DTY:HD1	8	0.2
(1,59)	1:A:7:SER:HA	1:A:8:DTY:HD1	14	0.2
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	5	0.2
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	5	0.2
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	5	0.2
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	16	0.2
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	16	0.2
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	16	0.2
(1,58)	1:A:7:SER:HB2	1:A:7:SER:H	10	0.19
(1,58)	1:A:7:SER:HB3	1:A:7:SER:H	10	0.19
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	17	0.19
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	17	0.19
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	17	0.19
(1,83)	1:A:10:PRO:HD2	1:A:9:DCY:HA	15	0.18
(1,61)	1:A:7:SER:HB2	1:A:8:DTY:HE1	18	0.18
(1,61)	1:A:7:SER:HB3	1:A:8:DTY:HE1	18	0.18
(1,14)	1:A:8:DTY:HA	1:A:4:DCY:H	13	0.18
(1,57)	1:A:6:ASP:HB2	1:A:6:ASP:H	17	0.17
(1,45)	1:A:3:DPR:HD3	1:A:2:GLN:HA	12	0.17
(1,35)	1:A:2:GLN:HB2	1:A:2:GLN:H	5	0.17
(1,14)	1:A:8:DTY:HA	1:A:4:DCY:H	3	0.17
(1,62)	1:A:7:SER:HB2	1:A:8:DTY:H	5	0.16
(1,62)	1:A:7:SER:HB3	1:A:8:DTY:H	5	0.16
(1,6)	1:A:4:DCY:HA	1:A:5:DLY:H	3	0.16
(1,46)	1:A:3:DPR:HD3	1:A:8:DTY:HD1	7	0.16
(1,2)	1:A:2:GLN:HA	1:A:2:GLN:H	8	0.16
(1,2)	1:A:2:GLN:HA	1:A:2:GLN:H	9	0.15
(1,51)	1:A:4:DCY:HB2	1:A:4:DCY:H	12	0.14
(1,50)	1:A:4:DCY:HB3	1:A:4:DCY:H	4	0.14
(1,41)	1:A:3:DPR:HB3	1:A:3:DPR:HA	4	0.14
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	19	0.14
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	19	0.14
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	19	0.14
(1,30)	1:A:1:DAL:HB1	1:A:9:DCY:HB3	7	0.14
(1,30)	1:A:1:DAL:HB2	1:A:9:DCY:HB3	7	0.14
(1,30)	1:A:1:DAL:HB3	1:A:9:DCY:HB3	7	0.14
(1,67)	1:A:8:DTY:HA	1:A:8:DTY:HD1	18	0.13
(1,50)	1:A:4:DCY:HB3	1:A:4:DCY:H	3	0.13
(1,41)	1:A:3:DPR:HB3	1:A:3:DPR:HA	7	0.13
(1,41)	1:A:3:DPR:HB3	1:A:3:DPR:HA	19	0.13
(1,29)	1:A:1:DAL:HB1	1:A:2:GLN:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:A:1:DAL:HB2	1:A:2:GLN:H	14	0.13
(1,29)	1:A:1:DAL:HB3	1:A:2:GLN:H	14	0.13
(1,70)	1:A:8:DTY:HB3	1:A:10:PRO:HD3	1	0.12
(1,59)	1:A:7:SER:HA	1:A:8:DTY:HD1	11	0.12
(1,57)	1:A:6:ASP:HB2	1:A:6:ASP:H	7	0.12
(1,57)	1:A:6:ASP:HB2	1:A:6:ASP:H	15	0.12
(1,32)	1:A:2:GLN:HE22	1:A:2:GLN:HE21	5	0.12
(1,31)	1:A:1:DAL:HB1	1:A:9:DCY:HB2	7	0.12
(1,31)	1:A:1:DAL:HB2	1:A:9:DCY:HB2	7	0.12
(1,31)	1:A:1:DAL:HB3	1:A:9:DCY:HB2	7	0.12
(1,50)	1:A:4:DCY:HB3	1:A:4:DCY:H	6	0.11
(1,41)	1:A:3:DPR:HB3	1:A:3:DPR:HA	13	0.11
(1,4)	1:A:3:DPR:HA	1:A:9:DCY:H	18	0.11
(1,32)	1:A:2:GLN:HE22	1:A:2:GLN:HE21	19	0.11
(1,11)	1:A:6:ASP:HA	1:A:6:ASP:H	17	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found