Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 07:17 pm BST

PDB ID	:	7OMK
BMRB ID	:	34630
Title	:	The NMR structure of the Zf-GRF domains from the mouse Endonuclease VIII-LIKE 3 (mNEIL3)
Authors	:	Dinesh, D.C.; Huskova, A.; Srb, P.; Veverka, V.; Silhan, J.
Deposited on	:	2021-05-24

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

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

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

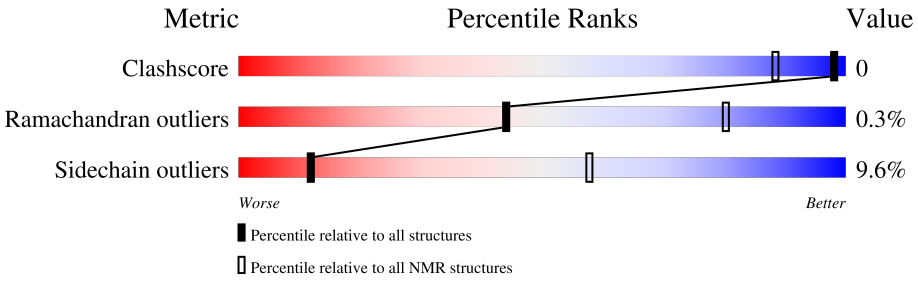
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 89%.

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	93	90% 6% ·

2 Ensemble composition and analysis (i)

This entry contains 35 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:505-A:553 (49)	0.59	1
2	A:554-A:594 (41)	0.29	9

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 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 6, 8, 10, 11, 12, 14, 23, 25, 26, 27, 31, 34, 35
2	7, 9, 13, 15, 16, 17, 19, 24, 28, 30
3	18, 20, 21, 29, 33
4	22, 32
Single-model clusters	4

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1509 atoms, of which 752 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Endonuclease 8-like 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	93	1509	482	752	142	124	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	556	LYS	ARG	variant	UNP Q8K203
A	585	GLU	LYS	variant	UNP Q8K203

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: Endonuclease 8-like 3

Chain A:

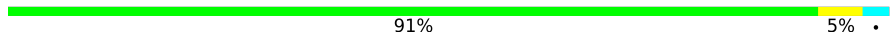
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Endonuclease 8-like 3

Chain A:



4.2.2 Score per residue for model 2

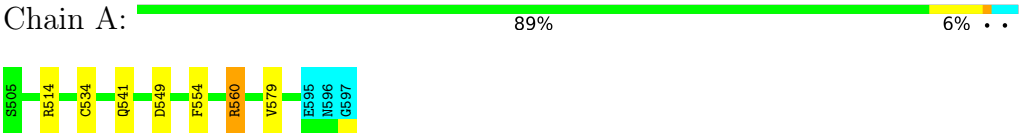
• Molecule 1: Endonuclease 8-like 3

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Endonuclease 8-like 3

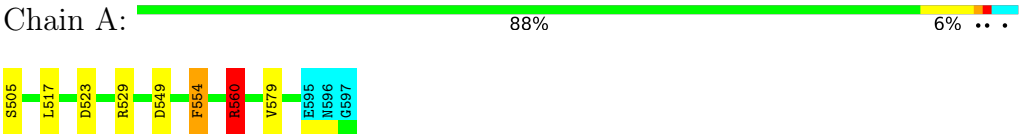
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Endonuclease 8-like 3

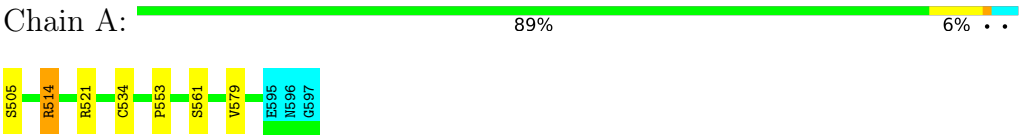
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Endonuclease 8-like 3

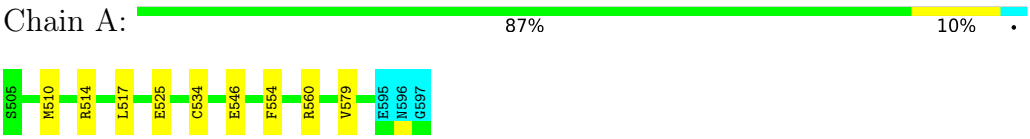
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Endonuclease 8-like 3

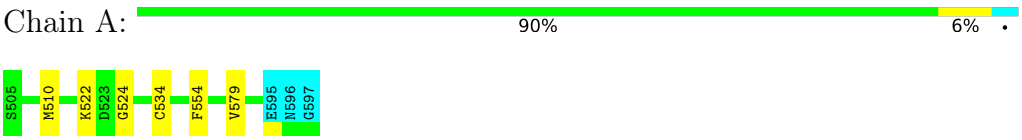
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Endonuclease 8-like 3

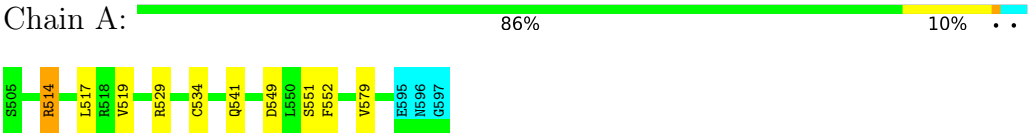
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Endonuclease 8-like 3

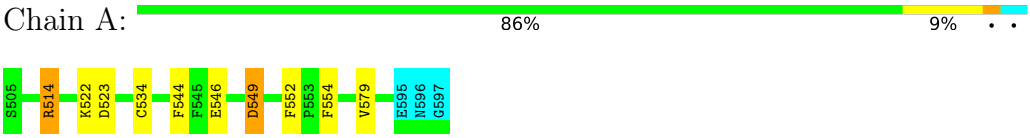
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Endonuclease 8-like 3

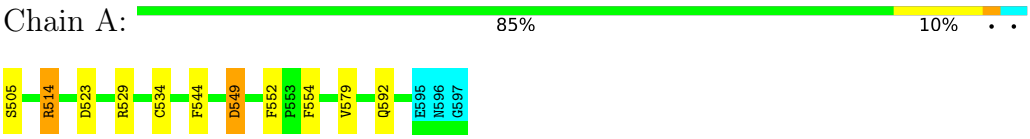
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Endonuclease 8-like 3

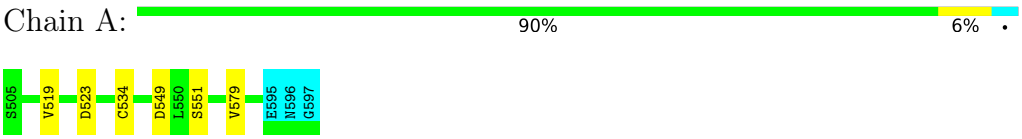
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Endonuclease 8-like 3

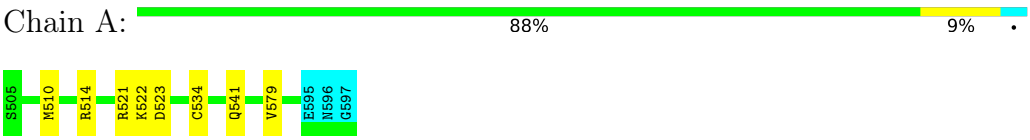
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Endonuclease 8-like 3

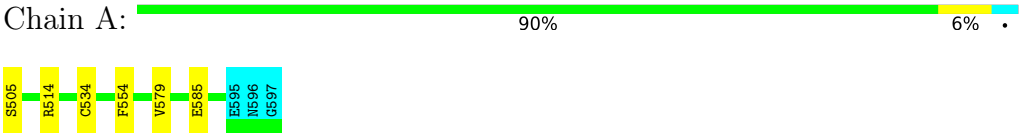
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Endonuclease 8-like 3

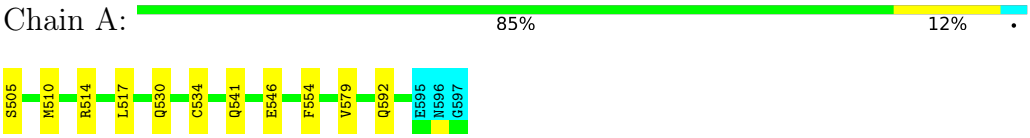
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Endonuclease 8-like 3

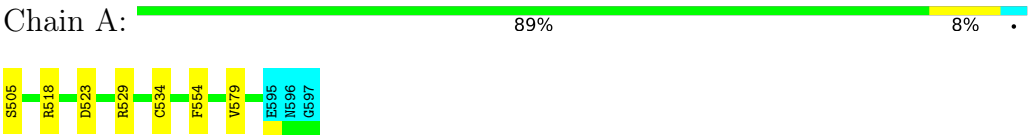
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Endonuclease 8-like 3

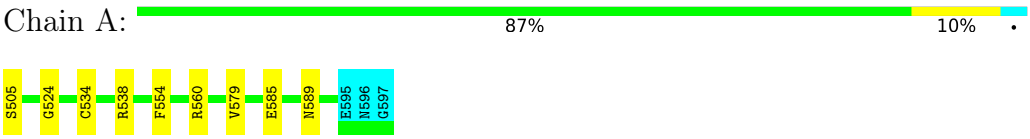
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Endonuclease 8-like 3

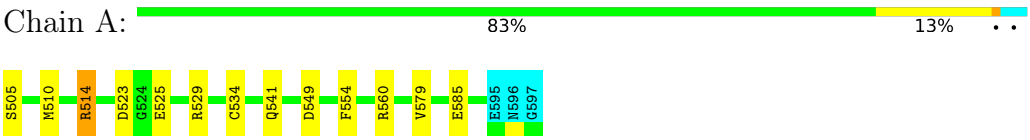
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Endonuclease 8-like 3

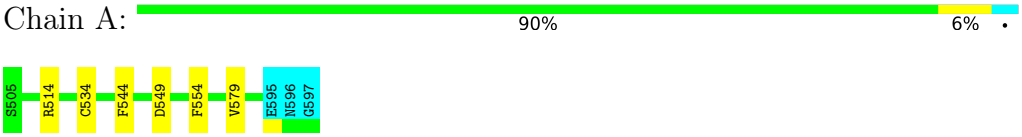
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Endonuclease 8-like 3

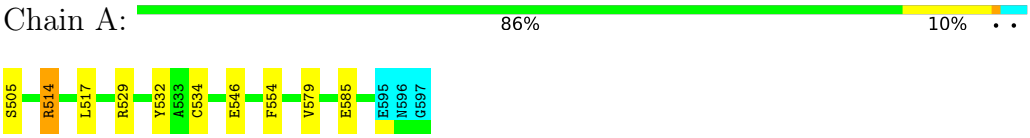
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Endonuclease 8-like 3

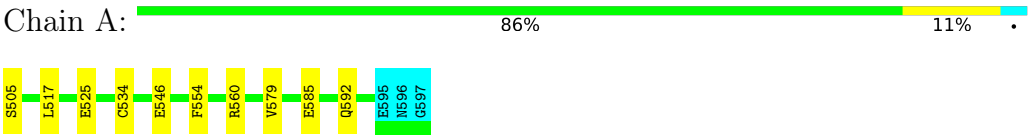
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Endonuclease 8-like 3

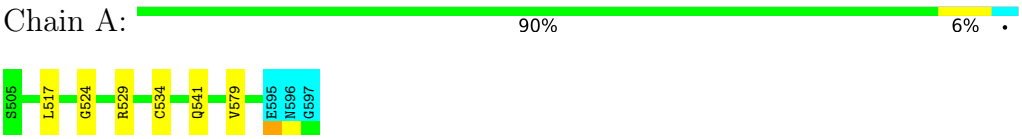
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Endonuclease 8-like 3

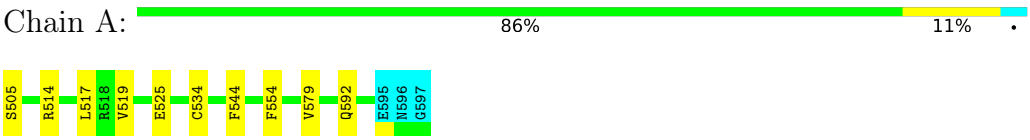
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Endonuclease 8-like 3

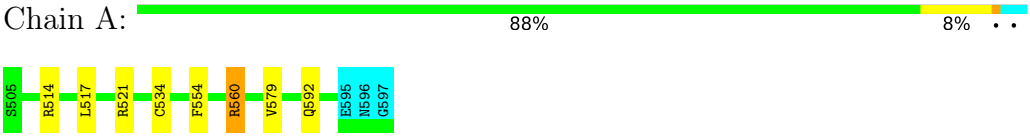
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Endonuclease 8-like 3

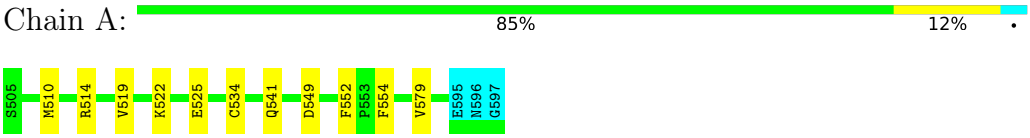
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Endonuclease 8-like 3

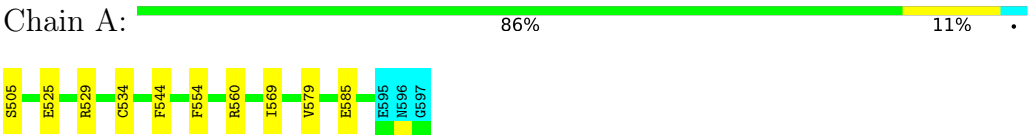
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Endonuclease 8-like 3

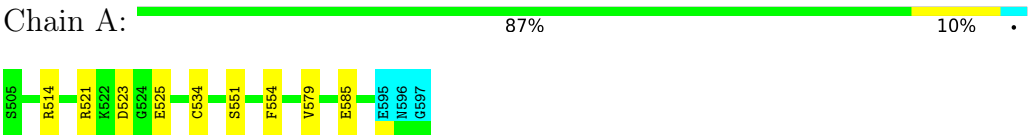
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: Endonuclease 8-like 3

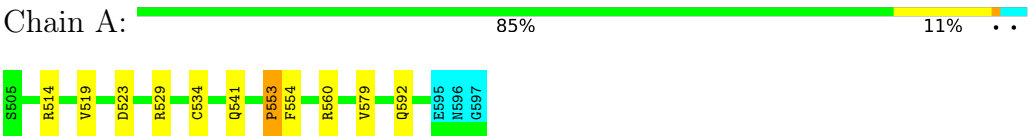
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: Endonuclease 8-like 3

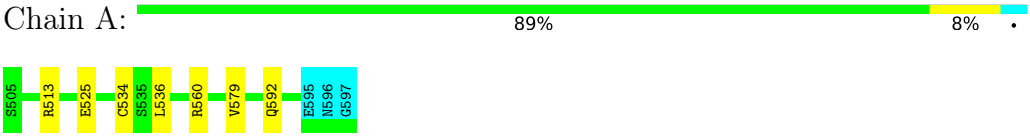
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: Endonuclease 8-like 3

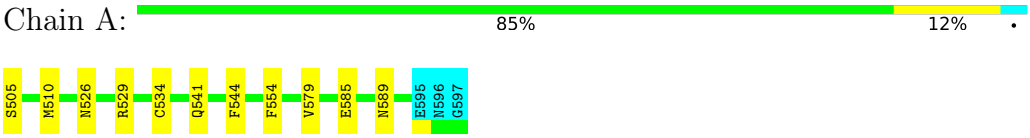
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: Endonuclease 8-like 3

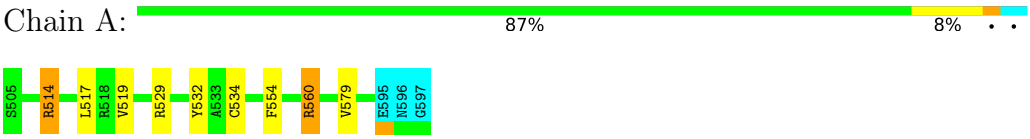
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: Endonuclease 8-like 3

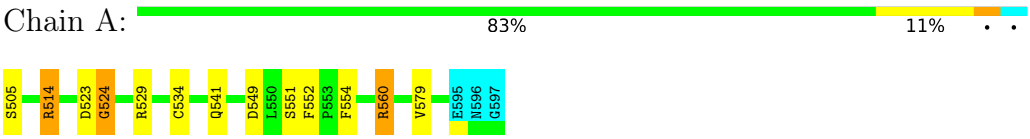
Chain A:



4.2.31 Score per residue for model 31

• Molecule 1: Endonuclease 8-like 3

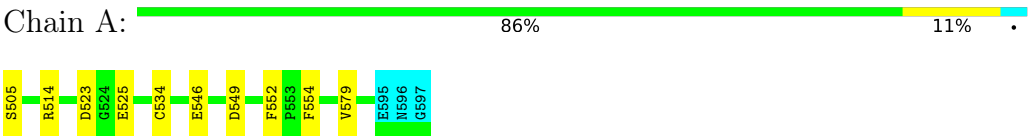
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: Endonuclease 8-like 3

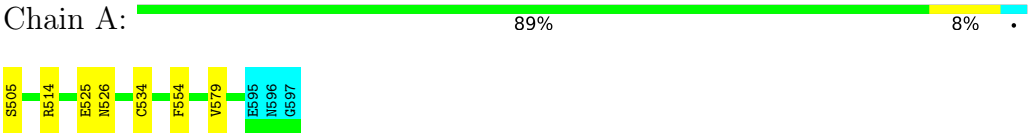
Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: Endonuclease 8-like 3

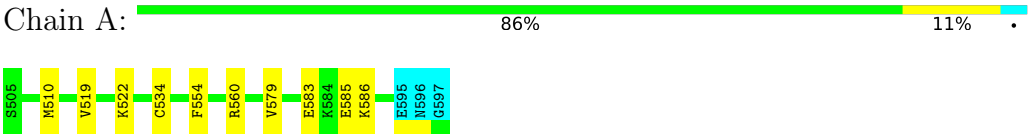
Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: Endonuclease 8-like 3

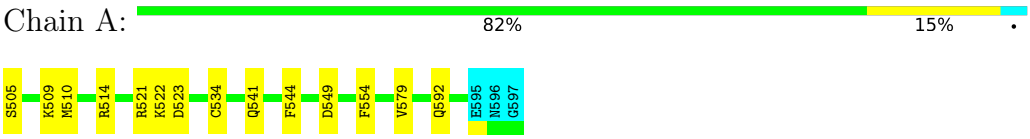
Chain A:



4.2.35 Score per residue for model 35

• Molecule 1: Endonuclease 8-like 3

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 35 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
CYANA	structure calculation	
YASARA	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	1163
Number of shifts mapped to atoms	1163
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality

6.1 Standard geometry

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±0/757 (0.0± 0.0%)	0.76±0.02	1±1/1013 (0.1± 0.1%)
All	All	0.71	0/26495 (0.0%)	0.77	35/35455 (0.1%)

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	514	ARG	NE-CZ-NH1	6.83	123.72	120.30	5	14
1	A	529	ARG	NE-CZ-NH1	6.15	123.37	120.30	29	13
1	A	513	ARG	NE-CZ-NH1	5.64	123.12	120.30	28	1
1	A	560	ARG	NE-CZ-NH1	5.39	123.00	120.30	25	6
1	A	514	ARG	NE-CZ-NH2	-5.04	117.78	120.30	10	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	735	737	734	0±1
All	All	25725	25795	25690	15

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:549:ASP:HA	1:A:552:PHE:CD1	0.51	2.40	32	3
1:A:585:GLU:CD	1:A:585:GLU:H	0.50	2.09	17	3
1:A:554:PHE:CD2	1:A:554:PHE:N	0.45	2.84	27	1
1:A:549:ASP:HA	1:A:552:PHE:CD2	0.43	2.48	10	3
1:A:517:LEU:HD13	1:A:532:TYR:CE1	0.43	2.48	19	2
1:A:517:LEU:HD11	1:A:530:GLN:HB3	0.41	1.92	14	1
1:A:554:PHE:HA	1:A:560:ARG:HA	0.41	1.91	4	1
1:A:523:ASP:CG	1:A:524:GLY:H	0.41	2.19	31	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	89/93 (96%)	86±1 (96±1%)	3±1 (3±1%)	0±0 (0±0%)	44	80
All	All	3115/3255 (96%)	3004 (96%)	103 (3%)	8 (0%)	44	80

All 3 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	524	GLY	4
1	A	553	PRO	2
1	A	523	ASP	2

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	79/81 (98%)	71±2 (90±3%)	8±2 (10±3%)	12	58
All	All	2765/2835 (98%)	2500 (90%)	265 (10%)	12	58

All 32 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	579	VAL	35
1	A	534	CYS	34
1	A	554	PHE	27
1	A	505	SER	19
1	A	514	ARG	18
1	A	560	ARG	12
1	A	541	GLN	11
1	A	525	GLU	10
1	A	592	GLN	9
1	A	523	ASP	9
1	A	510	MET	9
1	A	549	ASP	8
1	A	546	GLU	7
1	A	517	LEU	7
1	A	519	VAL	7
1	A	544	PHE	7
1	A	522	LYS	6
1	A	585	GLU	6
1	A	521	ARG	5
1	A	551	SER	4
1	A	536	LEU	2
1	A	589	ASN	2
1	A	526	ASN	2
1	A	584	LYS	1
1	A	561	SER	1
1	A	518	ARG	1
1	A	538	ARG	1
1	A	569	ILE	1
1	A	553	PRO	1
1	A	583	GLU	1
1	A	586	LYS	1
1	A	509	LYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	1163
Number of shifts mapped to atoms	1163
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	93	-0.03 ± 0.22	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	85	-0.45 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	91	0.04 ± 0.22	None needed (< 0.5 ppm)
^{15}N	87	-0.66 ± 0.52	None needed (imprecise)

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 89%, i.e. 1134 atoms were assigned a chemical shift out of a possible 1277. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	441/447 (99%)	179/182 (98%)	178/180 (99%)	84/85 (99%)
Sidechain	599/686 (87%)	406/440 (92%)	184/206 (89%)	9/40 (22%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	94/144 (65%)	58/73 (79%)	34/66 (52%)	2/5 (40%)
Overall	1134/1277 (89%)	643/695 (93%)	396/452 (88%)	95/130 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1162 atoms were assigned a chemical shift out of a possible 1307. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	457/463 (99%)	186/189 (98%)	184/186 (99%)	87/88 (99%)
Sidechain	611/700 (87%)	414/448 (92%)	187/211 (89%)	10/41 (24%)
Aromatic	94/144 (65%)	58/73 (79%)	34/66 (52%)	2/5 (40%)
Overall	1162/1307 (89%)	658/710 (93%)	405/463 (87%)	99/134 (74%)

7.1.4 Statistically unusual chemical shifts (i)

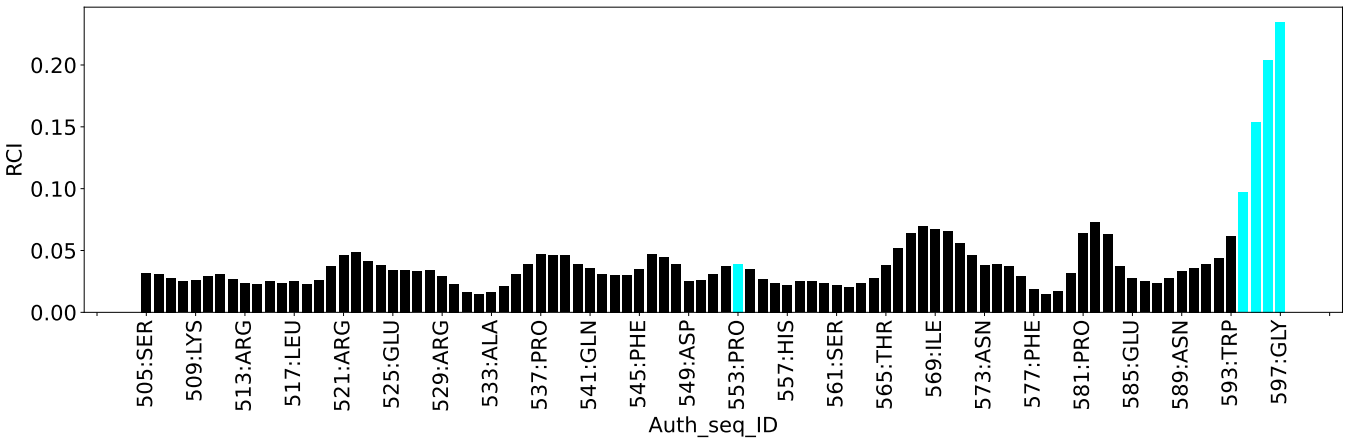
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	518	ARG	HB2	-0.03	0.52 – 3.08	-7.1
1	A	564	LYS	HB2	0.15	0.58 – 2.97	-6.8
1	A	545	PHE	HE1	5.24	5.56 – 8.62	-6.0
1	A	591	PHE	HZ	4.53	4.94 – 9.06	-6.0
1	A	545	PHE	HE2	5.24	5.54 – 8.63	-5.9
1	A	545	PHE	HZ	4.57	4.94 – 9.06	-5.9
1	A	553	PRO	HD2	1.71	1.93 – 5.38	-5.6
1	A	549	ASP	HA	2.93	3.04 – 6.12	-5.4
1	A	591	PHE	HE1	5.51	5.56 – 8.62	-5.1
1	A	591	PHE	HE2	5.51	5.54 – 8.63	-5.1

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.20
0.15
0.10
0.05
0.00
505:SER
509:LYS
513:ARG
517:LEU
521:ARG
525:GLU
529:ARG
533:ALA
537:PRO
541:GLN
545:PHE
549:ASP
553:PRO
557:HIS
561:SER
565:THR
569:ILE
573:ASN
577:PHE
581:PRO
585:GLU
589:ASN
593:TRP
597:GLY
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	1599
Intra-residue (|i-j|=0)	425
Sequential (|i-j|=1)	400
Medium range (|i-j|>1 and |i-j|<5)	167
Long range (|i-j|≥5)	565
Inter-chain	0
Hydrogen bond restraints	30
Disulfide bond restraints	12
Total dihedral-angle restraints	134
Number of unmapped restraints	0
Number of restraints per residue	18.6
Number of long range restraints per residue[1]	6.5

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.6	0.2
0.2-0.5 (Medium)	1.0	0.5
>0.5 (Large)	4.0	1.72

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.5	8.5
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

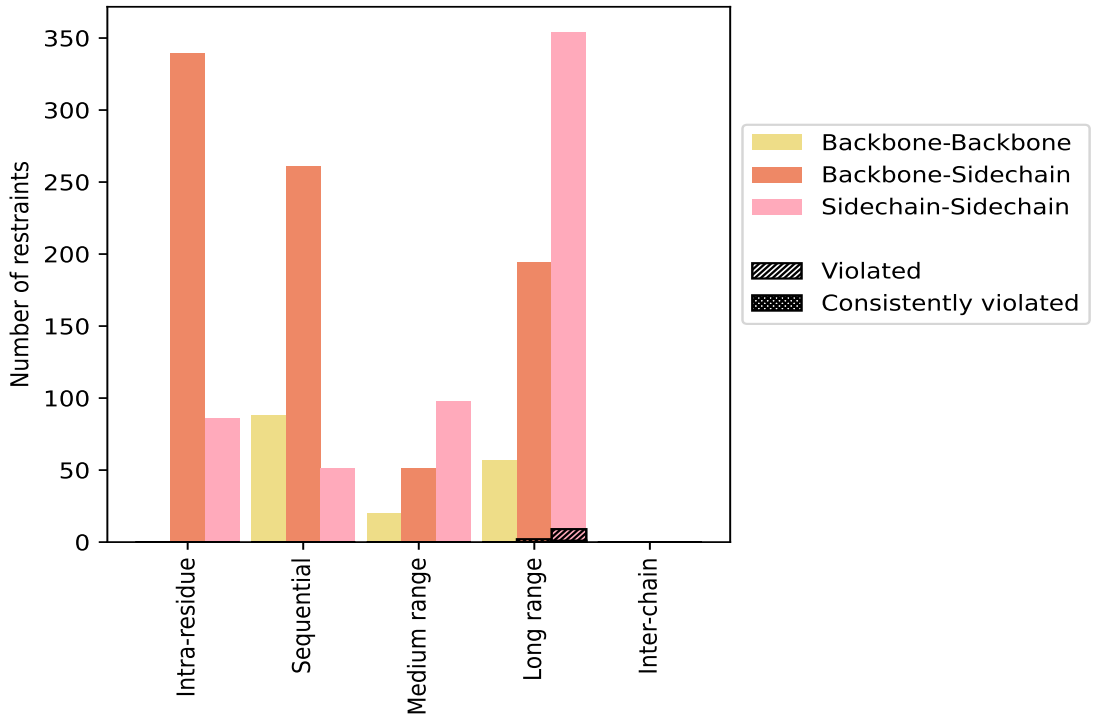
9.1 Summary of distance violations (i)

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)	425	26.6	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	339	21.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	86	5.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	400	25.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	88	5.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	261	16.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	51	3.2	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	167	10.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	20	1.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	51	3.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	96	6.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	565	35.3	11	1.9	0.7	1	0.2	0.1
Backbone-Backbone	27	1.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	194	12.1	2	1.0	0.1	0	0.0	0.0
Sidechain-Sidechain	344	21.5	9	2.6	0.6	1	0.3	0.1
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	30	1.9	0	0.0	0.0	0	0.0	0.0
Disulfide bond	12	0.8	0	0.0	0.0	0	0.0	0.0
Total	1599	100.0	11	0.7	0.7	1	0.1	0.1
Backbone-Backbone	165	10.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	845	52.8	2	0.2	0.1	0	0.0	0.0
Sidechain-Sidechain	589	36.8	9	1.5	0.6	1	0.2	0.1

[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	0	0	0	7	0	7	0.8	1.54	0.43	0.91
2	0	0	0	5	0	5	0.63	0.94	0.28	0.74
3	0	0	0	5	0	5	0.63	1.09	0.35	0.52
4	0	0	0	3	0	3	0.69	0.81	0.12	0.74
5	0	0	0	7	0	7	0.93	1.7	0.5	0.87
6	0	0	0	5	0	5	0.42	0.74	0.19	0.34
7	0	0	0	7	0	7	0.77	1.4	0.37	0.83
8	0	0	0	7	0	7	0.93	1.4	0.41	0.96
9	0	0	0	6	0	6	0.65	0.98	0.33	0.8
10	0	0	0	4	0	4	0.82	1.03	0.24	0.91
11	0	0	0	5	0	5	0.78	0.94	0.17	0.87

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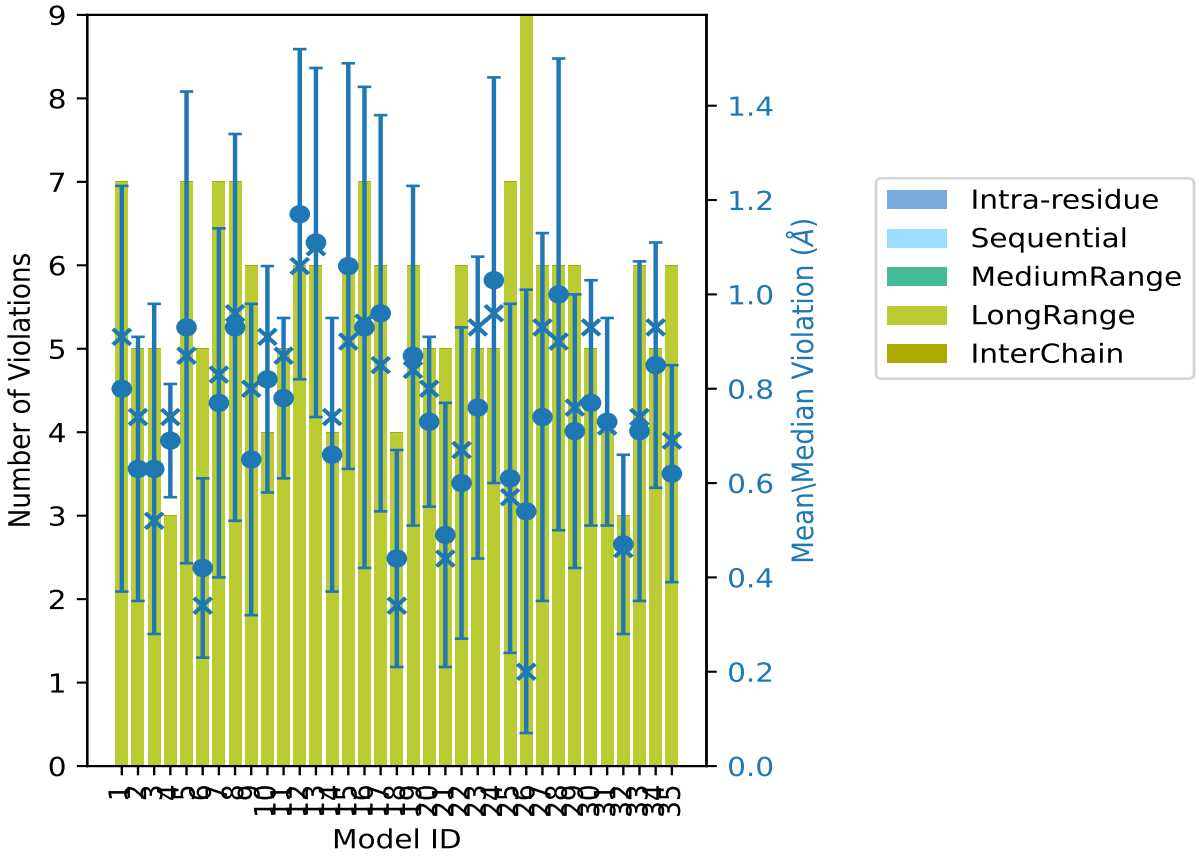
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	6	0	6	1.17	1.64	0.35	1.06
13	0	0	0	6	0	6	1.11	1.66	0.37	1.1
14	0	0	0	4	0	4	0.66	0.93	0.29	0.74
15	0	0	0	6	0	6	1.06	1.65	0.43	0.9
16	0	0	0	7	0	7	0.93	1.65	0.51	0.94
17	0	0	0	6	0	6	0.96	1.59	0.42	0.85
18	0	0	0	4	0	4	0.44	0.82	0.23	0.34
19	0	0	0	6	0	6	0.87	1.57	0.36	0.84
20	0	0	0	5	0	5	0.73	0.97	0.18	0.8
21	0	0	0	5	0	5	0.49	0.93	0.28	0.44
22	0	0	0	6	0	6	0.6	0.97	0.33	0.67
23	0	0	0	5	0	5	0.76	1.12	0.32	0.93
24	0	0	0	5	0	5	1.03	1.72	0.43	0.96
25	0	0	0	7	0	7	0.61	1.36	0.37	0.57
26	0	0	0	9	0	9	0.54	1.51	0.47	0.2
27	0	0	0	6	0	6	0.74	1.22	0.39	0.93
28	0	0	0	6	0	6	1.0	1.66	0.5	0.9
29	0	0	0	6	0	6	0.71	1.02	0.29	0.76
30	0	0	0	5	0	5	0.77	0.97	0.26	0.93
31	0	0	0	4	0	4	0.73	0.96	0.22	0.72
32	0	0	0	3	0	3	0.47	0.71	0.19	0.46
33	0	0	0	6	0	6	0.71	1.18	0.36	0.74
34	0	0	0	5	0	5	0.85	1.15	0.26	0.93
35	0	0	0	6	0	6	0.62	0.93	0.23	0.69

[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, 1546(IR:425, SQ:400, MR:167, LR:554, 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	0	0	2	0	2	1	2.9
0	0	0	1	0	1	2	5.7
0	0	0	0	0	0	3	8.6
0	0	0	1	0	1	4	11.4
0	0	0	0	0	0	5	14.3
0	0	0	0	0	0	6	17.1

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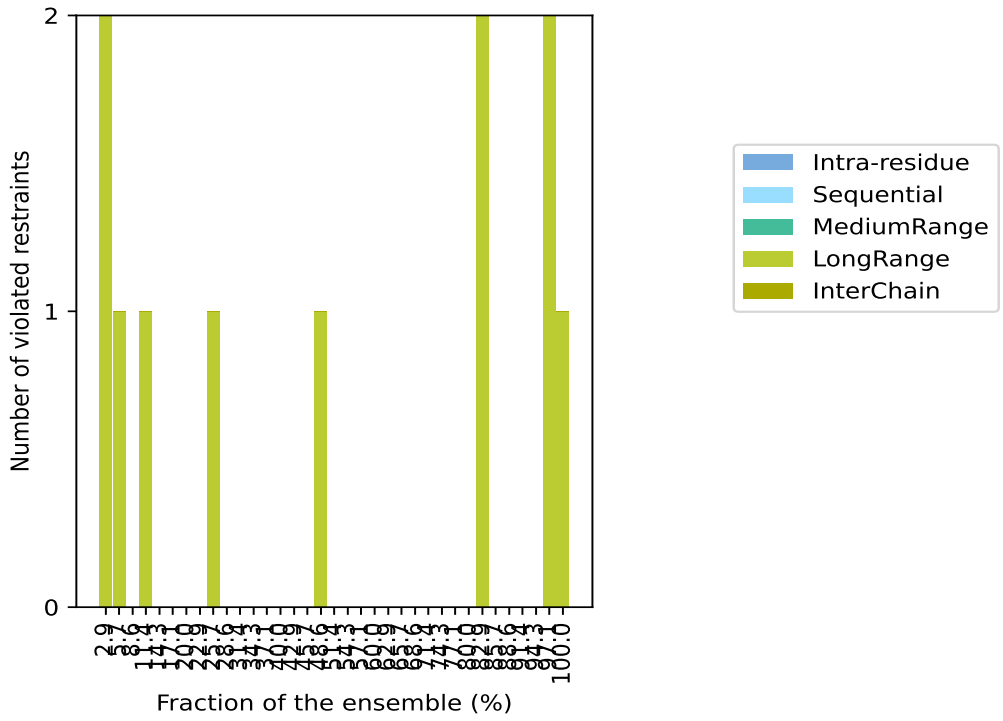
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	20.0
0	0	0	0	0	0	8	22.9
0	0	0	1	0	1	9	25.7
0	0	0	0	0	0	10	28.6
0	0	0	0	0	0	11	31.4
0	0	0	0	0	0	12	34.3
0	0	0	0	0	0	13	37.1
0	0	0	0	0	0	14	40.0
0	0	0	0	0	0	15	42.9
0	0	0	0	0	0	16	45.7
0	0	0	1	0	1	17	48.6
0	0	0	0	0	0	18	51.4
0	0	0	0	0	0	19	54.3
0	0	0	0	0	0	20	57.1
0	0	0	0	0	0	21	60.0
0	0	0	0	0	0	22	62.9
0	0	0	0	0	0	23	65.7
0	0	0	0	0	0	24	68.6
0	0	0	0	0	0	25	71.4
0	0	0	0	0	0	26	74.3
0	0	0	0	0	0	27	77.1
0	0	0	0	0	0	28	80.0
0	0	0	2	0	2	29	82.9
0	0	0	0	0	0	30	85.7
0	0	0	0	0	0	31	88.6
0	0	0	0	0	0	32	91.4
0	0	0	0	0	0	33	94.3
0	0	0	2	0	2	34	97.1
0	0	0	1	0	1	35	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

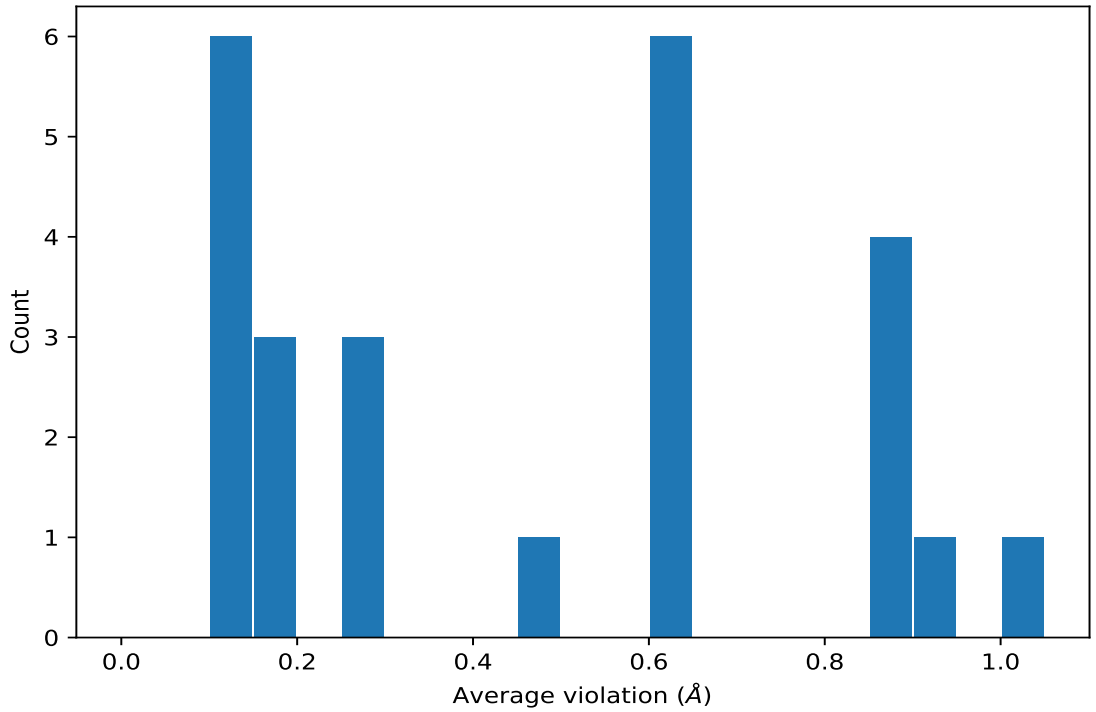
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (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)
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	35	0.89	0.07	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	35	0.89	0.07	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	35	0.89	0.07	0.93
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	34	1.0	0.42	0.96
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	34	0.61	0.24	0.55
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	34	0.61	0.24	0.55
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	34	0.61	0.24	0.55
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	34	0.61	0.24	0.55
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	34	0.61	0.24	0.55
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	34	0.61	0.24	0.55
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	29	0.95	0.45	0.92
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	29	0.87	0.41	0.86
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	17	0.49	0.28	0.47
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	9	0.26	0.15	0.19
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	9	0.26	0.15	0.19
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	9	0.26	0.15	0.19

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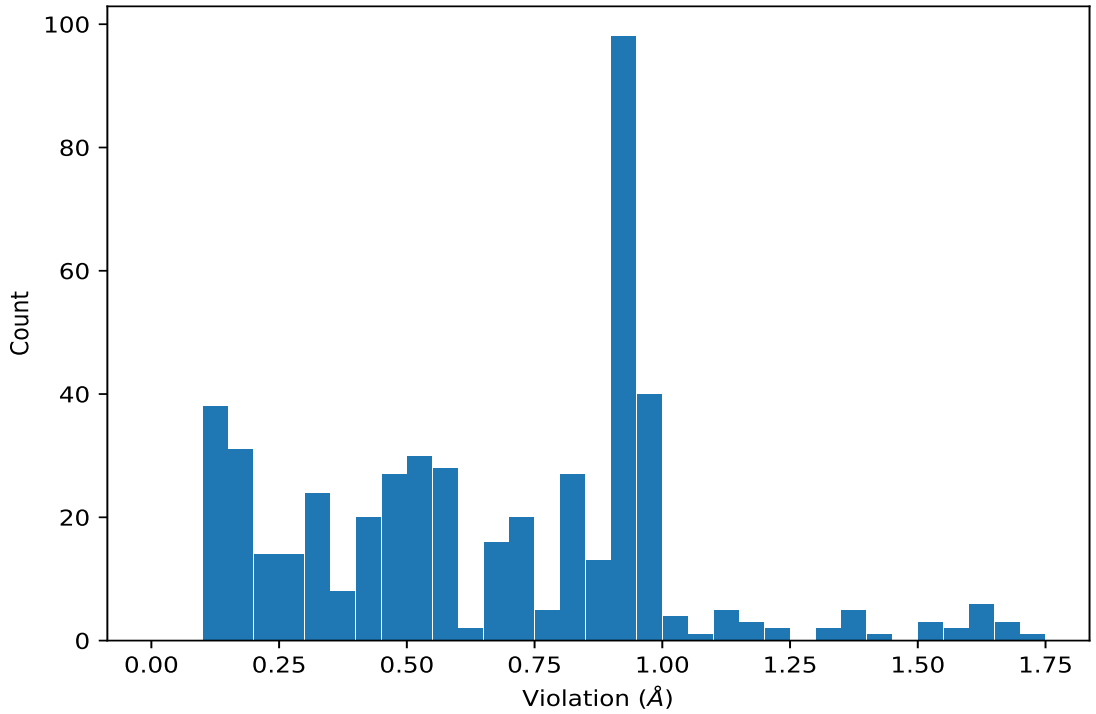
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1234)	1:A:507:LEU:HD11	1:A:515:CYS:H	4	0.13	0.01	0.12
(1,1234)	1:A:507:LEU:HD12	1:A:515:CYS:H	4	0.13	0.01	0.12
(1,1234)	1:A:507:LEU:HD13	1:A:515:CYS:H	4	0.13	0.01	0.12
(1,1234)	1:A:507:LEU:HD21	1:A:515:CYS:H	4	0.13	0.01	0.12
(1,1234)	1:A:507:LEU:HD22	1:A:515:CYS:H	4	0.13	0.01	0.12
(1,1234)	1:A:507:LEU:HD23	1:A:515:CYS:H	4	0.13	0.01	0.12
(1,867)	1:A:517:LEU:HD21	1:A:530:GLN:HE21	2	0.18	0.01	0.18
(1,867)	1:A:517:LEU:HD22	1:A:530:GLN:HE21	2	0.18	0.01	0.18
(1,867)	1:A:517:LEU:HD23	1:A:530:GLN:HE21	2	0.18	0.01	0.18

[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

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)
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	24	1.72
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	5	1.7
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	28	1.66
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	13	1.66
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	15	1.65
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	16	1.65
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	15	1.64
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	12	1.64
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	12	1.63
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	28	1.6
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	17	1.59
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	19	1.57
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	1	1.54
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	16	1.52
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	26	1.51
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	17	1.45
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	7	1.4
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	8	1.4
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	8	1.38
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	13	1.36
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	25	1.36
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	5	1.31
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	5	1.3
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	27	1.22
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	13	1.21
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	12	1.19
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	33	1.18
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	24	1.17
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	34	1.15
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	23	1.12
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	8	1.11
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	1	1.11
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	7	1.1
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	3	1.09
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	10	1.03
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	29	1.02
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	23	1.01
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	33	1.0
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	15	0.98
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	16	0.98
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	9	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	13	0.98
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	22	0.97
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	30	0.97
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	20	0.97
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	20	0.97
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	20	0.97
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	20	0.97
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	20	0.97
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	20	0.97
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	31	0.96
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	13	0.96
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	13	0.96
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	13	0.96
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	8	0.96
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	8	0.96
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	8	0.96
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	8	0.96
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	8	0.96
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	8	0.96
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	24	0.96
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	24	0.96
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	24	0.96
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	24	0.96
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	24	0.96
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	24	0.96
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	30	0.96
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	30	0.96
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	30	0.96
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	30	0.96
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	30	0.96
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	30	0.96
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	34	0.96
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	34	0.96
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	34	0.96
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	34	0.96
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	34	0.96
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	34	0.96
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	27	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	2	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	2	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	2	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	11	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	11	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	11	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	16	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	16	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	16	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	19	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	19	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	19	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	26	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	26	0.94
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	26	0.94
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	11	0.93
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	16	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	1	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	1	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	1	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	3	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	3	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	3	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	8	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	8	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	8	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	9	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	9	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	9	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	10	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	10	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	10	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	12	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	12	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	12	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	14	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	14	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	14	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	17	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	17	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	17	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	21	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	21	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	21	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	22	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	22	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	22	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	23	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	23	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	23	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	24	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	24	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	24	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	27	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	27	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	27	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	28	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	28	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	28	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	29	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	29	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	29	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	30	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	30	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	30	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	31	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	31	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	31	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	33	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	33	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	33	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	34	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	34	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	34	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	35	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	35	0.93
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	35	0.93
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	27	0.93
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	27	0.93
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	27	0.93
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	27	0.93
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	27	0.93
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	27	0.93
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	14	0.92
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	12	0.92
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	12	0.92
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	12	0.92
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	12	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	12	0.92
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	12	0.92
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	1	0.91
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	26	0.9
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	26	0.9
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	26	0.9
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	26	0.9
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	26	0.9
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	26	0.9
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	10	0.89
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	28	0.88
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	9	0.87
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	5	0.87
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	5	0.87
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	5	0.87
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	11	0.87
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	11	0.87
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	11	0.87
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	11	0.87
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	11	0.87
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	11	0.87
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	7	0.86
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	19	0.84
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	20	0.84
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	34	0.84
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	19	0.84
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	19	0.84
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	19	0.84
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	19	0.84
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	19	0.84
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	19	0.84
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	7	0.83
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	7	0.83
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	7	0.83
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	18	0.82
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	18	0.82
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	18	0.82
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	15	0.81
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	15	0.81
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	15	0.81
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	4	0.81
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	4	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	4	0.81
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	4	0.81
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	4	0.81
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	4	0.81
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	20	0.8
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	20	0.8
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	20	0.8
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	29	0.78
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	2	0.77
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	17	0.77
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	35	0.77
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	35	0.75
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	9	0.74
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	2	0.74
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	25	0.74
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	12	0.74
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	4	0.74
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	4	0.74
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	4	0.74
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	6	0.74
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	6	0.74
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	6	0.74
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	29	0.73
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	26	0.72
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	15	0.72
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	28	0.71
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	25	0.71
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	25	0.71
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	25	0.71
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB1	32	0.71
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB2	32	0.71
(1,276)	1:A:576:ASN:HD21	1:A:594:ALA:HB3	32	0.71
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	5	0.7
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	22	0.69
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	11	0.68
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	29	0.68
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	29	0.68
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	29	0.68
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	29	0.68
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	29	0.68
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	29	0.68
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	30	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	22	0.65
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	22	0.65
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	22	0.65
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	22	0.65
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	22	0.65
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	22	0.65
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	35	0.63
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	21	0.62
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	2	0.58
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	2	0.58
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	2	0.58
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	2	0.58
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	2	0.58
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	2	0.58
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	15	0.58
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	15	0.58
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	15	0.58
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	15	0.58
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	15	0.58
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	15	0.58
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	17	0.57
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	25	0.57
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	25	0.57
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	25	0.57
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	25	0.57
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	25	0.57
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	25	0.57
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	20	0.56
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	14	0.56
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	7	0.56
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	7	0.56
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	7	0.56
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	7	0.56
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	7	0.56
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	7	0.56
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	19	0.55
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	8	0.54
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	33	0.54
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	33	0.54
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	33	0.54
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	33	0.54
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	33	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	33	0.54
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	1	0.53
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	1	0.53
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	1	0.53
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	1	0.53
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	1	0.53
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	1	0.53
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	6	0.53
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	6	0.53
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	6	0.53
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	6	0.53
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	6	0.53
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	6	0.53
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	3	0.52
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	4	0.52
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	4	0.52
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	4	0.52
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	31	0.51
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	31	0.5
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	31	0.5
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	31	0.5
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	31	0.5
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	31	0.5
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	31	0.5
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	11	0.49
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	25	0.49
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	25	0.49
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	25	0.49
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	3	0.49
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	3	0.49
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	3	0.49
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	3	0.49
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	3	0.49
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	3	0.49
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	20	0.48
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	13	0.48
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	13	0.48
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	13	0.48
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	13	0.48
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	13	0.48
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	13	0.48
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	33	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	1	0.47
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	19	0.47
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	17	0.47
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	17	0.47
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	17	0.47
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	17	0.47
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	17	0.47
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	17	0.47
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	32	0.46
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	21	0.44
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	5	0.44
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	5	0.44
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	5	0.44
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	5	0.44
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	5	0.44
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	5	0.44
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	18	0.42
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	18	0.42
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	18	0.42
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	18	0.42
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	18	0.42
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	18	0.42
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	23	0.41
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	10	0.41
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	10	0.41
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	10	0.41
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	10	0.41
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	10	0.41
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	10	0.41
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	24	0.39
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	34	0.38
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	35	0.38
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	35	0.38
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	35	0.38
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	35	0.38
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	35	0.38
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	35	0.38
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	7	0.35
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	16	0.35
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	16	0.35
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	16	0.35
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	16	0.35
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	16	0.35
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	6	0.34
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	23	0.34
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	23	0.34
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	23	0.34
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	23	0.34
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	23	0.34
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	23	0.34
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	6	0.32
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	7	0.32
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	7	0.32
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	7	0.32
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	21	0.32
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	21	0.32
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	21	0.32
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	21	0.32
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	21	0.32
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	21	0.32
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	30	0.3
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	27	0.29
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	35	0.28
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	35	0.28
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	35	0.28
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	9	0.28
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	9	0.28
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	9	0.28
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	9	0.28
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	9	0.28
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	9	0.28
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	18	0.27
(1,545)	1:A:530:GLN:HE22	1:A:563:MET:HB2	18	0.26
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	25	0.25
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	32	0.24
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	28	0.24
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	28	0.24
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	28	0.24
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	28	0.24
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	28	0.24
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	28	0.24
(1,1313)	1:A:519:VAL:HG11	1:A:530:GLN:HE21	14	0.23
(1,1313)	1:A:519:VAL:HG12	1:A:530:GLN:HE21	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:A:519:VAL:HG13	1:A:530:GLN:HE21	14	0.23
(1,1313)	1:A:519:VAL:HG21	1:A:530:GLN:HE21	14	0.23
(1,1313)	1:A:519:VAL:HG22	1:A:530:GLN:HE21	14	0.23
(1,1313)	1:A:519:VAL:HG23	1:A:530:GLN:HE21	14	0.23
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	26	0.2
(1,867)	1:A:517:LEU:HD21	1:A:530:GLN:HE21	8	0.19
(1,867)	1:A:517:LEU:HD22	1:A:530:GLN:HE21	8	0.19
(1,867)	1:A:517:LEU:HD23	1:A:530:GLN:HE21	8	0.19
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	5	0.19
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	5	0.19
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	5	0.19
(1,1232)	1:A:507:LEU:HD11	1:A:514:ARG:HG2	26	0.19
(1,1232)	1:A:507:LEU:HD11	1:A:514:ARG:HG3	26	0.19
(1,1232)	1:A:507:LEU:HD12	1:A:514:ARG:HG2	26	0.19
(1,1232)	1:A:507:LEU:HD12	1:A:514:ARG:HG3	26	0.19
(1,1232)	1:A:507:LEU:HD13	1:A:514:ARG:HG2	26	0.19
(1,1232)	1:A:507:LEU:HD13	1:A:514:ARG:HG3	26	0.19
(1,1232)	1:A:507:LEU:HD21	1:A:514:ARG:HG2	26	0.19
(1,1232)	1:A:507:LEU:HD21	1:A:514:ARG:HG3	26	0.19
(1,1232)	1:A:507:LEU:HD22	1:A:514:ARG:HG2	26	0.19
(1,1232)	1:A:507:LEU:HD22	1:A:514:ARG:HG3	26	0.19
(1,1232)	1:A:507:LEU:HD23	1:A:514:ARG:HG2	26	0.19
(1,1232)	1:A:507:LEU:HD23	1:A:514:ARG:HG3	26	0.19
(1,551)	1:A:530:GLN:HE22	1:A:563:MET:HG2	6	0.18
(1,867)	1:A:517:LEU:HD21	1:A:530:GLN:HE21	22	0.17
(1,867)	1:A:517:LEU:HD22	1:A:530:GLN:HE21	22	0.17
(1,867)	1:A:517:LEU:HD23	1:A:530:GLN:HE21	22	0.17
(1,552)	1:A:519:VAL:HG11	1:A:530:GLN:HB2	26	0.17
(1,552)	1:A:519:VAL:HG11	1:A:530:GLN:HB3	26	0.17
(1,552)	1:A:519:VAL:HG12	1:A:530:GLN:HB2	26	0.17
(1,552)	1:A:519:VAL:HG12	1:A:530:GLN:HB3	26	0.17
(1,552)	1:A:519:VAL:HG13	1:A:530:GLN:HB2	26	0.17
(1,552)	1:A:519:VAL:HG13	1:A:530:GLN:HB3	26	0.17
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	22	0.16
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	22	0.16
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	22	0.16
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	25	0.15
(1,1234)	1:A:507:LEU:HD11	1:A:515:CYS:H	16	0.15
(1,1234)	1:A:507:LEU:HD12	1:A:515:CYS:H	16	0.15
(1,1234)	1:A:507:LEU:HD13	1:A:515:CYS:H	16	0.15
(1,1234)	1:A:507:LEU:HD21	1:A:515:CYS:H	16	0.15
(1,1234)	1:A:507:LEU:HD22	1:A:515:CYS:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1234)	1:A:507:LEU:HD23	1:A:515:CYS:H	16	0.15
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	33	0.13
(1,1234)	1:A:507:LEU:HD11	1:A:515:CYS:H	1	0.13
(1,1234)	1:A:507:LEU:HD12	1:A:515:CYS:H	1	0.13
(1,1234)	1:A:507:LEU:HD13	1:A:515:CYS:H	1	0.13
(1,1234)	1:A:507:LEU:HD21	1:A:515:CYS:H	1	0.13
(1,1234)	1:A:507:LEU:HD22	1:A:515:CYS:H	1	0.13
(1,1234)	1:A:507:LEU:HD23	1:A:515:CYS:H	1	0.13
(1,86)	1:A:530:GLN:HE22	1:A:563:MET:H	26	0.12
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	27	0.12
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	9	0.12
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	9	0.12
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	9	0.12
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	21	0.12
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	21	0.12
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	21	0.12
(1,1234)	1:A:507:LEU:HD11	1:A:515:CYS:H	26	0.12
(1,1234)	1:A:507:LEU:HD12	1:A:515:CYS:H	26	0.12
(1,1234)	1:A:507:LEU:HD13	1:A:515:CYS:H	26	0.12
(1,1234)	1:A:507:LEU:HD21	1:A:515:CYS:H	26	0.12
(1,1234)	1:A:507:LEU:HD22	1:A:515:CYS:H	26	0.12
(1,1234)	1:A:507:LEU:HD23	1:A:515:CYS:H	26	0.12
(1,542)	1:A:530:GLN:HE22	1:A:563:MET:HB3	29	0.11
(1,522)	1:A:565:THR:HG21	1:A:576:ASN:HD22	3	0.11
(1,522)	1:A:565:THR:HG22	1:A:576:ASN:HD22	3	0.11
(1,522)	1:A:565:THR:HG23	1:A:576:ASN:HD22	3	0.11
(1,1234)	1:A:507:LEU:HD11	1:A:515:CYS:H	2	0.11
(1,1234)	1:A:507:LEU:HD12	1:A:515:CYS:H	2	0.11
(1,1234)	1:A:507:LEU:HD13	1:A:515:CYS:H	2	0.11
(1,1234)	1:A:507:LEU:HD21	1:A:515:CYS:H	2	0.11
(1,1234)	1:A:507:LEU:HD22	1:A:515:CYS:H	2	0.11
(1,1234)	1:A:507:LEU:HD23	1:A:515:CYS:H	2	0.11

10 Dihedral-angle violation analysis

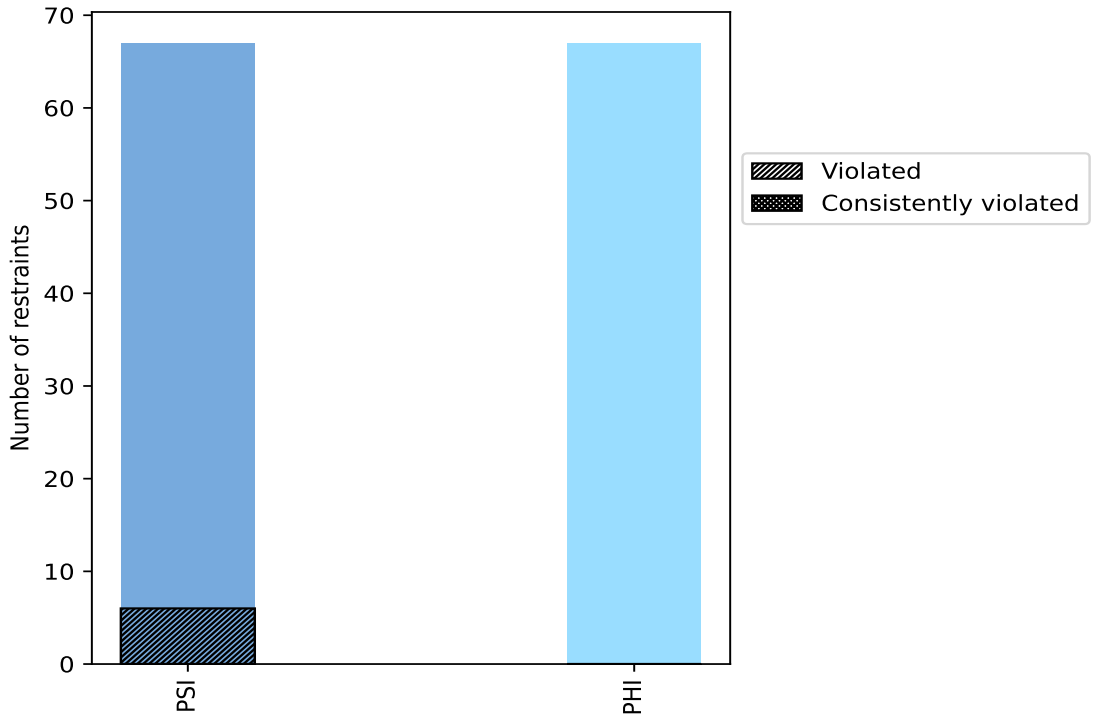
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	67	50.0	6	9.0	4.5	0	0.0	0.0
PHI	67	50.0	0	0.0	0.0	0	0.0	0.0
Total	134	100.0	6	4.5	4.5	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



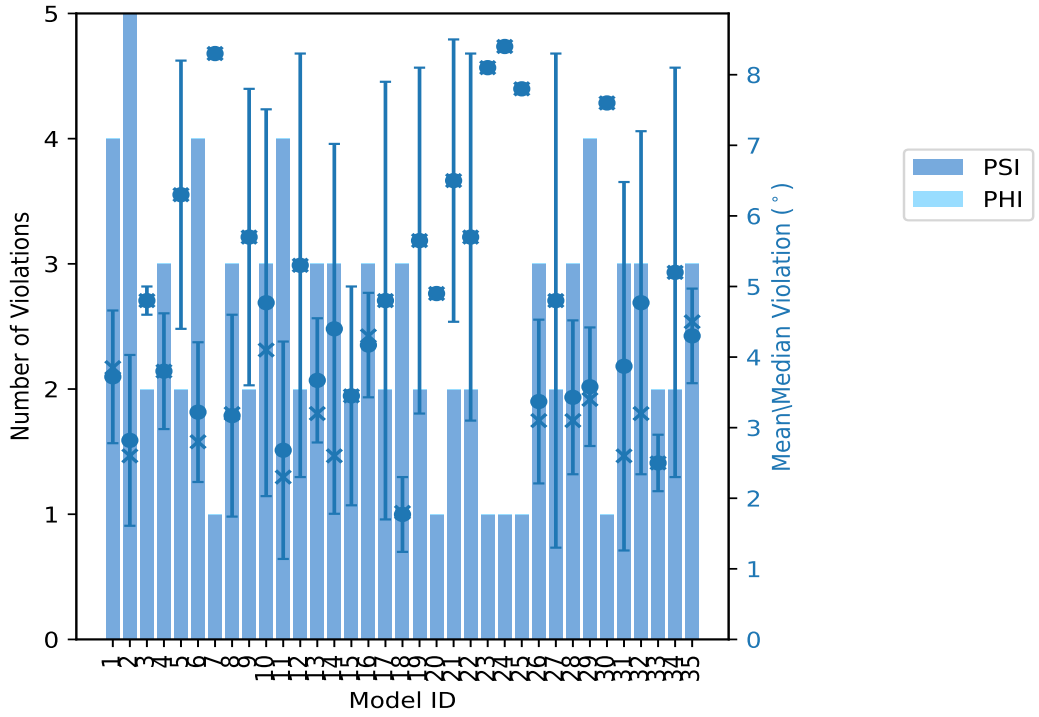
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	4	0	4	3.72	4.8	0.94	3.85
2	5	0	5	2.82	4.9	1.21	2.6
3	2	0	2	4.8	5.0	0.2	4.8
4	3	0	3	3.8	4.8	0.82	3.8
5	2	0	2	6.3	8.2	1.9	6.3
6	4	0	4	3.22	4.9	0.99	2.8
7	1	0	1	8.3	8.3	0.0	8.3
8	3	0	3	3.17	4.9	1.43	3.2
9	2	0	2	5.7	7.8	2.1	5.7
10	3	0	3	4.77	8.4	2.74	4.1
11	4	0	4	2.68	5.0	1.54	2.3
12	2	0	2	5.3	8.3	3.0	5.3
13	3	0	3	3.67	4.9	0.88	3.2
14	3	0	3	4.4	8.1	2.62	2.6
15	2	0	2	3.45	5.0	1.55	3.45
16	3	0	3	4.17	5.0	0.74	4.3
17	2	0	2	4.8	7.9	3.1	4.8
18	3	0	3	1.77	2.4	0.53	1.8
19	2	0	2	5.65	8.1	2.45	5.65
20	1	0	1	4.9	4.9	0.0	4.9
21	2	0	2	6.5	8.5	2.0	6.5
22	2	0	2	5.7	8.3	2.6	5.7
23	1	0	1	8.1	8.1	0.0	8.1
24	1	0	1	8.4	8.4	0.0	8.4
25	1	0	1	7.8	7.8	0.0	7.8
26	3	0	3	3.37	4.9	1.16	3.1
27	2	0	2	4.8	8.3	3.5	4.8
28	3	0	3	3.43	4.9	1.09	3.1
29	4	0	4	3.58	4.9	0.84	3.4
30	1	0	1	7.6	7.6	0.0	7.6
31	3	0	3	3.87	7.5	2.61	2.6
32	3	0	3	4.77	8.2	2.43	3.2
33	2	0	2	2.5	2.9	0.4	2.5
34	2	0	2	5.2	8.1	2.9	5.2
35	3	0	3	4.3	5.0	0.67	4.5

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	0	1	1	2.9
0	0	0	2	5.7
0	0	0	3	8.6
1	0	1	4	11.4
0	0	0	5	14.3
0	0	0	6	17.1
0	0	0	7	20.0
0	0	0	8	22.9
0	0	0	9	25.7
0	0	0	10	28.6
0	0	0	11	31.4

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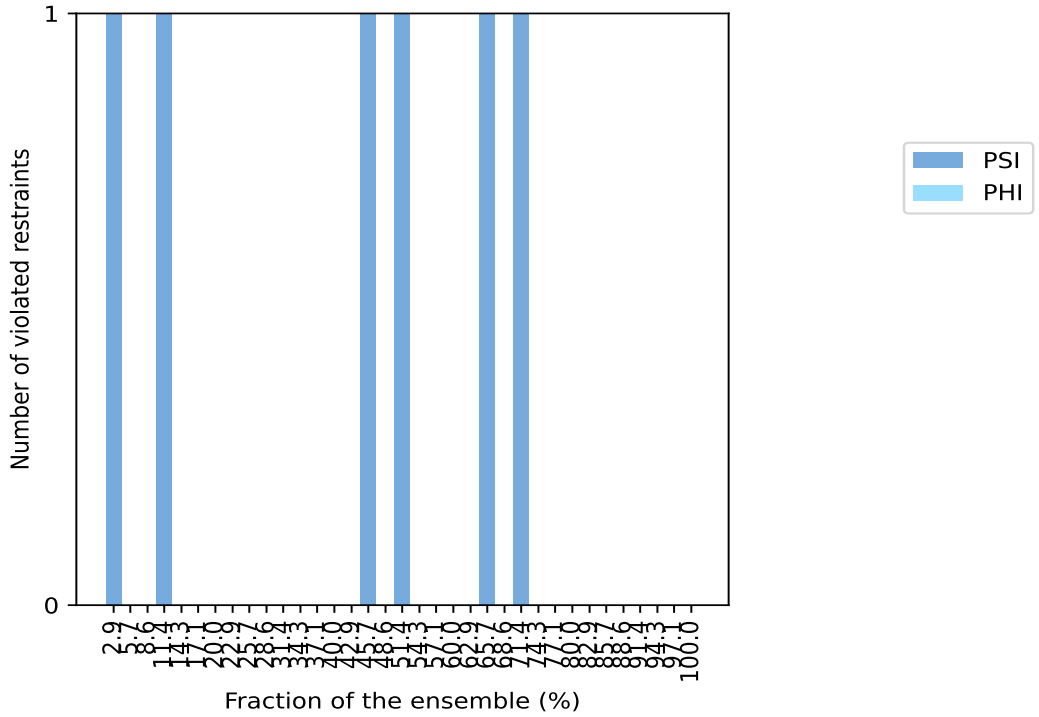
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	34.3
0	0	0	13	37.1
0	0	0	14	40.0
0	0	0	15	42.9
1	0	1	16	45.7
0	0	0	17	48.6
1	0	1	18	51.4
0	0	0	19	54.3
0	0	0	20	57.1
0	0	0	21	60.0
0	0	0	22	62.9
1	0	1	23	65.7
0	0	0	24	68.6
1	0	1	25	71.4
0	0	0	26	74.3
0	0	0	27	77.1
0	0	0	28	80.0
0	0	0	29	82.9
0	0	0	30	85.7
0	0	0	31	88.6
0	0	0	32	91.4
0	0	0	33	94.3
0	0	0	34	97.1
0	0	0	35	100.0

[1] Number of models with violations

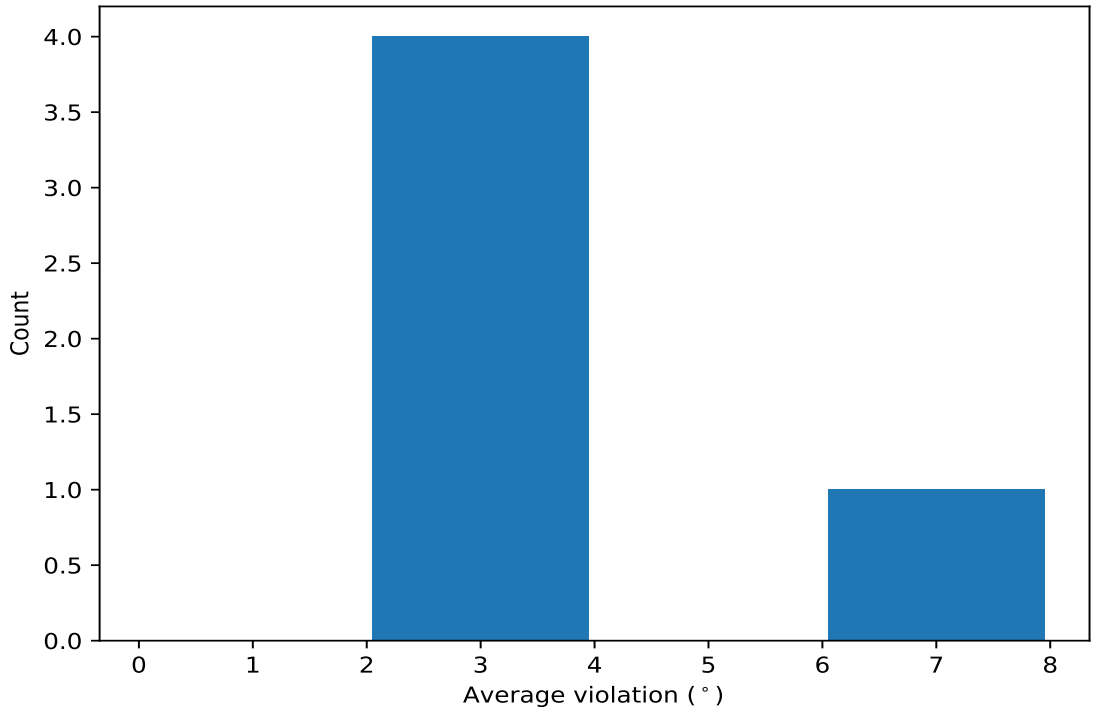
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

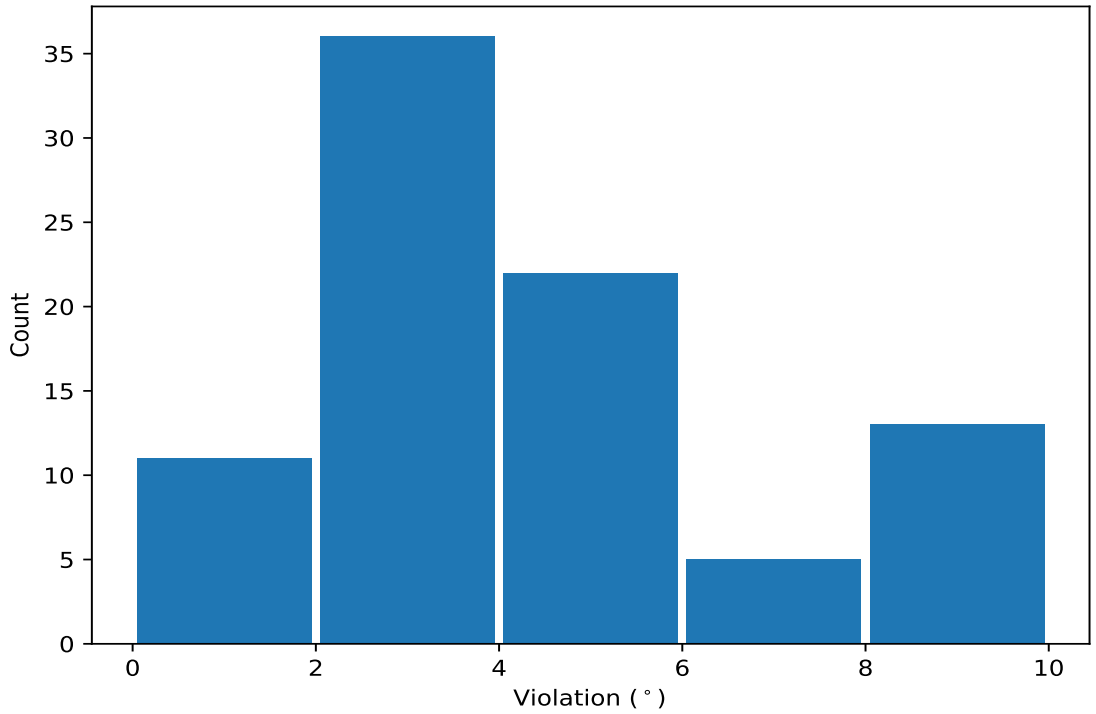
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	25	6.37	2.8	8.1
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	23	3.4	1.32	3.6
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	18	3.8	1.34	4.55
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	16	3.09	0.19	3.1
(1,78)	1:A:555:CYS:N	1:A:555:CYS:CA	1:A:555:CYS:C	1:A:556:LYS:N	4	2.35	0.05	2.35

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	21	8.5
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	10	8.4
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	24	8.4
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	7	8.3
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	12	8.3
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	22	8.3
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	27	8.3
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	5	8.2
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	32	8.2
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	14	8.1
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	19	8.1
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	23	8.1
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	34	8.1
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	17	7.9
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	9	7.8
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	25	7.8
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	30	7.6
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	31	7.5
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	15	5.0
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	16	5.0
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	3	5.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	11	5.0
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	35	5.0
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	8	4.9
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	20	4.9
(1,36)	1:A:527:LYS:N	1:A:527:LYS:CA	1:A:527:LYS:C	1:A:528:GLY:N	29	4.9
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	2	4.9
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	6	4.9
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	13	4.9
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	26	4.9
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	28	4.9
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	4	4.8
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	1	4.8
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	3	4.6
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	21	4.5
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	35	4.5
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	1	4.4
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	5	4.4
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	16	4.3
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	10	4.1
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	4	3.8
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	29	3.6
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	9	3.6
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	35	3.4
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	1	3.3
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	8	3.2
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	13	3.2
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	16	3.2
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	19	3.2
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	29	3.2
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	32	3.2
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	2	3.1
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	11	3.1
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	22	3.1
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	26	3.1
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	28	3.1
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	6	3.0
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	32	2.9
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	13	2.9
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	33	2.9
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	4	2.8
(1,80)	1:A:557:HIS:N	1:A:557:HIS:CA	1:A:557:HIS:C	1:A:558:GLY:N	14	2.6
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	2	2.6
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	6	2.6
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	31	2.6
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	29	2.6
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	14	2.5
(1,78)	1:A:555:CYS:N	1:A:555:CYS:CA	1:A:555:CYS:C	1:A:556:LYS:N	6	2.4
(1,78)	1:A:555:CYS:N	1:A:555:CYS:CA	1:A:555:CYS:C	1:A:556:LYS:N	18	2.4
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	1	2.4
(1,78)	1:A:555:CYS:N	1:A:555:CYS:CA	1:A:555:CYS:C	1:A:556:LYS:N	2	2.3
(1,78)	1:A:555:CYS:N	1:A:555:CYS:CA	1:A:555:CYS:C	1:A:556:LYS:N	34	2.3

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	12	2.3
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	28	2.3
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	26	2.1
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	33	2.1
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	15	1.9
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	10	1.8
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	18	1.8
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	17	1.7
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	31	1.5
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	11	1.5
(1,18)	1:A:515:CYS:N	1:A:515:CYS:CA	1:A:515:CYS:C	1:A:516:VAL:N	8	1.4
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	27	1.3
(1,112)	1:A:579:VAL:N	1:A:579:VAL:CA	1:A:579:VAL:C	1:A:580:CYS:N	2	1.2
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	11	1.1
(1,4)	1:A:508:CYS:N	1:A:508:CYS:CA	1:A:508:CYS:C	1:A:509:LYS:N	18	1.1