Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2N7A
BMRB ID	:	25798
Title	:	Solution structure of the human Siglec-8 lectin domain
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Deposited on	:	2015-09-07

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:

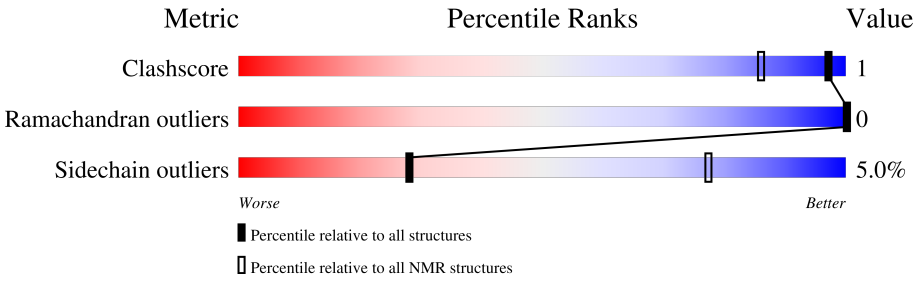
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 91%.

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	145	77% · 19%

2 Ensemble composition and analysis

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:8-A:53, A:61-A:67, A:71-A:121, A:125-A:137 (117)	0.21	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2289 atoms, of which 1114 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sialic acid-binding Ig-like lectin 8.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	145	2289	738	1114	209	224	4	0

There are 7 discrepancies between the modelled and reference sequences:

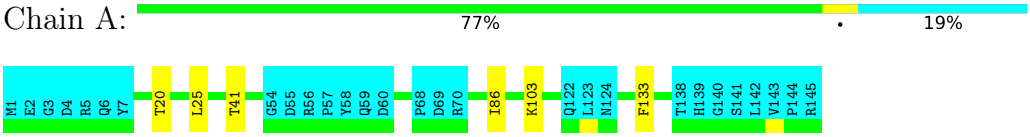
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	SER	CYS	engineered mutation	UNP Q9NYZ4
A	140	GLY	-	expression tag	UNP Q9NYZ4
A	141	SER	-	expression tag	UNP Q9NYZ4
A	142	LEU	-	expression tag	UNP Q9NYZ4
A	143	VAL	-	expression tag	UNP Q9NYZ4
A	144	PRO	-	expression tag	UNP Q9NYZ4
A	145	ARG	-	expression tag	UNP Q9NYZ4

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: Sialic acid-binding Ig-like lectin 8

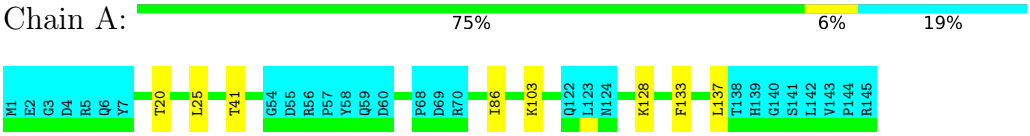


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

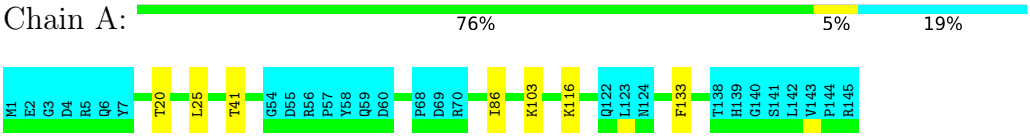
4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Sialic acid-binding Ig-like lectin 8



4.2.2 Score per residue for model 2

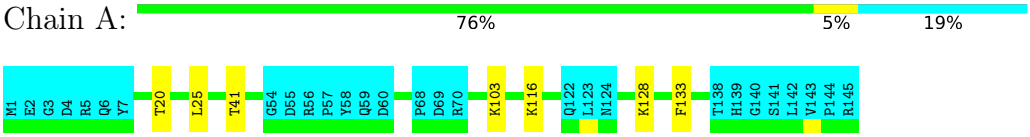
• Molecule 1: Sialic acid-binding Ig-like lectin 8



4.2.3 Score per residue for model 3

• Molecule 1: Sialic acid-binding Ig-like lectin 8

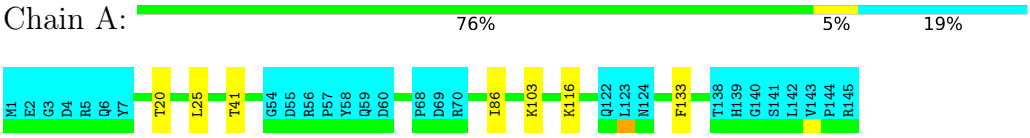
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Sialic acid-binding Ig-like lectin 8

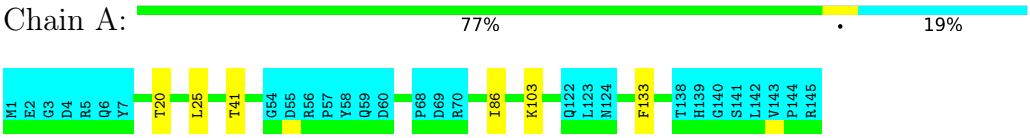
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Sialic acid-binding Ig-like lectin 8

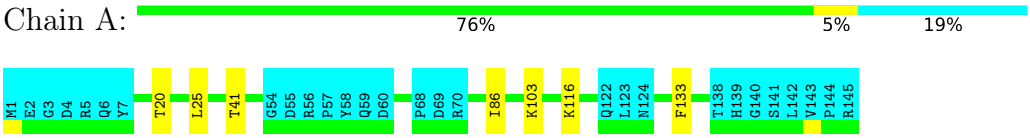
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Sialic acid-binding Ig-like lectin 8

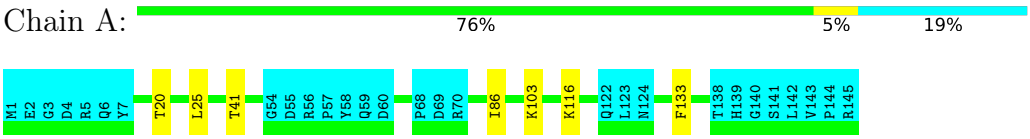
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Sialic acid-binding Ig-like lectin 8

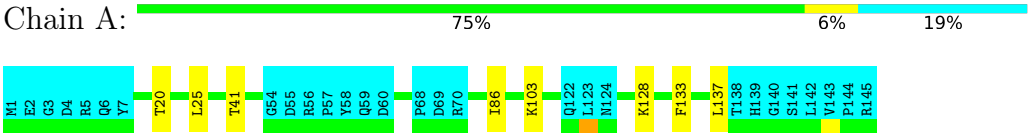
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Sialic acid-binding Ig-like lectin 8

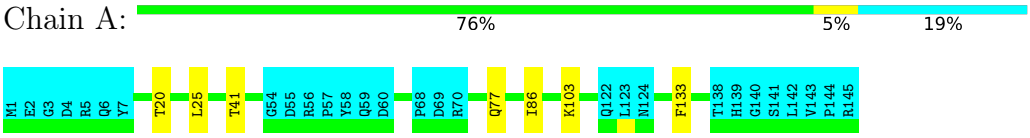
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Sialic acid-binding Ig-like lectin 8

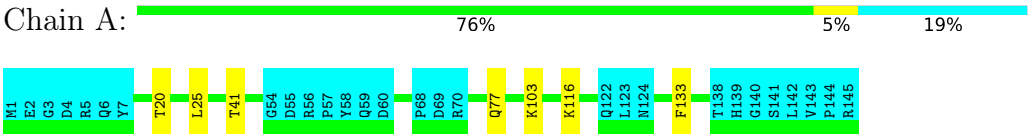
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Sialic acid-binding Ig-like lectin 8

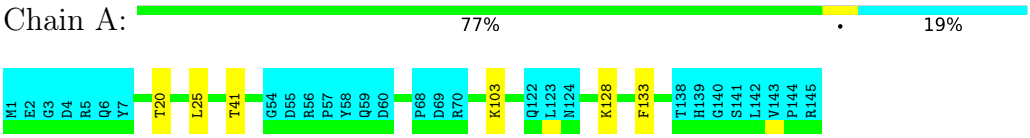
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Sialic acid-binding Ig-like lectin 8

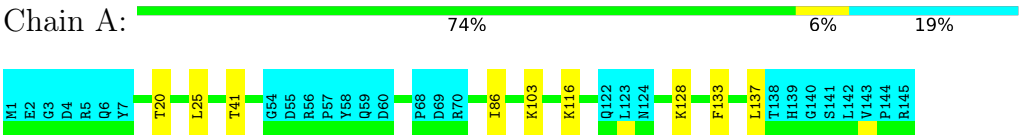
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Sialic acid-binding Ig-like lectin 8

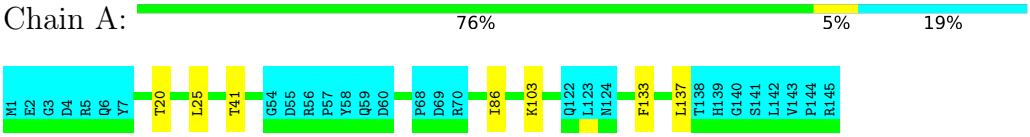
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Sialic acid-binding Ig-like lectin 8

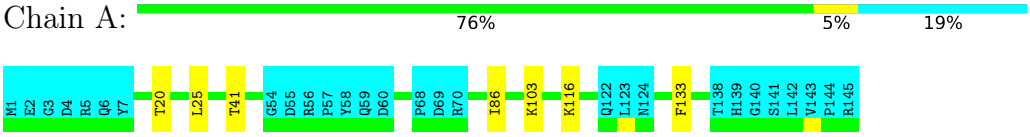
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Sialic acid-binding Ig-like lectin 8

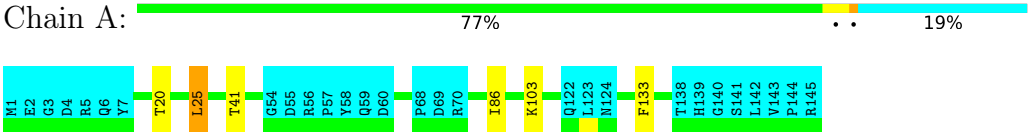
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Sialic acid-binding Ig-like lectin 8

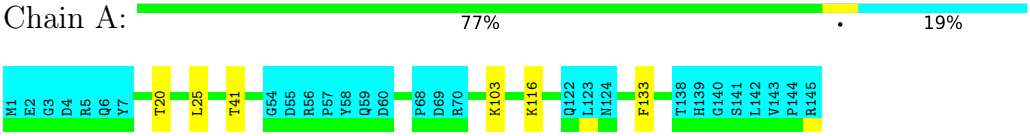
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Sialic acid-binding Ig-like lectin 8

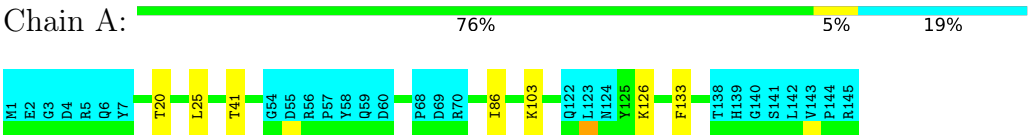
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Sialic acid-binding Ig-like lectin 8

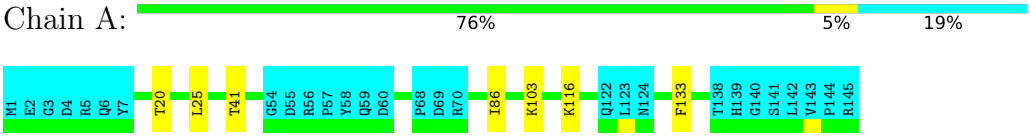
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Sialic acid-binding Ig-like lectin 8

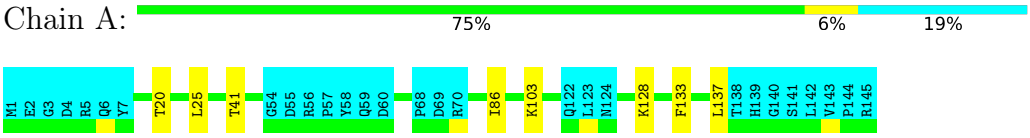
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Sialic acid-binding Ig-like lectin 8

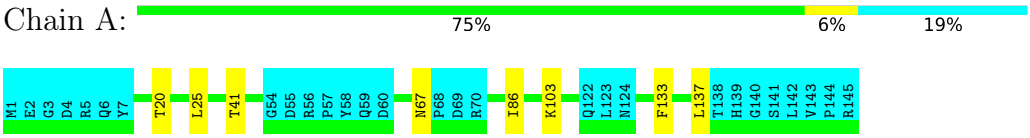
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Sialic acid-binding Ig-like lectin 8

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	structure calculation	3.0
Amber	refinement	12

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	1778
Number of shifts mapped to atoms	1778
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

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

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	944	901	901	1±0
All	All	18880	18020	18020	21

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:LYS:HE2	1:A:133:PHE:CD2	0.50	2.42	2	1
1:A:103:LYS:HE3	1:A:133:PHE:CD2	0.50	2.42	12	19
1:A:25:LEU:HD13	1:A:25:LEU:N	0.41	2.31	15	1

6.3 Torsion angles

6.3.1 Protein backbone

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	117/145 (81%)	117±1 (100±1%)	0±1 (0±1%)	0±0 (0±0%)	100	100
All	All	2340/2900 (81%)	2331 (100%)	9 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	102/127 (80%)	97±1 (95±1%)	5±1 (5±1%)	28	77
All	All	2040/2540 (80%)	1938 (95%)	102 (5%)	28	77

All 10 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	20	THR	20
1	A	25	LEU	20
1	A	41	THR	20
1	A	86	ILE	16
1	A	116	LYS	10
1	A	128	LYS	6
1	A	137	LEU	6
1	A	77	GLN	2
1	A	126	LYS	1
1	A	67	ASN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% 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

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	1778
Number of shifts mapped to atoms	1778
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	145	0.01 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	131	0.10 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	141	0.38 ± 0.13	None needed (< 0.5 ppm)
^{15}N	133	-1.17 ± 0.24	Should be applied

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 91%, i.e. 1455 atoms were assigned a chemical shift out of a possible 1592. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	577/586 (98%)	234/239 (98%)	232/234 (99%)	111/113 (98%)
Sidechain	744/830 (90%)	505/536 (94%)	223/256 (87%)	16/38 (42%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	134/176 (76%)	78/86 (91%)	52/84 (62%)	4/6 (67%)
Overall	1455/1592 (91%)	817/861 (95%)	507/574 (88%)	131/157 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1776 atoms were assigned a chemical shift out of a possible 1977. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	705/723 (98%)	286/295 (97%)	286/290 (99%)	133/138 (96%)
Sidechain	921/1053 (87%)	624/676 (92%)	276/323 (85%)	21/54 (39%)
Aromatic	150/201 (75%)	88/98 (90%)	58/96 (60%)	4/7 (57%)
Overall	1776/1977 (90%)	998/1069 (93%)	620/709 (87%)	158/199 (79%)

7.1.4 Statistically unusual chemical shifts (i)

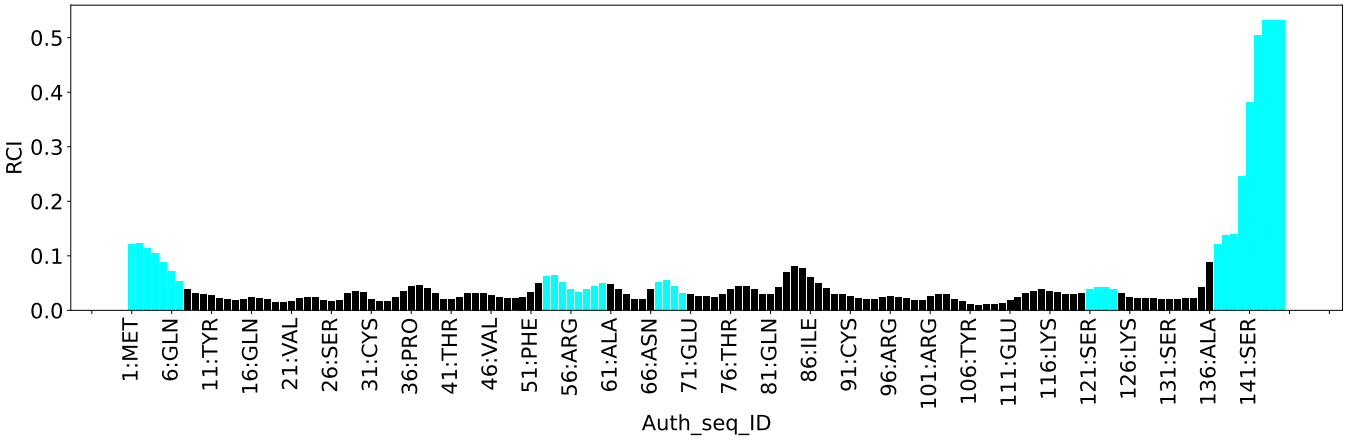
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	79	ARG	HH12	10.27	5.04 – 8.65	9.5
1	A	79	ARG	HH22	9.60	5.04 – 8.54	8.0
1	A	117	TRP	HD1	4.61	5.46 – 8.81	-7.6
1	A	117	TRP	HZ2	5.32	5.71 – 8.86	-6.2
1	A	95	ILE	HG13	-1.05	-0.82 – 3.23	-5.6
1	A	112	ARG	HD3	1.67	1.81 – 4.39	-5.6
1	A	108	PHE	HB3	1.01	1.03 – 4.85	-5.0
1	A	36	PRO	HD2	1.92	1.93 – 5.38	-5.0

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
0.0
0.1
0.2
0.3
0.4
0.5
1:MET
6:GLN
11:TYR
16:GLN
21:VAL
26:SER
31:CYS
36:PRO
41:THR
46:VAL
51:PHE
56:ARG
61:ALA
66:ASN
71:GLU
76:THR
81:GLN
86:ILE
91:CYS
96:ARG
101:ARG
106:TYR
111:GLU
116:LYS
121:SER
126:LYS
131:SER
136:ALA
141:SER
Auth_seq_ID

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	3213
Intra-residue (|i-j|=0)	544
Sequential (|i-j|=1)	804
Medium range (|i-j|>1 and |i-j|<5)	431
Long range (|i-j|≥5)	1358
Inter-chain	0
Hydrogen bond restraints	76
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	22.2
Number of long range restraints per residue[1]	9.8

[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)	5.3	0.2
0.2-0.5 (Medium)	1.1	0.36
>0.5 (Large)	3.8	2.26

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)

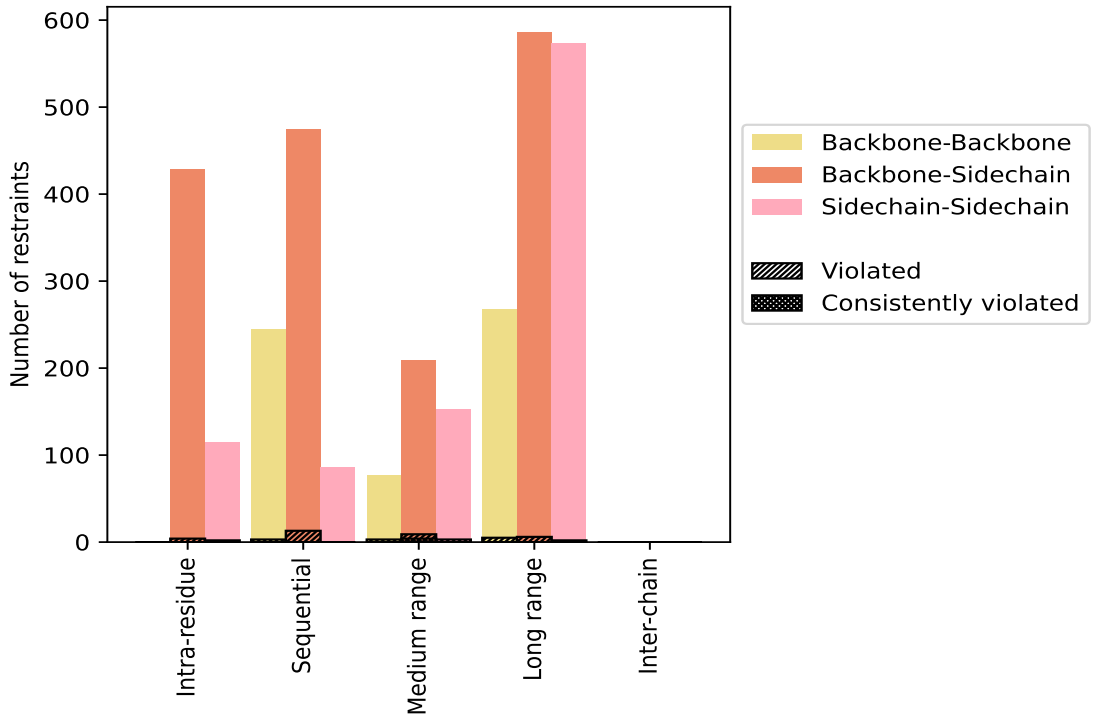
9.1 Summary of distance violations (i)

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)	544	16.9	6	1.1	0.2	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	428	13.3	4	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	115	3.6	2	1.7	0.1	0	0.0	0.0
Sequential (|i-j|=1)	804	25.0	16	2.0	0.5	0	0.0	0.0
Backbone-Backbone	244	7.6	3	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	474	14.8	13	2.7	0.4	0	0.0	0.0
Sidechain-Sidechain	86	2.7	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	431	13.4	15	3.5	0.5	4	0.9	0.1
Backbone-Backbone	71	2.2	3	4.2	0.1	0	0.0	0.0
Backbone-Sidechain	207	6.4	9	4.3	0.3	4	1.9	0.1
Sidechain-Sidechain	153	4.8	3	2.0	0.1	0	0.0	0.0
Long range (|i-j|≥5)	1358	42.3	13	1.0	0.4	0	0.0	0.0
Backbone-Backbone	201	6.3	5	2.5	0.2	0	0.0	0.0
Backbone-Sidechain	584	18.2	6	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	573	17.8	2	0.3	0.1	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	76	2.4	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	3213	100.0	50	1.6	1.6	4	0.1	0.1
Backbone-Backbone	589	18.3	11	1.9	0.3	0	0.0	0.0
Backbone-Sidechain	1697	52.8	32	1.9	1.0	4	0.2	0.1
Sidechain-Sidechain	927	28.9	7	0.8	0.2	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	1	2	5	2	0	10	0.74	2.1	0.76	0.23
2	1	2	4	3	0	10	0.66	1.78	0.62	0.24
3	2	3	6	3	0	14	0.5	1.82	0.58	0.15
4	1	4	4	1	0	10	0.57	1.59	0.54	0.2
5	0	2	8	3	0	13	0.61	2.26	0.76	0.16
6	1	3	5	0	0	9	0.62	1.5	0.53	0.21
7	0	2	5	1	0	8	0.74	1.74	0.63	0.68
8	2	3	4	3	0	12	0.37	1.73	0.52	0.13
9	1	4	4	0	0	9	0.6	1.62	0.55	0.2
10	0	2	5	0	0	7	0.84	1.77	0.62	1.12
11	2	4	6	1	0	13	0.47	1.55	0.49	0.19

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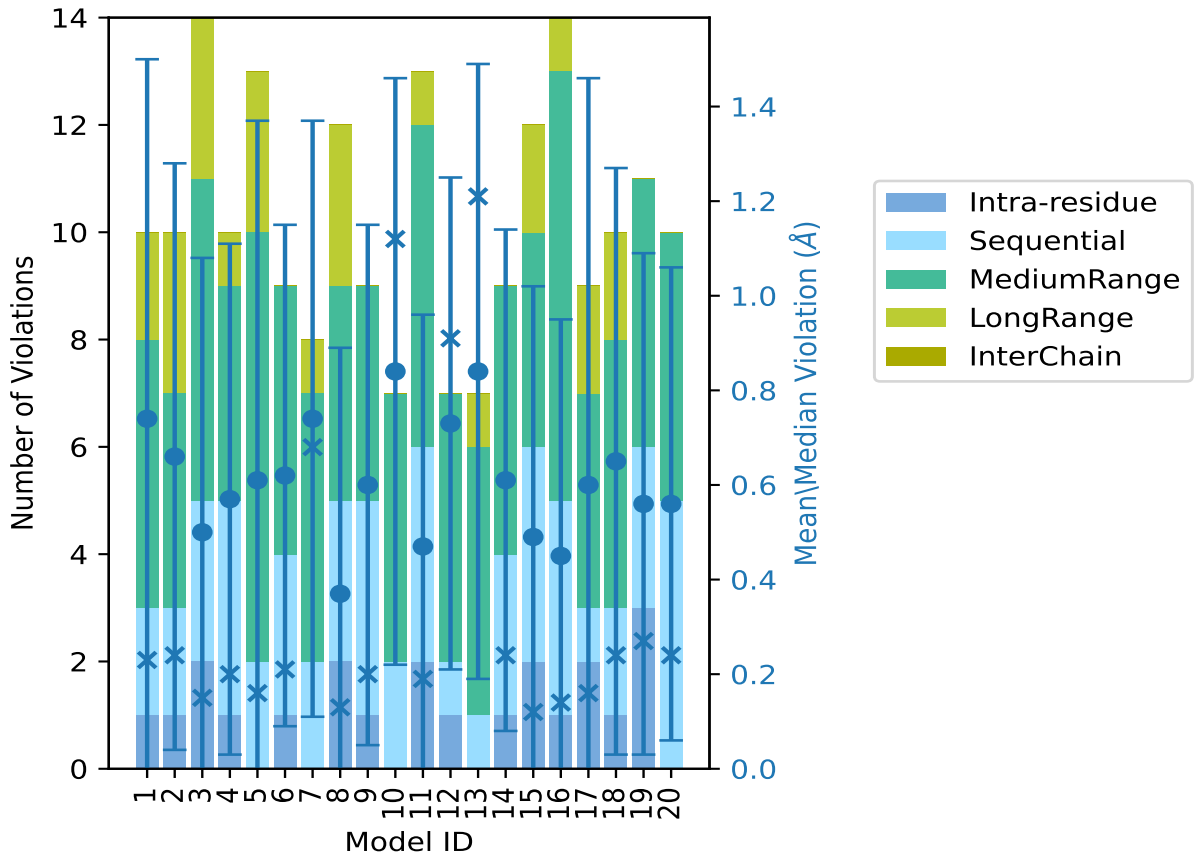
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	1	5	0	0	7	0.73	1.54	0.52	0.91
13	0	1	5	1	0	7	0.84	1.77	0.65	1.21
14	1	3	5	0	0	9	0.61	1.56	0.53	0.24
15	2	4	4	2	0	12	0.49	1.57	0.53	0.12
16	1	4	8	1	0	14	0.45	1.56	0.5	0.14
17	2	1	4	2	0	9	0.6	2.26	0.86	0.16
18	1	2	5	2	0	10	0.65	1.76	0.62	0.24
19	3	3	5	0	0	11	0.56	1.61	0.53	0.27
20	0	5	5	0	0	10	0.56	1.46	0.5	0.24

[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

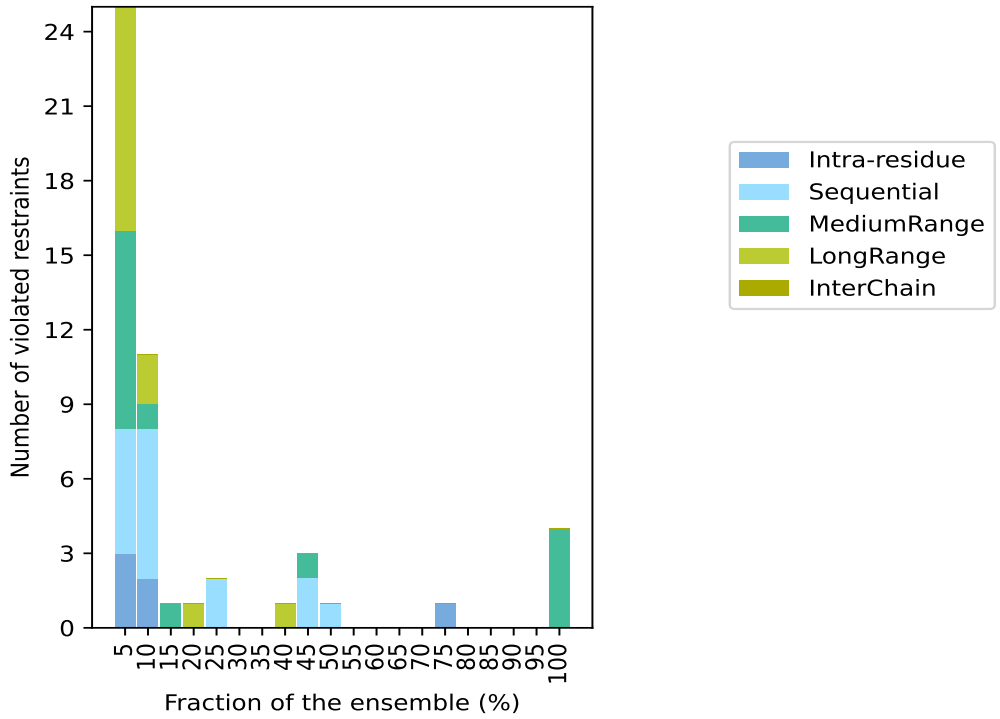
9.3 Distance violation statistics for the ensemble (i)

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, 3087(IR:538, SQ:788, MR:416, LR:1345, 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	5	8	9	0	25	1	5.0
2	6	1	2	0	11	2	10.0
0	0	1	0	0	1	3	15.0
0	0	0	1	0	1	4	20.0
0	2	0	0	0	2	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	1	0	1	8	40.0
0	2	1	0	0	3	9	45.0
0	1	0	0	0	1	10	50.0
0	0	0	0	0	0	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
1	0	0	0	0	1	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
0	0	4	0	0	4	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

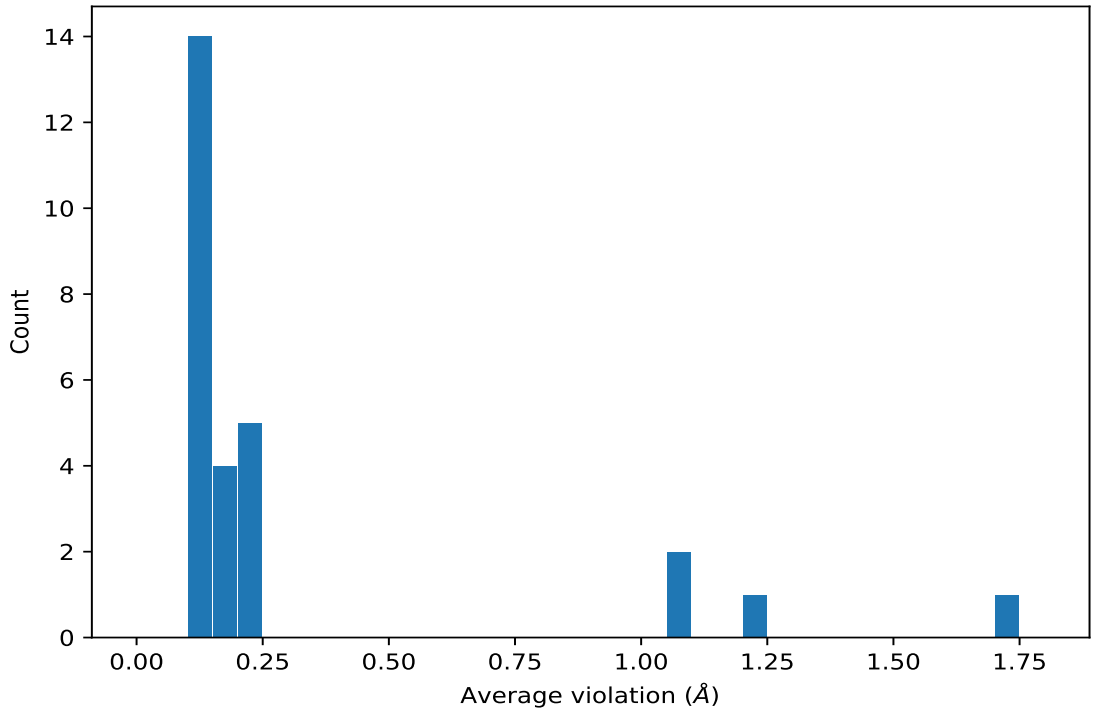
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	20	1.73	0.23	1.68
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	20	1.24	0.42	1.12
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	20	1.06	0.3	1.15
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	20	1.05	0.31	1.16
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	15	0.21	0.05	0.24
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	15	0.21	0.05	0.24
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	15	0.21	0.05	0.24
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	10	0.13	0.01	0.13
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	9	0.19	0.04	0.21
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	9	0.12	0.02	0.11
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	9	0.12	0.01	0.12
(1,2757)	1:A:53:ALA:H	1:A:107:PHE:H	8	0.14	0.03	0.12
(1,132)	1:A:96:ARG:H	1:A:97:ASP:HB2	5	0.18	0.02	0.18
(1,1707)	1:A:69:ASP:HB3	1:A:70:ARG:H	5	0.15	0.04	0.12
(2,74)	1:A:117:TRP:NE1	1:A:125:TYR:OH	4	0.12	0.01	0.12
(1,2649)	1:A:28:HIS:HD2	1:A:30:PRO:HG3	3	0.16	0.01	0.15

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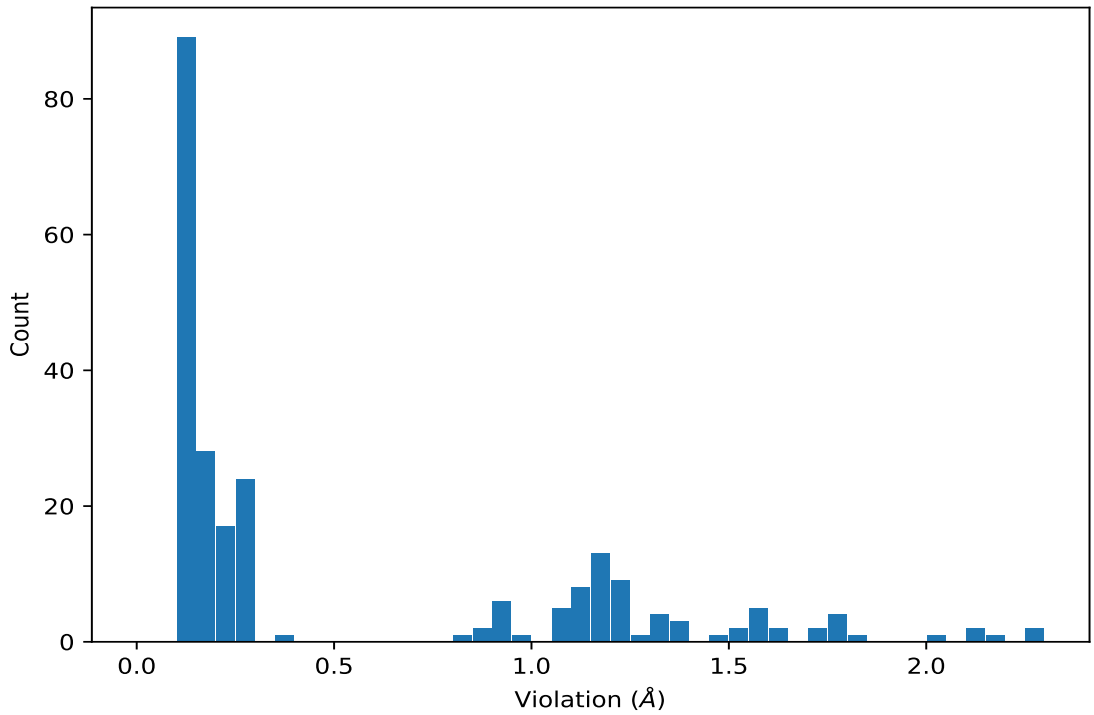
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,734)	1:A:5:ARG:H	1:A:6:GLN:HA	2	0.24	0.02	0.24
(1,1667)	1:A:4:ASP:H	1:A:5:ARG:H	2	0.21	0.01	0.21
(1,722)	1:A:43:SER:H	1:A:43:SER:HB2	2	0.16	0.02	0.16
(1,858)	1:A:5:ARG:H	1:A:6:GLN:HB3	2	0.14	0.02	0.14
(1,1521)	1:A:124:ASN:H	1:A:125:TYR:H	2	0.12	0.02	0.12
(1,853)	1:A:52:ARG:HB2	1:A:55:ASP:H	2	0.12	0.0	0.12
(1,1428)	1:A:71:GLU:HG2	1:A:72:VAL:H	2	0.12	0.0	0.12
(1,2415)	1:A:122:GLN:H	1:A:127:THR:H	2	0.12	0.0	0.12
(1,2670)	1:A:32:SER:HB3	1:A:91:CYS:H	2	0.12	0.0	0.12
(1,1499)	1:A:112:ARG:HB3	1:A:113:GLY:H	2	0.11	0.0	0.11
(1,2806)	1:A:6:GLN:HA	1:A:6:GLN:HE21	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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)
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	5	2.26
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	17	2.26
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	5	2.16
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	17	2.13
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	1	2.1
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	1	2.01
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	3	1.82
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	2	1.78
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	10	1.77
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	13	1.77
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	18	1.76
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	7	1.74
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	8	1.73
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	9	1.62
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	19	1.61
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	4	1.59
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	15	1.57
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	14	1.56
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	16	1.56
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	11	1.55
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	12	1.54
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	6	1.5
(2,33)	1:A:52:ARG:H	1:A:55:ASP:OD1	20	1.46
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	3	1.38
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	10	1.37
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	2	1.36
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	7	1.33
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	18	1.33
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	13	1.32
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	8	1.3
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	18	1.25
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	18	1.23
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	2	1.21
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	6	1.21
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	13	1.21
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	2	1.21
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	13	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	3	1.2
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	6	1.2
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	19	1.2
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	16	1.19
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	16	1.19
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	3	1.18
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	1	1.17
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	15	1.17
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	19	1.17
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	1	1.17
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	4	1.16
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	20	1.16
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	4	1.16
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	7	1.15
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	15	1.15
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	20	1.15
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	7	1.14
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	11	1.14
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	10	1.13
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	10	1.12
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	5	1.11
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	11	1.11
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	14	1.1
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	5	1.1
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	9	1.09
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	14	1.09
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	9	1.08
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	12	1.07
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	12	1.05
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	19	0.95
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	9	0.94
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	4	0.93
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	14	0.93
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	15	0.92
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	12	0.91
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	11	0.9
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	16	0.89
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	6	0.86
(2,34)	1:A:52:ARG:N	1:A:55:ASP:OD1	20	0.82
(1,470)	1:A:6:GLN:HG3	1:A:6:GLN:HE21	19	0.36
(1,582)	1:A:59:GLN:HB2	1:A:60:ASP:H	16	0.27
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	16	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	16	0.27
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	16	0.27
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	19	0.27
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	19	0.27
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	19	0.27
(1,734)	1:A:5:ARG:H	1:A:6:GLN:HA	20	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	1	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	1	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	1	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	2	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	2	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	2	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	18	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	18	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	18	0.26
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	11	0.25
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	11	0.25
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	11	0.25
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	12	0.25
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	12	0.25
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	12	0.25
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	10	0.25
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	14	0.24
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	14	0.24
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	14	0.24
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	5	0.24
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	3	0.23
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	3	0.23
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	3	0.23
(1,734)	1:A:5:ARG:H	1:A:6:GLN:HA	2	0.22
(1,1707)	1:A:69:ASP:HB3	1:A:70:ARG:H	11	0.22
(1,1667)	1:A:4:ASP:H	1:A:5:ARG:H	18	0.22
(1,132)	1:A:96:ARG:H	1:A:97:ASP:HB2	4	0.21
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	6	0.21
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	7	0.21
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	20	0.21
(1,471)	1:A:70:ARG:HA	1:A:71:GLU:HG2	9	0.2
(1,2757)	1:A:53:ALA:H	1:A:107:PHE:H	1	0.2
(1,1667)	1:A:4:ASP:H	1:A:5:ARG:H	3	0.2
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	8	0.19
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	8	0.19
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1427)	1:A:70:ARG:H	1:A:70:ARG:HB3	11	0.19
(1,132)	1:A:96:ARG:H	1:A:97:ASP:HB2	1	0.19
(1,722)	1:A:43:SER:H	1:A:43:SER:HB2	15	0.18
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	4	0.18
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	4	0.18
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	4	0.18
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	17	0.18
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	17	0.18
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	17	0.18
(1,132)	1:A:96:ARG:H	1:A:97:ASP:HB2	6	0.18
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	8	0.18
(1,2810)	1:A:6:GLN:HG3	1:A:6:GLN:HE22	19	0.17
(1,2649)	1:A:28:HIS:HD2	1:A:30:PRO:HG3	14	0.17
(1,1707)	1:A:69:ASP:HB3	1:A:70:ARG:H	20	0.17
(1,132)	1:A:96:ARG:H	1:A:97:ASP:HB2	2	0.17
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	8	0.16
(2,55)	1:A:99:ARG:H	1:A:102:ASP:OD1	17	0.16
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	6	0.16
(1,2757)	1:A:53:ALA:H	1:A:107:PHE:H	5	0.16
(1,1971)	1:A:16:GLN:HE21	1:A:20:THR:H	5	0.16
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	17	0.16
(1,858)	1:A:5:ARG:H	1:A:6:GLN:HB3	5	0.15
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	12	0.15
(1,2649)	1:A:28:HIS:HD2	1:A:30:PRO:HG3	3	0.15
(1,2649)	1:A:28:HIS:HD2	1:A:30:PRO:HG3	20	0.15
(1,829)	1:A:15:VAL:H	1:A:128:LYS:HE2	16	0.14
(1,829)	1:A:15:VAL:H	1:A:128:LYS:HE3	16	0.14
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	9	0.14
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	16	0.14
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	20	0.14
(1,2757)	1:A:53:ALA:H	1:A:107:PHE:H	18	0.14
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	3	0.14
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	11	0.14
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	6	0.14
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	6	0.14
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	6	0.14
(1,1581)	1:A:19:VAL:H	1:A:130:LEU:HA	5	0.14
(1,1521)	1:A:124:ASN:H	1:A:125:TYR:H	9	0.14
(1,132)	1:A:96:ARG:H	1:A:97:ASP:HB2	8	0.14
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	4	0.14
(2,74)	1:A:117:TRP:NE1	1:A:125:TYR:OH	4	0.13
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,861)	1:A:67:ASN:HD22	1:A:70:ARG:HB3	11	0.13
(1,722)	1:A:43:SER:H	1:A:43:SER:HB2	3	0.13
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	11	0.13
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	14	0.13
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	11	0.13
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	14	0.13
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	19	0.13
(1,2757)	1:A:53:ALA:H	1:A:107:PHE:H	17	0.13
(1,2698)	1:A:41:THR:H	1:A:114:SER:H	15	0.13
(2,74)	1:A:117:TRP:NE1	1:A:125:TYR:OH	3	0.12
(2,56)	1:A:99:ARG:N	1:A:102:ASP:OD1	8	0.12
(1,858)	1:A:5:ARG:H	1:A:6:GLN:HB3	16	0.12
(1,853)	1:A:52:ARG:HB2	1:A:55:ASP:H	16	0.12
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	10	0.12
(1,436)	1:A:7:TYR:HA	1:A:117:TRP:HH2	13	0.12
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	15	0.12
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	18	0.12
(1,2890)	1:A:8:GLY:HA2	1:A:117:TRP:HE1	5	0.12
(1,2775)	1:A:5:ARG:HB3	1:A:9:ASP:HB2	16	0.12
(1,2757)	1:A:53:ALA:H	1:A:107:PHE:H	2	0.12
(1,2670)	1:A:32:SER:HB3	1:A:91:CYS:H	18	0.12
(1,2415)	1:A:122:GLN:H	1:A:127:THR:H	15	0.12
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	5	0.12
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	6	0.12
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	10	0.12
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	9	0.12
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	9	0.12
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	9	0.12
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD21	15	0.12
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD22	15	0.12
(1,1874)	1:A:123:LEU:H	1:A:123:LEU:HD23	15	0.12
(1,1707)	1:A:69:ASP:HB3	1:A:70:ARG:H	14	0.12
(1,1428)	1:A:71:GLU:HG2	1:A:72:VAL:H	19	0.12
(1,1381)	1:A:40:TRP:H	1:A:114:SER:H	8	0.12
(1,1148)	1:A:123:LEU:HB2	1:A:124:ASN:H	15	0.12
(2,74)	1:A:117:TRP:NE1	1:A:125:TYR:OH	8	0.11
(2,74)	1:A:117:TRP:NE1	1:A:125:TYR:OH	17	0.11
(1,956)	1:A:37:GLN:HA	1:A:40:TRP:H	7	0.11
(1,853)	1:A:52:ARG:HB2	1:A:55:ASP:H	18	0.11
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	3	0.11
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	8	0.11
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	15	0.11
(1,666)	1:A:59:GLN:H	1:A:60:ASP:HB3	19	0.11
(1,596)	1:A:103:LYS:HG2	1:A:133:PHE:HA	2	0.11
(1,503)	1:A:41:THR:HB	1:A:43:SER:H	12	0.11
(1,479)	1:A:101:ARG:HB3	1:A:102:ASP:H	13	0.11
(1,318)	1:A:50:TRP:H	1:A:51:PHE:HZ	4	0.11
(1,2806)	1:A:6:GLN:HA	1:A:6:GLN:HE21	8	0.11
(1,2806)	1:A:6:GLN:HA	1:A:6:GLN:HE21	17	0.11
(1,2757)	1:A:53:ALA:H	1:A:107:PHE:H	3	0.11
(1,2757)	1:A:53:ALA:H	1:A:107:PHE:H	7	0.11
(1,2757)	1:A:53:ALA:H	1:A:107:PHE:H	8	0.11
(1,2686)	1:A:38:ASP:H	1:A:40:TRP:HD1	16	0.11
(1,2670)	1:A:32:SER:HB3	1:A:91:CYS:H	1	0.11
(1,2415)	1:A:122:GLN:H	1:A:127:THR:H	2	0.11
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	1	0.11
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	13	0.11
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	16	0.11
(1,2016)	1:A:22:GLN:H	1:A:25:LEU:HG	19	0.11
(1,1968)	1:A:16:GLN:HB3	1:A:17:GLU:H	11	0.11
(1,1950)	1:A:15:VAL:HA	1:A:17:GLU:H	5	0.11
(1,186)	1:A:79:ARG:HB3	1:A:97:ASP:HB3	3	0.11
(1,1707)	1:A:69:ASP:HB3	1:A:70:ARG:H	1	0.11
(1,1707)	1:A:69:ASP:HB3	1:A:70:ARG:H	4	0.11
(1,1689)	1:A:5:ARG:HG2	1:A:6:GLN:HA	3	0.11
(1,1521)	1:A:124:ASN:H	1:A:125:TYR:H	15	0.11
(1,1499)	1:A:112:ARG:HB3	1:A:113:GLY:H	7	0.11
(1,1499)	1:A:112:ARG:HB3	1:A:113:GLY:H	16	0.11
(1,1434)	1:A:7:TYR:H	1:A:124:ASN:HD22	11	0.11
(1,1428)	1:A:71:GLU:HG2	1:A:72:VAL:H	20	0.11
(1,1426)	1:A:6:GLN:H	1:A:9:ASP:H	5	0.11

10 Dihedral-angle violation analysis (i)

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