



Full wwPDB NMR Structure Validation Report ⓘ

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BMRB ID : 25900
Title : NRAS Isoform 5
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Deposited on : 2015-11-13

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

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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 : 4-5-2 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

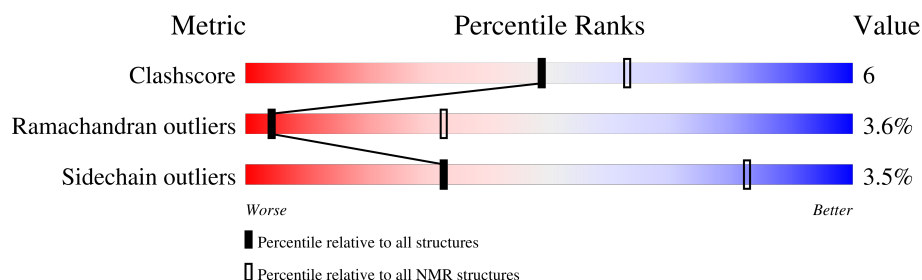
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 55%.

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	20	 85% 15%

2 Ensemble composition and analysis

This entry contains 25 models. Model 9 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:1-A:20 (20)	0.40	9

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 25
2	23, 24
Single-model clusters	22

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 300 atoms, of which 152 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GTPase NRas.

Mol	Chain	Residues	Atoms						Trace
1	A	20	Total	C	H	N	O	S	0
			300	97	152	25	25	1	

There are 3 discrepancies between the modelled and reference sequences:

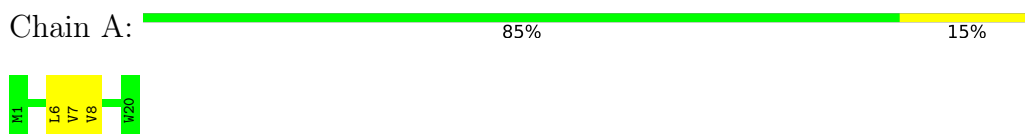
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	HIS	-	SEE REMARK 999	UNP P01111
A	19	VAL	-	SEE REMARK 999	UNP P01111
A	20	TRP	-	SEE REMARK 999	UNP P01111

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: GTPase NRas

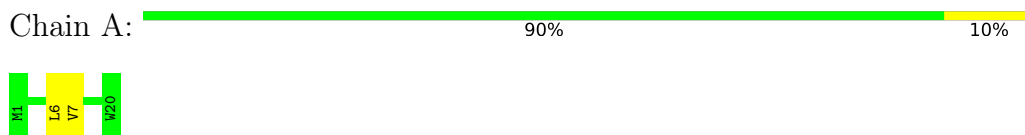


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

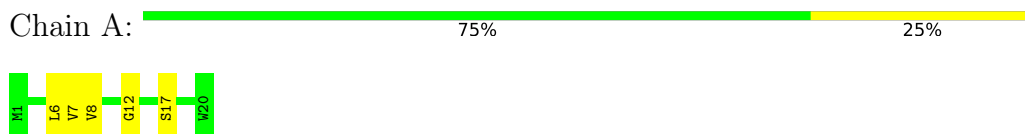
4.2.1 Score per residue for model 1

- Molecule 1: GTPase NRas



4.2.2 Score per residue for model 2

- Molecule 1: GTPase NRas



4.2.3 Score per residue for model 3

- Molecule 1: GTPase NRas

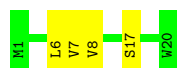
Chain A:  85% 15%



4.2.4 Score per residue for model 4

- Molecule 1: GTPase NRas

Chain A:  80% 20%



4.2.5 Score per residue for model 5

- Molecule 1: GTPase NRas

Chain A:  80% 20%



4.2.6 Score per residue for model 6

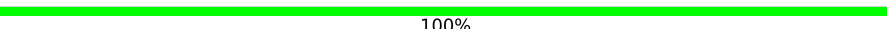
- Molecule 1: GTPase NRas

Chain A:  75% 20% 5%



4.2.7 Score per residue for model 7

- Molecule 1: GTPase NRas

Chain A:  100%

There are no outlier residues in this chain.

4.2.8 Score per residue for model 8

- Molecule 1: GTPase NRas

Chain A:  90% 10%



4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: GTPase NRas

Chain A:  95% 5%



4.2.10 Score per residue for model 10

- Molecule 1: GTPase NRas

Chain A:  75% 20% 5%



4.2.11 Score per residue for model 11

- Molecule 1: GTPase NRas

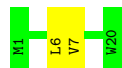
Chain A:  85% 10% 5%



4.2.12 Score per residue for model 12

- Molecule 1: GTPase NRas

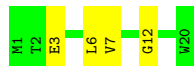
Chain A:  90% 10%



4.2.13 Score per residue for model 13

- Molecule 1: GTPase NRas

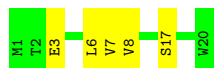
Chain A:  80% 20%



4.2.14 Score per residue for model 14

- Molecule 1: GTPase NRas

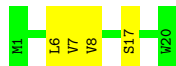
Chain A:  75% 25%



4.2.15 Score per residue for model 15

- Molecule 1: GTPase NRas

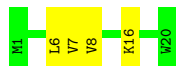
Chain A:  80% 20%



4.2.16 Score per residue for model 16

- Molecule 1: GTPase NRas

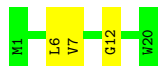
Chain A:  80% 20%



4.2.17 Score per residue for model 17

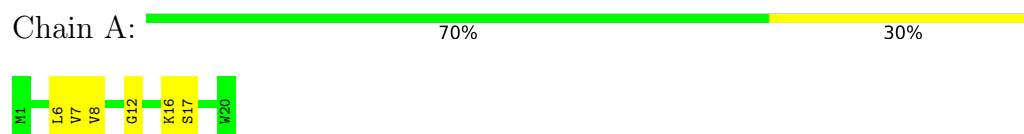
- Molecule 1: GTPase NRas

Chain A:  85% 15%



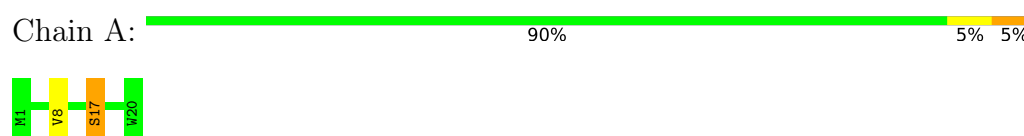
4.2.18 Score per residue for model 18

- Molecule 1: GTPase NRas



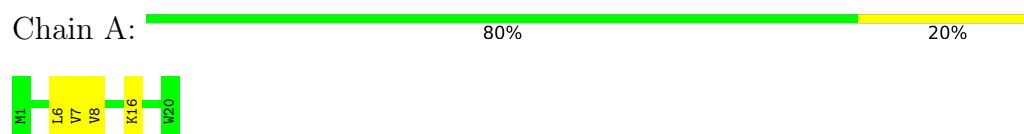
4.2.19 Score per residue for model 19

- Molecule 1: GTPase NRas



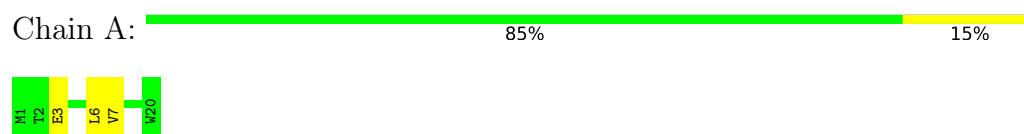
4.2.20 Score per residue for model 20

- Molecule 1: GTPase NRas



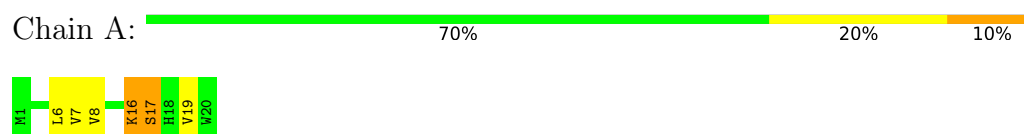
4.2.21 Score per residue for model 21

- Molecule 1: GTPase NRas



4.2.22 Score per residue for model 22

- Molecule 1: GTPase NRas



4.2.23 Score per residue for model 23

- Molecule 1: GTPase NRas

Chain A:  75% 25%



4.2.24 Score per residue for model 24

- Molecule 1: GTPase NRas

Chain A:  65% 35%



4.2.25 Score per residue for model 25

- Molecule 1: GTPase NRas

Chain A:  90% 10%



5 Refinement protocol and experimental data overview

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

Of the 25 calculated structures, 25 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	150
Number of shifts mapped to atoms	149
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	55%

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	148	152	154	2±1
All	All	3700	3800	3696	43

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD12	1:A:7:VAL:HG23	0.51	1.81	6	8
1:A:8:VAL:HG13	1:A:14:VAL:HB	0.50	1.83	10	4
1:A:8:VAL:HG11	1:A:16:LYS:HB2	0.49	1.84	20	3
1:A:16:LYS:O	1:A:19:VAL:HG23	0.48	2.07	23	3
1:A:8:VAL:HG11	1:A:17:SER:H	0.46	1.70	19	6
1:A:6:LEU:CD1	1:A:7:VAL:HG23	0.45	2.42	16	17
1:A:8:VAL:HG11	1:A:17:SER:HB2	0.45	1.88	22	1
1:A:8:VAL:HG21	1:A:16:LYS:HB2	0.41	1.91	11	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	18/20 (90%)	15±0 (82±2%)	3±1 (14±5%)	1±1 (4±4%)	4	32
All	All	450/500 (90%)	369 (82%)	65 (14%)	16 (4%)	4	32

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	12	GLY	9
1	A	3	GLU	7

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	15/15 (100%)	14±1 (97±4%)	1±1 (3±4%)	32	82
All	All	375/375 (100%)	362 (97%)	13 (3%)	32	82

All 5 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	16	LYS	4
1	A	17	SER	4
1	A	6	LEU	3
1	A	5	LYS	1
1	A	1	MET	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 55% for the well-defined parts and 55% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	150
Number of shifts mapped to atoms	149
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	HIS	HE2	7.142	.	4

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

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 55%, i.e. 143 atoms were assigned a chemical shift out of a possible 260. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	43/104 (41%)	43/44 (98%)	0/40 (0%)	0/20 (0%)
Sidechain	86/128 (67%)	86/86 (100%)	0/40 (0%)	0/2 (0%)
Aromatic	14/28 (50%)	14/14 (100%)	0/12 (0%)	0/2 (0%)
Overall	143/260 (55%)	143/144 (99%)	0/92 (0%)	0/24 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 143 atoms were assigned a chemical shift out of a possible 260. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	43/104 (41%)	43/44 (98%)	0/40 (0%)	0/20 (0%)
Sidechain	86/128 (67%)	86/86 (100%)	0/40 (0%)	0/2 (0%)
Aromatic	14/28 (50%)	14/14 (100%)	0/12 (0%)	0/2 (0%)
Overall	143/260 (55%)	143/144 (99%)	0/92 (0%)	0/24 (0%)

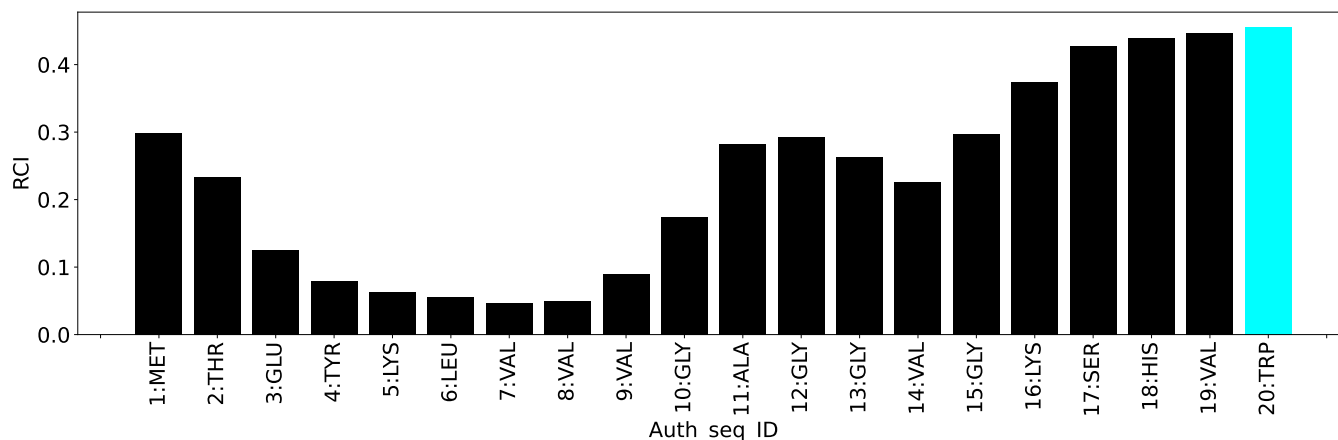
7.1.4 Statistically unusual chemical shifts [i](#)

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 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	181
Intra-residue ($ i-j =0$)	66
Sequential ($ i-j =1$)	67
Medium range ($ i-j >1$ and $ i-j <5$)	39
Long range ($ i-j \geq 5$)	9
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	9.1
Number of long range restraints per residue ¹	0.5

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)	0.4	0.19
0.2-0.5 (Medium)	1.2	0.5
>0.5 (Large)	15.1	3.19

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 ⓘ

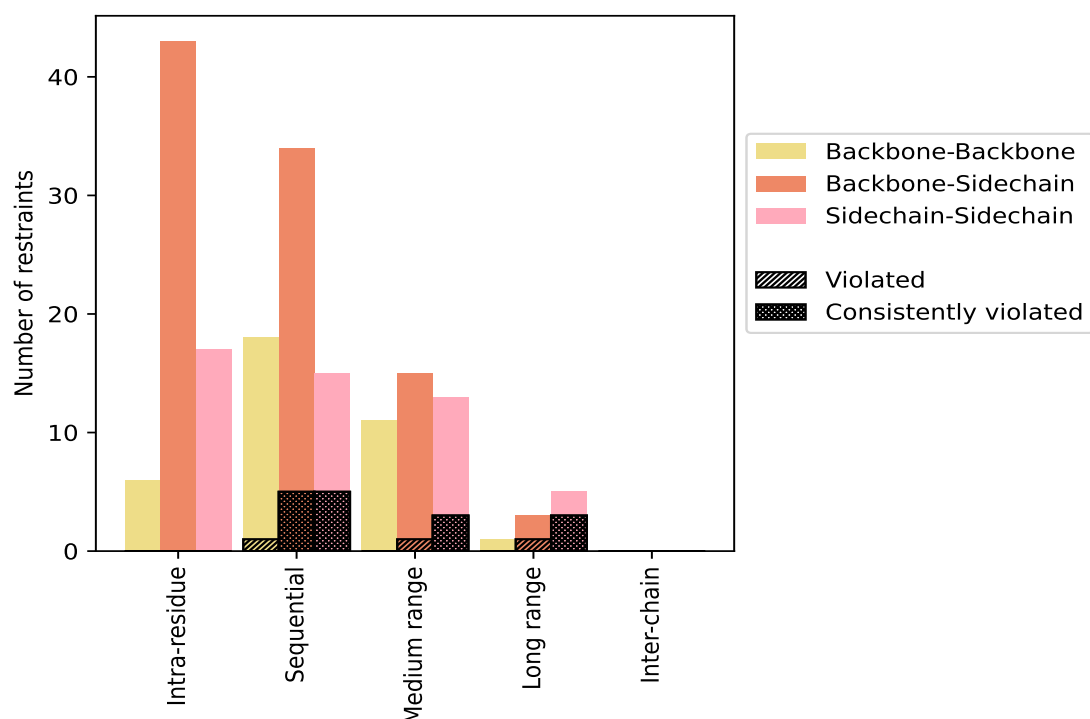
9.1 Summary of distance violations ⓘ

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)	66	36.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	6	3.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	43	23.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	17	9.4	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	67	37.0	11	16.4	6.1	10	14.9	5.5
Backbone-Backbone	18	9.9	1	5.6	0.6	0	0.0	0.0
Backbone-Sidechain	34	18.8	5	14.7	2.8	5	14.7	2.8
Sidechain-Sidechain	15	8.3	5	33.3	2.8	5	33.3	2.8
Medium range (i-j >1 & i-j <5)	39	21.5	4	10.3	2.2	3	7.7	1.7
Backbone-Backbone	11	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	15	8.3	1	6.7	0.6	0	0.0	0.0
Sidechain-Sidechain	13	7.2	3	23.1	1.7	3	23.1	1.7
Long range (i-j ≥5)	9	5.0	4	44.4	2.2	3	33.3	1.7
Backbone-Backbone	1	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	1.7	1	33.3	0.6	0	0.0	0.0
Sidechain-Sidechain	5	2.8	3	60.0	1.7	3	60.0	1.7
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	181	100.0	19	10.5	10.5	16	8.8	8.8
Backbone-Backbone	36	19.9	1	2.8	0.6	0	0.0	0.0
Backbone-Sidechain	95	52.5	7	7.4	3.9	5	5.3	2.8
Sidechain-Sidechain	50	27.6	11	22.0	6.1	11	22.0	6.1

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	10	3	4	0	17	1.55	3.14	0.85	1.44
2	0	11	3	4	0	18	1.46	3.14	0.88	1.31
3	0	10	4	4	0	18	1.4	3.14	0.91	1.31
4	0	10	3	3	0	16	1.59	3.14	0.85	1.38
5	0	10	4	4	0	18	1.41	3.13	0.89	1.34
6	0	10	3	4	0	17	1.54	3.13	0.93	1.4
7	0	10	3	4	0	17	1.49	3.14	0.88	1.41
8	0	10	3	3	0	16	1.57	3.14	0.84	1.36
9	0	10	3	3	0	16	1.61	3.14	0.85	1.44
10	0	10	3	4	0	17	1.5	3.14	0.87	1.32

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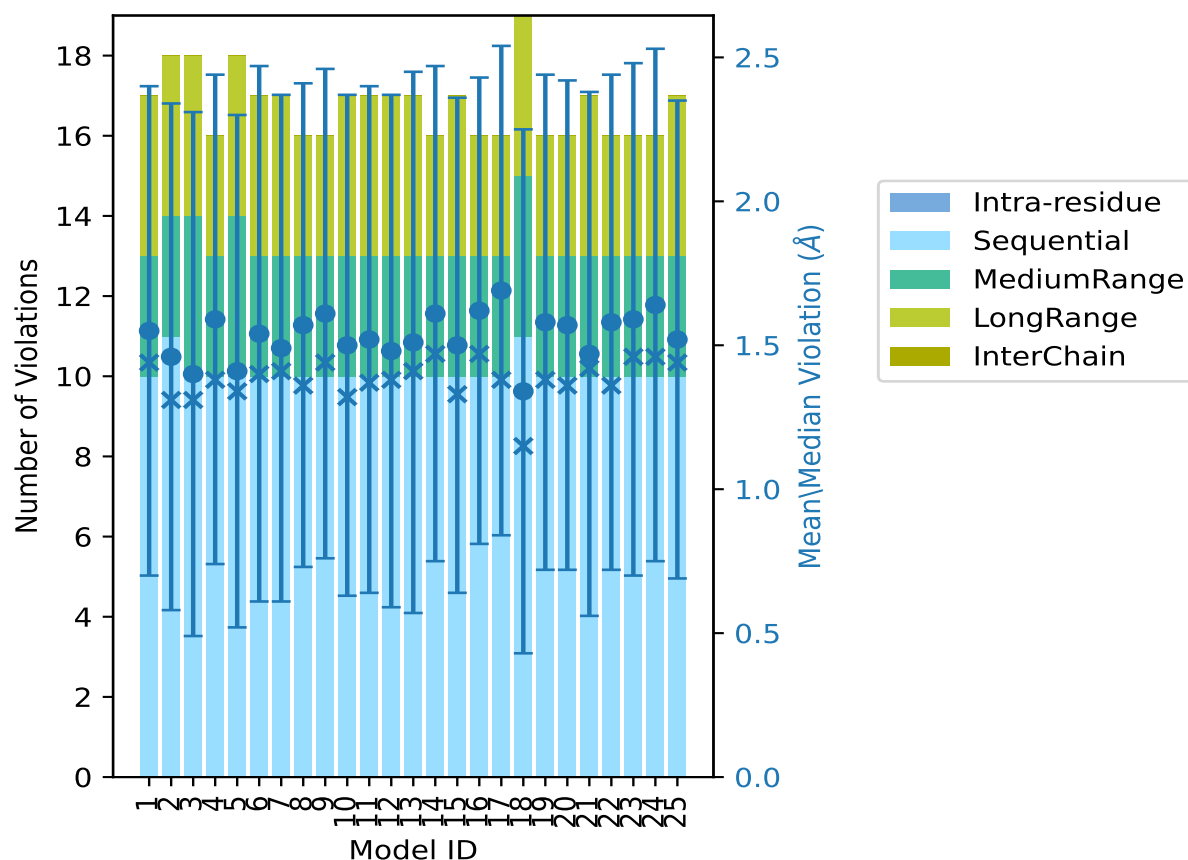
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	10	3	4	0	17	1.52	3.14	0.88	1.37
12	0	10	3	4	0	17	1.48	3.15	0.89	1.38
13	0	10	3	4	0	17	1.51	3.19	0.94	1.41
14	0	10	3	3	0	16	1.61	3.13	0.86	1.47
15	0	10	3	4	0	17	1.5	3.16	0.86	1.33
16	0	10	3	3	0	16	1.62	3.16	0.81	1.47
17	0	10	3	3	0	16	1.69	3.16	0.85	1.38
18	0	11	4	4	0	19	1.34	3.16	0.91	1.15
19	0	10	3	3	0	16	1.58	3.15	0.86	1.38
20	0	10	3	3	0	16	1.57	3.16	0.85	1.36
21	0	10	3	4	0	17	1.47	3.13	0.91	1.42
22	0	10	3	3	0	16	1.58	3.16	0.86	1.36
23	0	10	3	3	0	16	1.59	3.13	0.89	1.46
24	0	10	3	3	0	16	1.64	3.14	0.89	1.46
25	0	10	3	4	0	17	1.52	3.14	0.83	1.44

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 [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 162(IR:66, SQ:56, MR:35, LR:5, 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	0	0	0	1	4.0
0	1	0	0	0	1	2	8.0
0	0	1	0	0	1	3	12.0
0	0	0	0	0	0	4	16.0
0	0	0	0	0	0	5	20.0
0	0	0	0	0	0	6	24.0

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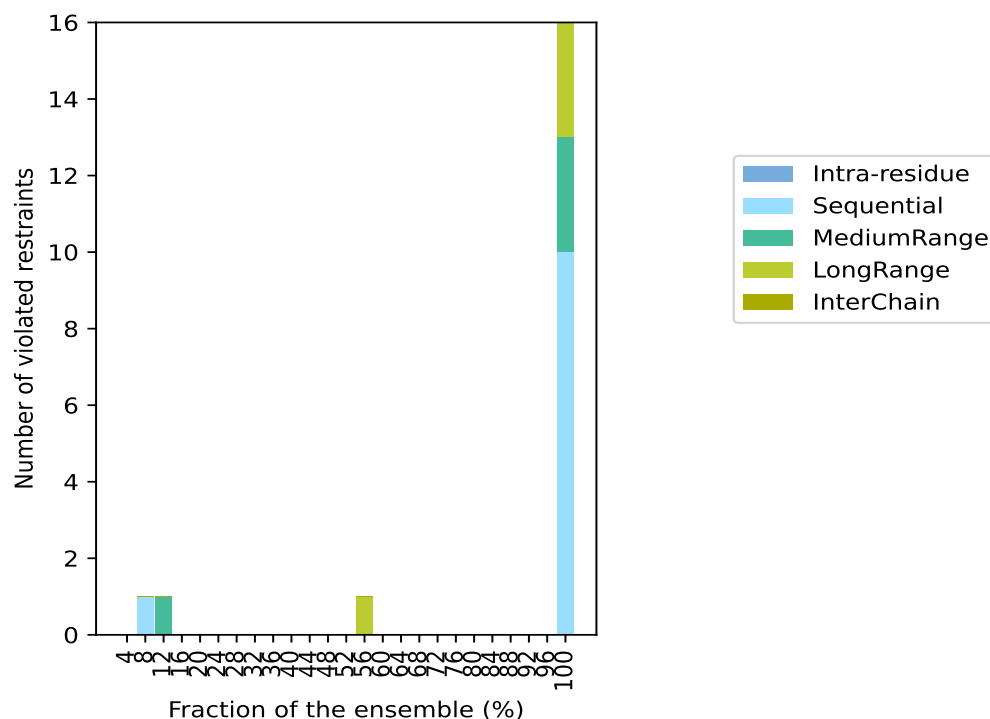
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	7	28.0
0	0	0	0	0	0	8	32.0
0	0	0	0	0	0	9	36.0
0	0	0	0	0	0	10	40.0
0	0	0	0	0	0	11	44.0
0	0	0	0	0	0	12	48.0
0	0	0	0	0	0	13	52.0
0	0	0	1	0	1	14	56.0
0	0	0	0	0	0	15	60.0
0	0	0	0	0	0	16	64.0
0	0	0	0	0	0	17	68.0
0	0	0	0	0	0	18	72.0
0	0	0	0	0	0	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	0	0	0	21	84.0
0	0	0	0	0	0	22	88.0
0	0	0	0	0	0	23	92.0
0	0	0	0	0	0	24	96.0
0	10	3	3	0	16	25	100.0

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

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

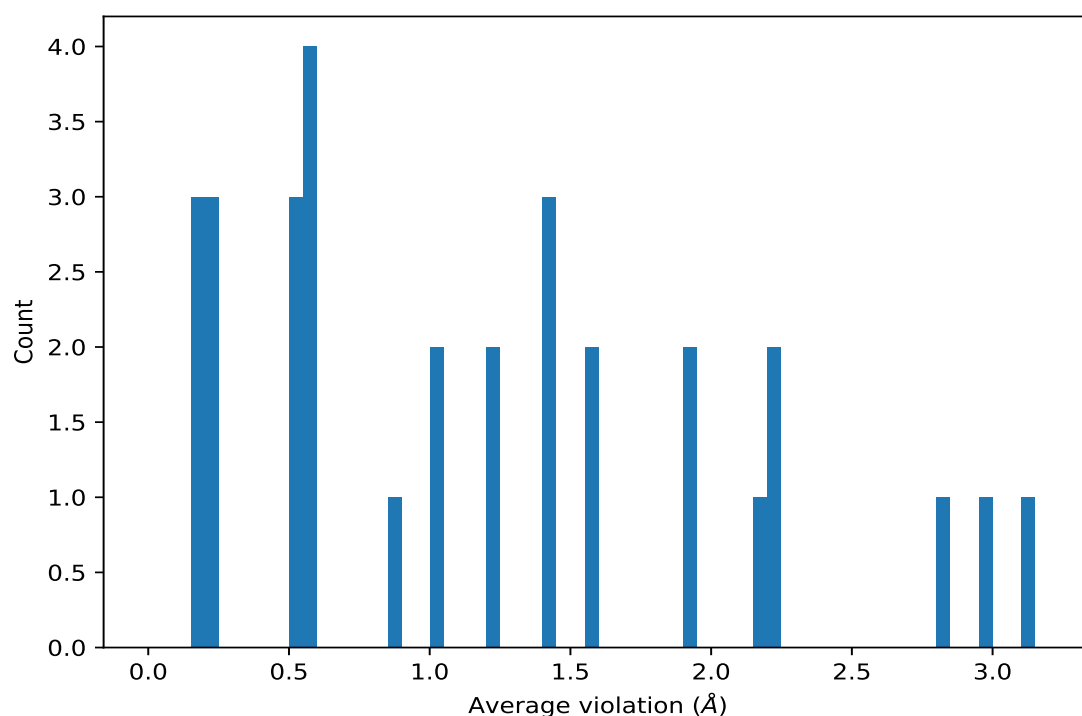
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	25	3.14	0.01	3.14
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	25	2.98	0.14	3.01
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	25	2.81	0.02	2.81
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	25	2.23	0.02	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	25	2.23	0.02	2.22
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	25	2.19	0.35	2.23
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	25	1.93	0.12	1.87
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	25	1.93	0.12	1.87
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	25	1.55	0.03	1.54
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	25	1.55	0.03	1.54
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	25	1.44	0.11	1.38
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	25	1.44	0.11	1.38
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	25	1.41	0.0	1.41
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	25	1.22	0.06	1.22
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	25	1.22	0.06	1.22
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	25	1.03	0.22	0.99

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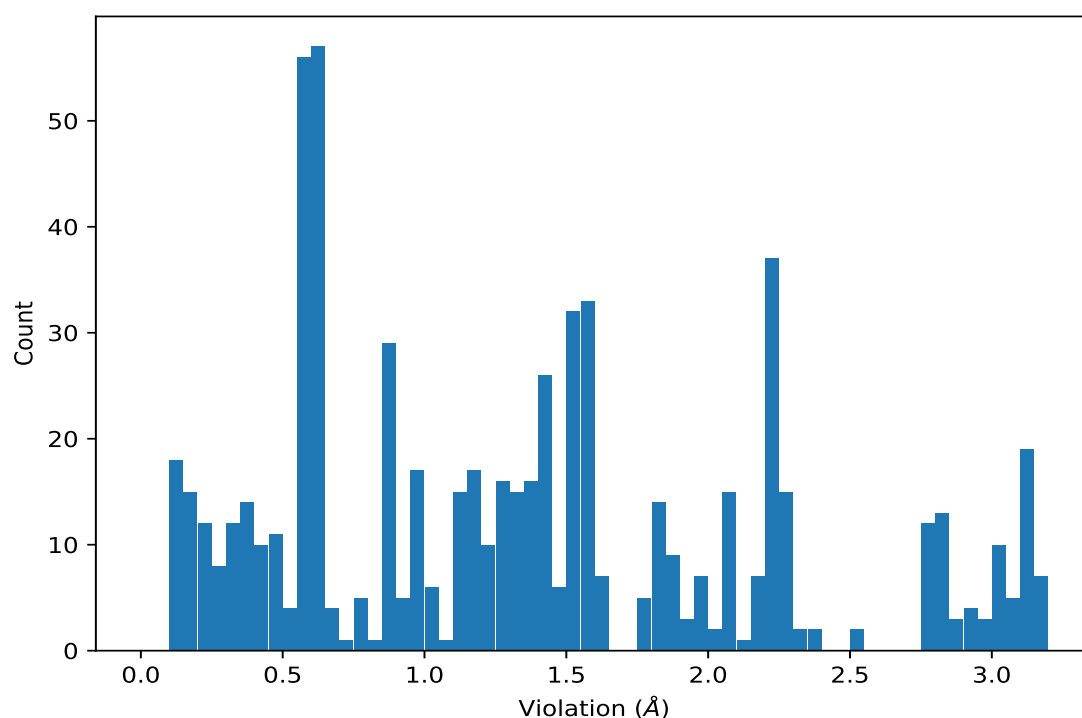
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	25	1.03	0.08	0.98
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	25	0.87	0.01	0.87
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	25	0.58	0.2	0.55
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	25	0.57	0.1	0.62
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	25	0.57	0.1	0.62
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	25	0.57	0.1	0.62
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	25	0.53	0.11	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	25	0.53	0.11	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	25	0.53	0.11	0.59
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	14	0.17	0.05	0.16
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	14	0.17	0.05	0.16
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	14	0.17	0.05	0.16
(1,120)	1:9:A:VAL:HG11	1:12:A:GLY:H	3	0.23	0.07	0.19
(1,120)	1:9:A:VAL:HG12	1:12:A:GLY:H	3	0.23	0.07	0.19
(1,120)	1:9:A:VAL:HG13	1:12:A:GLY:H	3	0.23	0.07	0.19

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)
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	13	3.19
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	15	3.16
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	16	3.16
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	17	3.16
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	18	3.16
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	20	3.16
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	22	3.16
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	12	3.15
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	19	3.15
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	1	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	2	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	3	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	4	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	7	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	8	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	9	3.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	10	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	11	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	24	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	25	3.14
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	5	3.13
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	6	3.13
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	13	3.13
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	14	3.13
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	21	3.13
(1,44)	1:4:A:TYR:HD2	1:5:A:LYS:HA	23	3.13
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	9	3.08
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	17	3.07
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	23	3.07
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	6	3.06
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	7	3.06
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	3	3.05
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	14	3.05
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	21	3.04
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	12	3.03
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	1	3.02
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	4	3.02
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	19	3.02
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	2	3.01
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	24	3.01
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	11	3.0
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	5	2.98
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	18	2.96
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	8	2.95
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	16	2.94
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	20	2.94
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	15	2.93
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	10	2.91
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	17	2.9
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	22	2.9
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	24	2.86
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	15	2.84
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	16	2.84
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	17	2.84
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	20	2.84
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	22	2.84
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	12	2.83
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	18	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	19	2.83
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	2	2.81
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	4	2.81
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	8	2.81
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	9	2.81
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	10	2.81
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	1	2.8
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	3	2.8
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	7	2.8
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	11	2.8
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	24	2.8
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	5	2.79
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	6	2.79
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	13	2.79
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	14	2.79
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	23	2.79
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	25	2.78
(1,53)	1:4:A:TYR:HE2	1:5:A:LYS:HA	21	2.77
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	22	2.52
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	6	2.51
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	23	2.4
(1,48)	1:4:A:TYR:HD2	1:8:A:VAL:HB	25	2.36
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	19	2.34
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	20	2.31
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	11	2.3
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	14	2.29
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	9	2.28
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	13	2.27
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	8	2.27
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	8	2.27
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	10	2.27
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	10	2.27
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	4	2.26
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	2	2.26
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	2	2.26
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	4	2.26
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	4	2.26
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	11	2.26
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	11	2.26
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	10	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	3	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	3	2.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	19	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	19	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	20	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	20	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	21	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	21	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	22	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	22	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	23	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	23	2.23
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	1	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	1	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	9	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	9	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	13	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	13	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	15	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	15	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	17	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	17	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	18	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	18	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	24	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	24	2.22
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	12	2.21
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	12	2.21
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	16	2.21
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	16	2.21
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	5	2.2
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	5	2.2
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	14	2.2
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	14	2.2
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	25	2.2
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	25	2.2
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	16	2.19
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	6	2.19
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	6	2.19
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB2	7	2.19
(1,46)	1:4:A:TYR:HD2	1:5:A:LYS:HB3	7	2.19
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	25	2.18
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	2	2.16
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	8	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	5	2.09
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	5	2.09
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	6	2.09
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	6	2.09
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	14	2.09
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	14	2.09
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	21	2.09
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	21	2.09
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	25	2.09
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	25	2.09
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	1	2.08
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	7	2.08
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	7	2.08
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	13	2.07
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	13	2.07
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	23	2.01
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	23	2.01
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	15	1.99
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	24	1.99
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	24	1.99
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	1	1.97
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	1	1.97
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	9	1.96
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	9	1.96
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	12	1.95
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	3	1.95
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	3	1.95
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	18	1.87
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	11	1.87
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	11	1.87
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	2	1.85
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	2	1.85
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	4	1.85
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	4	1.85
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	12	1.85
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	12	1.85
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	19	1.84
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	19	1.84
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	16	1.83
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	16	1.83
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	18	1.83
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	18	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	8	1.82
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	8	1.82
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	10	1.81
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	10	1.81
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	17	1.81
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	17	1.81
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	15	1.8
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	15	1.8
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	21	1.78
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	20	1.78
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	20	1.78
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG2	22	1.78
(1,45)	1:4:A:TYR:HD2	1:5:A:LYS:HG3	22	1.78
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	7	1.63
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	8	1.6
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	8	1.6
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	10	1.6
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	10	1.6
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	11	1.6
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	11	1.6
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	2	1.59
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	2	1.59
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	4	1.59
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	4	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	5	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	5	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	6	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	6	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	14	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	14	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	21	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	21	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	25	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	25	1.59
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	7	1.58
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	7	1.58
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	21	1.57
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	21	1.57
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	23	1.57
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	23	1.57
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	13	1.57
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	13	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	3	1.56
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	3	1.56
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	13	1.56
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	13	1.56
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	1	1.55
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	1	1.55
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	9	1.55
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	9	1.55
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	24	1.55
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	24	1.55
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	16	1.55
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	19	1.54
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	19	1.54
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	22	1.54
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	22	1.54
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	25	1.54
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	25	1.54
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	3	1.54
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	5	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	5	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	6	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	6	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	14	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	14	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	18	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	18	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	20	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	20	1.53
(1,51)	1:4:A:TYR:HE1	1:20:A:TRP:HE3	5	1.53
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	12	1.52
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	12	1.52
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	15	1.52
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	15	1.52
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	16	1.52
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	16	1.52
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	17	1.52
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	17	1.52
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB2	7	1.51
(1,55)	1:4:A:TYR:HE2	1:5:A:LYS:HB3	7	1.51
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	23	1.51
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	23	1.51
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	24	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	24	1.5
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	1	1.47
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	1	1.47
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	3	1.46
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	3	1.46
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	9	1.46
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	9	1.46
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	1	1.44
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	25	1.44
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	15	1.42
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	16	1.42
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	17	1.42
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	21	1.42
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	22	1.42
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	25	1.42
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	1	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	2	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	3	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	4	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	5	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	7	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	8	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	9	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	10	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	11	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	12	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	13	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	14	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	18	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	19	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	20	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	23	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	24	1.41
(1,43)	1:4:A:TYR:HD2	1:5:A:LYS:H	6	1.4
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	12	1.38
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	12	1.38
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	11	1.37
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	11	1.37
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	2	1.36
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	2	1.36
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	4	1.36
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	4	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	19	1.36
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	19	1.36
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	16	1.35
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	16	1.35
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	18	1.35
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	18	1.35
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	17	1.35
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	17	1.34
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	17	1.34
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	15	1.33
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	8	1.32
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	8	1.32
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	10	1.32
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	10	1.32
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	15	1.32
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	15	1.32
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	7	1.32
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	7	1.32
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	20	1.3
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	20	1.3
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG2	22	1.3
(1,54)	1:4:A:TYR:HE2	1:5:A:LYS:HG3	22	1.3
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	1	1.29
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	1	1.29
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	6	1.29
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	6	1.29
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	9	1.29
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	9	1.29
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	25	1.28
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	25	1.28
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	14	1.27
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	14	1.27
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	2	1.26
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	2	1.26
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	5	1.26
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	5	1.26
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	4	1.25
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	4	1.25
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	11	1.24
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	11	1.24
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	8	1.23
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	8	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	10	1.23
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	10	1.23
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	22	1.22
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	22	1.22
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	3	1.21
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	3	1.21
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	15	1.2
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	15	1.2
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	20	1.2
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	20	1.2
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	23	1.19
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	24	1.19
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	17	1.18
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	24	1.17
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	24	1.17
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	17	1.16
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	17	1.16
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	19	1.16
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	19	1.16
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	21	1.16
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	21	1.16
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	6	1.16
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	21	1.16
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	18	1.15
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	12	1.15
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	12	1.15
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	13	1.15
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	13	1.15
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	16	1.14
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	16	1.14
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	18	1.14
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	18	1.14
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	13	1.14
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	14	1.14
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD2	23	1.13
(1,47)	1:4:A:TYR:HD2	1:5:A:LYS:HD3	23	1.13
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	25	1.11
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	3	1.1
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	2	1.07
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	6	1.04
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	5	1.03
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	10	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	1	1.0
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	5	1.0
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	19	1.0
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	7	0.99
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	14	0.99
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	12	0.99
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	2	0.98
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	18	0.98
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	22	0.98
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	3	0.97
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	4	0.97
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	8	0.97
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	9	0.97
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	10	0.97
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	11	0.97
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	15	0.97
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	17	0.97
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	20	0.97
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	7	0.96
(1,24)	1:3:A:GLU:H	1:4:A:TYR:HD2	16	0.96
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	8	0.93
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	11	0.93
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	9	0.92
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	12	0.92
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	24	0.9
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	21	0.89
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	25	0.89
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	24	0.89
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	25	0.89
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	11	0.88
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	15	0.88
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	16	0.88
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	17	0.88
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	18	0.88
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	20	0.88
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	22	0.88
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	4	0.88
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	1	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	2	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	3	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	4	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	5	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	6	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	7	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	8	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	9	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	10	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	12	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	13	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	14	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	19	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	23	0.87
(1,52)	1:4:A:TYR:HE2	1:5:A:LYS:H	24	0.87
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	20	0.87
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	19	0.82
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	13	0.79
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	23	0.78
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	21	0.77
(1,50)	1:4:A:TYR:HE1	1:20:A:TRP:HD1	22	0.77
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	6	0.77
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	16	0.74
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	5	0.66
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	5	0.66
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	5	0.66
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	1	0.65
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	1	0.64
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	1	0.64
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	1	0.64
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	2	0.64
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	2	0.64
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	2	0.64
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	4	0.64
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	4	0.64
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	4	0.64
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	10	0.64
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	10	0.64
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	10	0.64
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	11	0.64
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	11	0.64
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	11	0.64
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	3	0.63
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	3	0.63
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	3	0.63
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	7	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	7	0.63
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	7	0.63
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	8	0.63
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	8	0.63
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	8	0.63
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	9	0.63
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	9	0.63
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	9	0.63
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	12	0.62
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	12	0.62
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	12	0.62
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	15	0.62
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	15	0.62
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	15	0.62
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	16	0.62
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	16	0.62
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	16	0.62
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	17	0.62
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	17	0.62
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	17	0.62
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	19	0.62
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	19	0.62
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	19	0.62
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	20	0.62
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	20	0.62
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	20	0.62
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	22	0.62
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	22	0.62
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	22	0.62
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	18	0.61
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	18	0.61
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	18	0.61
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	1	0.61
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	1	0.61
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	1	0.61
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	2	0.61
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	2	0.61
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	2	0.61
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	14	0.6
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	4	0.6
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	4	0.6
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	5	0.6
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	5	0.6
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	5	0.6
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	11	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	3	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	3	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	3	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	7	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	7	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	7	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	8	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	8	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	8	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	9	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	9	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	9	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	10	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	10	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	10	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	11	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	11	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	11	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	12	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	12	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	12	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	15	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	15	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	15	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	16	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	16	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	16	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	17	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	17	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	17	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	19	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	19	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	19	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	20	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	20	0.59
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	20	0.59
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	22	0.59
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	22	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	22	0.59
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	10	0.58
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	18	0.58
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	18	0.58
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	18	0.58
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	2	0.57
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	9	0.57
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	20	0.56
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	13	0.55
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	23	0.55
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	4	0.54
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	19	0.54
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	22	0.51
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	12	0.5
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	15	0.49
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	8	0.46
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	13	0.46
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	13	0.46
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	13	0.46
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	14	0.46
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	14	0.46
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	14	0.46
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	21	0.45
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	21	0.45
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	21	0.45
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	23	0.43
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	23	0.43
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	23	0.43
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	14	0.42
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	14	0.42
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	14	0.42
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	21	0.41
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	25	0.4
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	25	0.4
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	25	0.4
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	24	0.39
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	24	0.39
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	24	0.39
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	7	0.38
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	13	0.38
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	13	0.38
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	13	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	24	0.37
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	24	0.37
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	24	0.37
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	18	0.36
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	21	0.36
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	21	0.36
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	21	0.36
(1,15)	1:2:A:THR:HG21	1:4:A:TYR:HE2	6	0.35
(1,15)	1:2:A:THR:HG22	1:4:A:TYR:HE2	6	0.35
(1,15)	1:2:A:THR:HG23	1:4:A:TYR:HE2	6	0.35
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	23	0.35
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	23	0.35
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	23	0.35
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	25	0.34
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	25	0.34
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	25	0.34
(1,120)	1:9:A:VAL:HG11	1:12:A:GLY:H	5	0.33
(1,120)	1:9:A:VAL:HG12	1:12:A:GLY:H	5	0.33
(1,120)	1:9:A:VAL:HG13	1:12:A:GLY:H	5	0.33
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	3	0.28
(1,42)	1:4:A:TYR:HD1	1:20:A:TRP:HB2	5	0.28
(1,14)	1:2:A:THR:HG21	1:4:A:TYR:HD2	6	0.28
(1,14)	1:2:A:THR:HG22	1:4:A:TYR:HD2	6	0.28
(1,14)	1:2:A:THR:HG23	1:4:A:TYR:HD2	6	0.28
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	2	0.27
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	2	0.27
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	2	0.27
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	1	0.24
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	1	0.24
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	1	0.24
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	15	0.23
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	15	0.23
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	15	0.23
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	7	0.22
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	7	0.22
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	7	0.22
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	18	0.22
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	18	0.22
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	18	0.22
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	3	0.19
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	3	0.19
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:9:A:VAL:HG11	1:12:A:GLY:H	3	0.19
(1,120)	1:9:A:VAL:HG12	1:12:A:GLY:H	3	0.19
(1,120)	1:9:A:VAL:HG13	1:12:A:GLY:H	3	0.19
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	11	0.17
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	11	0.17
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	11	0.17
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	10	0.16
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	10	0.16
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	10	0.16
(1,120)	1:9:A:VAL:HG11	1:12:A:GLY:H	18	0.16
(1,120)	1:9:A:VAL:HG12	1:12:A:GLY:H	18	0.16
(1,120)	1:9:A:VAL:HG13	1:12:A:GLY:H	18	0.16
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	5	0.15
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	5	0.15
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	5	0.15
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	21	0.13
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	21	0.13
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	21	0.13
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	25	0.13
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	25	0.13
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	25	0.13
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	6	0.12
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	6	0.12
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	6	0.12
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	12	0.11
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	12	0.11
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	12	0.11
(1,121)	1:9:A:VAL:HG11	1:14:A:VAL:H	13	0.1
(1,121)	1:9:A:VAL:HG12	1:14:A:VAL:H	13	0.1
(1,121)	1:9:A:VAL:HG13	1:14:A:VAL:H	13	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found