



Full wwPDB NMR Structure Validation Report ⓘ

Jul 18, 2023 – 10:09 AM JST

PDB ID : 7YB4
BMRB ID : 51157
Title : Solution structure of homeodomain of EXTRADENTICLE
Authors : Acharya, B.; Basak, A.J.; Lee, W.; De, S.
Deposited on : 2022-06-28

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 ⓘ 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 ⓘ](#)) 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) : 2.34

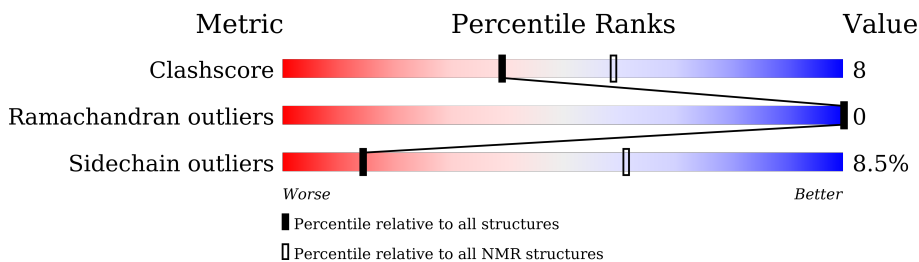
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	67	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:246-A:296 (51)	0.42	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, 4, 5, 6, 8, 10, 11, 12, 17, 18
2	2, 3, 7, 14, 15, 16, 19, 20
Single-model clusters	9; 13

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1120 atoms, of which 559 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Homeobox protein extradenticle.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	67	1120	350	559	108	101	2	0

There are 4 discrepancies between the modelled and reference sequences:

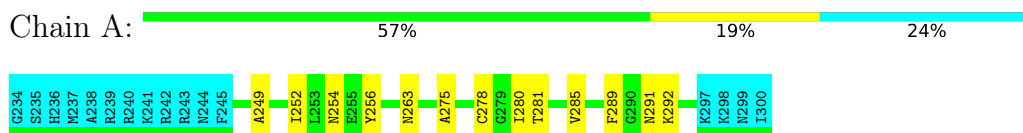
Chain	Residue	Modelled	Actual	Comment	Reference
A	234	GLY	-	expression tag	UNP P40427
A	235	SER	-	expression tag	UNP P40427
A	236	HIS	-	expression tag	UNP P40427
A	237	MET	-	expression tag	UNP P40427

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: Homeobox protein extradenticle

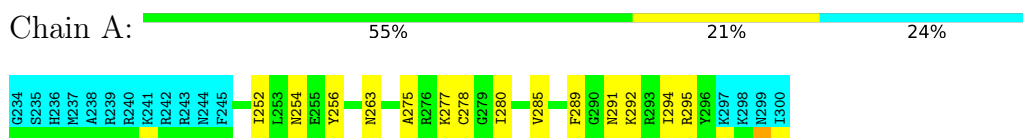


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

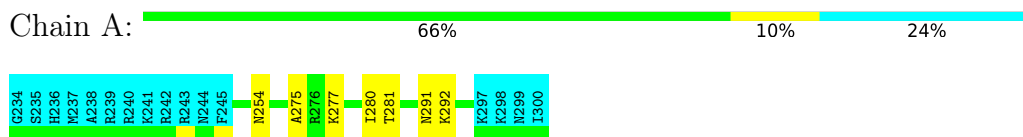
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Homeobox protein extradenticle



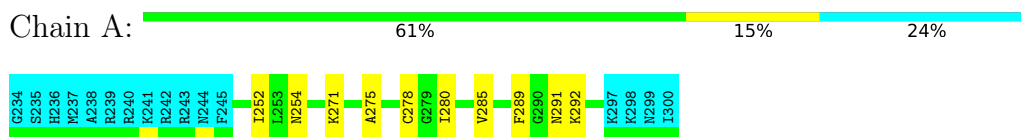
4.2.2 Score per residue for model 2

- Molecule 1: Homeobox protein extradenticle



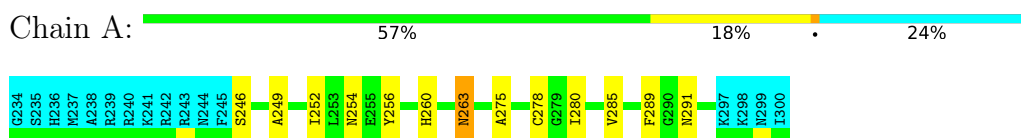
4.2.3 Score per residue for model 3

- Molecule 1: Homeobox protein extradenticle



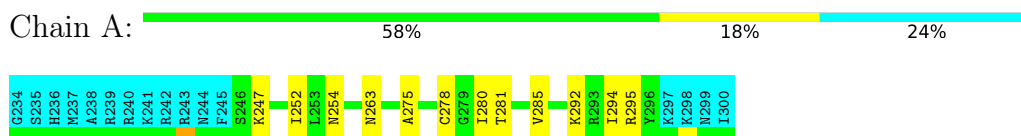
4.2.4 Score per residue for model 4

- Molecule 1: Homeobox protein extradenticle



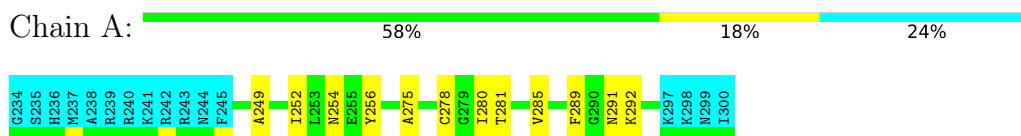
4.2.5 Score per residue for model 5

- Molecule 1: Homeobox protein extradenticle



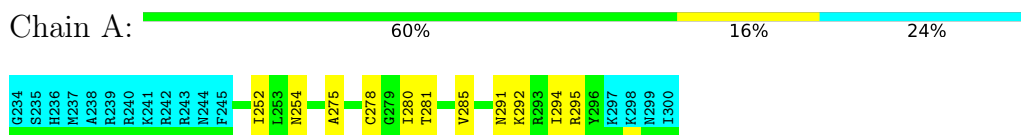
4.2.6 Score per residue for model 6

- Molecule 1: Homeobox protein extradenticle



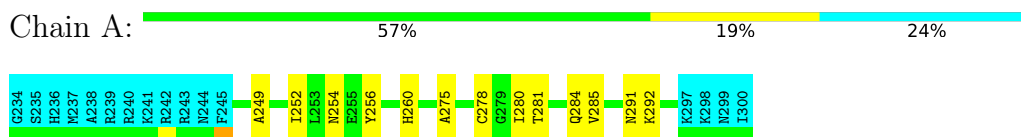
4.2.7 Score per residue for model 7

- Molecule 1: Homeobox protein extradenticle



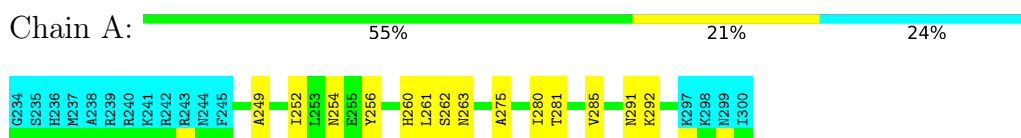
4.2.8 Score per residue for model 8

- Molecule 1: Homeobox protein extradenticle



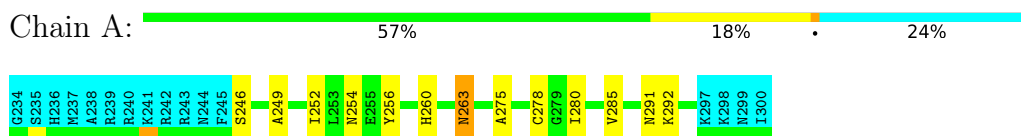
4.2.9 Score per residue for model 9

- Molecule 1: Homeobox protein extradenticle



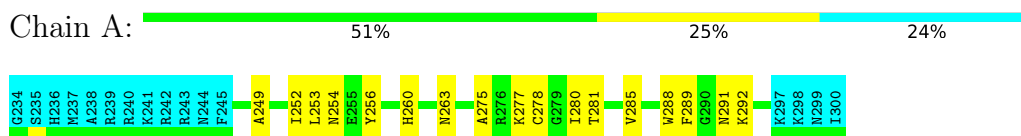
4.2.10 Score per residue for model 10

- Molecule 1: Homeobox protein extradenticle



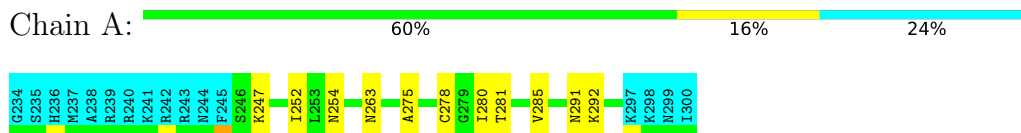
4.2.11 Score per residue for model 11

- Molecule 1: Homeobox protein extradenticle



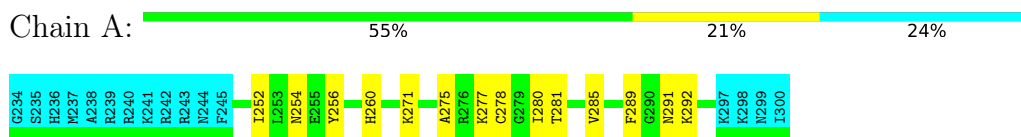
4.2.12 Score per residue for model 12

- Molecule 1: Homeobox protein extradenticle



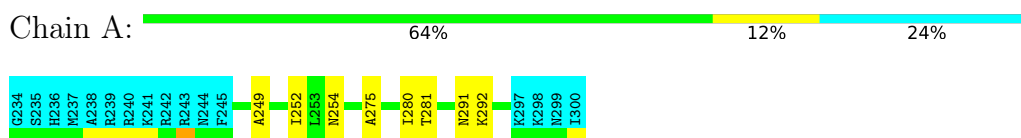
4.2.13 Score per residue for model 13

- Molecule 1: Homeobox protein extradenticle



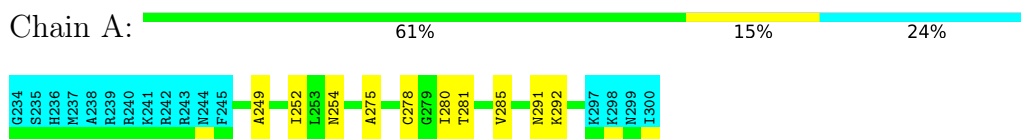
4.2.14 Score per residue for model 14

- Molecule 1: Homeobox protein extradenticle



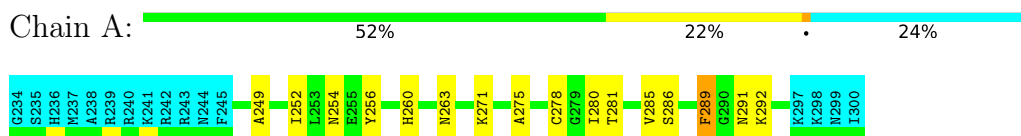
4.2.15 Score per residue for model 15

- Molecule 1: Homeobox protein extradenticle



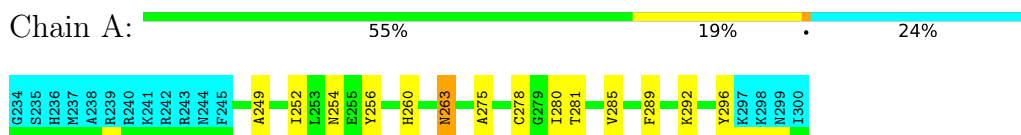
4.2.16 Score per residue for model 16

- Molecule 1: Homeobox protein extradenticle



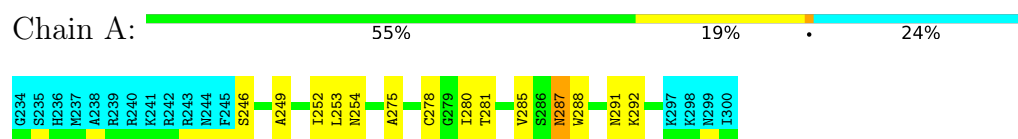
4.2.17 Score per residue for model 17

- Molecule 1: Homeobox protein extradenticle



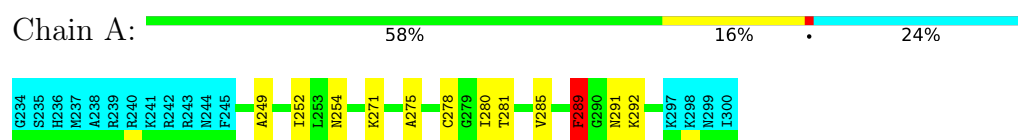
4.2.18 Score per residue for model 18

- Molecule 1: Homeobox protein extradenticle



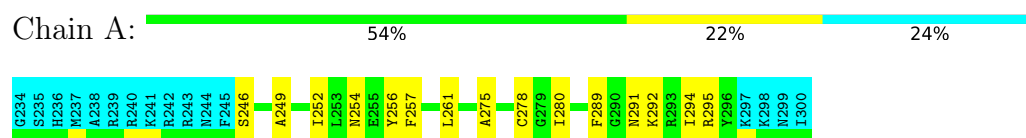
4.2.19 Score per residue for model 19

- Molecule 1: Homeobox protein extradenticle



4.2.20 Score per residue for model 20

- Molecule 1: Homeobox protein extradenticle



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
PONDEROSA-C/S	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	855
Number of shifts mapped to atoms	855
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 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	0.91±0.02	0±0/432 (0.0± 0.0%)	0.77±0.03	0±0/583 (0.0± 0.1%)
All	All	0.91	0/8640 (0.0%)	0.77	2/11660 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	289	PHE	CB-CG-CD2	7.58	126.11	120.80	19	1
1	A	289	PHE	CB-CG-CD1	-7.22	115.74	120.80	19	1

There are no chirality outliers.

There are no planarity outliers.

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	421	405	404	6±2
All	All	8420	8100	8080	129

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:252:ILE:HD11	1:A:285:VAL:HG22	0.86	1.42	19	10
1:A:252:ILE:HD12	1:A:278:CYS:SG	0.80	2.17	15	5
1:A:249:ALA:O	1:A:252:ILE:HG22	0.76	1.81	6	11
1:A:252:ILE:HD11	1:A:285:VAL:CG2	0.68	2.17	13	2
1:A:252:ILE:CD1	1:A:285:VAL:HG22	0.66	2.20	15	8
1:A:294:ILE:HD12	1:A:295:ARG:N	0.63	2.08	20	4
1:A:252:ILE:HD12	1:A:278:CYS:CB	0.63	2.23	12	3
1:A:252:ILE:HD12	1:A:278:CYS:HB2	0.59	1.74	5	9
1:A:275:ALA:HB1	1:A:280:ILE:O	0.58	1.99	9	20
1:A:281:THR:O	1:A:285:VAL:HG23	0.57	2.00	7	6
1:A:252:ILE:HD12	1:A:278:CYS:HB3	0.56	1.78	6	3
1:A:271:LYS:HA	1:A:285:VAL:HG11	0.53	1.79	16	4
1:A:256:TYR:HH	1:A:260:HIS:CE1	0.51	2.24	16	3
1:A:287:ASN:OD1	1:A:288:TRP:N	0.51	2.44	18	1
1:A:246:SER:O	1:A:249:ALA:HB3	0.50	2.06	18	2
1:A:281:THR:HG23	1:A:284:GLN:H	0.50	1.67	8	1
1:A:286:SER:HA	1:A:289:PHE:CD2	0.50	2.41	16	1
1:A:257:PHE:O	1:A:261:LEU:HD23	0.48	2.08	20	1
1:A:261:LEU:HD12	1:A:262:SER:N	0.47	2.24	9	1
1:A:289:PHE:CD2	1:A:289:PHE:C	0.47	2.88	19	1
1:A:253:LEU:HD22	1:A:288:TRP:CE3	0.45	2.46	18	2
1:A:256:TYR:CE2	1:A:289:PHE:CD1	0.45	3.04	20	2
1:A:246:SER:H	1:A:249:ALA:HB3	0.45	1.70	4	1
1:A:280:ILE:HG22	1:A:285:VAL:HG23	0.45	1.87	1	1
1:A:280:ILE:HG22	1:A:281:THR:N	0.44	2.28	13	11
1:A:252:ILE:HG21	1:A:280:ILE:HD12	0.43	1.90	14	1
1:A:256:TYR:CZ	1:A:260:HIS:CG	0.43	3.07	9	2
1:A:256:TYR:CE1	1:A:289:PHE:CZ	0.43	3.07	17	5
1:A:294:ILE:HD12	1:A:294:ILE:C	0.43	2.35	1	3
1:A:260:HIS:CE1	1:A:263:ASN:O	0.40	2.74	4	3
1:A:256:TYR:OH	1:A:260:HIS:CE1	0.40	2.74	11	2

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	51/67 (76%)	50±1 (98±2%)	1±1 (2±2%)	0±0 (0±0%)	100	100
All	All	1020/1340 (76%)	995 (98%)	25 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	46/60 (77%)	42±1 (92±2%)	4±1 (8±2%)	14	61
All	All	920/1200 (77%)	842 (92%)	78 (8%)	14	61

All 10 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	254	ASN	20
1	A	292	LYS	19
1	A	291	ASN	18
1	A	263	ASN	9
1	A	277	LYS	4
1	A	289	PHE	3
1	A	247	LYS	2
1	A	296	TYR	1
1	A	287	ASN	1
1	A	246	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chem_shift_list_1*

7.1.1 Bookkeeping i

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

Total number of shifts	855
Number of shifts mapped to atoms	855
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 46 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	238	ALA	HB2	1.287	0.00	.
1	A	238	ALA	HB3	1.287	0.00	.
1	A	249	ALA	HB2	1.253	0.01	.
1	A	249	ALA	HB3	1.253	0.01	.
1	A	252	ILE	HD12	0.659	0.01	.
1	A	252	ILE	HD13	0.659	0.01	.
1	A	252	ILE	HG22	0.792	0.04	.
1	A	252	ILE	HG23	0.792	0.04	.
1	A	253	LEU	HD12	-0.387	0.01	.
1	A	253	LEU	HD13	-0.387	0.01	.
1	A	253	LEU	HD22	0.312	0.01	.
1	A	253	LEU	HD23	0.312	0.01	.
1	A	261	LEU	HD12	0.752	0.01	.
1	A	261	LEU	HD13	0.752	0.01	.
1	A	261	LEU	HD22	0.372	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	261	LEU	HD23	0.372	0.01	.
1	A	270	ALA	HB2	1.216	0.01	.
1	A	270	ALA	HB3	1.216	0.01	.
1	A	274	LEU	HD12	-0.024	0.01	.
1	A	274	LEU	HD13	-0.024	0.01	.
1	A	274	LEU	HD22	0.515	0.00	.
1	A	274	LEU	HD23	0.515	0.00	.
1	A	275	ALA	HB2	1.343	0.01	.
1	A	275	ALA	HB3	1.343	0.01	.
1	A	280	ILE	HD12	0.428	0.01	.
1	A	280	ILE	HD13	0.428	0.01	.
1	A	280	ILE	HG22	0.570	0.02	.
1	A	280	ILE	HG23	0.570	0.02	.
1	A	281	THR	HG22	1.209	0.01	.
1	A	281	THR	HG23	1.209	0.01	.
1	A	282	VAL	HG12	0.887	0.01	.
1	A	282	VAL	HG13	0.887	0.01	.
1	A	282	VAL	HG22	0.913	0.01	.
1	A	282	VAL	HG23	0.913	0.01	.
1	A	285	VAL	HG12	0.987	0.01	.
1	A	285	VAL	HG13	0.987	0.01	.
1	A	285	VAL	HG22	0.919	0.01	.
1	A	285	VAL	HG23	0.919	0.01	.
1	A	294	ILE	HD12	0.789	0.01	.
1	A	294	ILE	HD13	0.789	0.01	.
1	A	294	ILE	HG22	0.794	0.01	.
1	A	294	ILE	HG23	0.794	0.01	.
1	A	300	ILE	HD12	0.762	0.01	.
1	A	300	ILE	HD13	0.762	0.01	.
1	A	300	ILE	HG22	0.769	0.00	.
1	A	300	ILE	HG23	0.769	0.00	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	65	-0.36 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	62	0.19 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	64	-0.57 ± 0.10	Should be applied
^{15}N	60	-0.18 ± 0.37	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 89%, i.e. 632 atoms were assigned a chemical shift out of a possible 707. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	250/253 (99%)	101/102 (99%)	101/102 (99%)	48/49 (98%)
Sidechain	342/378 (90%)	235/242 (97%)	101/117 (86%)	6/19 (32%)
Aromatic	40/76 (53%)	26/36 (72%)	13/37 (35%)	1/3 (33%)
Overall	632/707 (89%)	362/380 (95%)	215/256 (84%)	55/71 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 794 atoms were assigned a chemical shift out of a possible 966. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	313/334 (94%)	124/135 (92%)	129/134 (96%)	60/65 (92%)
Sidechain	439/539 (81%)	297/343 (87%)	134/160 (84%)	8/36 (22%)
Aromatic	42/93 (45%)	28/45 (62%)	13/44 (30%)	1/4 (25%)
Overall	794/966 (82%)	449/523 (86%)	276/338 (82%)	69/105 (66%)

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.

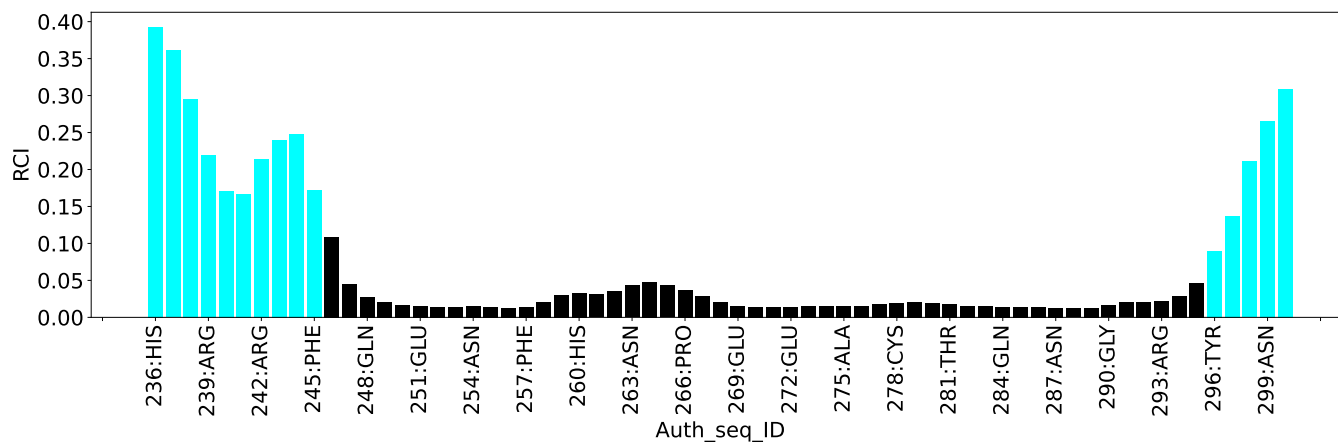
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	260	HIS	CD2	49.71	103.95 – 136.66	-21.6
1	A	237	MET	CG	16.68	25.46 – 38.60	-11.7
1	A	253	LEU	HB3	-1.18	-0.26 – 3.31	-7.6
1	A	292	LYS	HG2	-0.43	0.13 – 2.61	-7.3
1	A	292	LYS	HG3	-0.43	0.04 – 2.67	-6.8
1	A	292	LYS	HB3	0.08	0.46 – 3.04	-6.5
1	A	292	LYS	HD2	0.41	0.58 – 2.64	-5.8
1	A	266	PRO	HG3	0.22	0.33 – 3.48	-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:



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	702
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	578
Inter-chain	0
Hydrogen bond restraints	124
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	10.5
Number of long range restraints per residue ¹	8.6

¹Long 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)	18.2	0.2
0.2-0.5 (Medium)	5.5	0.5
>0.5 (Large)	0.1	0.99

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

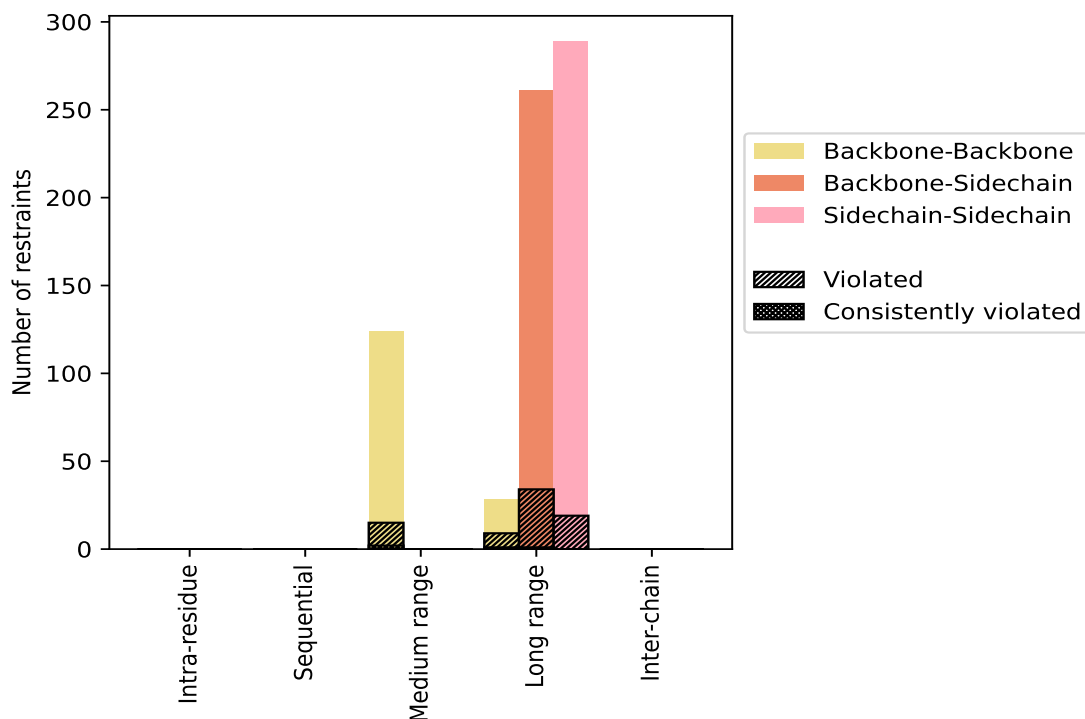
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	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
Sequential (i-j =1)	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
Medium range (i-j >1 & i-j <5)	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
Long range (i-j ≥5)	578	82.3	62	10.7	8.8	2	0.3	0.3
Backbone-Backbone	28	4.0	9	32.1	1.3	1	3.6	0.1
Backbone-Sidechain	261	37.2	34	13.0	4.8	1	0.4	0.1
Sidechain-Sidechain	289	41.2	19	6.6	2.7	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	124	17.7	15	12.1	2.1	2	1.6	0.3
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	702	100.0	77	11.0	11.0	4	0.6	0.6
Backbone-Backbone	152	21.7	24	15.8	3.4	3	2.0	0.4
Backbone-Sidechain	261	37.2	34	13.0	4.8	1	0.4	0.1
Sidechain-Sidechain	289	41.2	19	6.6	2.7	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 disulfid 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	0	7	14	0	21	0.18	0.34	0.07	0.16
2	0	0	8	16	0	24	0.17	0.33	0.06	0.15
3	0	0	8	17	0	25	0.16	0.3	0.04	0.15
4	0	0	8	12	0	20	0.16	0.26	0.04	0.16
5	0	0	8	14	0	22	0.17	0.37	0.07	0.14
6	0	0	7	18	0	25	0.17	0.35	0.06	0.14
7	0	0	8	12	0	20	0.15	0.32	0.05	0.13
8	0	0	6	17	0	23	0.2	0.99	0.17	0.17
9	0	0	5	21	0	26	0.19	0.35	0.06	0.18
10	0	0	5	14	0	19	0.17	0.25	0.04	0.17
11	0	0	5	18	0	23	0.18	0.37	0.07	0.18

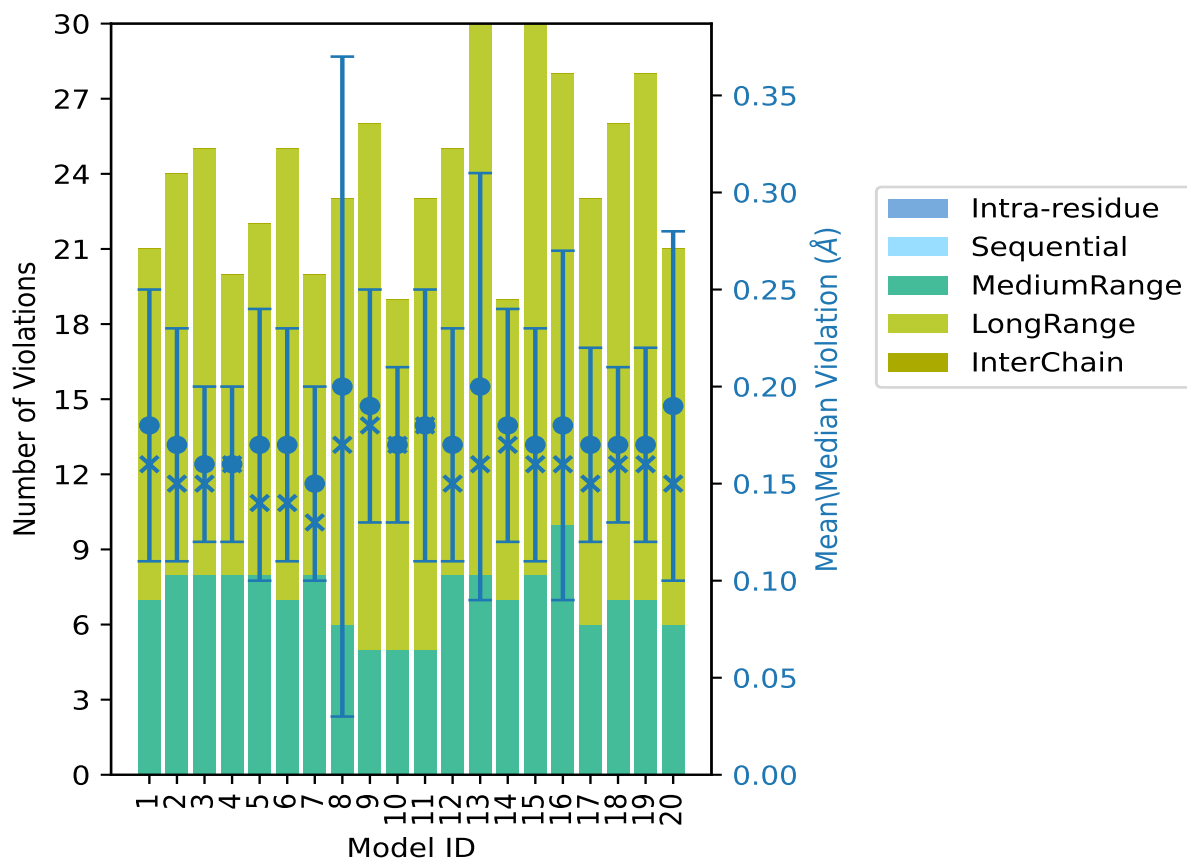
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
12	0	0	8	17	0	25	0.17	0.39	0.06	0.15
13	0	0	8	22	0	30	0.2	0.58	0.11	0.16
14	0	0	7	12	0	19	0.18	0.33	0.06	0.17
15	0	0	8	22	0	30	0.17	0.34	0.06	0.16
16	0	0	10	18	0	28	0.18	0.5	0.09	0.16
17	0	0	6	17	0	23	0.17	0.31	0.05	0.15
18	0	0	7	19	0	26	0.17	0.27	0.04	0.16
19	0	0	7	21	0	28	0.17	0.3	0.05	0.16
20	0	0	6	15	0	21	0.19	0.43	0.09	0.15

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard 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

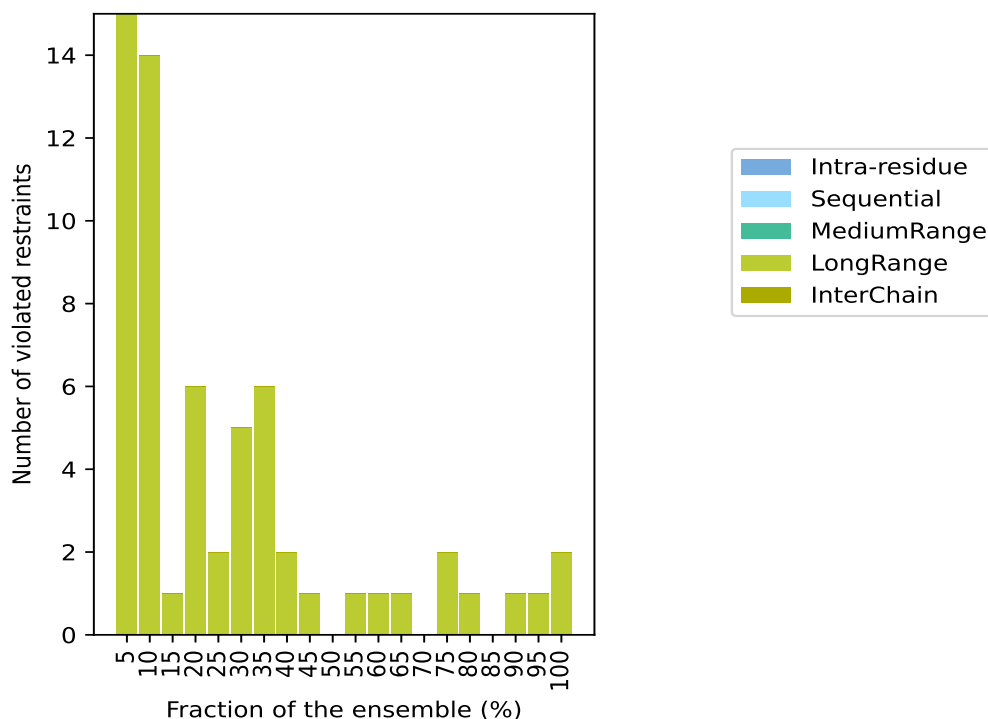
9.3 Distance violation statistics for the ensemble

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, 516(IR:0, SQ:0, MR:0, LR:516, 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	15	0	15	1	5.0
0	0	0	14	0	14	2	10.0
0	0	0	1	0	1	3	15.0
0	0	0	6	0	6	4	20.0
0	0	0	2	0	2	5	25.0
0	0	0	5	0	5	6	30.0
0	0	0	6	0	6	7	35.0
0	0	0	2	0	2	8	40.0
0	0	0	1	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	1	0	1	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	1	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	2	0	2	15	75.0
0	0	0	1	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	1	0	1	18	90.0
0	0	0	1	0	1	19	95.0
0	0	0	2	0	2	20	100.0

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

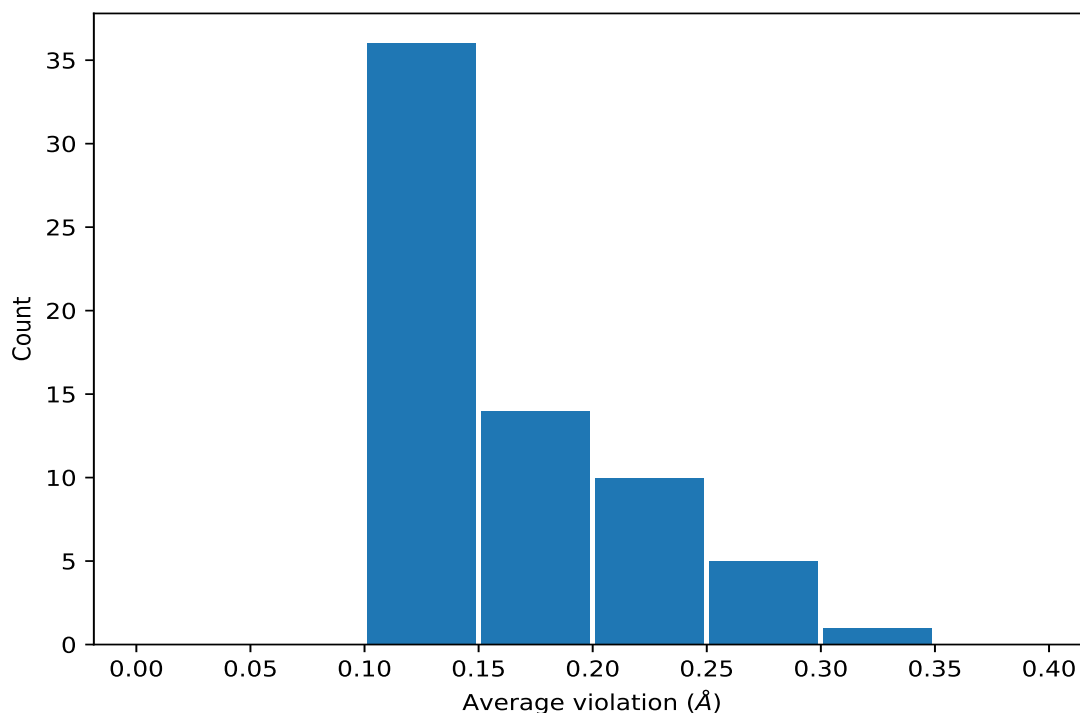
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	20	0.29	0.09	0.3
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	20	0.24	0.03	0.24
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	20	0.22	0.03	0.22
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	20	0.18	0.02	0.18
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	19	0.21	0.04	0.2
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	18	0.16	0.04	0.15
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	17	0.21	0.02	0.2
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	16	0.17	0.03	0.18
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	15	0.22	0.07	0.22
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	15	0.18	0.06	0.16
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	15	0.15	0.03	0.15
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	14	0.15	0.02	0.16
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	13	0.13	0.01	0.13
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	12	0.12	0.01	0.12
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	11	0.22	0.05	0.22
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	10	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	10	0.14	0.02	0.14
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	9	0.13	0.02	0.13
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	9	0.13	0.02	0.11
(4,146)	1:A:275:ALA:H	1:A:280:ILE:H	8	0.14	0.03	0.14
(4,2)	1:A:248:GLN:HE22	1:A:277:LYS:HA	8	0.13	0.01	0.13
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	7	0.25	0.12	0.16
(5,87)	1:A:266:PRO:HB2	1:A:290:GLY:H	7	0.2	0.11	0.14
(4,30)	1:A:252:ILE:HA	1:A:274:LEU:HG	7	0.13	0.03	0.12
(4,117)	1:A:272:GLU:HA	1:A:282:VAL:H	7	0.13	0.01	0.13
(5,114)	1:A:274:LEU:HB3	1:A:279:GLY:H	7	0.13	0.03	0.11
(5,106)	1:A:271:LYS:HB3	1:A:289:PHE:HD1	7	0.13	0.02	0.12
(2,7)	1:A:254:ASN:H	1:A:250:SER:O	7	0.12	0.01	0.12
(5,59)	1:A:256:TYR:H	1:A:292:LYS:HB3	6	0.23	0.06	0.25
(4,47)	1:A:254:ASN:HA	1:A:288:TRP:HH2	6	0.17	0.03	0.16
(5,62)	1:A:257:PHE:H	1:A:295:ARG:HE	6	0.16	0.02	0.16
(2,52)	1:A:291:ASN:H	1:A:287:ASN:O	6	0.15	0.03	0.16
(5,55)	1:A:256:TYR:HE2	1:A:267:SER:H	6	0.13	0.01	0.12
(5,119)	1:A:275:ALA:H	1:A:281:THR:H	6	0.13	0.02	0.12
(4,80)	1:A:260:HIS:HD2	1:A:265:TYR:H	5	0.15	0.03	0.16
(4,60)	1:A:256:TYR:HB2	1:A:288:TRP:HB3	5	0.13	0.02	0.13
(2,16)	1:A:258:TYR:H	1:A:254:ASN:O	5	0.11	0.0	0.11
(5,126)	1:A:281:THR:HB	1:A:286:SER:H	4	0.34	0.38	0.12
(5,76)	1:A:262:SER:H	1:A:293:ARG:HD2	4	0.2	0.05	0.18
(4,20)	1:A:252:ILE:HD11	1:A:278:CYS:HB2	4	0.18	0.07	0.16
(4,20)	1:A:252:ILE:HD12	1:A:278:CYS:HB2	4	0.18	0.07	0.16
(4,20)	1:A:252:ILE:HD13	1:A:278:CYS:HB2	4	0.18	0.07	0.16
(5,11)	1:A:252:ILE:HB	1:A:279:GLY:H	4	0.17	0.03	0.16
(4,81)	1:A:260:HIS:HA	1:A:292:LYS:HD3	4	0.16	0.03	0.16
(5,102)	1:A:271:LYS:HB2	1:A:287:ASN:H	4	0.14	0.02	0.14
(2,43)	1:A:287:ASN:H	1:A:283:SER:O	4	0.12	0.01	0.12
(4,10)	1:A:252:ILE:HG13	1:A:278:CYS:HB3	3	0.13	0.01	0.14
(4,70)	1:A:258:TYR:H	1:A:292:LYS:HZ1	2	0.25	0.08	0.25
(4,70)	1:A:258:TYR:H	1:A:292:LYS:HZ2	2	0.25	0.08	0.25
(4,70)	1:A:258:TYR:H	1:A:292:LYS:HZ3	2	0.25	0.08	0.25
(4,79)	1:A:260:HIS:HD2	1:A:293:ARG:HD2	2	0.24	0.12	0.24
(4,46)	1:A:254:ASN:HB2	1:A:288:TRP:HH2	2	0.17	0.06	0.17
(4,110)	1:A:271:LYS:HE3	1:A:286:SER:HA	2	0.17	0.02	0.17
(4,16)	1:A:252:ILE:HG12	1:A:274:LEU:HB2	2	0.16	0.02	0.16
(5,58)	1:A:256:TYR:HB2	1:A:288:TRP:HZ2	2	0.15	0.02	0.15
(5,79)	1:A:262:SER:H	1:A:292:LYS:HD2	2	0.14	0.03	0.14
(2,40)	1:A:285:VAL:H	1:A:281:THR:O	2	0.14	0.01	0.14
(5,44)	1:A:253:LEU:H	1:A:274:LEU:HB3	2	0.14	0.02	0.14

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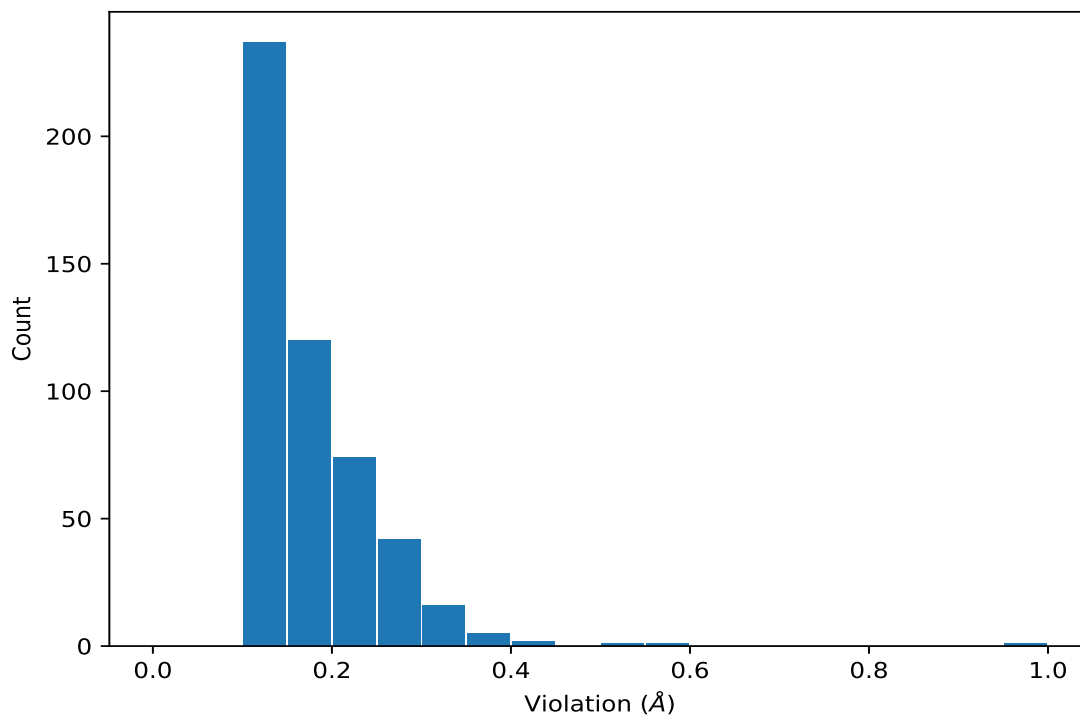
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,45)	1:A:254:ASN:H	1:A:288:TRP:HH2	2	0.13	0.0	0.13
(5,56)	1:A:256:TYR:HA	1:A:261:LEU:H	2	0.13	0.02	0.13
(2,2)	1:A:251:GLU:H	1:A:247:LYS:O	2	0.12	0.01	0.12
(4,48)	1:A:254:ASN:HB2	1:A:288:TRP:HZ2	2	0.12	0.01	0.12
(4,144)	1:A:275:ALA:HA	1:A:285:VAL:HB	2	0.12	0.0	0.12
(4,35)	1:A:253:LEU:HA	1:A:288:TRP:HD1	2	0.11	0.0	0.11
(5,13)	1:A:252:ILE:H	1:A:277:LYS:HE2	2	0.11	0.0	0.11
(5,13)	1:A:252:ILE:H	1:A:277:LYS:HE3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,126)	1:A:281:THR:HB	1:A:286:SER:H	8	0.99
(5,54)	1:A:256:TYR:HD1	1:A:266:PRO:HB3	13	0.58
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	16	0.5
(5,87)	1:A:266:PRO:HB2	1:A:290:GLY:H	13	0.44
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	20	0.43
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	12	0.39
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	16	0.37
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	5	0.37
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	11	0.37
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	13	0.36
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	9	0.35
(4,79)	1:A:260:HIS:HD2	1:A:293:ARG:HD2	20	0.35
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	6	0.35
(4,84)	1:A:266:PRO:HD3	1:A:293:ARG:HG2	13	0.34
(4,84)	1:A:266:PRO:HD3	1:A:293:ARG:HG3	13	0.34
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	1	0.34
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	15	0.34
(4,70)	1:A:258:TYR:H	1:A:292:LYS:HZ1	1	0.33
(4,70)	1:A:258:TYR:H	1:A:292:LYS:HZ2	1	0.33
(4,70)	1:A:258:TYR:H	1:A:292:LYS:HZ3	1	0.33
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	14	0.33
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	2	0.33
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	20	0.33
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	7	0.32
(5,87)	1:A:266:PRO:HB2	1:A:290:GLY:H	16	0.31
(5,59)	1:A:256:TYR:H	1:A:292:LYS:HB3	17	0.31
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	1	0.3
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	9	0.3
(4,20)	1:A:252:ILE:HD11	1:A:278:CYS:HB2	11	0.3
(4,20)	1:A:252:ILE:HD12	1:A:278:CYS:HB2	11	0.3
(4,20)	1:A:252:ILE:HD13	1:A:278:CYS:HB2	11	0.3
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	3	0.3
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	19	0.3
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	19	0.28
(4,61)	1:A:256:TYR:HB3	1:A:274:LEU:HD21	16	0.28
(4,61)	1:A:256:TYR:HB3	1:A:274:LEU:HD22	16	0.28
(4,61)	1:A:256:TYR:HB3	1:A:274:LEU:HD23	16	0.28
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	14	0.28
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	15	0.28
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	13	0.28
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	9	0.28
(5,59)	1:A:256:TYR:H	1:A:292:LYS:HB3	9	0.27
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	5	0.27
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	9	0.27
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	18	0.27
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	15	0.27
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	17	0.27
(5,76)	1:A:262:SER:H	1:A:293:ARG:HD2	15	0.26
(5,59)	1:A:256:TYR:H	1:A:292:LYS:HB3	2	0.26
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	20	0.26
(4,8)	1:A:252:ILE:HG13	1:A:280:ILE:HD11	2	0.26
(4,8)	1:A:252:ILE:HG13	1:A:280:ILE:HD12	2	0.26
(4,8)	1:A:252:ILE:HG13	1:A:280:ILE:HD13	2	0.26
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	4	0.26
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	19	0.26
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	12	0.26
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	18	0.26
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	1	0.26
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	5	0.26
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	8	0.26
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	12	0.26
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	2	0.25
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	3	0.25
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	12	0.25
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	20	0.25
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	10	0.25
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	11	0.25
(5,59)	1:A:256:TYR:H	1:A:292:LYS:HB3	11	0.24
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	9	0.24
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	13	0.24
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	1	0.24
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	5	0.24
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	6	0.24
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	17	0.24
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	13	0.24
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	4	0.24
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	17	0.24
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	6	0.24
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	11	0.24
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	14	0.24
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	20	0.24
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	6	0.23
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	13	0.23
(4,46)	1:A:254:ASN:HB2	1:A:288:TRP:HH2	8	0.23
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	1	0.23
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	2	0.23
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	15	0.23
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	9	0.23
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	1	0.23
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	18	0.23
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	4	0.23
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	7	0.23
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	11	0.23
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	19	0.23
(5,76)	1:A:262:SER:H	1:A:293:ARG:HD2	14	0.22
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	16	0.22
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	2	0.22
(5,11)	1:A:252:ILE:HB	1:A:279:GLY:H	10	0.22
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	15	0.22
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	18	0.22
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	14	0.22
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	19	0.22
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	11	0.22
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	8	0.22
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	10	0.22
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	10	0.22
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	13	0.22
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	3	0.21
(5,59)	1:A:256:TYR:H	1:A:292:LYS:HB3	3	0.21
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	10	0.21
(4,81)	1:A:260:HIS:HA	1:A:292:LYS:HD3	11	0.21
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	10	0.21
(4,47)	1:A:254:ASN:HA	1:A:288:TRP:HH2	10	0.21
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	9	0.21
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	11	0.21
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	15	0.21
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	7	0.21
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	14	0.21
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	3	0.21
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	16	0.21
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	8	0.2
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	12	0.2
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	8	0.2
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	11	0.2
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	18	0.2
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	18	0.2
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	12	0.2
(4,30)	1:A:252:ILE:HA	1:A:274:LEU:HG	16	0.2
(4,146)	1:A:275:ALA:H	1:A:280:ILE:H	6	0.2
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	8	0.2
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	13	0.2
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	19	0.2
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	20	0.2
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	6	0.2
(2,50)	1:A:290:GLY:H	1:A:286:SER:O	16	0.2
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	9	0.2
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	15	0.2
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	17	0.2
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	18	0.2
(5,62)	1:A:257:PHE:H	1:A:295:ARG:HE	1	0.19
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	4	0.19
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	14	0.19
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	8	0.19
(4,47)	1:A:254:ASN:HA	1:A:288:TRP:HH2	11	0.19
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	4	0.19
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	6	0.19
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	15	0.19
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	19	0.19
(4,110)	1:A:271:LYS:HE3	1:A:286:SER:HA	19	0.19
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	9	0.19
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	17	0.19
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	18	0.19
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	9	0.19
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	3	0.19
(2,52)	1:A:291:ASN:H	1:A:287:ASN:O	16	0.19
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	3	0.19
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	5	0.19
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	12	0.19
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	2	0.19
(5,79)	1:A:262:SER:H	1:A:292:LYS:HD2	16	0.18
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	5	0.18
(5,119)	1:A:275:ALA:H	1:A:281:THR:H	9	0.18
(4,80)	1:A:260:HIS:HD2	1:A:265:TYR:H	8	0.18
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	7	0.18
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	8	0.18
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	16	0.18
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	20	0.18
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	19	0.18
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	11	0.18
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	12	0.18
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	14	0.18
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	17	0.18
(4,14)	1:A:252:ILE:HA	1:A:277:LYS:HG2	9	0.18
(4,14)	1:A:252:ILE:HA	1:A:277:LYS:HG3	9	0.18
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	8	0.18
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	10	0.18
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	17	0.18
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	12	0.18
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	14	0.18
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	18	0.18
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	19	0.18
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	2	0.18
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	19	0.18
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	7	0.18
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	9	0.18
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	19	0.17
(5,114)	1:A:274:LEU:HB3	1:A:279:GLY:H	9	0.17
(5,114)	1:A:274:LEU:HB3	1:A:279:GLY:H	18	0.17
(5,11)	1:A:252:ILE:HB	1:A:279:GLY:H	20	0.17
(4,80)	1:A:260:HIS:HD2	1:A:265:TYR:H	2	0.17
(4,70)	1:A:258:TYR:H	1:A:292:LYS:HZ1	16	0.17
(4,70)	1:A:258:TYR:H	1:A:292:LYS:HZ2	16	0.17
(4,70)	1:A:258:TYR:H	1:A:292:LYS:HZ3	16	0.17
(4,47)	1:A:254:ASN:HA	1:A:288:TRP:HH2	6	0.17
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	13	0.17
(4,16)	1:A:252:ILE:HG12	1:A:274:LEU:HB2	19	0.17
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	10	0.17
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	18	0.17
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	14	0.17
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	10	0.17
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	20	0.17
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	4	0.17
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	5	0.17
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	6	0.17
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	2	0.17
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	8	0.17
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	16	0.17
(2,52)	1:A:291:ASN:H	1:A:287:ASN:O	3	0.17
(2,52)	1:A:291:ASN:H	1:A:287:ASN:O	13	0.17
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	4	0.17
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	2	0.17
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	15	0.17
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	19	0.17
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	12	0.16
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	11	0.16
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	12	0.16
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	18	0.16
(5,62)	1:A:257:PHE:H	1:A:295:ARG:HE	13	0.16
(5,62)	1:A:257:PHE:H	1:A:295:ARG:HE	15	0.16
(5,62)	1:A:257:PHE:H	1:A:295:ARG:HE	17	0.16
(5,6)	1:A:249:ALA:HA	1:A:277:LYS:HD2	4	0.16
(5,6)	1:A:249:ALA:HA	1:A:277:LYS:HD3	4	0.16
(5,58)	1:A:256:TYR:HB2	1:A:288:TRP:HZ2	16	0.16
(5,51)	1:A:256:TYR:HE1	1:A:266:PRO:HB2	13	0.16
(5,44)	1:A:253:LEU:H	1:A:274:LEU:HB3	15	0.16
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	1	0.16
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	17	0.16
(5,11)	1:A:252:ILE:HB	1:A:279:GLY:H	15	0.16
(5,106)	1:A:271:LYS:HB3	1:A:289:PHE:HD1	8	0.16
(5,102)	1:A:271:LYS:HB2	1:A:287:ASN:H	9	0.16
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	9	0.16
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	17	0.16
(4,81)	1:A:260:HIS:HA	1:A:292:LYS:HD3	9	0.16
(4,80)	1:A:260:HIS:HD2	1:A:265:TYR:H	3	0.16
(4,73)	1:A:260:HIS:HB2	1:A:288:TRP:HD1	15	0.16
(4,60)	1:A:256:TYR:HB2	1:A:288:TRP:HB3	10	0.16
(4,30)	1:A:252:ILE:HA	1:A:274:LEU:HG	6	0.16
(4,20)	1:A:252:ILE:HD11	1:A:278:CYS:HB2	15	0.16
(4,20)	1:A:252:ILE:HD12	1:A:278:CYS:HB2	15	0.16
(4,20)	1:A:252:ILE:HD13	1:A:278:CYS:HB2	15	0.16
(4,20)	1:A:252:ILE:HD11	1:A:278:CYS:HB2	18	0.16
(4,20)	1:A:252:ILE:HD12	1:A:278:CYS:HB2	18	0.16
(4,20)	1:A:252:ILE:HD13	1:A:278:CYS:HB2	18	0.16
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	4	0.16
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	4	0.16
(4,117)	1:A:272:GLU:HA	1:A:282:VAL:H	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	3	0.16
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	1	0.16
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	7	0.16
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	16	0.16
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	1	0.16
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	10	0.16
(2,52)	1:A:291:ASN:H	1:A:287:ASN:O	18	0.16
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	13	0.16
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	16	0.16
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	1	0.16
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	14	0.16
(5,87)	1:A:266:PRO:HB2	1:A:290:GLY:H	3	0.15
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	10	0.15
(5,76)	1:A:262:SER:H	1:A:293:ARG:HD2	7	0.15
(5,76)	1:A:262:SER:H	1:A:293:ARG:HD2	19	0.15
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	6	0.15
(5,56)	1:A:256:TYR:HA	1:A:261:LEU:H	18	0.15
(5,55)	1:A:256:TYR:HE2	1:A:267:SER:H	15	0.15
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	7	0.15
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	20	0.15
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	3	0.15
(5,106)	1:A:271:LYS:HB3	1:A:289:PHE:HD1	18	0.15
(4,81)	1:A:260:HIS:HA	1:A:292:LYS:HD3	3	0.15
(4,60)	1:A:256:TYR:HB2	1:A:288:TRP:HB3	12	0.15
(4,47)	1:A:254:ASN:HA	1:A:288:TRP:HH2	18	0.15
(4,47)	1:A:254:ASN:HA	1:A:288:TRP:HH2	20	0.15
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	1	0.15
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	17	0.15
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	8	0.15
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	18	0.15
(4,131)	1:A:274:LEU:HB2	1:A:285:VAL:HA	2	0.15
(4,110)	1:A:271:LYS:HE3	1:A:286:SER:HA	1	0.15
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	3	0.15
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	12	0.15
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	8	0.15
(2,40)	1:A:285:VAL:H	1:A:281:THR:O	13	0.15
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	19	0.15
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	4	0.15
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	12	0.15
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	17	0.15
(5,87)	1:A:266:PRO:HB2	1:A:290:GLY:H	9	0.14
(5,87)	1:A:266:PRO:HB2	1:A:290:GLY:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	6	0.14
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	2	0.14
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	17	0.14
(5,62)	1:A:257:PHE:H	1:A:295:ARG:HE	19	0.14
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	6	0.14
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	11	0.14
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	2	0.14
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	5	0.14
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	8	0.14
(5,114)	1:A:274:LEU:HB3	1:A:279:GLY:H	15	0.14
(5,106)	1:A:271:LYS:HB3	1:A:289:PHE:HD1	10	0.14
(5,102)	1:A:271:LYS:HB2	1:A:287:ASN:H	8	0.14
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	9	0.14
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	12	0.14
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	13	0.14
(4,2)	1:A:248:GLN:HE22	1:A:277:LYS:HA	3	0.14
(4,2)	1:A:248:GLN:HE22	1:A:277:LYS:HA	6	0.14
(4,16)	1:A:252:ILE:HG12	1:A:274:LEU:HB2	13	0.14
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	3	0.14
(4,146)	1:A:275:ALA:H	1:A:280:ILE:H	5	0.14
(4,146)	1:A:275:ALA:H	1:A:280:ILE:H	12	0.14
(4,146)	1:A:275:ALA:H	1:A:280:ILE:H	13	0.14
(4,117)	1:A:272:GLU:HA	1:A:282:VAL:H	6	0.14
(4,10)	1:A:252:ILE:HG13	1:A:278:CYS:HB3	9	0.14
(4,10)	1:A:252:ILE:HG13	1:A:278:CYS:HB3	20	0.14
(2,7)	1:A:254:ASN:H	1:A:250:SER:O	5	0.14
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	13	0.14
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	14	0.14
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	2	0.14
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	11	0.14
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	12	0.14
(2,43)	1:A:287:ASN:H	1:A:283:SER:O	19	0.14
(5,87)	1:A:266:PRO:HB2	1:A:290:GLY:H	20	0.13
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	1	0.13
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	11	0.13
(5,58)	1:A:256:TYR:HB2	1:A:288:TRP:HZ2	13	0.13
(5,55)	1:A:256:TYR:HE2	1:A:267:SER:H	2	0.13
(5,55)	1:A:256:TYR:HE2	1:A:267:SER:H	13	0.13
(5,45)	1:A:253:LEU:HA	1:A:274:LEU:HB3	15	0.13
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	14	0.13
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	15	0.13
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	9	0.13
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	12	0.13
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	14	0.13
(5,119)	1:A:275:ALA:H	1:A:281:THR:H	4	0.13
(5,11)	1:A:252:ILE:HB	1:A:279:GLY:H	5	0.13
(5,102)	1:A:271:LYS:HB2	1:A:287:ASN:H	3	0.13
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	16	0.13
(4,81)	1:A:260:HIS:HA	1:A:292:LYS:HD3	2	0.13
(4,80)	1:A:260:HIS:HD2	1:A:265:TYR:H	6	0.13
(4,60)	1:A:256:TYR:HB2	1:A:288:TRP:HB3	6	0.13
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	16	0.13
(4,48)	1:A:254:ASN:HB2	1:A:288:TRP:HZ2	8	0.13
(4,47)	1:A:254:ASN:HA	1:A:288:TRP:HH2	3	0.13
(4,45)	1:A:254:ASN:H	1:A:288:TRP:HH2	3	0.13
(4,45)	1:A:254:ASN:H	1:A:288:TRP:HH2	18	0.13
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	5	0.13
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	16	0.13
(4,31)	1:A:252:ILE:HG13	1:A:280:ILE:H	6	0.13
(4,2)	1:A:248:GLN:HE22	1:A:277:LYS:HA	12	0.13
(4,2)	1:A:248:GLN:HE22	1:A:277:LYS:HA	15	0.13
(4,2)	1:A:248:GLN:HE22	1:A:277:LYS:HA	16	0.13
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	1	0.13
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	5	0.13
(4,146)	1:A:275:ALA:H	1:A:280:ILE:H	17	0.13
(4,117)	1:A:272:GLU:HA	1:A:282:VAL:H	5	0.13
(4,117)	1:A:272:GLU:HA	1:A:282:VAL:H	7	0.13
(4,117)	1:A:272:GLU:HA	1:A:282:VAL:H	8	0.13
(4,117)	1:A:272:GLU:HA	1:A:282:VAL:H	17	0.13
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	7	0.13
(2,7)	1:A:254:ASN:H	1:A:250:SER:O	16	0.13
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	7	0.13
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	17	0.13
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	4	0.13
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	18	0.13
(2,43)	1:A:287:ASN:H	1:A:283:SER:O	11	0.13
(2,40)	1:A:285:VAL:H	1:A:281:THR:O	16	0.13
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	3	0.13
(2,2)	1:A:251:GLU:H	1:A:247:LYS:O	18	0.13
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	5	0.13
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	13	0.13
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	16	0.13
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	17	0.12
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	20	0.12
(5,72)	1:A:261:LEU:HG	1:A:292:LYS:HD2	20	0.12
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	14	0.12
(5,69)	1:A:260:HIS:HB2	1:A:292:LYS:HB3	13	0.12
(5,62)	1:A:257:PHE:H	1:A:295:ARG:HE	4	0.12
(5,55)	1:A:256:TYR:HE2	1:A:267:SER:H	9	0.12
(5,55)	1:A:256:TYR:HE2	1:A:267:SER:H	12	0.12
(5,55)	1:A:256:TYR:HE2	1:A:267:SER:H	16	0.12
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	3	0.12
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	4	0.12
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	18	0.12
(5,126)	1:A:281:THR:HB	1:A:286:SER:H	15	0.12
(5,126)	1:A:281:THR:HB	1:A:286:SER:H	17	0.12
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	10	0.12
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	15	0.12
(5,119)	1:A:275:ALA:H	1:A:281:THR:H	19	0.12
(5,106)	1:A:271:LYS:HB3	1:A:289:PHE:HD1	4	0.12
(5,106)	1:A:271:LYS:HB3	1:A:289:PHE:HD1	16	0.12
(5,101)	1:A:271:LYS:HB2	1:A:283:SER:H	4	0.12
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	15	0.12
(4,79)	1:A:260:HIS:HD2	1:A:293:ARG:HD2	19	0.12
(4,74)	1:A:260:HIS:HD2	1:A:293:ARG:HD3	20	0.12
(4,65)	1:A:257:PHE:H	1:A:288:TRP:HH2	13	0.12
(4,60)	1:A:256:TYR:HB2	1:A:288:TRP:HB3	18	0.12
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	6	0.12
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	11	0.12
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	2	0.12
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	6	0.12
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	10	0.12
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	14	0.12
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	18	0.12
(4,30)	1:A:252:ILE:HA	1:A:274:LEU:HG	3	0.12
(4,30)	1:A:252:ILE:HA	1:A:274:LEU:HG	12	0.12
(4,30)	1:A:252:ILE:HA	1:A:274:LEU:HG	19	0.12
(4,20)	1:A:252:ILE:HD11	1:A:278:CYS:HB2	13	0.12
(4,20)	1:A:252:ILE:HD12	1:A:278:CYS:HB2	13	0.12
(4,20)	1:A:252:ILE:HD13	1:A:278:CYS:HB2	13	0.12
(4,2)	1:A:248:GLN:HE22	1:A:277:LYS:HA	19	0.12
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	7	0.12
(4,146)	1:A:275:ALA:H	1:A:280:ILE:H	15	0.12
(4,146)	1:A:275:ALA:H	1:A:280:ILE:H	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,144)	1:A:275:ALA:HA	1:A:285:VAL:HB	2	0.12
(4,10)	1:A:252:ILE:HG13	1:A:278:CYS:HB3	10	0.12
(2,7)	1:A:254:ASN:H	1:A:250:SER:O	2	0.12
(2,7)	1:A:254:ASN:H	1:A:250:SER:O	4	0.12
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	5	0.12
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	7	0.12
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	3	0.12
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	13	0.12
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	14	0.12
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	20	0.12
(2,52)	1:A:291:ASN:H	1:A:287:ASN:O	12	0.12
(2,16)	1:A:258:TYR:H	1:A:254:ASN:O	4	0.12
(2,16)	1:A:258:TYR:H	1:A:254:ASN:O	14	0.12
(2,13)	1:A:257:PHE:H	1:A:253:LEU:O	8	0.12
(5,87)	1:A:266:PRO:HB2	1:A:290:GLY:H	12	0.11
(5,83)	1:A:265:TYR:HE1	1:A:293:ARG:HB3	9	0.11
(5,79)	1:A:262:SER:H	1:A:292:LYS:HD2	8	0.11
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	7	0.11
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	13	0.11
(5,59)	1:A:256:TYR:H	1:A:292:LYS:HB3	15	0.11
(5,56)	1:A:256:TYR:HA	1:A:261:LEU:H	5	0.11
(5,44)	1:A:253:LEU:H	1:A:274:LEU:HB3	11	0.11
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	8	0.11
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	19	0.11
(5,13)	1:A:252:ILE:H	1:A:277:LYS:HE2	17	0.11
(5,13)	1:A:252:ILE:H	1:A:277:LYS:HE3	17	0.11
(5,13)	1:A:252:ILE:H	1:A:277:LYS:HE2	20	0.11
(5,13)	1:A:252:ILE:H	1:A:277:LYS:HE3	20	0.11
(5,126)	1:A:281:THR:HB	1:A:286:SER:H	7	0.11
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	1	0.11
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	6	0.11
(5,120)	1:A:276:ARG:H	1:A:282:VAL:HA	17	0.11
(5,119)	1:A:275:ALA:H	1:A:281:THR:H	11	0.11
(5,119)	1:A:275:ALA:H	1:A:281:THR:H	14	0.11
(5,119)	1:A:275:ALA:H	1:A:281:THR:H	17	0.11
(5,114)	1:A:274:LEU:HB3	1:A:279:GLY:H	10	0.11
(5,114)	1:A:274:LEU:HB3	1:A:279:GLY:H	11	0.11
(5,114)	1:A:274:LEU:HB3	1:A:279:GLY:H	16	0.11
(5,114)	1:A:274:LEU:HB3	1:A:279:GLY:H	19	0.11
(5,106)	1:A:271:LYS:HB3	1:A:289:PHE:HD1	9	0.11
(5,106)	1:A:271:LYS:HB3	1:A:289:PHE:HD1	17	0.11
(5,102)	1:A:271:LYS:HB2	1:A:287:ASN:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,80)	1:A:260:HIS:HD2	1:A:265:TYR:H	18	0.11
(4,60)	1:A:256:TYR:HB2	1:A:288:TRP:HB3	5	0.11
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	5	0.11
(4,48)	1:A:254:ASN:HB2	1:A:288:TRP:HZ2	11	0.11
(4,46)	1:A:254:ASN:HB2	1:A:288:TRP:HH2	15	0.11
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	7	0.11
(4,37)	1:A:253:LEU:HA	1:A:288:TRP:HB3	11	0.11
(4,35)	1:A:253:LEU:HA	1:A:288:TRP:HD1	13	0.11
(4,35)	1:A:253:LEU:HA	1:A:288:TRP:HD1	19	0.11
(4,30)	1:A:252:ILE:HA	1:A:274:LEU:HG	1	0.11
(4,30)	1:A:252:ILE:HA	1:A:274:LEU:HG	2	0.11
(4,2)	1:A:248:GLN:HE22	1:A:277:LYS:HA	2	0.11
(4,2)	1:A:248:GLN:HE22	1:A:277:LYS:HA	8	0.11
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	1	0.11
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	16	0.11
(4,146)	1:A:275:ALA:H	1:A:280:ILE:H	18	0.11
(4,144)	1:A:275:ALA:HA	1:A:285:VAL:HB	3	0.11
(4,117)	1:A:272:GLU:HA	1:A:282:VAL:H	9	0.11
(2,7)	1:A:254:ASN:H	1:A:250:SER:O	1	0.11
(2,7)	1:A:254:ASN:H	1:A:250:SER:O	7	0.11
(2,7)	1:A:254:ASN:H	1:A:250:SER:O	15	0.11
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	4	0.11
(2,62)	1:A:296:TYR:H	1:A:292:LYS:O	15	0.11
(2,58)	1:A:294:ILE:H	1:A:290:GLY:O	15	0.11
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	5	0.11
(2,56)	1:A:293:ARG:H	1:A:289:PHE:O	6	0.11
(2,52)	1:A:291:ASN:H	1:A:287:ASN:O	6	0.11
(2,43)	1:A:287:ASN:H	1:A:283:SER:O	1	0.11
(2,43)	1:A:287:ASN:H	1:A:283:SER:O	2	0.11
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	5	0.11
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	6	0.11
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	12	0.11
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	15	0.11
(2,28)	1:A:274:LEU:H	1:A:270:ALA:O	20	0.11
(2,2)	1:A:251:GLU:H	1:A:247:LYS:O	20	0.11
(2,16)	1:A:258:TYR:H	1:A:254:ASN:O	2	0.11
(2,16)	1:A:258:TYR:H	1:A:254:ASN:O	7	0.11
(2,16)	1:A:258:TYR:H	1:A:254:ASN:O	16	0.11

10 Dihedral-angle violation analysis

No dihedral-angle restraints found