Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 08:55 PM EDT

PDB ID	:	2MZS
BMRB ID	:	25498
Title	:	NMR structure of the RRM2 domain of Hrb1
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Deposited on	:	2015-02-23

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:

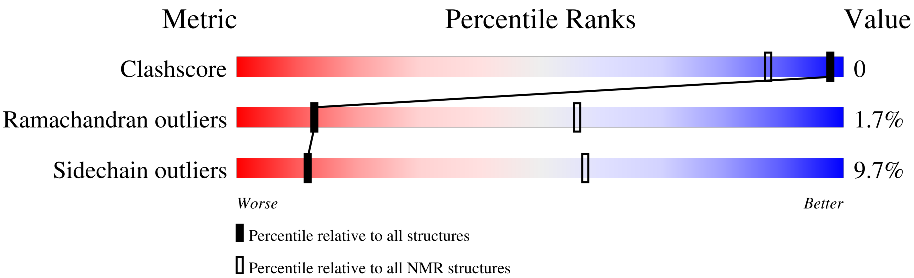
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 94%.

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	99	 71% 5% 24%

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:262-A:336 (75)	0.87	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 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1459 atoms, of which 707 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein HRB1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	99	1459	463	707	126	161	2	0

There are 2 discrepancies between the modelled and reference sequences:

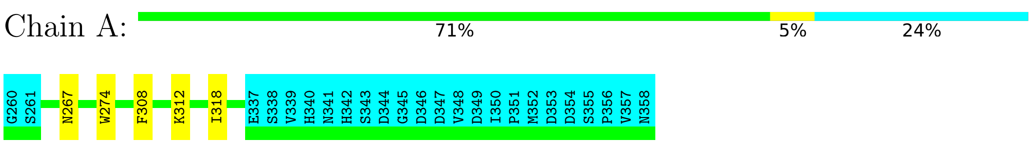
Chain	Residue	Modelled	Actual	Comment	Reference
A	260	GLY	-	expression tag	UNP P38922
A	261	SER	-	expression tag	UNP P38922

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: Protein HRB1

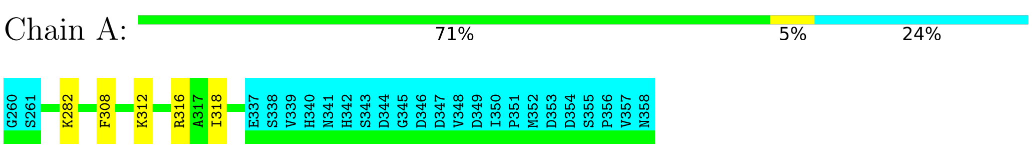


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

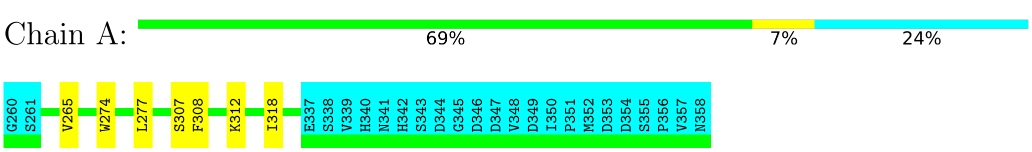
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Protein HRB1



4.2.2 Score per residue for model 2

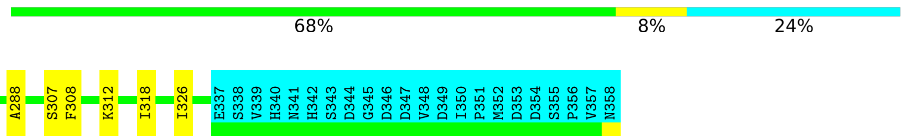
- Molecule 1: Protein HRB1



4.2.3 Score per residue for model 3

• Molecule 1: Protein HRB1

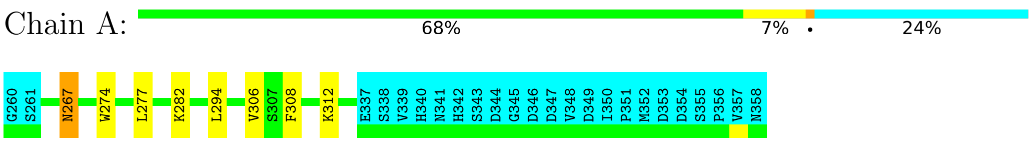
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Protein HRB1

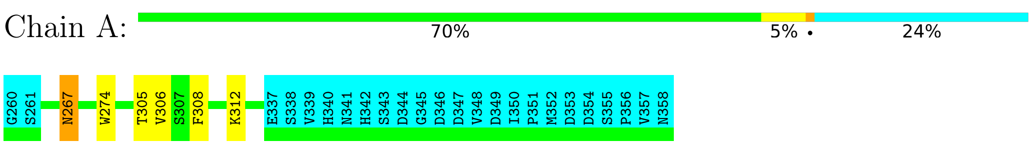
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Protein HRB1

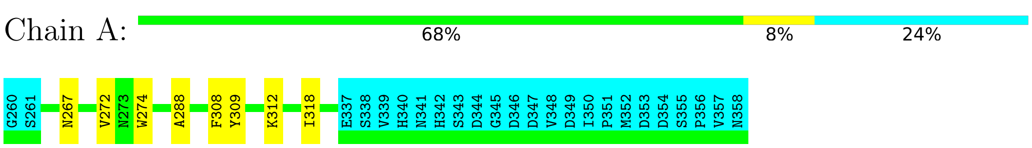
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Protein HRB1

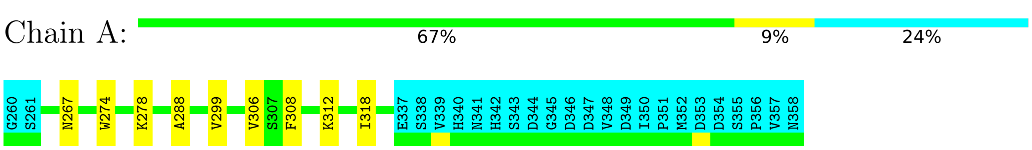
Chain A:



4.2.7 Score per residue for model 7

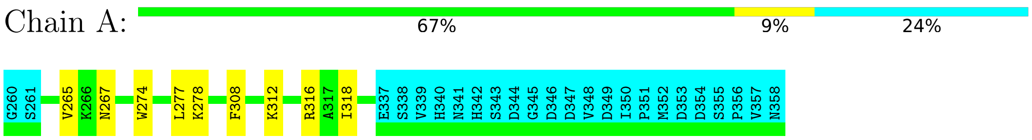
• Molecule 1: Protein HRB1

Chain A:



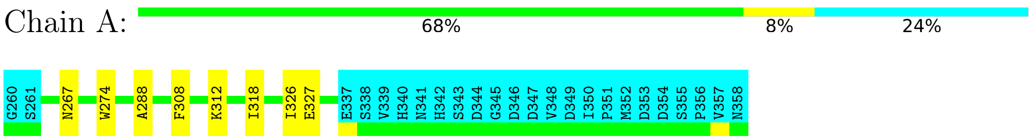
4.2.8 Score per residue for model 8

- Molecule 1: Protein HRB1



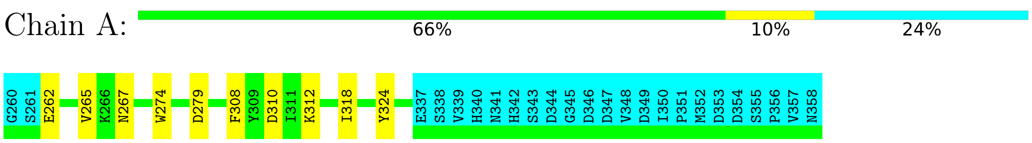
4.2.9 Score per residue for model 9

- Molecule 1: Protein HRB1



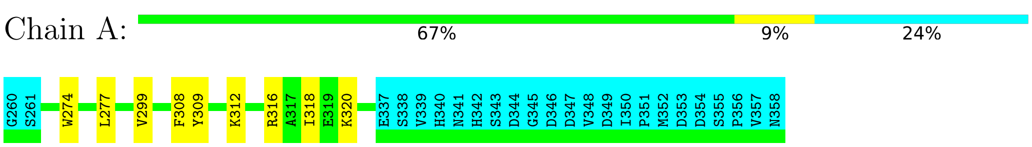
4.2.10 Score per residue for model 10

- Molecule 1: Protein HRB1



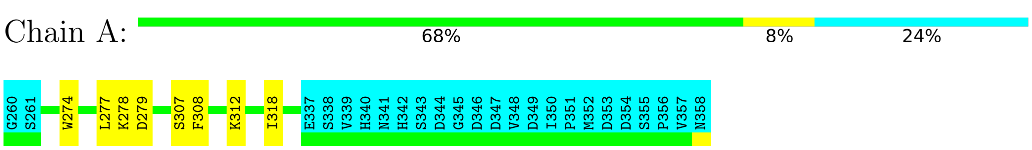
4.2.11 Score per residue for model 11

- Molecule 1: Protein HRB1



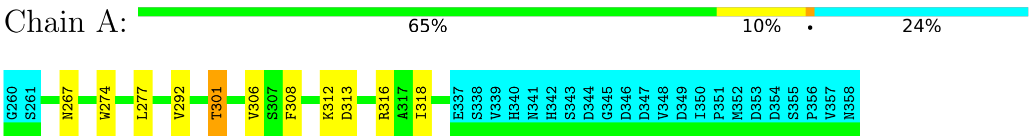
4.2.12 Score per residue for model 12

- Molecule 1: Protein HRB1



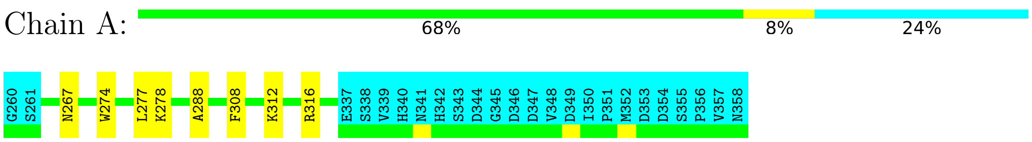
4.2.13 Score per residue for model 13

• Molecule 1: Protein HRB1



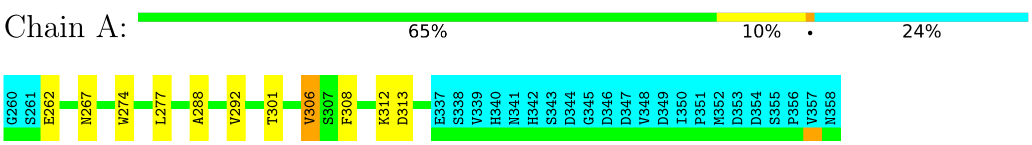
4.2.14 Score per residue for model 14

• Molecule 1: Protein HRB1



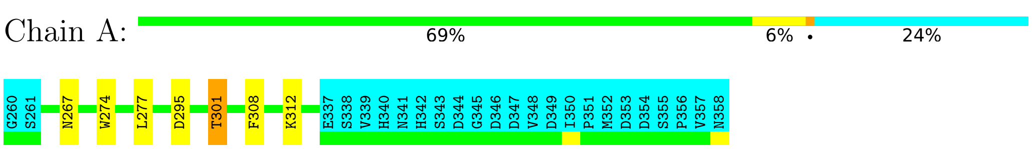
4.2.15 Score per residue for model 15

• Molecule 1: Protein HRB1



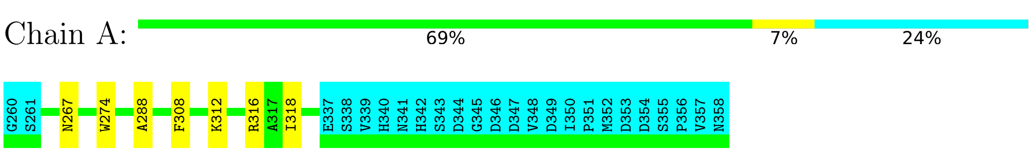
4.2.16 Score per residue for model 16

• Molecule 1: Protein HRB1



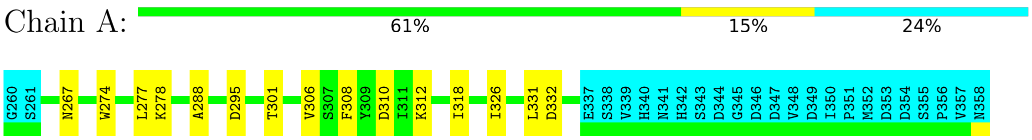
4.2.17 Score per residue for model 17

• Molecule 1: Protein HRB1



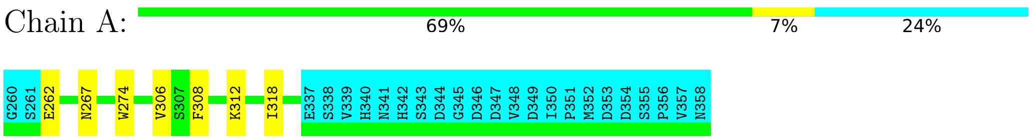
4.2.18 Score per residue for model 18

- Molecule 1: Protein HRB1



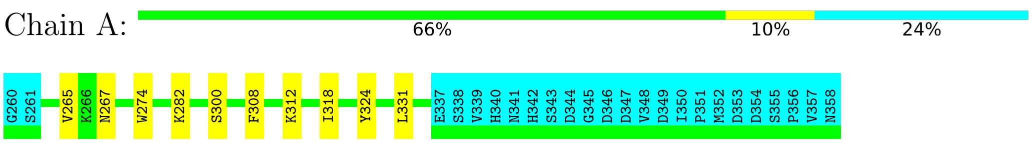
4.2.19 Score per residue for model 19

- Molecule 1: Protein HRB1



4.2.20 Score per residue for model 20

- Molecule 1: Protein HRB1



5 Refinement protocol and experimental data overview (i)

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	**Classification**	**Version**
CYANA	structure solution	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1146
Number of shifts mapped to atoms	1146
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality (i)

6.1 Standard geometry (i)

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	0.71±0.01	0±0/585 (0.0± 0.0%)	0.95±0.02	0±1/792 (0.0± 0.1%)
All	All	0.71	0/11700 (0.0%)	0.95	6/15840 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.6±0.7
All	All	0	11

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	316	ARG	NE-CZ-NH1	5.91	123.26	120.30	8	5
1	A	316	ARG	NE-CZ-NH2	-5.13	117.74	120.30	8	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	265	VAL	Peptide	4
1	A	307	SER	Peptide	3
1	A	267	ASN	Peptide	2
1	A	309	TYR	Peptide	1
1	A	331	LEU	Peptide	1

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	575	562	562	0±1
All	All	11500	11240	11240	9

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:277:LEU:HD21	1:A:306:VAL:HG12	0.61	1.72	18	2
1:A:277:LEU:HD21	1:A:306:VAL:CG1	0.48	2.38	13	3
1:A:277:LEU:HD23	1:A:277:LEU:C	0.44	2.33	2	4

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	75/99 (76%)	66±3 (88±4%)	7±3 (10±3%)	1±1 (2±1%)	13	56
All	All	1500/1980 (76%)	1326 (88%)	148 (10%)	26 (2%)	13	56

All 4 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	267	ASN	14
1	A	288	ALA	8
1	A	301	THR	3
1	A	299	VAL	1

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	63/85 (74%)	57±2 (90±3%)	6±2 (10±3%)	12	57
All	All	1260/1700 (74%)	1138 (90%)	122 (10%)	12	57

All 29 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	308	PHE	20
1	A	312	LYS	20
1	A	274	TRP	19
1	A	318	ILE	15
1	A	278	LYS	5
1	A	306	VAL	4
1	A	282	LYS	3
1	A	326	ILE	3
1	A	262	GLU	3
1	A	301	THR	3
1	A	267	ASN	2
1	A	277	LEU	2
1	A	279	ASP	2
1	A	310	ASP	2
1	A	324	TYR	2
1	A	292	VAL	2
1	A	313	ASP	2
1	A	295	ASP	2
1	A	294	LEU	1
1	A	305	THR	1
1	A	272	VAL	1
1	A	309	TYR	1
1	A	327	GLU	1
1	A	299	VAL	1
1	A	320	LYS	1
1	A	316	ARG	1
1	A	331	LEU	1
1	A	332	ASP	1
1	A	300	SER	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 (i)

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1146
Number of shifts mapped to atoms	1146
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	98	-0.25 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	90	0.13 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	91	0.01 ± 0.12	None needed (< 0.5 ppm)
^{15}N	92	-0.26 ± 0.39	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 94%, i.e. 915 atoms were assigned a chemical shift out of a possible 976. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	376/380 (99%)	155/156 (99%)	148/150 (99%)	73/74 (99%)
Sidechain	477/523 (91%)	321/339 (95%)	149/168 (89%)	7/16 (44%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	62/73 (85%)	32/36 (89%)	29/34 (85%)	1/3 (33%)
Overall	915/976 (94%)	508/531 (96%)	326/352 (93%)	81/93 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1146 atoms were assigned a chemical shift out of a possible 1242. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	479/498 (96%)	198/204 (97%)	189/198 (95%)	92/96 (96%)
Sidechain	597/657 (91%)	401/424 (95%)	187/215 (87%)	9/18 (50%)
Aromatic	70/87 (80%)	36/44 (82%)	33/38 (87%)	1/5 (20%)
Overall	1146/1242 (92%)	635/672 (94%)	409/451 (91%)	102/119 (86%)

7.1.4 Statistically unusual chemical shifts (i)

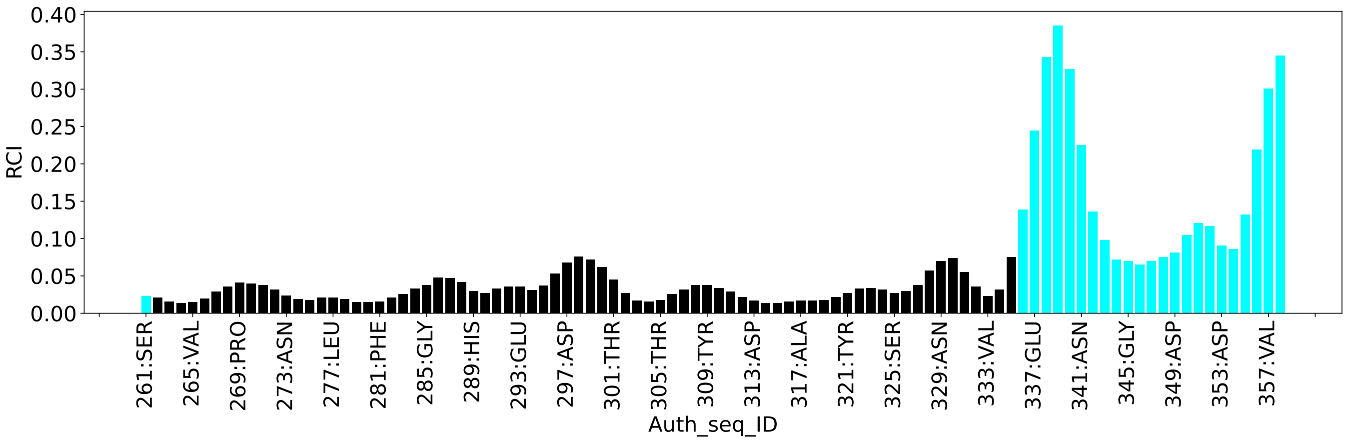
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	275	GLN	HG3	0.86	0.91 – 3.68	-5.2

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
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
261:SER
265:VAL
269:PRO
273:ASN
277:LEU
281:PHE
285:GLY
289:HIS
293:GLU
297:ASP
301:THR
305:THR
309:TYR
313:ASP
317:ALA
321:TYR
325:SER
329:ASN
333:VAL
337:GLU
341:ASN
345:GLY
349:ASP
353:ASP
357:VAL
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	627
Intra-residue (|i-j|=0)	163
Sequential (|i-j|=1)	127
Medium range (|i-j|>1 and |i-j|<5)	114
Long range (|i-j|≥5)	223
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	6.3
Number of long range restraints per residue[1]	2.3

[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)	1.4	0.18
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

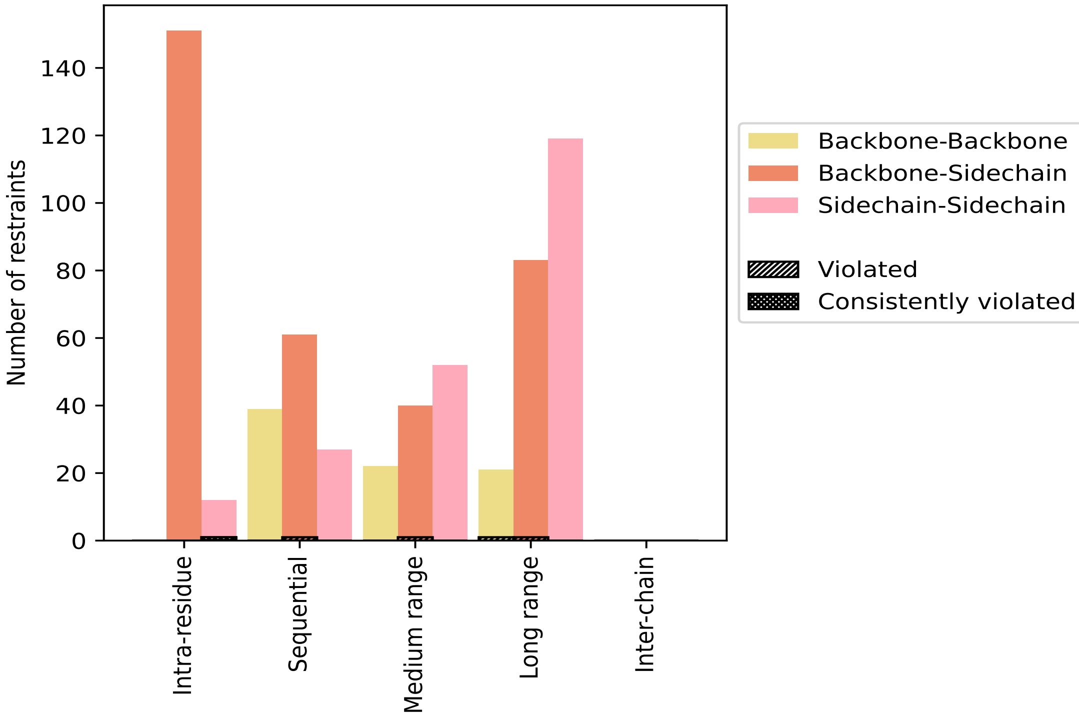
9.1 Summary of distance violations (i)

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)	163	26.0	1	0.6	0.2	1	0.6	0.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	151	24.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	12	1.9	1	8.3	0.2	1	8.3	0.2
Sequential (|i-j|=1)	127	20.3	1	0.8	0.2	0	0.0	0.0
Backbone-Backbone	39	6.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	61	9.7	1	1.6	0.2	0	0.0	0.0
Sidechain-Sidechain	27	4.3	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	114	18.2	1	0.9	0.2	0	0.0	0.0
Backbone-Backbone	22	3.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	40	6.4	1	2.5	0.2	0	0.0	0.0
Sidechain-Sidechain	52	8.3	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	223	35.6	2	0.9	0.3	0	0.0	0.0
Backbone-Backbone	21	3.3	1	4.8	0.2	0	0.0	0.0
Backbone-Sidechain	83	13.2	1	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	119	19.0	0	0.0	0.0	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	627	100.0	5	0.8	0.8	1	0.2	0.2
Backbone-Backbone	82	13.1	1	1.2	0.2	0	0.0	0.0
Backbone-Sidechain	335	53.4	3	0.9	0.5	0	0.0	0.0
Sidechain-Sidechain	210	33.5	1	0.5	0.2	1	0.5	0.2

[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	1	0	0	0	0	1	0.18	0.18	0.0	0.18
2	1	0	0	0	0	1	0.18	0.18	0.0	0.18
3	1	0	0	0	0	1	0.18	0.18	0.0	0.18
4	1	0	1	0	0	2	0.16	0.18	0.02	0.16
5	1	0	1	0	0	2	0.16	0.18	0.02	0.16
6	1	0	0	0	0	1	0.17	0.17	0.0	0.17
7	1	0	0	0	0	1	0.17	0.17	0.0	0.17
8	1	0	0	0	0	1	0.18	0.18	0.0	0.18
9	1	0	0	0	0	1	0.18	0.18	0.0	0.18
10	1	0	0	0	0	1	0.18	0.18	0.0	0.18
11	1	1	0	0	0	2	0.14	0.18	0.03	0.14

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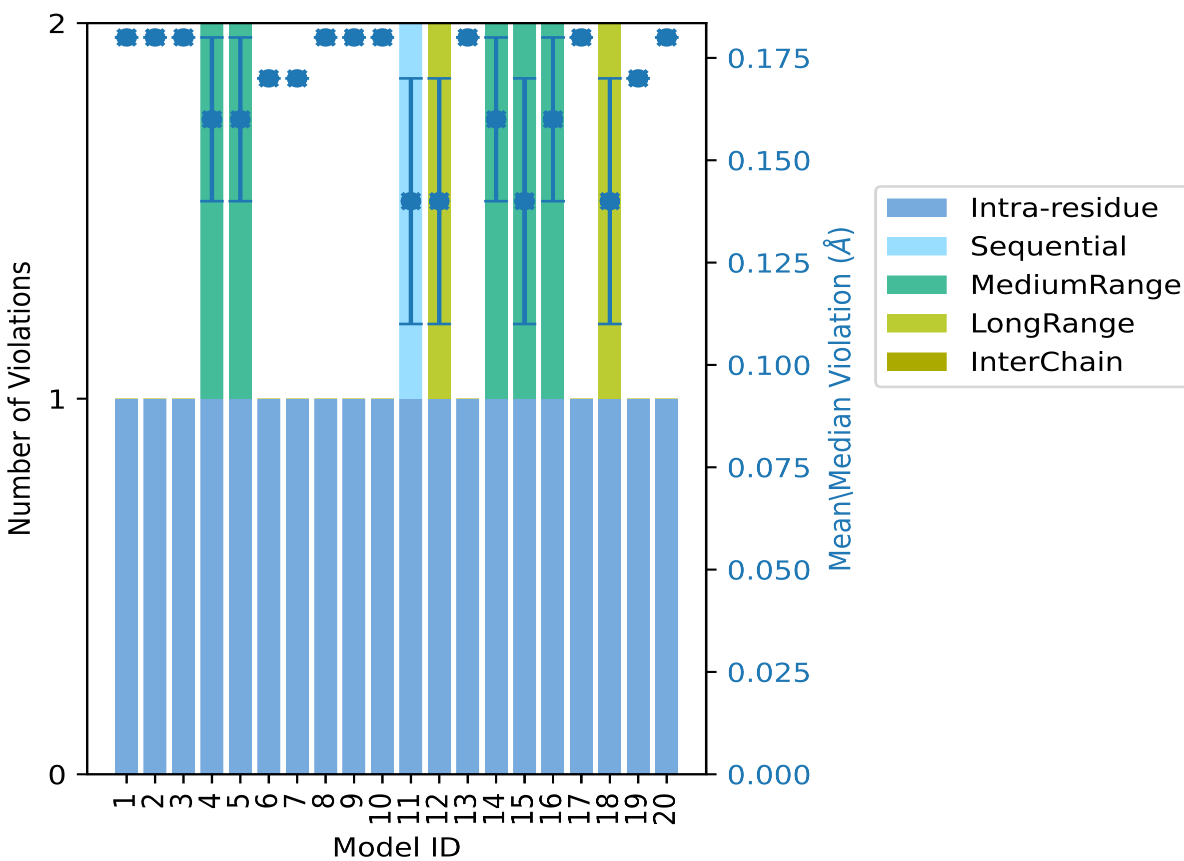
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	0	0	1	0	2	0.14	0.18	0.03	0.14
13	1	0	0	0	0	1	0.18	0.18	0.0	0.18
14	1	0	1	0	0	2	0.16	0.18	0.02	0.16
15	1	0	1	0	0	2	0.14	0.18	0.03	0.14
16	1	0	1	0	0	2	0.16	0.18	0.02	0.16
17	1	0	0	0	0	1	0.18	0.18	0.0	0.18
18	1	0	0	1	0	2	0.14	0.17	0.03	0.14
19	1	0	0	0	0	1	0.17	0.17	0.0	0.17
20	1	0	0	0	0	1	0.18	0.18	0.0	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

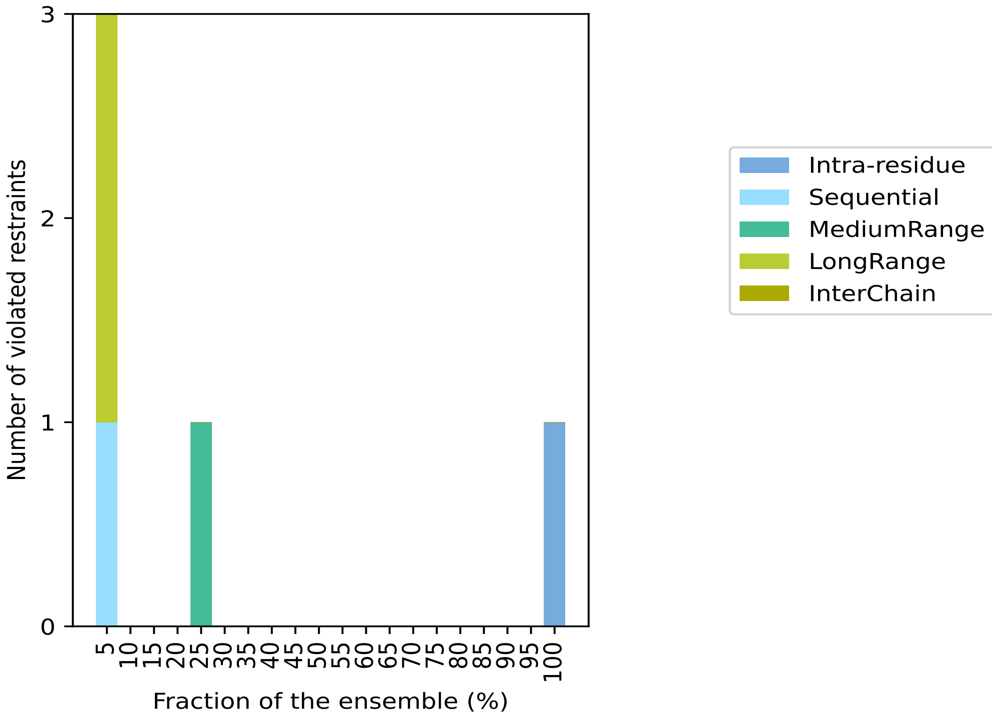
9.3 Distance violation statistics for the ensemble (i)

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, 622(IR:162, SQ:126, MR:113, LR:221, 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]	%
0	1	0	2	0	3	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	1	0	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	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
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	0	0	0	0	1	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

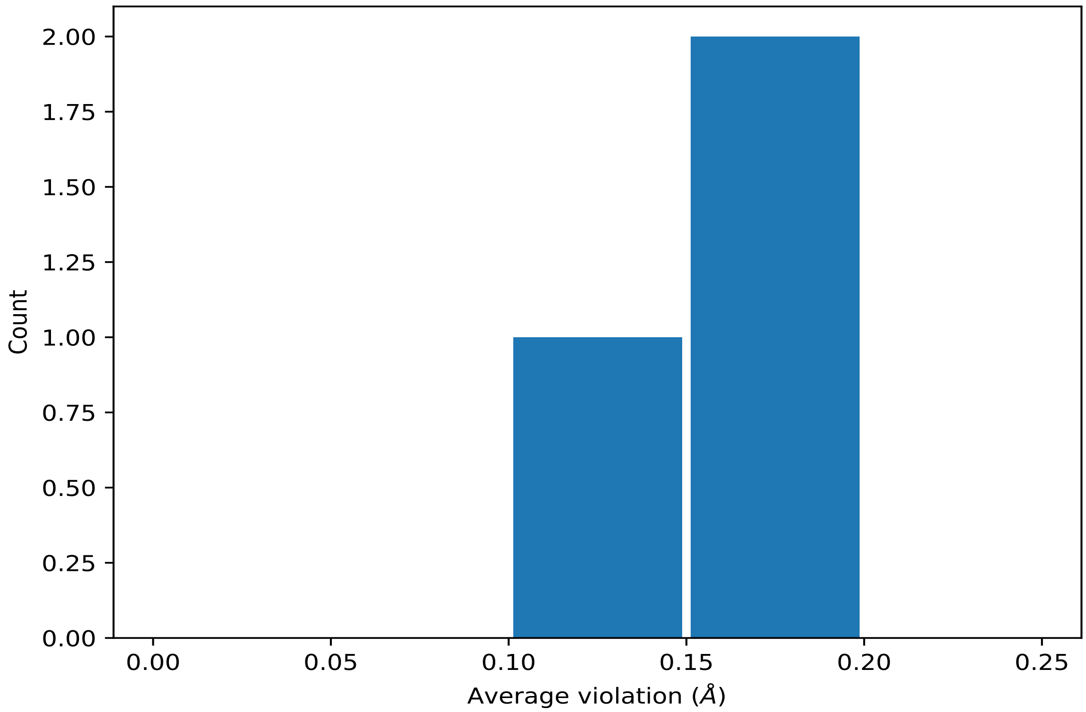
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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 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.

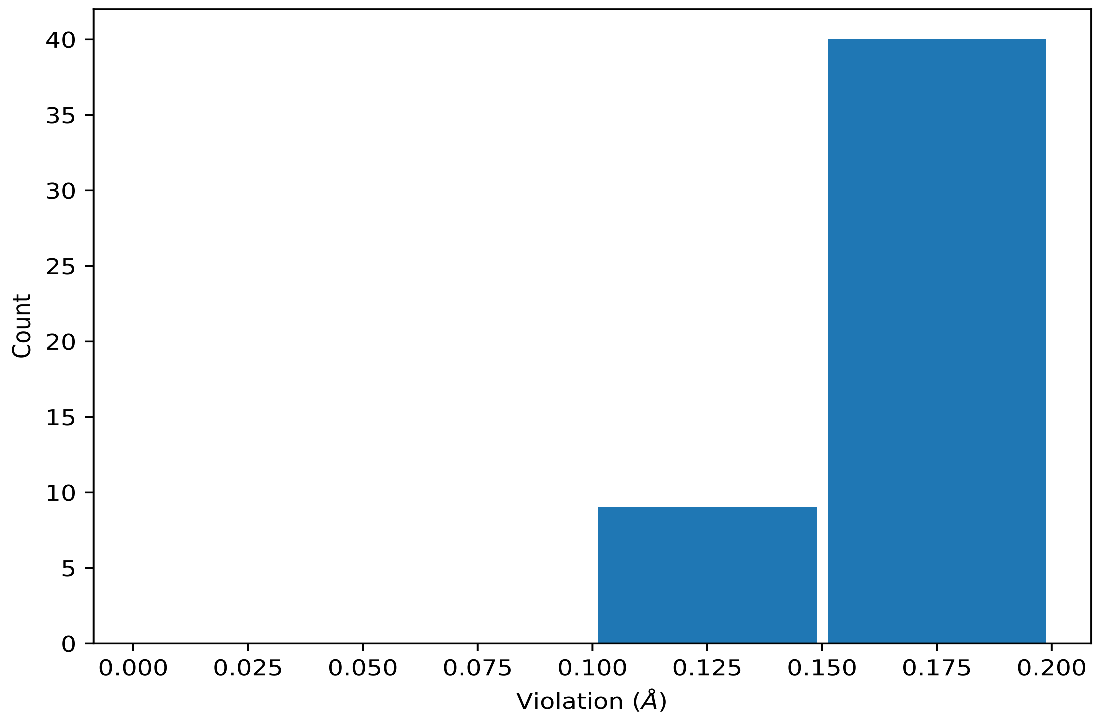
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	20	0.18	0.0	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	20	0.18	0.0	0.18
(1,294)	1:A:315:HIS:HA	1:A:318:ILE:HB	5	0.13	0.01	0.13

[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

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)
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	1	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	1	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	2	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	2	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	3	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	3	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	4	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	4	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	5	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	5	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	8	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	8	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	9	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	9	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	10	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	11	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	11	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	12	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	12	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	13	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	13	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	14	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	14	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	15	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	15	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	16	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	16	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	17	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	17	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	20	0.18
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	20	0.18
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	6	0.17
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	6	0.17
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	7	0.17
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	7	0.17
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	18	0.17
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	18	0.17
(1,159)	1:A:308:PHE:HD1	1:A:308:PHE:HZ	19	0.17
(1,159)	1:A:308:PHE:HD2	1:A:308:PHE:HZ	19	0.17
(1,294)	1:A:315:HIS:HA	1:A:318:ILE:HB	4	0.13
(1,294)	1:A:315:HIS:HA	1:A:318:ILE:HB	5	0.13
(1,294)	1:A:315:HIS:HA	1:A:318:ILE:HB	14	0.13
(1,294)	1:A:315:HIS:HA	1:A:318:ILE:HB	16	0.13
(1,549)	1:A:312:LYS:HB2	1:A:313:ASP:HA	11	0.11
(1,549)	1:A:312:LYS:HB3	1:A:313:ASP:HA	11	0.11
(1,294)	1:A:315:HIS:HA	1:A:318:ILE:HB	15	0.11
(1,235)	1:A:272:VAL:HB	1:A:327:GLU:HA	18	0.11
(1,202)	1:A:267:ASN:H	1:A:303:SER:H	12	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found