wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	5N6R
BMRB ID	:	34101
Title	:	Solution structure of the Dbl-homology domain of Bcr-Abl
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

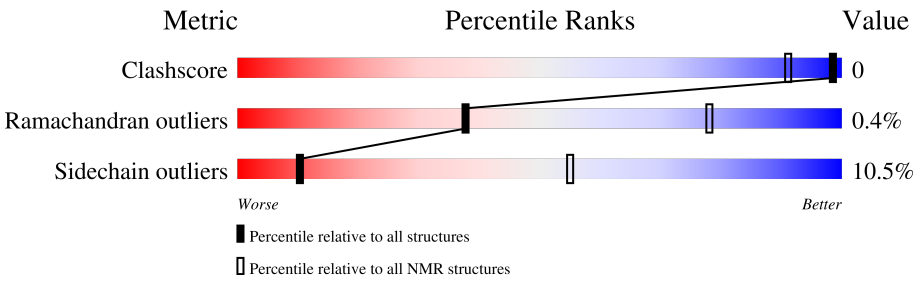
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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	218	79% · 17%

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:496-A:619, A:638-A:693 (180)	1.08	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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3500 atoms, of which 1756 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Breakpoint cluster region protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	218	3500	1105	1756	302	329	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	485	ALA	-	expression tag	UNP P11274
A	486	MET	-	expression tag	UNP P11274

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: Breakpoint cluster region protein

Chain A: 79% • 17%

A485 M486 A487 S488 E489 L490 D491 L492 E493 K494 G495 W501 L514 F560 R576 Y598 E620 N621 L622 R623 A624 R625 S626 N627 K628 D629 A630 K631 D632 P633 T634 T635 K636 N637 L655 V656 H668 P694 R695 R696 Q697 S698 M699 T700 V701 K702

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

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

- Molecule 1: Breakpoint cluster region protein

Chain A: 73% 10% 17%

A485 M486 A487 S488 E489 L490 D491 L492 E493 K494 G495 M498 W501 L507 K528 S540 E544 F560 Q575 L588 G589 V590 Y598 E606 E620 N621 L622 R623 A624 R625 S626 N627 K628 D629 A630 K631 D632 P633 T634 T635 K636 N637 S638 L639 R649 L655

V656 D659 L660 L661 S667 E691 I692 T693 P694 R695 R696 Q697 S698 M699 T700 V701 K702

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *TORSION ANGLE DYNAMICS ONFORMERS, NUMBER CALCULATED : NULL.*

Of the 200 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 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	2893
Number of shifts mapped to atoms	2893
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	0.58±0.00	0±0/1481 (0.0± 0.0%)	0.96±0.02	1±1/2013 (0.0± 0.1%)
All	All	0.58	0/29620 (0.0%)	0.96	18/40260 (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	1.8±1.0
All	All	0	35

There are no bond-length outliers.

5 of 13 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	592	ARG	NE-CZ-NH2	-7.64	116.48	120.30	3	2
1	A	679	ARG	NE-CZ-NH1	7.46	124.03	120.30	20	1
1	A	567	ARG	NE-CZ-NH2	-6.09	117.25	120.30	2	1
1	A	652	ARG	NE-CZ-NH1	5.95	123.28	120.30	19	1
1	A	681	SER	N-CA-CB	-5.89	101.66	110.50	2	2

There are no chirality outliers.

5 of 11 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	598	TYR	Sidechain	8
1	A	592	ARG	Sidechain	6
1	A	649	ARG	Sidechain	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	644	TYR	Sidechain	3
1	A	499	ARG	Sidechain	3

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	1447	1450	1450	0±0
All	All	28940	29000	29000	5

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:514:LEU:HD22	1:A:558:LYS:HG2	0.47	1.84	2	1
1:A:654:THR:HG21	1:A:685:LEU:HD23	0.47	1.86	12	1
1:A:514:LEU:HD21	1:A:557:HIS:CB	0.45	2.41	9	1
1:A:514:LEU:HD13	1:A:558:LYS:HG2	0.43	1.90	4	1
1:A:575:GLN:NE2	1:A:576:ARG:H	0.43	2.11	8	1

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	180/218 (83%)	173±2 (96±1%)	7±2 (4±1%)	1±1 (0±0%)	38	78
All	All	3600/4360 (83%)	3452 (96%)	134 (4%)	14 (0%)	38	78

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occur-

rence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	578	GLY	8
1	A	534	SER	3
1	A	693	THR	2
1	A	688	ILE	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	161/194 (83%)	144±3 (90±2%)	17±3 (10±2%)	10	55
All	All	3220/3880 (83%)	2882 (90%)	338 (10%)	10	55

5 of 99 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	501	TRP	17
1	A	560	PHE	16
1	A	656	VAL	14
1	A	655	LEU	13
1	A	576	ARG	12

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 94% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *dh_final_NMR-STAR.str*

7.1.1 Bookkeeping (i)

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

Total number of shifts	2893
Number of shifts mapped to atoms	2893
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	218	-0.70 ± 0.11	Should be checked
$^{13}C_{\beta}$	212	0.18 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	218	-0.45 ± 0.08	None needed (< 0.5 ppm)
^{15}N	207	0.06 ± 0.15	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. 2387 atoms were assigned a chemical shift out of a possible 2527. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	887/887 (100%)	356/356 (100%)	360/360 (100%)	171/171 (100%)
Sidechain	1313/1433 (92%)	910/938 (97%)	402/448 (90%)	1/47 (2%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	187/207 (90%)	97/104 (93%)	88/94 (94%)	2/9 (22%)
Overall	2387/2527 (94%)	1363/1398 (97%)	850/902 (94%)	174/227 (77%)

7.1.4 Statistically unusual chemical shifts (i)

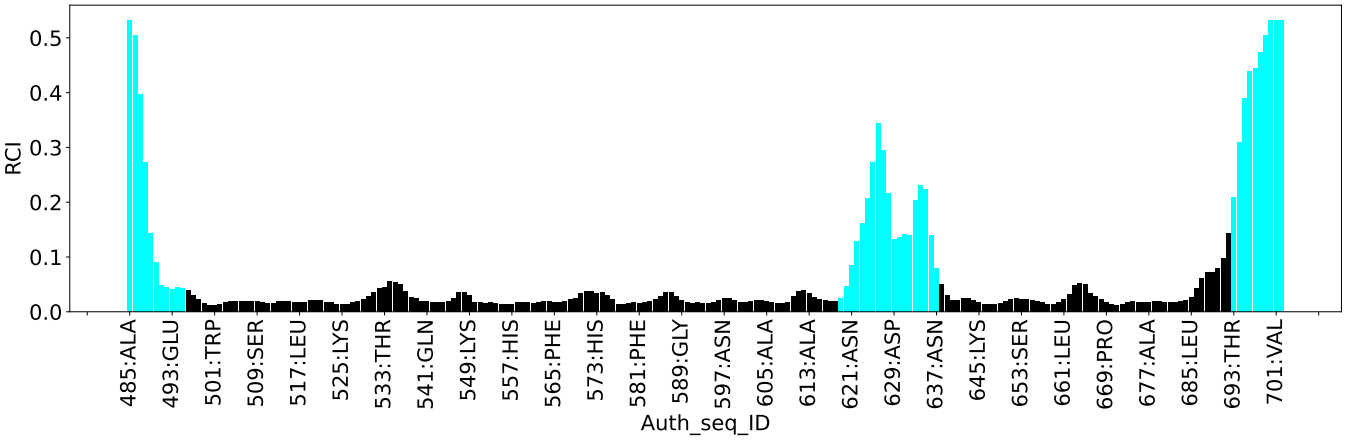
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	539	THR	HG1	7.66	0.08 – 2.19	30.9
1	A	693	THR	HG1	7.65	0.08 – 2.19	30.9
1	A	533	THR	HG1	5.58	0.08 – 2.19	21.1
1	A	634	THR	HG1	4.73	0.08 – 2.19	17.0
1	A	635	THR	HG1	4.73	0.08 – 2.19	17.0
1	A	700	THR	HG1	4.73	0.08 – 2.19	17.0
1	A	641	THR	HG1	4.73	0.08 – 2.19	17.0
1	A	664	THR	HG1	4.73	0.08 – 2.19	17.0
1	A	512	THR	HG1	4.35	0.08 – 2.19	15.2
1	A	532	THR	HG1	4.20	0.08 – 2.19	14.5
1	A	545	THR	HG1	3.90	0.08 – 2.19	13.1
1	A	625	ARG	HE	4.30	4.52 – 10.19	-5.4

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
485:ALA
493:GLU
501:TRP
509:SER
517:LEU
525:LYS
533:THR
541:GLN
549:LYS
557:HIS
565:PHE
573:HIS
581:PHE
589:GLY
597:ASN
605:ALA
613:ALA
621:ASN
629:ASP
637:ASN
645:LYS
653:SER
661:LEU
669:PRO
677:ALA
685:LEU
693:THR
701: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	3682
Intra-residue (|i-j|=0)	667
Sequential (|i-j|=1)	1137
Medium range (|i-j|>1 and |i-j|<5)	1192
Long range (|i-j|≥5)	686
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	2
Number of restraints per residue	16.9
Number of long range restraints per residue[1]	3.1

[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)	5.3	0.16
0.2-0.5 (Medium)	0.1	0.32
>0.5 (Large)	0.2	0.93

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)

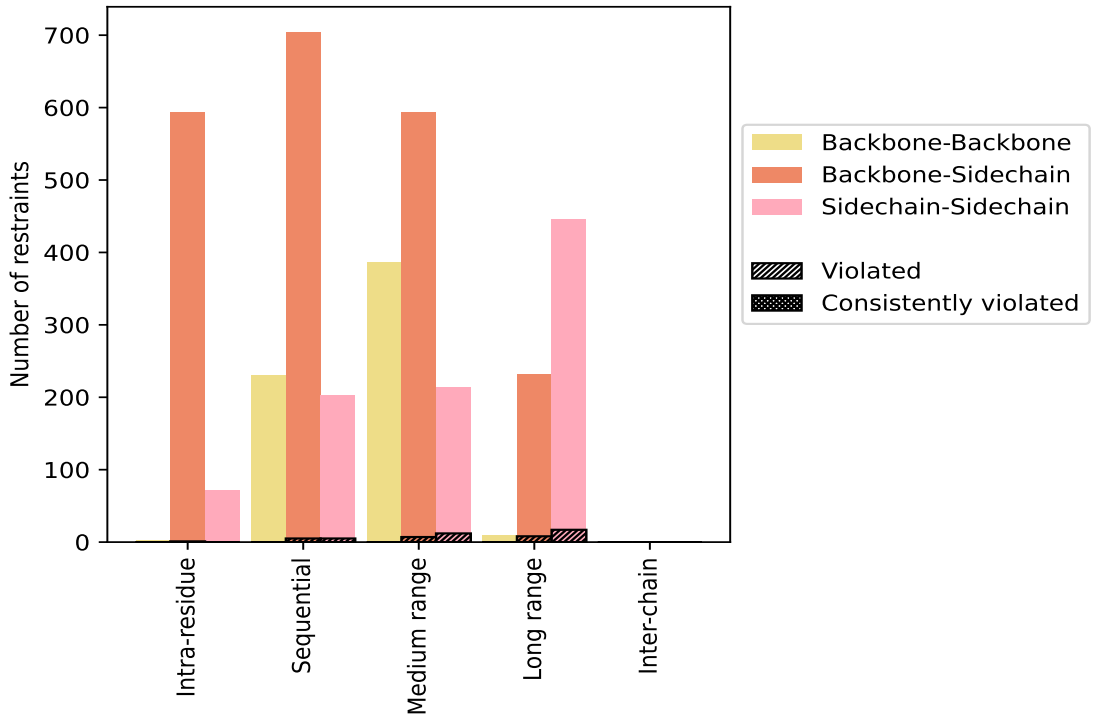
9.1 Summary of distance violations (i)

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)	667	18.1	1	0.1	0.0	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	594	16.1	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	71	1.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1137	30.9	10	0.9	0.3	0	0.0	0.0
Backbone-Backbone	230	6.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	704	19.1	5	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	203	5.5	5	2.5	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	1192	32.4	19	1.6	0.5	0	0.0	0.0
Backbone-Backbone	386	10.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	593	16.1	7	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	213	5.8	12	5.6	0.3	0	0.0	0.0
Long range (|i-j|≥5)	686	18.6	25	3.6	0.7	0	0.0	0.0
Backbone-Backbone	9	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	232	6.3	8	3.4	0.2	0	0.0	0.0
Sidechain-Sidechain	445	12.1	17	3.8	0.5	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	3682	100.0	55	1.5	1.5	0	0.0	0.0
Backbone-Backbone	627	17.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2123	57.7	21	1.0	0.6	0	0.0	0.0
Sidechain-Sidechain	932	25.3	34	3.6	0.9	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 (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	0	1	0	4	0	5	0.12	0.14	0.01	0.11
2	0	1	2	5	0	8	0.12	0.13	0.01	0.12
3	0	0	3	4	0	7	0.26	0.91	0.28	0.12
4	0	1	4	4	0	9	0.12	0.13	0.01	0.12
5	0	1	3	2	0	6	0.12	0.13	0.01	0.11
6	0	0	2	4	0	6	0.11	0.12	0.0	0.11
7	0	0	5	1	0	6	0.12	0.13	0.01	0.11
8	0	1	2	2	0	5	0.11	0.12	0.0	0.11
9	0	1	2	3	0	6	0.33	0.93	0.32	0.12
10	0	0	3	3	0	6	0.25	0.75	0.23	0.14
11	1	3	1	1	0	6	0.11	0.12	0.0	0.11

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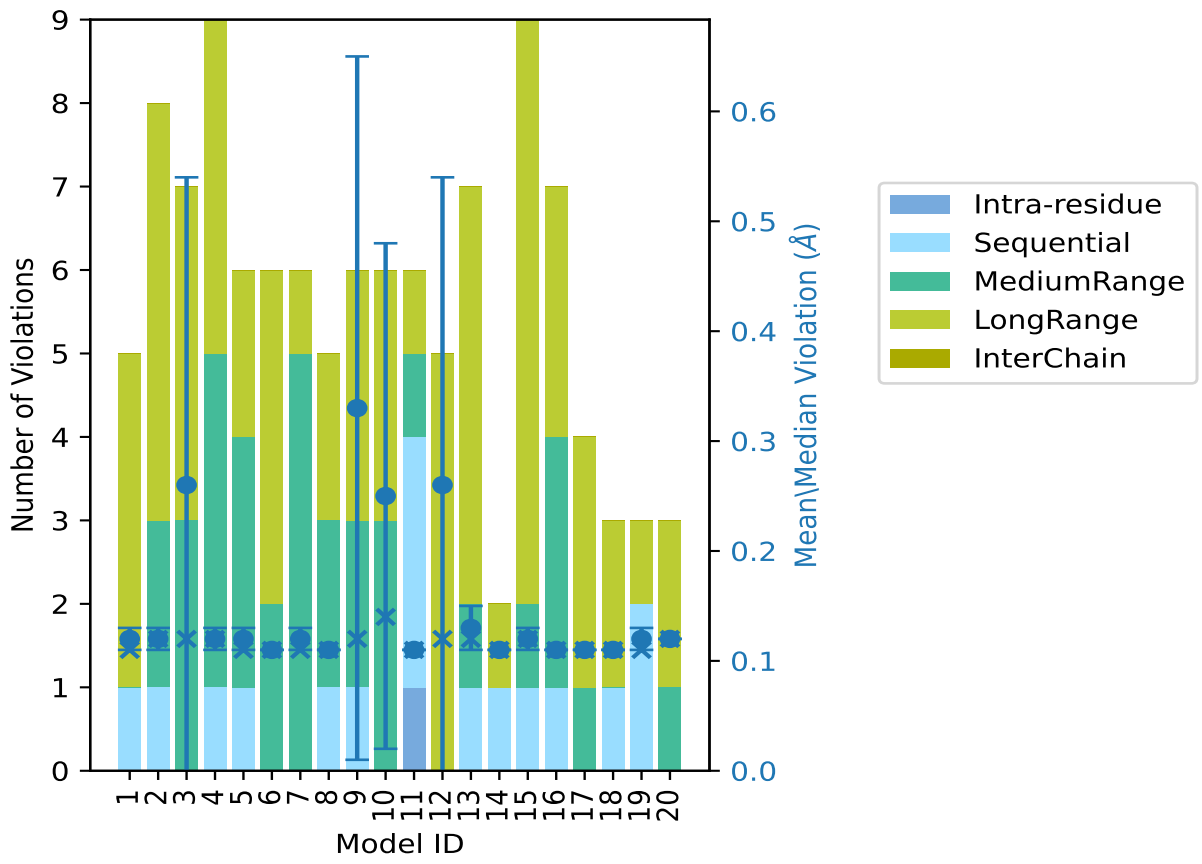
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	5	0	5	0.26	0.81	0.28	0.12
13	0	1	1	5	0	7	0.13	0.16	0.02	0.12
14	0	1	0	1	0	2	0.11	0.11	0.0	0.11
15	0	1	1	7	0	9	0.12	0.13	0.01	0.12
16	0	1	3	3	0	7	0.11	0.12	0.0	0.11
17	0	0	1	3	0	4	0.11	0.12	0.0	0.11
18	0	1	0	2	0	3	0.11	0.11	0.0	0.11
19	0	2	0	1	0	3	0.12	0.13	0.01	0.11
20	0	0	1	2	0	3	0.12	0.12	0.0	0.12

[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

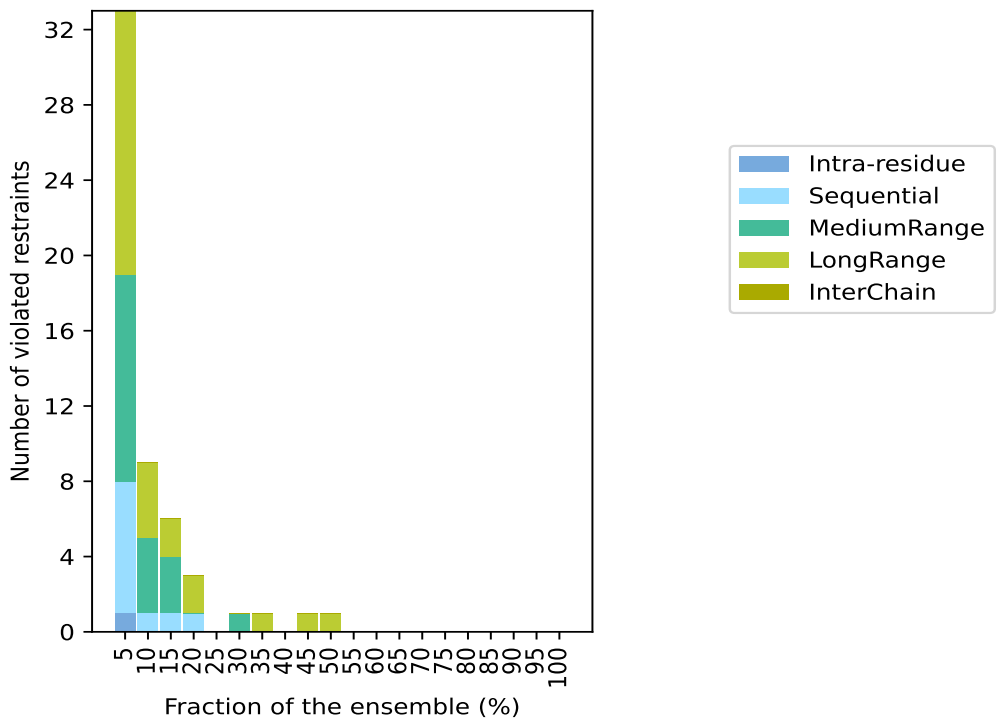
9.3 Distance violation statistics for the ensemble (i)

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, 3627(IR:666, SQ:1127, MR:1173, LR:661, 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]	%
1	7	11	14	0	33	1	5.0
0	1	4	4	0	9	2	10.0
0	1	3	2	0	6	3	15.0
0	1	0	2	0	3	4	20.0
0	0	0	0	0	0	5	25.0
0	0	1	0	0	1	6	30.0
0	0	0	1	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	1	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
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
0	0	0	0	0	0	20	100.0

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

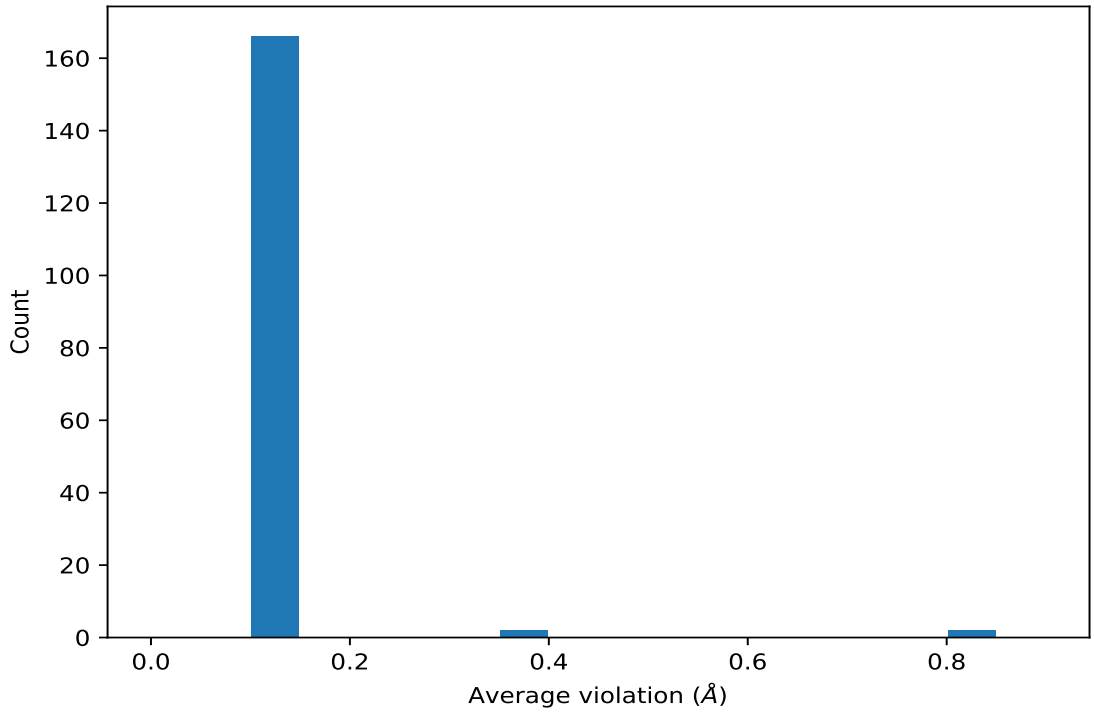
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2138)	1:A:522:LEU:H	1:A:550:VAL:HG11	10	0.12	0.01	0.11
(1,2138)	1:A:522:LEU:H	1:A:550:VAL:HG12	10	0.12	0.01	0.11
(1,2138)	1:A:522:LEU:H	1:A:550:VAL:HG13	10	0.12	0.01	0.11
(1,2138)	1:A:522:LEU:H	1:A:550:VAL:HG21	10	0.12	0.01	0.11
(1,2138)	1:A:522:LEU:H	1:A:550:VAL:HG22	10	0.12	0.01	0.11
(1,2138)	1:A:522:LEU:H	1:A:550:VAL:HG23	10	0.12	0.01	0.11
(1,2228)	1:A:563:GLY:H	1:A:580:LEU:HD11	9	0.12	0.01	0.12
(1,2228)	1:A:563:GLY:H	1:A:580:LEU:HD12	9	0.12	0.01	0.12
(1,2228)	1:A:563:GLY:H	1:A:580:LEU:HD13	9	0.12	0.01	0.12
(1,2228)	1:A:563:GLY:H	1:A:580:LEU:HD21	9	0.12	0.01	0.12
(1,2228)	1:A:563:GLY:H	1:A:580:LEU:HD22	9	0.12	0.01	0.12
(1,2228)	1:A:563:GLY:H	1:A:580:LEU:HD23	9	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG11	1:A:692:ILE:HD11	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG11	1:A:692:ILE:HD12	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG11	1:A:692:ILE:HD13	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG12	1:A:692:ILE:HD11	7	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2317)	1:A:595:VAL:HG12	1:A:692:ILE:HD12	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG12	1:A:692:ILE:HD13	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG13	1:A:692:ILE:HD11	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG13	1:A:692:ILE:HD12	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG13	1:A:692:ILE:HD13	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG21	1:A:692:ILE:HD11	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG21	1:A:692:ILE:HD12	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG21	1:A:692:ILE:HD13	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG22	1:A:692:ILE:HD11	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG22	1:A:692:ILE:HD12	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG22	1:A:692:ILE:HD13	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG23	1:A:692:ILE:HD11	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG23	1:A:692:ILE:HD12	7	0.12	0.01	0.12
(1,2317)	1:A:595:VAL:HG23	1:A:692:ILE:HD13	7	0.12	0.01	0.12
(1,2447)	1:A:659:ASP:H	1:A:661:LEU:HD11	6	0.12	0.0	0.12
(1,2447)	1:A:659:ASP:H	1:A:661:LEU:HD12	6	0.12	0.0	0.12
(1,2447)	1:A:659:ASP:H	1:A:661:LEU:HD13	6	0.12	0.0	0.12
(1,2447)	1:A:659:ASP:H	1:A:661:LEU:HD21	6	0.12	0.0	0.12
(1,2447)	1:A:659:ASP:H	1:A:661:LEU:HD22	6	0.12	0.0	0.12
(1,2447)	1:A:659:ASP:H	1:A:661:LEU:HD23	6	0.12	0.0	0.12
(2,1030)	1:A:553:LEU:HB2	1:A:591:TYR:HE2	4	0.85	0.07	0.86
(2,1030)	1:A:553:LEU:HB3	1:A:591:TYR:HE2	4	0.85	0.07	0.86
(1,2362)	1:A:620:GLU:HG2	1:A:621:ASN:HD21	4	0.12	0.0	0.12
(1,2362)	1:A:620:GLU:HG2	1:A:621:ASN:HD22	4	0.12	0.0	0.12
(1,2362)	1:A:620:GLU:HG3	1:A:621:ASN:HD21	4	0.12	0.0	0.12
(1,2362)	1:A:620:GLU:HG3	1:A:621:ASN:HD22	4	0.12	0.0	0.12
(1,2547)	1:A:506:ILE:HG21	1:A:564:LEU:HD11	4	0.11	0.0	0.11
(1,2547)	1:A:506:ILE:HG21	1:A:564:LEU:HD12	4	0.11	0.0	0.11
(1,2547)	1:A:506:ILE:HG21	1:A:564:LEU:HD13	4	0.11	0.0	0.11
(1,2547)	1:A:506:ILE:HG22	1:A:564:LEU:HD11	4	0.11	0.0	0.11
(1,2547)	1:A:506:ILE:HG22	1:A:564:LEU:HD12	4	0.11	0.0	0.11
(1,2547)	1:A:506:ILE:HG22	1:A:564:LEU:HD13	4	0.11	0.0	0.11
(1,2547)	1:A:506:ILE:HG23	1:A:564:LEU:HD11	4	0.11	0.0	0.11
(1,2547)	1:A:506:ILE:HG23	1:A:564:LEU:HD12	4	0.11	0.0	0.11
(1,2547)	1:A:506:ILE:HG23	1:A:564:LEU:HD13	4	0.11	0.0	0.11
(2,859)	1:A:588:LEU:HB2	1:A:591:TYR:HD1	3	0.39	0.16	0.32
(2,859)	1:A:588:LEU:HB3	1:A:591:TYR:HD1	3	0.39	0.16	0.32
(1,2099)	1:A:514:LEU:HD11	1:A:561:TYR:H	3	0.12	0.01	0.13
(1,2099)	1:A:514:LEU:HD12	1:A:561:TYR:H	3	0.12	0.01	0.13
(1,2099)	1:A:514:LEU:HD13	1:A:561:TYR:H	3	0.12	0.01	0.13
(1,2099)	1:A:514:LEU:HD21	1:A:561:TYR:H	3	0.12	0.01	0.13
(1,2099)	1:A:514:LEU:HD22	1:A:561:TYR:H	3	0.12	0.01	0.13

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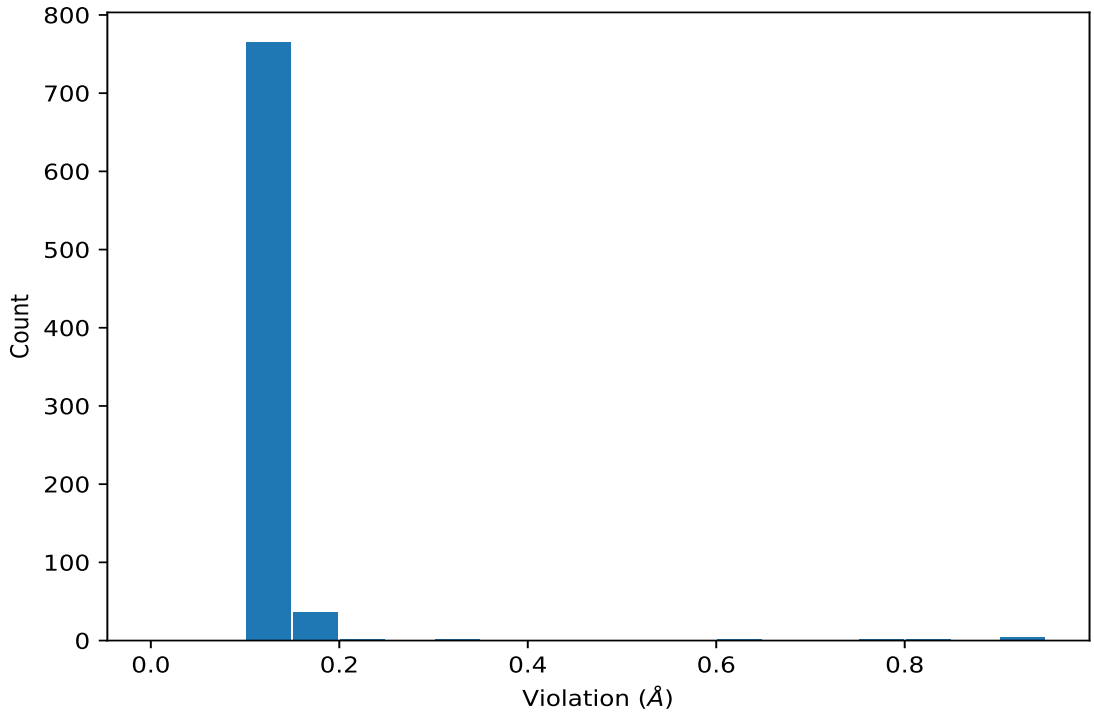
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2099)	1:A:514:LEU:HD23	1:A:561:TYR:H	3	0.12	0.01	0.13
(1,464)	1:A:601:ALA:HB1	1:A:604:MET:HE1	3	0.12	0.01	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1030)	1:A:553:LEU:HB2	1:A:591:TYR:HE2	9	0.93
(2,1030)	1:A:553:LEU:HB3	1:A:591:TYR:HE2	9	0.93
(2,1030)	1:A:553:LEU:HB2	1:A:591:TYR:HE2	3	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1030)	1:A:553:LEU:HB3	1:A:591:TYR:HE2	3	0.91
(2,1030)	1:A:553:LEU:HB2	1:A:591:TYR:HE2	12	0.81
(2,1030)	1:A:553:LEU:HB3	1:A:591:TYR:HE2	12	0.81
(2,1030)	1:A:553:LEU:HB2	1:A:591:TYR:HE2	10	0.75
(2,1030)	1:A:553:LEU:HB3	1:A:591:TYR:HE2	10	0.75
(2,859)	1:A:588:LEU:HB2	1:A:591:TYR:HD1	9	0.62
(2,859)	1:A:588:LEU:HB3	1:A:591:TYR:HD1	9	0.62
(2,859)	1:A:588:LEU:HB2	1:A:591:TYR:HD1	3	0.32
(2,859)	1:A:588:LEU:HB3	1:A:591:TYR:HD1	3	0.32
(2,859)	1:A:588:LEU:HB2	1:A:591:TYR:HD1	10	0.24
(2,859)	1:A:588:LEU:HB3	1:A:591:TYR:HD1	10	0.24
(1,2484)	1:A:673:LEU:HD11	1:A:677:ALA:HB1	13	0.16
(1,2484)	1:A:673:LEU:HD11	1:A:677:ALA:HB2	13	0.16
(1,2484)	1:A:673:LEU:HD11	1:A:677:ALA:HB3	13	0.16
(1,2484)	1:A:673:LEU:HD12	1:A:677:ALA:HB1	13	0.16
(1,2484)	1:A:673:LEU:HD12	1:A:677:ALA:HB2	13	0.16
(1,2484)	1:A:673:LEU:HD12	1:A:677:ALA:HB3	13	0.16
(1,2484)	1:A:673:LEU:HD13	1:A:677:ALA:HB1	13	0.16
(1,2484)	1:A:673:LEU:HD13	1:A:677:ALA:HB2	13	0.16
(1,2484)	1:A:673:LEU:HD13	1:A:677:ALA:HB3	13	0.16
(1,2484)	1:A:673:LEU:HD21	1:A:677:ALA:HB1	13	0.16
(1,2484)	1:A:673:LEU:HD21	1:A:677:ALA:HB2	13	0.16
(1,2484)	1:A:673:LEU:HD21	1:A:677:ALA:HB3	13	0.16
(1,2484)	1:A:673:LEU:HD22	1:A:677:ALA:HB1	13	0.16
(1,2484)	1:A:673:LEU:HD22	1:A:677:ALA:HB2	13	0.16
(1,2484)	1:A:673:LEU:HD22	1:A:677:ALA:HB3	13	0.16
(1,2484)	1:A:673:LEU:HD23	1:A:677:ALA:HB1	13	0.16
(1,2484)	1:A:673:LEU:HD23	1:A:677:ALA:HB2	13	0.16
(1,2484)	1:A:673:LEU:HD23	1:A:677:ALA:HB3	13	0.16
(1,2317)	1:A:595:VAL:HG11	1:A:692:ILE:HD11	13	0.15
(1,2317)	1:A:595:VAL:HG11	1:A:692:ILE:HD12	13	0.15
(1,2317)	1:A:595:VAL:HG11	1:A:692:ILE:HD13	13	0.15
(1,2317)	1:A:595:VAL:HG12	1:A:692:ILE:HD11	13	0.15
(1,2317)	1:A:595:VAL:HG12	1:A:692:ILE:HD12	13	0.15
(1,2317)	1:A:595:VAL:HG12	1:A:692:ILE:HD13	13	0.15
(1,2317)	1:A:595:VAL:HG13	1:A:692:ILE:HD11	13	0.15
(1,2317)	1:A:595:VAL:HG13	1:A:692:ILE:HD12	13	0.15
(1,2317)	1:A:595:VAL:HG13	1:A:692:ILE:HD13	13	0.15
(1,2317)	1:A:595:VAL:HG21	1:A:692:ILE:HD11	13	0.15
(1,2317)	1:A:595:VAL:HG21	1:A:692:ILE:HD12	13	0.15
(1,2317)	1:A:595:VAL:HG21	1:A:692:ILE:HD13	13	0.15
(1,2317)	1:A:595:VAL:HG22	1:A:692:ILE:HD11	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2317)	1:A:595:VAL:HG22	1:A:692:ILE:HD12	13	0.15
(1,2317)	1:A:595:VAL:HG22	1:A:692:ILE:HD13	13	0.15
(1,2317)	1:A:595:VAL:HG23	1:A:692:ILE:HD11	13	0.15
(1,2317)	1:A:595:VAL:HG23	1:A:692:ILE:HD12	13	0.15
(1,2317)	1:A:595:VAL:HG23	1:A:692:ILE:HD13	13	0.15
(1,2228)	1:A:563:GLY:H	1:A:580:LEU:HD11	1	0.14

10 Dihedral-angle violation analysis (i)

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