



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 07:44 AM UTC

PDB ID : 5ZAU / pdb_00005zau
BMRB ID : 36164
Title : Complex of the human FYN SH3 and monobody binder
Authors : Reddy, P.P.; Gulyani, A.; Das, R.
Deposited on : 2018-02-09

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

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<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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

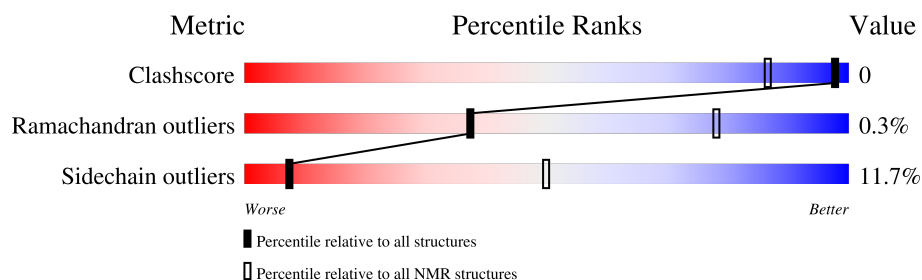
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 7%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	57	 88% 12%
2	B	64	 97% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:85-A:141, B:1-B:64 (121)	0.76	5

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 4 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1961 atoms, of which 978 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tyrosine-protein kinase Fyn.

Mol	Chain	Residues	Atoms					Trace
1	A	57	Total	C	H	N	O	0
			889	296	426	72	95	

- Molecule 2 is a protein called Monobody Binder.

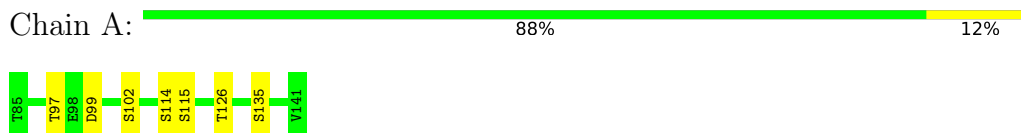
Mol	Chain	Residues	Atoms						Trace
2	B	64	Total	C	H	N	O	S	0
			1072	340	552	87	92	1	

4 Residue-property plots [i](#)

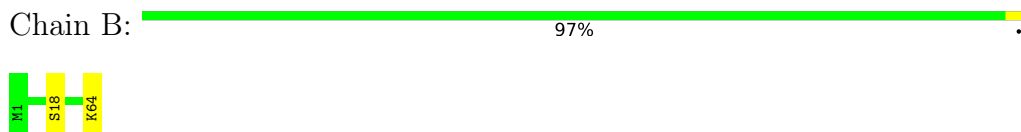
4.1 Average score per residue in the NMR ensemble

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: Tyrosine-protein kinase Fyn



- Molecule 2: Monobody Binder

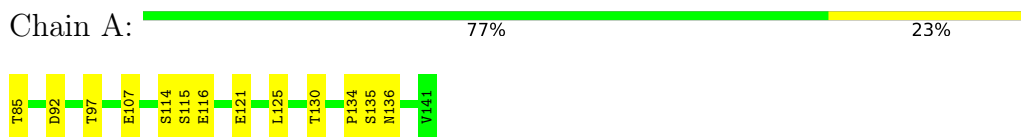


4.2 Scores per residue for each member of the ensemble

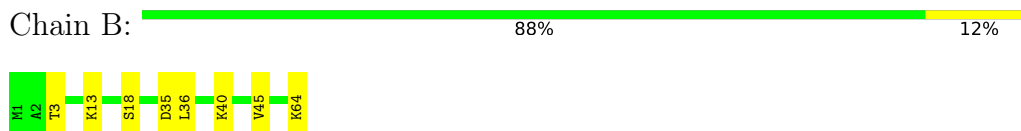
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Tyrosine-protein kinase Fyn



- Molecule 2: Monobody Binder



4.2.2 Score per residue for model 2

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  82% 18%



- Molecule 2: Monobody Binder

Chain B:  92% 8%



4.2.3 Score per residue for model 3

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  89% 11%



- Molecule 2: Monobody Binder

Chain B:  89% 11%



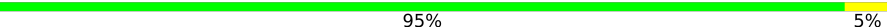
4.2.4 Score per residue for model 4

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  77% 23%



- Molecule 2: Monobody Binder

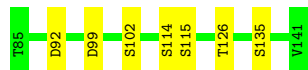
Chain B:  95% 5%



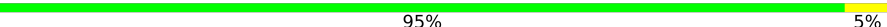
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  88% 12%



- Molecule 2: Monobody Binder

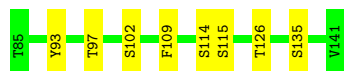
Chain B:  95% 5%



4.2.6 Score per residue for model 6

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  86% 14%



- Molecule 2: Monobody Binder

Chain B:  89% 11%



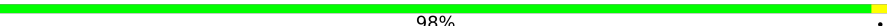
4.2.7 Score per residue for model 7

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  86% 14%



- Molecule 2: Monobody Binder

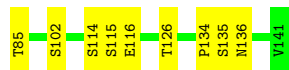
Chain B:  98% 2%



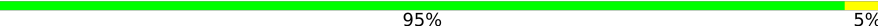
4.2.8 Score per residue for model 8

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  84% 16%



- Molecule 2: Monobody Binder

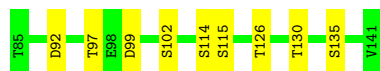
Chain B:  95% 5%



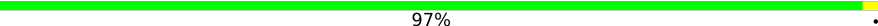
4.2.9 Score per residue for model 9

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  84% 16%



- Molecule 2: Monobody Binder

Chain B:  97% .



4.2.10 Score per residue for model 10

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  86% 14%



- Molecule 2: Monobody Binder

Chain B:  91% 8% .



4.2.11 Score per residue for model 11

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  82% 18%



- Molecule 2: Monobody Binder

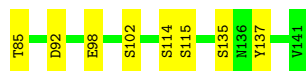
Chain B:  92% 8%



4.2.12 Score per residue for model 12

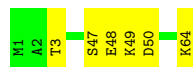
- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  86% 14%



- Molecule 2: Monobody Binder

Chain B:  91% 9%



4.2.13 Score per residue for model 13

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  84% 16%



- Molecule 2: Monobody Binder

Chain B:  89% 11%



4.2.14 Score per residue for model 14

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  86% 14%



- Molecule 2: Monobody Binder

Chain B:  91% 9%



4.2.15 Score per residue for model 15

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  79% 21%



- Molecule 2: Monobody Binder

Chain B:  92% 8%



4.2.16 Score per residue for model 16

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  89% 11%



- Molecule 2: Monobody Binder

Chain B:  94% 6%



4.2.17 Score per residue for model 17

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  79% 21%



- Molecule 2: Monobody Binder

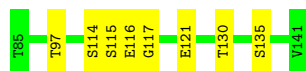
Chain B:  92% 8%



4.2.18 Score per residue for model 18

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  86% 14%



- Molecule 2: Monobody Binder

Chain B:  91% 9%



4.2.19 Score per residue for model 19

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  82% 18%



- Molecule 2: Monobody Binder

Chain B:  95% 5%



4.2.20 Score per residue for model 20

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A:  82% 18%



- Molecule 2: Monobody Binder

Chain B:  91% 9%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 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
HADDOCK	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	114
Number of shifts mapped to atoms	114
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	7%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [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	463	426	423	1±1
2	B	520	552	552	1±1
All	All	19660	19560	19500	18

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:119:TRP:HB2	2:B:43:PHE:CD2	0.48	2.44	14	2
1:A:113:ASN:ND2	1:A:116:GLU:HG3	0.48	2.24	15	1
1:A:134:PRO:HB2	1:A:136:ASN:OD1	0.47	2.09	4	5
2:B:25:ARG:HD2	2:B:48:GLU:OE1	0.46	2.10	3	2
2:B:25:ARG:HD2	2:B:48:GLU:OE2	0.44	2.11	10	1
1:A:93:TYR:CE1	2:B:24:THR:HG21	0.43	2.48	17	2
1:A:119:TRP:HB2	2:B:43:PHE:CE2	0.43	2.49	3	2
1:A:110:GLN:HB2	1:A:125:LEU:HD21	0.42	1.89	16	1
2:B:36:LEU:HB2	2:B:40:LYS:O	0.41	2.14	1	1
1:A:117:GLY:HA2	2:B:8:TYR:OH	0.40	2.16	18	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	55/57 (96%)	52±1 (95±2%)	3±1 (5±2%)	0±0 (0±0%)	49 83
2	B	62/64 (97%)	58±1 (93±2%)	4±2 (7±2%)	0±0 (0±1%)	31 76
All	All	2340/2420 (97%)	2190 (94%)	144 (6%)	6 (0%)	37 78

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)
2	B	21	VAL	4
2	B	49	LYS	1
1	A	116	GLU	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	49/49 (100%)	41±2 (83±4%)	8±2 (17±4%)	4 39
2	B	55/55 (100%)	51±1 (93±3%)	4±1 (7±3%)	15 63
All	All	2080/2080 (100%)	1837 (88%)	243 (12%)	7 50

All 46 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	114	SER	18
2	B	64	LYS	18
1	A	135	SER	17
1	A	97	THR	16

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Mol	Chain	Res	Type	Models (Total)
2	B	18	SER	15
1	A	102	SER	15
1	A	115	SER	13
1	A	99	ASP	13
1	A	126	THR	12
2	B	3	THR	10
1	A	85	THR	8
1	A	109	PHE	8
1	A	92	ASP	7
1	A	130	THR	6
2	B	54	GLU	6
2	B	47	SER	5
1	A	121	GLU	4
1	A	118	ASP	4
2	B	50	ASP	4
1	A	94	GLU	4
1	A	98	GLU	4
1	A	91	TYR	3
2	B	29	GLN	3
1	A	116	GLU	2
2	B	45	VAL	2
2	B	49	LYS	2
1	A	100	ASP	2
2	B	25	ARG	2
1	A	96	ARG	2
2	B	46	VAL	2
1	A	107	GLU	1
1	A	125	LEU	1
2	B	13	LYS	1
2	B	35	ASP	1
1	A	123	ARG	1
2	B	9	LYS	1
2	B	33	ARG	1
1	A	137	TYR	1
2	B	48	GLU	1
2	B	1	MET	1
2	B	7	LYS	1
2	B	14	GLN	1
2	B	61	LYS	1
2	B	62	GLN	1
2	B	24	THR	1
1	A	104	HIS	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 7% for the well-defined parts and 7% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *F29-bound-nmrstar-final.str*

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	114
Number of shifts mapped to atoms	114
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	57	-0.40 ± 0.84	None needed (< 0.5 ppm)

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 7%, i.e. 114 atoms were assigned a chemical shift out of a possible 1677. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	114/608 (19%)	57/249 (23%)	0/242 (0%)	57/117 (49%)
Sidechain	0/895 (0%)	0/576 (0%)	0/285 (0%)	0/34 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/174 (0%)	0/84 (0%)	0/87 (0%)	0/3 (0%)
Overall	114/1677 (7%)	57/909 (6%)	0/614 (0%)	57/154 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 114 atoms were assigned a chemical shift out of a possible 1677. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	114/608 (19%)	57/249 (23%)	0/242 (0%)	57/117 (49%)
Sidechain	0/895 (0%)	0/576 (0%)	0/285 (0%)	0/34 (0%)
Aromatic	0/174 (0%)	0/84 (0%)	0/87 (0%)	0/3 (0%)
Overall	114/1677 (7%)	57/909 (6%)	0/614 (0%)	57/154 (37%)

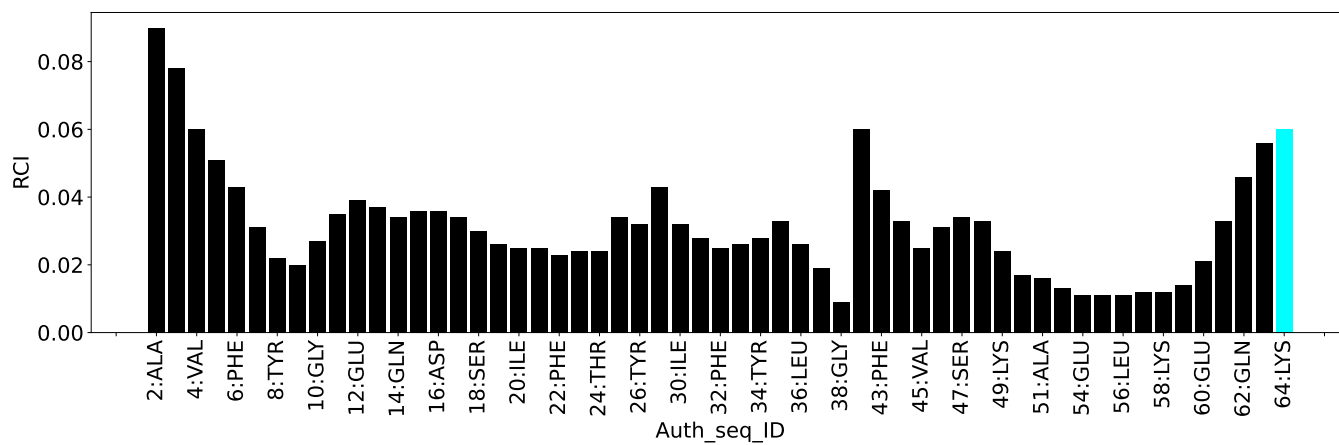
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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 B:



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	22
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$)	0
Inter-chain	22
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.2
Number of long range restraints per residue ¹	0.0

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)	2.6	0.2
0.2-0.5 (Medium)	3.6	0.5
>0.5 (Large)	5.5	11.82

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

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

9 Distance violation analysis

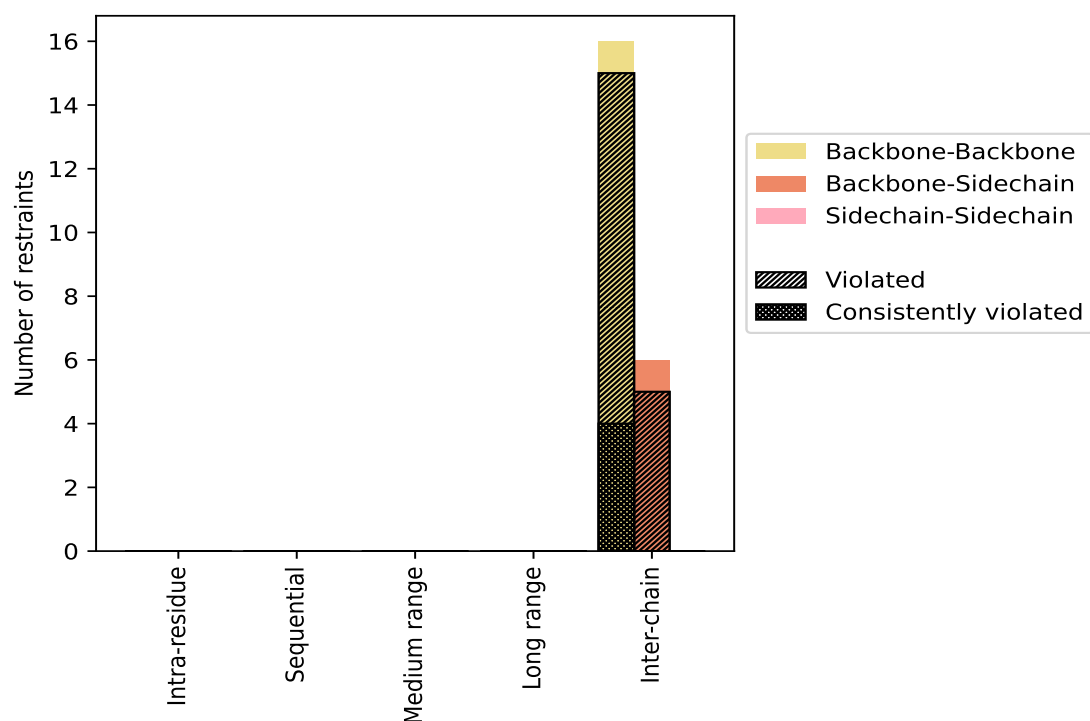
9.1 Summary of distance violations

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)	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
Inter-chain	22	100.0	20	90.9	90.9	4	18.2	18.2
Backbone-Backbone	16	72.7	15	93.8	68.2	4	25.0	18.2
Backbone-Sidechain	6	27.3	5	83.3	22.7	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	22	100.0	20	90.9	90.9	4	18.2	18.2
Backbone-Backbone	16	72.7	15	93.8	68.2	4	25.0	18.2
Backbone-Sidechain	6	27.3	5	83.3	22.7	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	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	0	0	12	12	1.59	10.76	2.92	0.32
2	0	0	0	0	10	10	1.85	10.8	3.09	0.55
3	0	0	0	0	12	12	1.51	10.85	2.94	0.25
4	0	0	0	0	12	12	1.46	10.26	2.72	0.52
5	0	0	0	0	8	8	2.36	10.59	3.24	0.78
6	0	0	0	0	8	8	2.09	11.02	3.44	0.7
7	0	0	0	0	14	14	1.5	11.82	2.95	0.44
8	0	0	0	0	15	15	1.35	11.08	2.68	0.34
9	0	0	0	0	13	13	1.49	10.91	2.83	0.55
10	0	0	0	0	11	11	1.58	10.62	2.97	0.29

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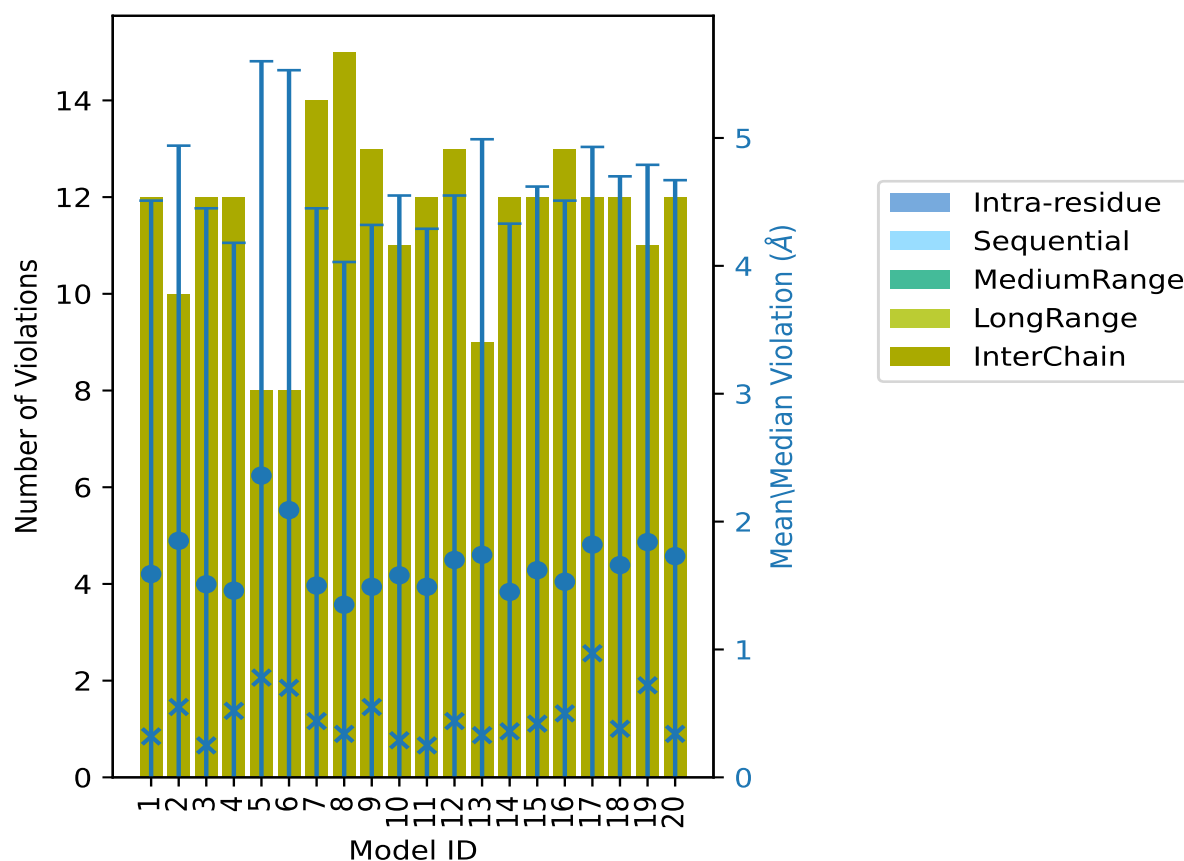
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	12	12	1.49	10.36	2.8	0.25
12	0	0	0	0	13	13	1.7	10.91	2.85	0.44
13	0	0	0	0	9	9	1.74	10.74	3.25	0.33
14	0	0	0	0	12	12	1.45	10.71	2.88	0.36
15	0	0	0	0	12	12	1.62	11.23	3.0	0.42
16	0	0	0	0	13	13	1.53	11.55	2.98	0.5
17	0	0	0	0	12	12	1.82	11.77	3.11	0.97
18	0	0	0	0	12	12	1.66	11.35	3.04	0.38
19	0	0	0	0	11	11	1.84	10.74	2.95	0.72
20	0	0	0	0	12	12	1.73	10.82	2.94	0.34

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 ⓘ



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

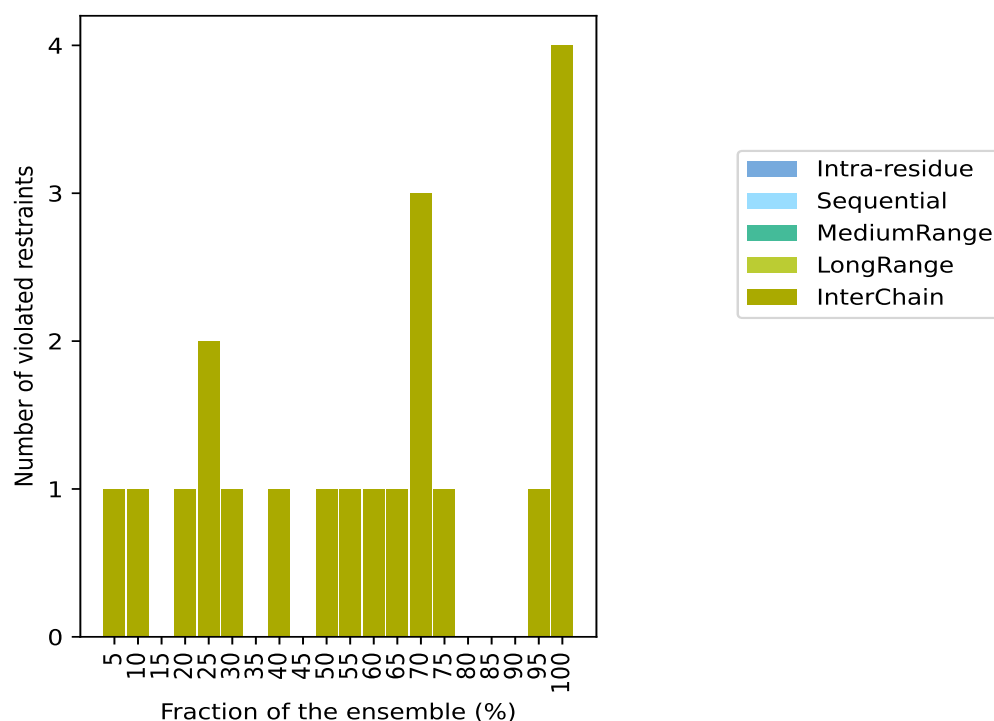
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2(IR:0, SQ:0, MR:0, LR:0, IC:2) restraints are not violated 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	0	1	1	1	5.0
0	0	0	0	1	1	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	1	1	4	20.0
0	0	0	0	2	2	5	25.0
0	0	0	0	1	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	1	1	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	1	1	10	50.0
0	0	0	0	1	1	11	55.0
0	0	0	0	1	1	12	60.0
0	0	0	0	1	1	13	65.0
0	0	0	0	3	3	14	70.0
0	0	0	0	1	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	1	1	19	95.0
0	0	0	0	4	4	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

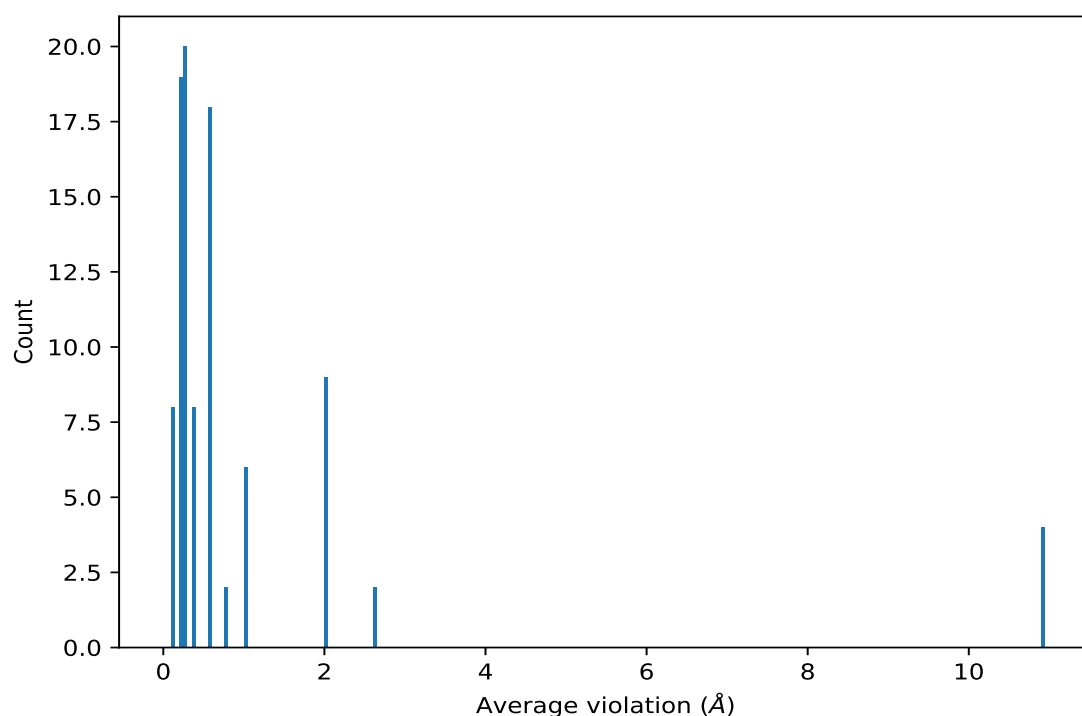
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	20	10.94	0.41	10.84
(2,3)	1:123:A:ARG:HA	2:33:B:ARG:HH12	20	10.94	0.41	10.84
(2,3)	1:123:A:ARG:N	2:22:B:PHE:HZ	20	10.94	0.41	10.84
(2,3)	1:123:A:ARG:N	2:33:B:ARG:HH21	20	10.94	0.41	10.84
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	20	2.64	0.48	2.7
(2,10)	2:27:B:GLY:HA3	1:91:A:TYR:HE2	20	2.64	0.48	2.7
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD2	20	1.03	0.26	0.94
(2,11)	2:45:B:VAL:HG12	1:118:A:ASP:OD1	20	1.03	0.26	0.94
(2,11)	2:45:B:VAL:HG13	1:118:A:ASP:OD1	20	1.03	0.26	0.94
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD2	20	1.03	0.26	0.94
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD1	20	1.03	0.26	0.94
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD1	20	1.03	0.26	0.94
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HD2	20	0.55	0.28	0.48
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HD2	20	0.55	0.28	0.48
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HE2	20	0.55	0.28	0.48
(2,1)	1:97:A:THR:HG22	2:21:B:VAL:HG13	20	0.55	0.28	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1)	1:97:A:THR:HG22	2:21:B:VAL:HG12	20	0.55	0.28	0.48
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:CD2	20	0.55	0.28	0.48
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HE2	20	0.55	0.28	0.48
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG22	19	0.56	0.33	0.53
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG21	19	0.56	0.33	0.53
(2,9)	1:134:A:PRO:HB3	2:24:B:THR:HG22	19	0.56	0.33	0.53
(2,9)	1:134:A:PRO:HA	2:31:B:PHE:HD2	19	0.56	0.33	0.53
(2,9)	1:134:A:PRO:HG2	2:24:B:THR:HG22	19	0.56	0.33	0.53
(2,9)	1:134:A:PRO:HB3	2:31:B:PHE:HD2	19	0.56	0.33	0.53
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG23	19	0.56	0.33	0.53
(2,15)	2:22:B:PHE:HE2	1:99:A:ASP:HB2	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HB3	1:96:A:ARG:HB2	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HD2	1:97:A:THR:OG1	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HD2	1:97:A:THR:HG1	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HE2	1:97:A:THR:OG1	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HB3	1:96:A:ARG:HD3	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HB3	1:96:A:ARG:HD2	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HE2	1:99:A:ASP:HB3	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HB3	1:96:A:ARG:HB3	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HE1	1:119:A:TRP:HH2	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HE2	1:97:A:THR:HG1	15	0.3	0.16	0.23
(2,15)	2:22:B:PHE:HA	1:96:A:ARG:HH21	15	0.3	0.16	0.23
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	14	0.6	0.33	0.46
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	14	0.6	0.33	0.46
(2,4)	1:93:A:TYR:OH	2:24:B:THR:HG1	14	0.39	0.14	0.38
(2,4)	1:93:A:TYR:HD1	2:24:B:THR:HG23	14	0.39	0.14	0.38
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG1	14	0.39	0.14	0.38
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG22	14	0.39	0.14	0.38
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:OG1	14	0.39	0.14	0.38
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG23	14	0.39	0.14	0.38
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	14	0.25	0.14	0.22
(2,5)	1:91:A:TYR:HE2	2:26:B:TYR:HE1	14	0.25	0.14	0.22
(2,5)	1:91:A:TYR:HB2	2:26:B:TYR:HE1	14	0.25	0.14	0.22
(2,2)	1:94:A:GLU:O	2:64:B:LYS:HZ1	13	2.03	1.26	2.53
(2,2)	1:94:A:GLU:H	2:64:B:LYS:HZ2	13	2.03	1.26	2.53
(2,2)	1:94:A:GLU:HB3	2:64:B:LYS:HZ1	13	2.03	1.26	2.53
(2,2)	1:94:A:GLU:HB3	2:64:B:LYS:HZ3	13	2.03	1.26	2.53
(2,2)	1:94:A:GLU:HB2	2:64:B:LYS:HZ3	13	2.03	1.26	2.53
(2,2)	1:94:A:GLU:H	2:24:B:THR:HG23	13	2.03	1.26	2.53
(2,2)	1:94:A:GLU:HG2	2:64:B:LYS:HZ1	13	2.03	1.26	2.53
(2,2)	1:94:A:GLU:O	2:64:B:LYS:HZ3	13	2.03	1.26	2.53
(2,2)	1:94:A:GLU:H	2:64:B:LYS:HZ3	13	2.03	1.26	2.53

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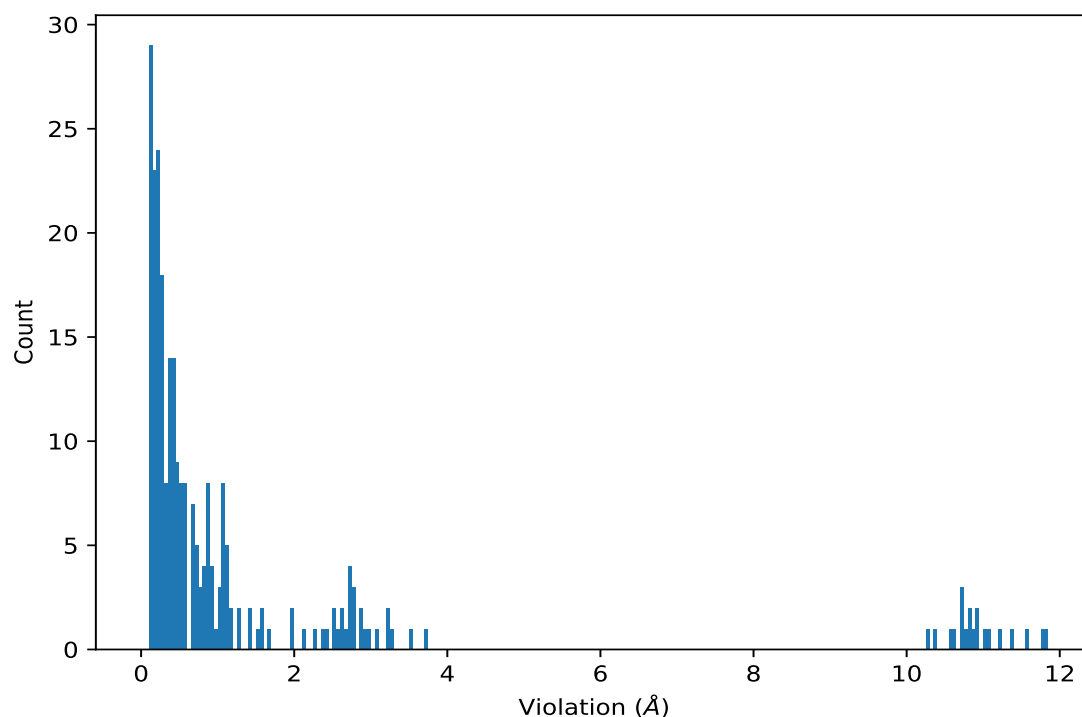
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,6)	1:136:A:ASN:HD21	2:29:B:GLN:O	12	0.26	0.09	0.24
(2,6)	1:136:A:ASN:HB3	2:31:B:PHE:HE1	12	0.26	0.09	0.24
(2,6)	1:136:A:ASN:HD21	2:26:B:TYR:HB2	12	0.26	0.09	0.24
(2,6)	1:136:A:ASN:HD22	2:24:B:THR:O	12	0.26	0.09	0.24
(2,6)	1:136:A:ASN:HD21	2:26:B:TYR:HB3	12	0.26	0.09	0.24
(2,12)	2:26:B:TYR:HE1	1:91:A:TYR:HD2	11	0.2	0.06	0.22
(2,12)	2:26:B:TYR:HH	1:90:A:LEU:HD11	11	0.2	0.06	0.22
(2,12)	2:26:B:TYR:HB2	1:136:A:ASN:HD21	11	0.2	0.06	0.22
(2,12)	2:26:B:TYR:HA	1:137:A:TYR:HE1	11	0.2	0.06	0.22
(2,12)	2:26:B:TYR:HD1	1:137:A:TYR:HA	11	0.2	0.06	0.22
(2,12)	2:26:B:TYR:HB2	1:137:A:TYR:HE1	11	0.2	0.06	0.22
(2,16)	2:24:B:THR:HG22	1:134:A:PRO:HG3	10	0.21	0.08	0.18
(2,16)	2:24:B:THR:HG23	1:137:A:TYR:HE1	10	0.21	0.08	0.18
(2,16)	2:24:B:THR:HG1	1:119:A:TRP:HH2	10	0.21	0.08	0.18
(2,16)	2:24:B:THR:OG1	1:93:A:TYR:HE1	10	0.21	0.08	0.18
(2,16)	2:24:B:THR:OG1	1:119:A:TRP:HH2	10	0.21	0.08	0.18
(2,16)	2:24:B:THR:HG1	1:93:A:TYR:HE1	10	0.21	0.08	0.18
(2,16)	2:24:B:THR:O	1:136:A:ASN:HD22	10	0.21	0.08	0.18
(2,16)	2:24:B:THR:HG22	1:137:A:TYR:HE1	10	0.21	0.08	0.18
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD2	8	0.79	0.6	0.57
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD3	8	0.79	0.6	0.57
(2,13)	2:43:B:PHE:HE2	1:119:A:TRP:HB2	6	0.2	0.11	0.16
(2,13)	2:43:B:PHE:HB3	1:119:A:TRP:HD1	6	0.2	0.11	0.16
(2,13)	2:43:B:PHE:HE1	1:116:A:GLU:HG3	6	0.2	0.11	0.16
(2,13)	2:43:B:PHE:HB2	1:118:A:ASP:OD2	6	0.2	0.11	0.16
(2,13)	2:43:B:PHE:HD1	1:117:A:GLY:HA3	6	0.2	0.11	0.16
(2,8)	1:119:A:TRP:HH2	2:24:B:THR:HG1	5	0.15	0.03	0.13
(2,8)	1:119:A:TRP:HB2	2:43:B:PHE:HE2	5	0.15	0.03	0.13
(2,8)	1:119:A:TRP:HH2	2:24:B:THR:OG1	5	0.15	0.03	0.13
(2,8)	1:119:A:TRP:HE1	2:31:B:PHE:HB3	5	0.15	0.03	0.13
(2,8)	1:119:A:TRP:HZ2	2:31:B:PHE:HB3	5	0.15	0.03	0.13
(2,14)	2:31:B:PHE:HE2	1:135:A:SER:OG	5	0.15	0.03	0.15
(2,14)	2:31:B:PHE:HB3	1:119:A:TRP:HE1	5	0.15	0.03	0.15
(2,14)	2:31:B:PHE:HB3	1:119:A:TRP:HZ2	5	0.15	0.03	0.15
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE2	4	0.38	0.32	0.24
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE3	4	0.38	0.32	0.24
(1,3)	1:117:A:GLY:H	2:8:B:TYR:HE1	2	0.59	0.25	0.59
(1,3)	1:117:A:GLY:H	2:8:B:TYR:HE2	2	0.59	0.25	0.59

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)
(2,3)	1:123:A:ARG:N	2:33:B:ARG:HH21	7	11.82
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	17	11.77
(2,3)	1:123:A:ARG:HA	2:33:B:ARG:HH12	16	11.55
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	18	11.35
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	15	11.23
(2,3)	1:123:A:ARG:HA	2:33:B:ARG:HH12	8	11.08
(2,3)	1:123:A:ARG:N	2:22:B:PHE:HZ	6	11.02
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	9	10.91
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	12	10.91
(2,3)	1:123:A:ARG:HA	2:33:B:ARG:HH12	3	10.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	20	10.82
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	2	10.8
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	1	10.76
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	13	10.74
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	19	10.74
(2,3)	1:123:A:ARG:HA	2:33:B:ARG:HH12	14	10.71
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	10	10.62
(2,3)	1:123:A:ARG:N	2:43:B:PHE:HZ	5	10.59
(2,3)	1:123:A:ARG:HA	2:33:B:ARG:HH12	11	10.36
(2,3)	1:123:A:ARG:HA	2:33:B:ARG:HH12	4	10.26
(2,2)	1:94:A:GLU:H	2:24:B:THR:HG23	12	3.74
(2,2)	1:94:A:GLU:H	2:64:B:LYS:HZ3	20	3.5
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	9	3.28
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	17	3.24
(2,2)	1:94:A:GLU:O	2:64:B:LYS:HZ3	15	3.2
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	18	3.06
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	10	2.97
(2,2)	1:94:A:GLU:HB3	2:64:B:LYS:HZ3	19	2.93
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	20	2.87
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	1	2.86
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	7	2.77
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	12	2.77
(2,2)	1:94:A:GLU:HB2	2:64:B:LYS:HZ3	5	2.77
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	11	2.74
(2,2)	1:94:A:GLU:O	2:64:B:LYS:HZ1	1	2.72
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	16	2.71
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	14	2.7
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	8	2.67
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	5	2.64
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	3	2.62
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	19	2.56
(2,2)	1:94:A:GLU:H	2:64:B:LYS:HZ2	2	2.53
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	4	2.51
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	13	2.41
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	6	2.37
(2,2)	1:94:A:GLU:HB3	2:64:B:LYS:HZ1	3	2.25
(2,10)	2:27:B:GLY:H	1:136:A:ASN:HD21	2	2.14
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD2	11	1.98
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD3	11	1.98
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD1	16	1.65
(2,2)	1:94:A:GLU:HB3	2:64:B:LYS:HZ3	18	1.59
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD2	18	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD1	7	1.53
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD2	8	1.42
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD3	8	1.42
(2,9)	1:134:A:PRO:HB3	2:31:B:PHE:HD2	17	1.26
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HD2	7	1.26
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:CD2	17	1.17
(2,11)	2:45:B:VAL:HG12	1:118:A:ASP:OD1	2	1.16
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	8	1.14
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	8	1.14
(2,11)	2:45:B:VAL:HG12	1:118:A:ASP:OD1	14	1.13
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD1	11	1.1
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD1	20	1.1
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD1	17	1.09
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	17	1.09
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	17	1.09
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	16	1.07
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	16	1.07
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG22	6	1.05
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD2	9	1.05
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD3	9	1.05
(2,9)	1:134:A:PRO:HB3	2:24:B:THR:HG22	10	1.04
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD2	19	1.01
(2,9)	1:134:A:PRO:HB3	2:24:B:THR:HG22	7	1.0
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD2	4	0.95
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD2	10	0.94
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE2	12	0.93
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE3	12	0.93
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD2	1	0.9
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD1	5	0.89
(2,10)	2:27:B:GLY:HA3	1:91:A:TYR:HE2	15	0.89
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	9	0.89
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	9	0.89
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD1	13	0.88
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD1	9	0.87
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD2	15	0.86
(2,9)	1:134:A:PRO:HA	2:31:B:PHE:HD2	15	0.85
(1,3)	1:117:A:GLY:H	2:8:B:TYR:HE1	17	0.84
(1,3)	1:117:A:GLY:H	2:8:B:TYR:HE2	17	0.84
(2,11)	2:45:B:VAL:HG13	1:118:A:ASP:OD1	3	0.83
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HD2	8	0.83
(2,11)	2:45:B:VAL:HG11	1:118:A:ASP:OD2	12	0.79
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	19	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	19	0.79
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HD2	16	0.73
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HD2	18	0.73
(2,11)	2:45:B:VAL:HB	1:118:A:ASP:OD1	8	0.72
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG23	19	0.72
(2,11)	2:45:B:VAL:HG12	1:118:A:ASP:OD1	6	0.71
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HD2	6	0.69
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	7	0.69
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	7	0.69
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:OG1	20	0.68
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD2	14	0.68
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD3	14	0.68
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG22	5	0.66
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG21	4	0.58
(2,9)	1:134:A:PRO:HB3	2:24:B:THR:HG22	9	0.58
(2,15)	2:22:B:PHE:HE2	1:97:A:THR:OG1	5	0.57
(2,4)	1:93:A:TYR:HD1	2:24:B:THR:HG23	2	0.57
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HE2	5	0.57
(2,15)	2:22:B:PHE:HD2	1:97:A:THR:HG1	4	0.55
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	9	0.55
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HD2	4	0.55
(2,4)	1:93:A:TYR:HD1	2:24:B:THR:HG23	14	0.54
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HD2	2	0.54
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG22	8	0.53
(2,4)	1:93:A:TYR:OH	2:24:B:THR:HG1	1	0.52
(2,15)	2:22:B:PHE:HB3	1:96:A:ARG:HD3	7	0.51
(2,15)	2:22:B:PHE:HB3	1:96:A:ARG:HB3	16	0.51
(1,4)	1:118:A:ASP:H	2:9:B:LYS:HD2	16	0.5
(1,4)	1:118:A:ASP:H	2:9:B:LYS:HD3	16	0.5
(2,5)	1:91:A:TYR:HE2	2:26:B:TYR:HE1	12	0.49
(2,1)	1:97:A:THR:HG22	2:21:B:VAL:HG12	10	0.49
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	4	0.49
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	4	0.49
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HD2	14	0.47
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD2	4	0.47
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD3	4	0.47
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HD2	13	0.46
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HD2	1	0.45
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:OG1	19	0.44
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	12	0.44
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	12	0.44
(2,13)	2:43:B:PHE:HB2	1:118:A:ASP:OD2	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG22	12	0.43
(2,6)	1:136:A:ASN:HD21	2:26:B:TYR:HB3	12	0.43
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	6	0.43
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	6	0.43
(2,15)	2:22:B:PHE:HD2	1:97:A:THR:OG1	15	0.42
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HD2	12	0.42
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HD2	15	0.42
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG23	15	0.41
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	11	0.41
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	11	0.41
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG23	18	0.39
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HD2	20	0.39
(2,6)	1:136:A:ASN:HD21	2:29:B:GLN:O	4	0.38
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG1	12	0.38
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD2	7	0.38
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD3	7	0.38
(2,5)	1:91:A:TYR:HB2	2:26:B:TYR:HE1	18	0.37
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	15	0.37
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	15	0.37
(2,16)	2:24:B:THR:HG22	1:137:A:TYR:HE1	19	0.36
(2,15)	2:22:B:PHE:HE2	1:99:A:ASP:HB2	6	0.36
(2,6)	1:136:A:ASN:HD21	2:26:B:TYR:HB3	17	0.35
(2,5)	1:91:A:TYR:HB2	2:26:B:TYR:HE1	15	0.35
(2,2)	1:94:A:GLU:HB3	2:64:B:LYS:HZ3	4	0.35
(2,16)	2:24:B:THR:OG1	1:93:A:TYR:HE1	8	0.34
(2,9)	1:134:A:PRO:HG2	2:24:B:THR:HG22	16	0.34
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:OG1	8	0.34
(1,3)	1:117:A:GLY:H	2:8:B:TYR:HE1	16	0.34
(1,3)	1:117:A:GLY:H	2:8:B:TYR:HE2	16	0.34
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG1	3	0.33
(2,2)	1:94:A:GLU:HG2	2:64:B:LYS:HZ1	13	0.33
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG22	13	0.31
(2,9)	1:134:A:PRO:HB3	2:24:B:THR:HG22	20	0.29
(2,6)	1:136:A:ASN:HD21	2:26:B:TYR:HB2	10	0.29
(2,2)	1:94:A:GLU:O	2:64:B:LYS:HZ1	9	0.29
(2,1)	1:97:A:THR:HG22	2:21:B:VAL:HG13	9	0.29
(2,12)	2:26:B:TYR:HE1	1:91:A:TYR:HD2	20	0.28
(2,6)	1:136:A:ASN:HD21	2:29:B:GLN:O	3	0.28
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	20	0.28
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	2	0.28
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	2	0.28
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG21	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	2:26:B:TYR:HE1	1:91:A:TYR:HD2	8	0.26
(2,12)	2:26:B:TYR:HD1	1:137:A:TYR:HA	15	0.26
(2,6)	1:136:A:ASN:HD21	2:29:B:GLN:O	14	0.26
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	8	0.26
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG22	4	0.26
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG22	7	0.26
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE2	19	0.25
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE3	19	0.25
(2,15)	2:22:B:PHE:HE2	1:97:A:THR:HG1	19	0.24
(2,12)	2:26:B:TYR:HE1	1:91:A:TYR:HD2	10	0.24
(2,12)	2:26:B:TYR:HB2	1:137:A:TYR:HE1	18	0.24
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	10	0.24
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HE2	19	0.24
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE2	14	0.24
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE3	14	0.24
(2,16)	2:24:B:THR:HG23	1:137:A:TYR:HE1	4	0.23
(2,15)	2:22:B:PHE:HE1	1:119:A:TRP:HH2	17	0.23
(2,2)	1:94:A:GLU:HB3	2:64:B:LYS:HZ1	11	0.23
(2,1)	1:97:A:THR:HG1	2:22:B:PHE:HD2	11	0.23
(2,12)	2:26:B:TYR:HB2	1:136:A:ASN:HD21	9	0.22
(2,6)	1:136:A:ASN:HD21	2:26:B:TYR:HB2	9	0.22
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD2	3	0.22
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD3	3	0.22
(2,16)	2:24:B:THR:HG1	1:93:A:TYR:HE1	13	0.21
(2,12)	2:26:B:TYR:HA	1:137:A:TYR:HE1	12	0.21
(2,6)	1:136:A:ASN:HD21	2:29:B:GLN:O	8	0.21
(2,6)	1:136:A:ASN:HD22	2:24:B:THR:O	11	0.21
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG1	13	0.21
(2,15)	2:22:B:PHE:HB3	1:96:A:ARG:HB2	2	0.2
(2,13)	2:43:B:PHE:HD1	1:117:A:GLY:HA3	18	0.2
(2,9)	1:134:A:PRO:HB3	2:24:B:THR:HG22	18	0.2
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	5	0.2
(2,15)	2:22:B:PHE:HA	1:96:A:ARG:HH21	20	0.19
(2,14)	2:31:B:PHE:HB3	1:119:A:TRP:HZ2	17	0.19
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG22	3	0.19
(2,8)	1:119:A:TRP:HZ2	2:31:B:PHE:HB3	17	0.19
(2,4)	1:93:A:TYR:HE1	2:24:B:THR:HG22	10	0.19
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	20	0.19
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	20	0.19
(2,16)	2:24:B:THR:HG22	1:134:A:PRO:HG3	1	0.18
(2,16)	2:24:B:THR:HG1	1:119:A:TRP:HH2	7	0.18
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG22	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8)	1:119:A:TRP:HH2	2:24:B:THR:HG1	7	0.18
(2,6)	1:136:A:ASN:HB3	2:31:B:PHE:HE1	7	0.18
(2,16)	2:24:B:THR:OG1	1:119:A:TRP:HH2	12	0.17
(2,15)	2:22:B:PHE:HE2	1:99:A:ASP:HB2	1	0.17
(2,14)	2:31:B:PHE:HE2	1:135:A:SER:OG	8	0.17
(2,13)	2:43:B:PHE:HB3	1:119:A:TRP:HD1	14	0.17
(2,16)	2:24:B:THR:HG22	1:134:A:PRO:HG3	14	0.16
(2,15)	2:22:B:PHE:HB3	1:96:A:ARG:HD3	10	0.16
(2,13)	2:43:B:PHE:HB3	1:119:A:TRP:HD1	10	0.16
(2,9)	1:134:A:PRO:HG3	2:24:B:THR:HG22	14	0.16
(2,14)	2:31:B:PHE:HB3	1:119:A:TRP:HE1	15	0.15
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG2	18	0.15
(1,6)	1:119:A:TRP:H	2:9:B:LYS:HG3	18	0.15
(2,15)	2:22:B:PHE:HB3	1:96:A:ARG:HD2	13	0.14
(2,15)	2:22:B:PHE:HE2	1:99:A:ASP:HB3	14	0.14
(2,6)	1:136:A:ASN:HD21	2:29:B:GLN:O	2	0.14
(2,16)	2:24:B:THR:OG1	1:119:A:TRP:HH2	9	0.13
(2,16)	2:24:B:THR:O	1:136:A:ASN:HD22	18	0.13
(2,15)	2:22:B:PHE:HD2	1:97:A:THR:OG1	3	0.13
(2,13)	2:43:B:PHE:HE1	1:116:A:GLU:HG3	16	0.13
(2,12)	2:26:B:TYR:HE1	1:91:A:TYR:HD2	1	0.13
(2,12)	2:26:B:TYR:HE1	1:91:A:TYR:HD2	7	0.13
(2,8)	1:119:A:TRP:HH2	2:24:B:THR:OG1	9	0.13
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	1	0.13
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	2	0.13
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	3	0.13
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	7	0.13
(2,1)	1:97:A:THR:OG1	2:22:B:PHE:HD2	3	0.13
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD2	1	0.13
(1,2)	1:99:A:ASP:H	2:33:B:ARG:HD3	1	0.13
(2,14)	2:31:B:PHE:HB3	1:119:A:TRP:HE1	11	0.12
(2,13)	2:43:B:PHE:HE2	1:119:A:TRP:HB2	8	0.12
(2,8)	1:119:A:TRP:HB2	2:43:B:PHE:HE2	8	0.12
(2,8)	1:119:A:TRP:HE1	2:31:B:PHE:HB3	11	0.12
(2,6)	1:136:A:ASN:HD21	2:29:B:GLN:O	6	0.12
(2,14)	2:31:B:PHE:HB3	1:119:A:TRP:HE1	16	0.11
(2,12)	2:26:B:TYR:HH	1:90:A:LEU:HD11	3	0.11
(2,12)	2:26:B:TYR:HE1	1:91:A:TYR:HD2	16	0.11
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	11	0.11
(2,5)	1:91:A:TYR:HD2	2:26:B:TYR:HE1	16	0.11
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE2	20	0.11
(1,1)	1:94:A:GLU:H	2:64:B:LYS:HE3	20	0.11

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found