



Full wwPDB NMR Structure Validation Report ⓘ

Oct 15, 2026 – 05:50 pm BST

PDB ID : 29KP / pdb_000029kp
BMRB ID : 35045
Title : Peptide-Conjugated Aggregation-Induced-Emission (AIE) Fluorophore DS-TPO-PRO-ALA-NH2
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Deposited on : 2026-03-18

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
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	:	v1.3.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

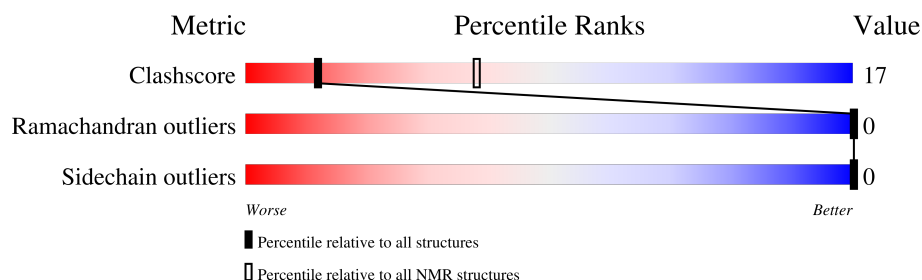
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 53%.

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	1	6	 83%17%

2 Ensemble composition and analysis ⓘ

This entry contains 30 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (2) was below the domain threshold value (8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 122 atoms, of which 54 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DS-TPO-PRO-ALA-NH2.

Mol	Chain	Residues	Atoms							Trace
1	1	6	Total	C	H	N	O	P	S	1
			122	44	54	11	10	1	2	

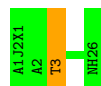
4 Residue-property plots

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: DS-TPO-PRO-ALA-NH2

Chain 1: 



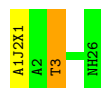
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: DS-TPO-PRO-ALA-NH2

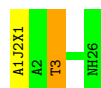
Chain 1: 



4.2.2 Score per residue for model 2

- Molecule 1: DS-TPO-PRO-ALA-NH2

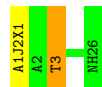
Chain 1: 



4.2.3 Score per residue for model 3

- Molecule 1: DS-TPO-PRO-ALA-NH2

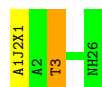
Chain 1:  67% 17% 17%



4.2.4 Score per residue for model 4

- Molecule 1: DS-TPO-PRO-ALA-NH2

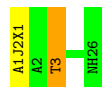
Chain 1:  67% 17% 17%



4.2.5 Score per residue for model 5

- Molecule 1: DS-TPO-PRO-ALA-NH2

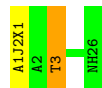
Chain 1:  67% 17% 17%



4.2.6 Score per residue for model 6

- Molecule 1: DS-TPO-PRO-ALA-NH2

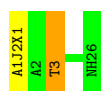
Chain 1:  67% 17% 17%



4.2.7 Score per residue for model 7

- Molecule 1: DS-TPO-PRO-ALA-NH2

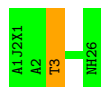
Chain 1:  67% 17% 17%



4.2.8 Score per residue for model 8

- Molecule 1: DS-TPO-PRO-ALA-NH2

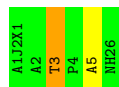
Chain 1:
83% 17%



4.2.9 Score per residue for model 9

- Molecule 1: DS-TPO-PRO-ALA-NH2

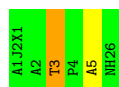
Chain 1:
67% 17% 17%



4.2.10 Score per residue for model 10

- Molecule 1: DS-TPO-PRO-ALA-NH2

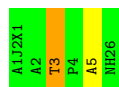
Chain 1:
67% 17% 17%



4.2.11 Score per residue for model 11

- Molecule 1: DS-TPO-PRO-ALA-NH2

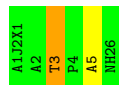
Chain 1:
67% 17% 17%



4.2.12 Score per residue for model 12

- Molecule 1: DS-TPO-PRO-ALA-NH2

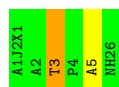
Chain 1:  67% 17% 17%



4.2.13 Score per residue for model 13

- Molecule 1: DS-TPO-PRO-ALA-NH2

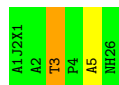
Chain 1:  67% 17% 17%



4.2.14 Score per residue for model 14

- Molecule 1: DS-TPO-PRO-ALA-NH2

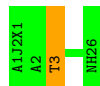
Chain 1:  67% 17% 17%



4.2.15 Score per residue for model 15

- Molecule 1: DS-TPO-PRO-ALA-NH2

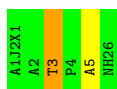
Chain 1:  83% 17%



4.2.16 Score per residue for model 16

- Molecule 1: DS-TPO-PRO-ALA-NH2

Chain 1:  67% 17% 17%



4.2.17 Score per residue for model 17

- Molecule 1: DS-TPO-PRO-ALA-NH2

Chain 1: 83% 17%



4.2.18 Score per residue for model 18

- Molecule 1: DS-TPO-PRO-ALA-NH2

Chain 1: 67% 17% 17%



4.2.19 Score per residue for model 19

- Molecule 1: DS-TPO-PRO-ALA-NH2

Chain 1: 67% 17% 17%



4.2.20 Score per residue for model 20

- Molecule 1: DS-TPO-PRO-ALA-NH2

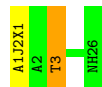
Chain 1: 67% 17% 17%



4.2.21 Score per residue for model 21

- Molecule 1: DS-TPO-PRO-ALA-NH2

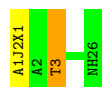
Chain 1:  67% 17% 17%



4.2.22 Score per residue for model 22

- Molecule 1: DS-TPO-PRO-ALA-NH2

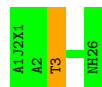
Chain 1:  67% 17% 17%



4.2.23 Score per residue for model 23

- Molecule 1: DS-TPO-PRO-ALA-NH2

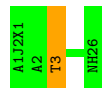
Chain 1:  83% 17%



4.2.24 Score per residue for model 24

- Molecule 1: DS-TPO-PRO-ALA-NH2

Chain 1:  83% 17%

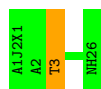


4.2.25 Score per residue for model 25

- Molecule 1: DS-TPO-PRO-ALA-NH2

Chain 1:  83% 17%

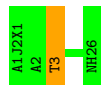




4.2.26 Score per residue for model 26

- Molecule 1: DS-TPO-PRO-ALA-NH2

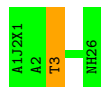
Chain 1:
83% 17%



4.2.27 Score per residue for model 27

- Molecule 1: DS-TPO-PRO-ALA-NH2

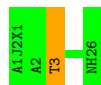
Chain 1:
83% 17%



4.2.28 Score per residue for model 28

- Molecule 1: DS-TPO-PRO-ALA-NH2

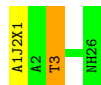
Chain 1:
83% 17%



4.2.29 Score per residue for model 29

- Molecule 1: DS-TPO-PRO-ALA-NH2

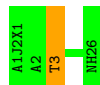
Chain 1:
67% 17% 17%



4.2.30 Score per residue for model 30

- Molecule 1: DS-TPO-PRO-ALA-NH2

Chain 1:  83% 17%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 30 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	
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	52
Number of shifts mapped to atoms	51
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	53%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1J2X, TPO, NH2

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	1	68	54	22	2±1
All	All	2040	1620	660	47

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:1:A1J2X:C19	1:1:3:TPO:HG23	0.66	2.21	21	7
1:1:1:A1J2X:C23	1:1:3:TPO:HG23	0.64	2.22	7	6
1:1:3:TPO:O2P	1:1:5:ALA:HB2	0.55	2.02	13	2
1:1:3:TPO:O3P	1:1:5:ALA:HB2	0.51	2.05	16	3
1:1:3:TPO:O1P	1:1:5:ALA:HB2	0.49	2.08	11	2
1:1:3:TPO:O2P	1:1:3:TPO:HG21	0.45	2.12	21	14
1:1:3:TPO:O3P	1:1:3:TPO:HG21	0.45	2.12	23	9
1:1:3:TPO:O1P	1:1:3:TPO:HG21	0.42	2.15	14	3
1:1:3:TPO:HG21	1:1:3:TPO:O1P	0.41	2.15	16	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	1	2/6 (33%)	1±1 (67±27%)	1±1 (33±27%)	0±0 (0±0%)	100	100
All	All	60/180 (33%)	40 (67%)	20 (33%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	1/1 (100%)	1±0 (100±0%)	0±0 (0±0%)	100	100
All	All	30/30 (100%)	30 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	TPO	1	3	1	8,10,11	1.07±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
1	TPO	1	3	1	10,14,16	2.06±0.00	2±0 (20±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	1	3	1	-	0±0,9,11,13	-

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	1	3	TPO	P-OG1-CB	5.45	106.74	123.21	6	30
1	1	3	TPO	O-C-CA	2.69	117.74	124.78	19	30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 53% for the well-defined parts and 53% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *D_1292155099_cs_P1.str.V1*

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	52
Number of shifts mapped to atoms	51
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	1	2	ALA	HB1	2.527	0.02	1

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 53%, i.e. 16 atoms were assigned a chemical shift out of a possible 30. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	4/13 (31%)	4/5 (80%)	0/6 (0%)	0/2 (0%)
Sidechain	12/17 (71%)	12/12 (100%)	0/5 (0%)	0/0 (—%)
Overall	16/30 (53%)	16/17 (94%)	0/11 (0%)	0/2 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 53%, i.e. 16 atoms were assigned a chemical shift out of a possible 30. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	4/13 (31%)	4/5 (80%)	0/6 (0%)	0/2 (0%)
Sidechain	12/17 (71%)	12/12 (100%)	0/5 (0%)	0/0 (—%)
Overall	16/30 (53%)	16/17 (94%)	0/11 (0%)	0/2 (0%)

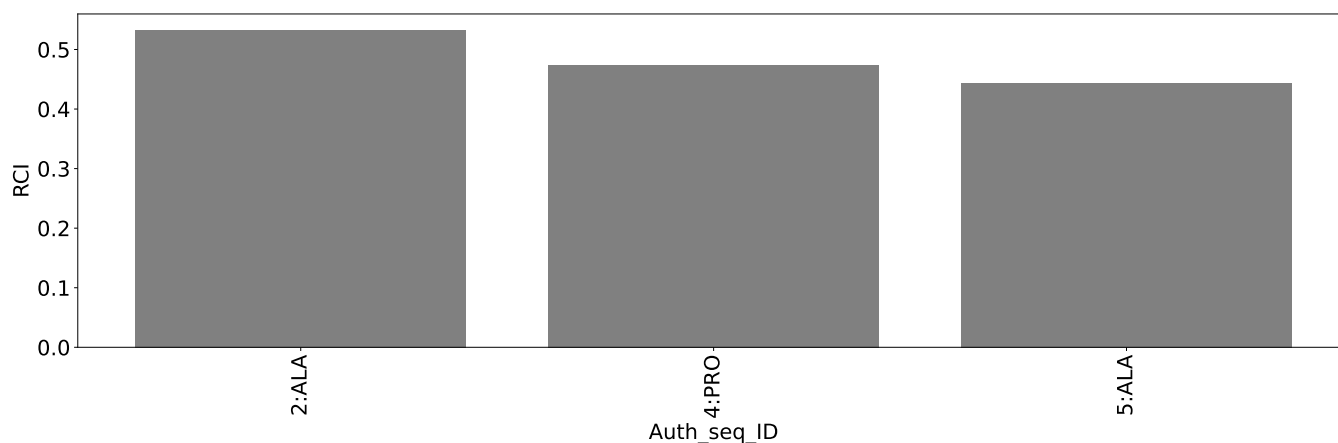
7.1.4 Statistically unusual chemical shifts [i](#)

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 1:



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	58
Intra-residue ($ i-j =0$)	7
Sequential ($ i-j =1$)	23
Medium range ($ i-j >1$ and $ i-j <5$)	28
Long range ($ i-j \geq 5$)	0
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	9.7
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)	0.6	0.2
0.2-0.5 (Medium)	3.2	0.5
>0.5 (Large)	8.9	1.92

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 ⓘ

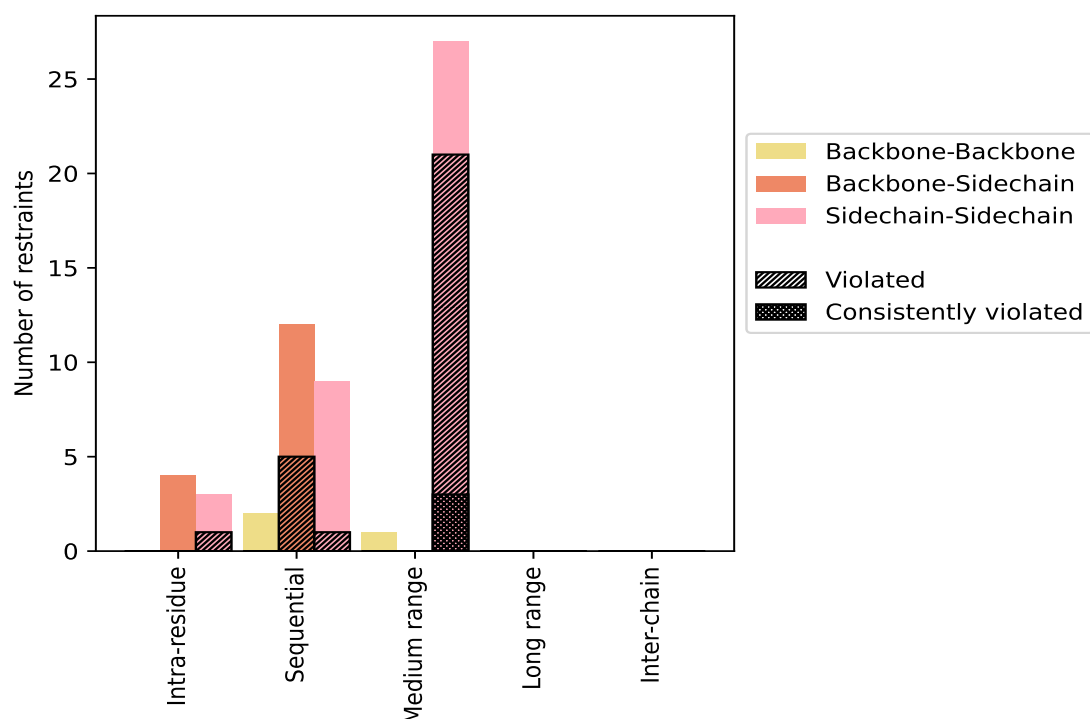
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	7	12.1	1	14.3	1.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	6.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	3	5.2	1	33.3	1.7	0	0.0	0.0
Sequential ($i-j =1$)	23	39.7	6	26.1	10.3	0	0.0	0.0
Backbone-Backbone	2	3.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	12	20.7	5	41.7	8.6	0	0.0	0.0
Sidechain-Sidechain	9	15.5	1	11.1	1.7	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	28	48.3	21	75.0	36.2	3	10.7	5.2
Backbone-Backbone	1	1.7	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	27	46.6	21	77.8	36.2	3	11.1	5.2
Long range ($i-j \geq 5$)	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	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	58	100.0	28	48.3	48.3	3	5.2	5.2
Backbone-Backbone	3	5.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	16	27.6	5	31.2	8.6	0	0.0	0.0
Sidechain-Sidechain	39	67.2	23	59.0	39.7	3	7.7	5.2

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	1	1	4	0	0	6	0.49	1.09	0.31	0.45
2	1	1	3	0	0	5	0.49	1.05	0.3	0.41
3	1	1	3	0	0	5	0.56	1.22	0.36	0.41
4	1	1	3	0	0	5	0.51	1.14	0.34	0.4
5	1	1	4	0	0	6	0.49	1.14	0.33	0.44
6	1	1	4	0	0	6	0.49	1.0	0.29	0.4
7	1	1	3	0	0	5	0.52	1.05	0.28	0.46
8	0	0	16	0	0	16	0.84	1.74	0.48	0.88
9	0	0	19	0	0	19	0.92	1.92	0.56	0.92
10	0	0	16	0	0	16	0.84	1.74	0.48	0.88

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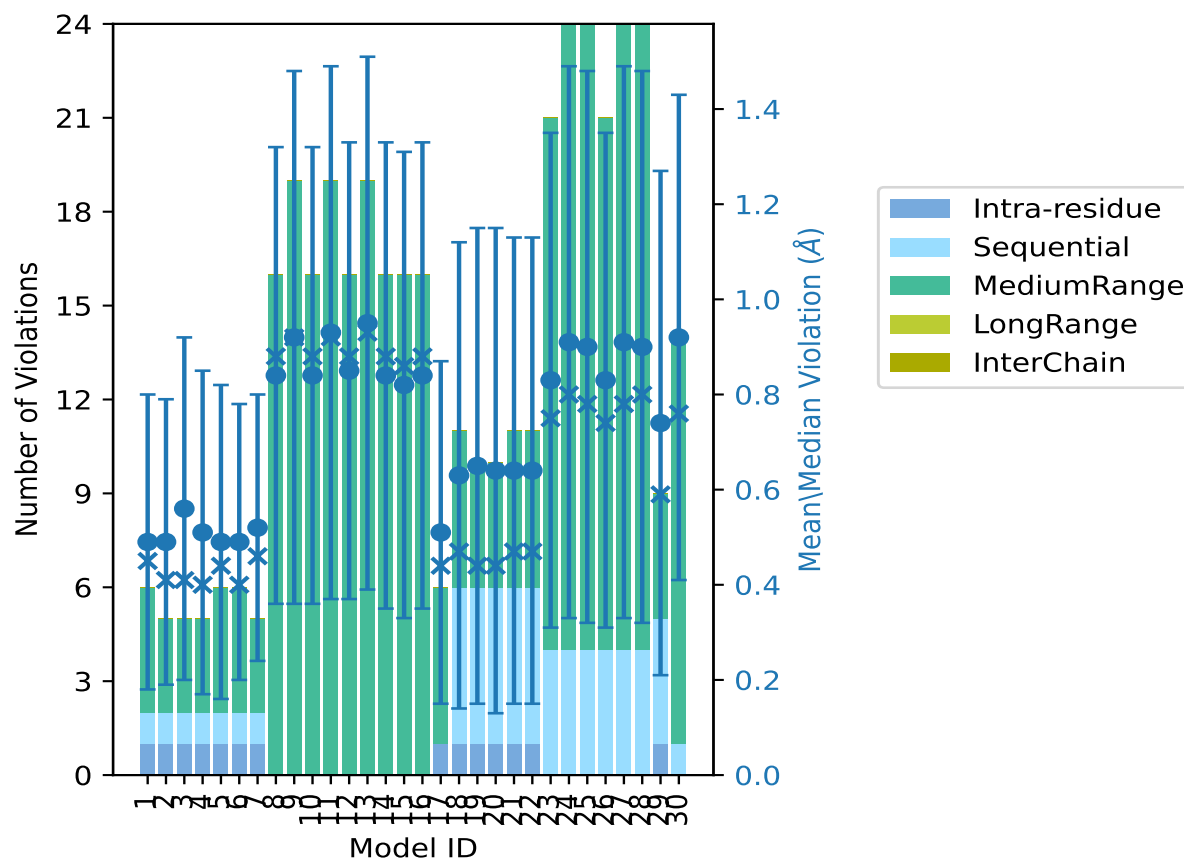
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	19	0	0	19	0.93	1.92	0.56	0.92
12	0	0	16	0	0	16	0.85	1.74	0.48	0.88
13	0	0	19	0	0	19	0.95	1.92	0.56	0.93
14	0	0	16	0	0	16	0.84	1.75	0.49	0.88
15	0	0	16	0	0	16	0.82	1.75	0.49	0.86
16	0	0	16	0	0	16	0.84	1.75	0.49	0.88
17	1	0	5	0	0	6	0.51	1.17	0.36	0.44
18	1	5	5	0	0	11	0.63	1.82	0.49	0.47
19	1	5	4	0	0	10	0.65	1.82	0.5	0.44
20	1	5	4	0	0	10	0.64	1.82	0.51	0.44
21	1	5	5	0	0	11	0.64	1.82	0.49	0.47
22	1	5	5	0	0	11	0.64	1.82	0.49	0.47
23	0	4	17	0	0	21	0.83	1.82	0.52	0.75
24	0	4	20	0	0	24	0.91	1.92	0.58	0.8
25	0	4	20	0	0	24	0.9	1.92	0.58	0.78
26	0	4	17	0	0	21	0.83	1.82	0.52	0.74
27	0	4	20	0	0	24	0.91	1.92	0.58	0.78
28	0	4	20	0	0	24	0.9	1.92	0.58	0.8
29	1	4	4	0	0	9	0.74	1.89	0.53	0.59
30	0	1	13	0	0	14	0.92	1.9	0.51	0.76

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, 30(IR:6, SQ:17, MR:7, LR:0, 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	1	1	0	0	2	1	3.3
0	0	0	0	0	0	2	6.7
0	0	0	0	0	0	3	10.0
0	0	0	0	0	0	4	13.3
0	0	0	0	0	0	5	16.7
0	0	0	0	0	0	6	20.0

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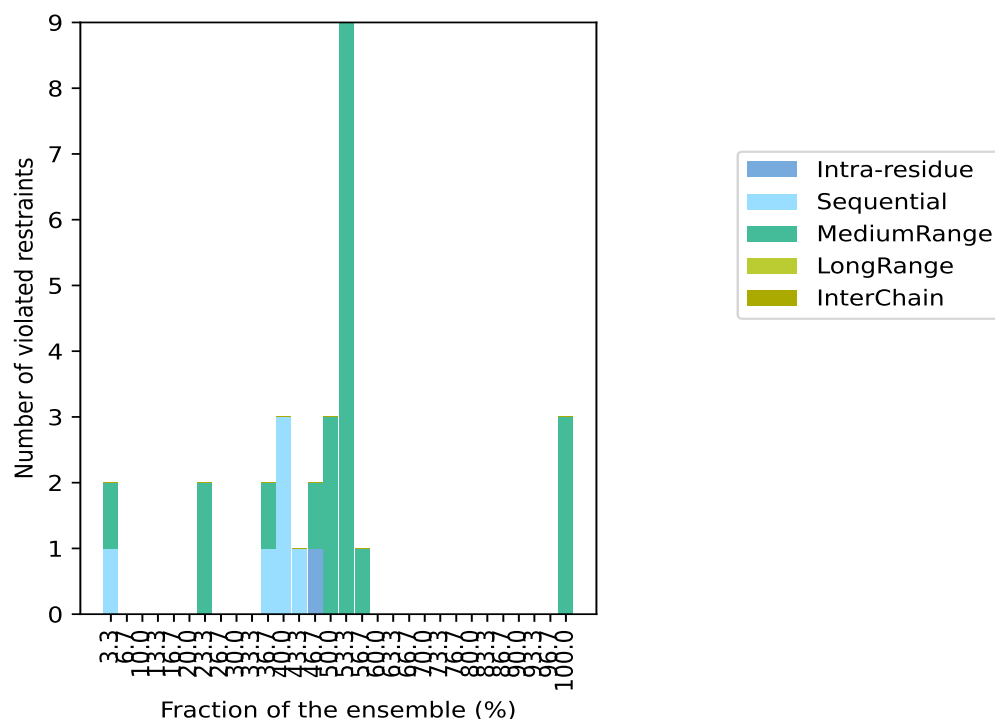
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	2	0	0	2	7	23.3
0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	0	0	0	10	33.3
0	1	1	0	0	2	11	36.7
0	3	0	0	0	3	12	40.0
0	1	0	0	0	1	13	43.3
1	0	1	0	0	2	14	46.7
0	0	3	0	0	3	15	50.0
0	0	9	0	0	9	16	53.3
0	0	1	0	0	1	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
0	0	3	0	0	3	30	100.0

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

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

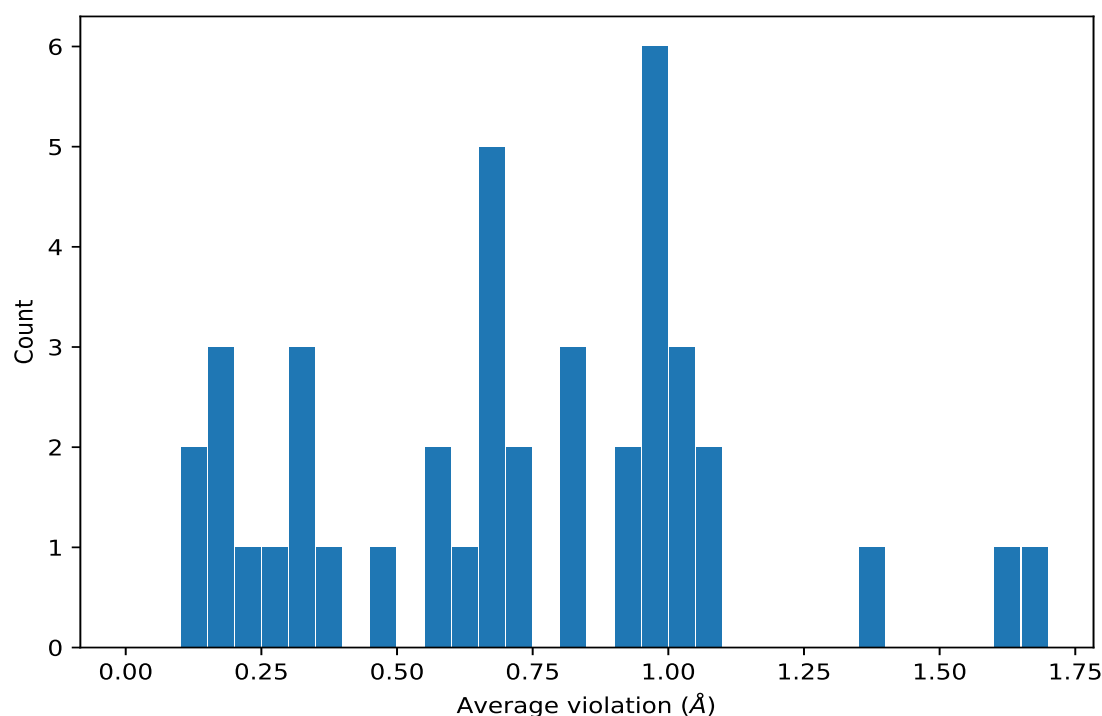
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	30	1.39	0.36	1.17
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	30	1.0	0.57	1.5
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	30	0.84	0.42	0.55
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	17	1.65	0.38	1.75
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	16	1.6	0.05	1.61
(1,43)	1:1:1:A1J2X:H23	1:4:1:PRO:HD2	16	1.08	0.74	0.51
(1,43)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	16	1.08	0.74	0.51
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	16	0.97	0.06	0.99
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	16	0.96	0.08	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	16	0.96	0.08	0.94
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	16	0.96	0.15	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	16	0.96	0.15	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	16	0.96	0.15	1.0
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	16	0.94	0.08	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	16	0.94	0.08	0.92
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	16	0.83	0.01	0.83

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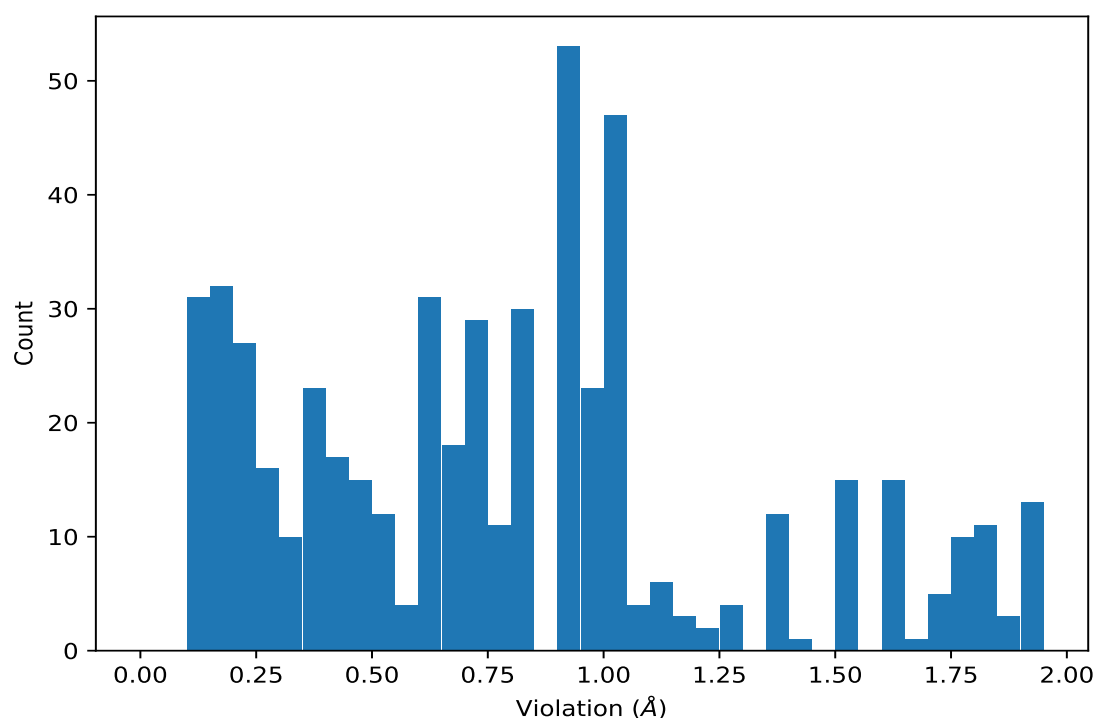
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	16	0.83	0.01	0.83
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	16	0.74	0.01	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	16	0.74	0.01	0.74
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	16	0.62	0.04	0.63
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	15	0.25	0.0	0.25
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	15	0.1	0.0	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	15	0.1	0.0	0.1
(1,45)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	14	1.04	0.86	1.03
(1,45)	1:1:1:A1J2X:H20	1:3:1:TPO:HB	14	1.04	0.86	1.03
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H20	14	0.55	0.15	0.6
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H23	14	0.55	0.15	0.6
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	13	0.18	0.03	0.17
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	13	0.18	0.03	0.17
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	13	0.18	0.03	0.17
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	12	0.67	0.0	0.67
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	12	0.65	0.03	0.64
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	12	0.39	0.05	0.38
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	11	0.47	0.0	0.47
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	11	0.21	0.0	0.21
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG23	7	0.66	0.02	0.67
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG22	7	0.66	0.02	0.67
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG21	7	0.66	0.02	0.67
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG23	7	0.3	0.02	0.31
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG22	7	0.3	0.02	0.31
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG21	7	0.3	0.02	0.31

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)
(1,45)	1:1:1:A1J2X:H20	1:3:1:TPO:HB	13	1.92
(1,45)	1:1:1:A1J2X:H20	1:3:1:TPO:HB	24	1.92
(1,45)	1:1:1:A1J2X:H20	1:3:1:TPO:HB	25	1.92
(1,45)	1:1:1:A1J2X:H20	1:3:1:TPO:HB	27	1.92
(1,45)	1:1:1:A1J2X:H20	1:3:1:TPO:HB	28	1.92
(1,43)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	9	1.92
(1,43)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	11	1.92
(1,43)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	13	1.92
(1,43)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	24	1.92
(1,43)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	25	1.92
(1,43)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	27	1.92
(1,43)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	28	1.92
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	30	1.9
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	29	1.89
(1,45)	1:1:1:A1J2X:H20	1:3:1:TPO:HB	9	1.86
(1,45)	1:1:1:A1J2X:H20	1:3:1:TPO:HB	11	1.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	18	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	19	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	20	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	21	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	22	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	23	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	24	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	25	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	26	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	27	1.82
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	28	1.82
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	13	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	14	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	15	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	16	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	23	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	24	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	25	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	26	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	27	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	28	1.75
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	8	1.74
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	9	1.74
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	10	1.74
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	11	1.74
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	12	1.74
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	30	1.69
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	8	1.63
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	9	1.63
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	10	1.63
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	11	1.63
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	12	1.63
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	13	1.61
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	14	1.61
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	15	1.61
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	16	1.61
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	23	1.61
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	24	1.61
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	25	1.61
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	26	1.61
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	27	1.61
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	28	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	11	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	12	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	13	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	14	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	15	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	16	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	23	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	24	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	25	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	26	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	27	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	28	1.51
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	8	1.5
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	9	1.5
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	10	1.5
(1,46)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	30	1.43
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	29	1.39
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	18	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	19	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	20	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	21	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	22	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	23	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	24	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	25	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	26	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	27	1.35
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	28	1.35
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	30	1.29
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	30	1.29
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	30	1.27
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	30	1.27
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	3	1.22
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	13	1.21
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	30	1.18
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	14	1.17
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	17	1.17
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	4	1.14
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	5	1.14
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	12	1.14
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	10	1.1
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	11	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	16	1.1
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	1	1.09
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	8	1.07
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	2	1.05
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	7	1.05
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	14	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	14	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	14	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	16	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	16	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	16	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	24	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	24	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	24	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	27	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	27	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	27	1.01
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	8	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	8	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	8	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	9	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	9	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	9	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	10	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	10	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	10	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	11	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	11	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	11	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	12	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	12	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	12	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	13	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	13	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	13	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	15	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	15	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	15	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	23	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	23	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	23	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	25	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	25	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	25	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	26	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	26	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	26	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	28	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	28	1.0
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	28	1.0
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	6	1.0
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	9	1.0
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	8	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	9	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	10	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	11	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	12	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	13	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	14	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	15	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	16	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	23	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	24	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	25	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	26	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	27	0.99
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	28	0.99
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	13	0.95
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	13	0.95
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	15	0.95
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	15	0.95
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	25	0.95
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	25	0.95
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	26	0.95
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	26	0.95
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	8	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	8	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	9	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	9	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	10	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	10	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	11	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	11	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	12	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	12	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	14	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	14	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	16	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	16	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	23	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	23	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	24	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	24	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	27	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	27	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	28	0.94
(1,40)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	28	0.94
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	13	0.93
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	13	0.93
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	15	0.93
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	15	0.93
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	25	0.93
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	25	0.93
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	26	0.93
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	26	0.93
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	8	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	8	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	9	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	9	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	10	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	10	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	11	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	11	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	12	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	12	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	14	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	14	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	16	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	16	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	23	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	23	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	24	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	24	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	27	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	27	0.92
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	28	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	28	0.92
(1,22)	1:4:1:PRO:HD2	1:6:1:NH2:HN1	15	0.9
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	16	0.84
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	16	0.84
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	23	0.84
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	23	0.84
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	24	0.84
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	24	0.84
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	28	0.84
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	28	0.84
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	8	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	8	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	9	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	9	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	10	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	10	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	11	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	11	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	12	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	12	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	13	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	13	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	14	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	14	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	15	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	15	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	25	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	25	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	26	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	26	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	27	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	27	0.83
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	30	0.79
(1,42)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	30	0.79
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	29	0.76
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	16	0.75
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	16	0.75
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	23	0.75
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	23	0.75
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	24	0.75
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	24	0.75
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	28	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	28	0.75
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H23	17	0.74
(1,44)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	30	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	8	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	8	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	9	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	9	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	10	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	10	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	11	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	11	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	12	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	12	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	13	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	13	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	14	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	14	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	15	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	15	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	25	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	25	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	26	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	26	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	27	0.74
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	27	0.74
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H20	21	0.73
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H20	22	0.73
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H20	6	0.72
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	30	0.7
(1,28)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	30	0.7
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG21	24	0.68
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG21	27	0.68
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG23	9	0.67
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG23	13	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	18	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	19	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	20	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	21	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	22	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	23	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	24	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	25	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	26	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	27	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	28	0.67
(1,5)	1:4:1:PRO:HG3	1:5:1:ALA:H	29	0.67
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG21	25	0.66
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG23	28	0.66
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	18	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	19	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	20	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	21	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	22	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	23	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	24	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	25	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	26	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	27	0.64
(1,7)	1:4:1:PRO:HD3	1:5:1:ALA:H	28	0.64
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	8	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	9	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	10	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	11	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	12	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	13	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	14	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	15	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	16	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	23	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	24	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	25	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	26	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	27	0.63
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	28	0.63
(1,31)	1:1:1:A1J2X:H20	1:3:1:TPO:HG22	11	0.63
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	3	0.61
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H20	1	0.6
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H20	5	0.6
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H20	18	0.6
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H20	29	0.59
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	13	0.58
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	29	0.57
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	30	0.55
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	14	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	17	0.54
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	10	0.53
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	12	0.53
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H23	7	0.52
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	4	0.52
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	11	0.52
(1,43)	1:1:1:A1J2X:H23	1:4:1:PRO:HD2	8	0.51
(1,43)	1:1:1:A1J2X:H23	1:4:1:PRO:HD2	10	0.51
(1,43)	1:1:1:A1J2X:H23	1:4:1:PRO:HD2	12	0.51
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	16	0.51
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	1	0.5
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	5	0.49
(1,36)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	30	0.48
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	18	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	19	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	20	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	21	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	22	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	23	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	24	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	25	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	26	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	27	0.47
(1,38)	1:4:1:PRO:HG3	1:6:1:NH2:HN2	28	0.47
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	2	0.46
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	7	0.46
(1,43)	1:1:1:A1J2X:H23	1:4:1:PRO:HD2	15	0.44
(1,43)	1:1:1:A1J2X:H23	1:4:1:PRO:HD2	23	0.44
(1,43)	1:1:1:A1J2X:H23	1:4:1:PRO:HD2	26	0.44
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	9	0.44
(1,43)	1:1:1:A1J2X:H23	1:4:1:PRO:HD2	14	0.43
(1,43)	1:1:1:A1J2X:H23	1:4:1:PRO:HD2	16	0.43
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	6	0.43
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	8	0.43
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	1	0.41
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	2	0.41
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	3	0.41
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	18	0.41
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	19	0.41
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	29	0.41
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	4	0.4
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	20	0.4
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	7	0.38
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	21	0.38
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	22	0.38
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG21	30	0.38
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG22	30	0.38
(1,25)	1:1:1:A1J2X:H1	1:3:1:TPO:HG23	30	0.38
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	18	0.38
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	20	0.38
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	21	0.38
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	23	0.38
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	24	0.38
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H23	2	0.37
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H23	3	0.37
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H23	19	0.37
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	6	0.37
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	19	0.37
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	22	0.37
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	25	0.37
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	26	0.37
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	27	0.37
(1,10)	1:4:1:PRO:HD2	1:5:1:ALA:H	28	0.37
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H23	20	0.36
(1,52)	1:1:1:A1J2X:H1	1:1:1:A1J2X:H23	4	0.35
(1,33)	1:1:1:A1J2X:H1	1:4:1:PRO:HB2	17	0.34
(1,20)	1:4:1:PRO:HG3	1:6:1:NH2:HN1	15	0.34
(1,29)	1:1:1:A1J2X:H1	1:4:1:PRO:HB3	30	0.33
(1,29)	1:1:1:A1J2X:H1	1:4:1:PRO:HB3	30	0.33
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG21	24	0.32
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG21	27	0.32
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG23	9	0.31
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG23	13	0.31
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG21	25	0.3
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG23	28	0.3
(1,23)	1:1:1:A1J2X:H20	1:3:1:TPO:HG22	11	0.27
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	8	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	9	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	10	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	11	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	12	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	13	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	15	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	16	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	23	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	24	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	25	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	26	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	27	0.25
(1,47)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	28	0.25
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	21	0.22
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	21	0.22
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	21	0.22
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	22	0.22
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	22	0.22
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	22	0.22
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	6	0.21
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	6	0.21
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	6	0.21
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	7	0.21
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	7	0.21
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	7	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	18	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	19	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	20	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	21	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	22	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	23	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	24	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	25	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	26	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	27	0.21
(1,21)	1:5:1:ALA:HA	1:6:1:NH2:HN1	28	0.21
(1,13)	1:2:1:ALA:HA	1:1:1:A1J2X:H1	30	0.21
(1,45)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	6	0.2
(1,45)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	21	0.2
(1,45)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	22	0.2
(1,45)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	5	0.19
(1,45)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	1	0.18
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	1	0.17
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	1	0.17
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	1	0.17
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	2	0.17
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	2	0.17
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	3	0.17
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	3	0.17
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	3	0.17
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	18	0.17
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	18	0.17
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	18	0.17
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	19	0.17
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	19	0.17
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	19	0.17
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	29	0.17
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	29	0.17
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	29	0.17
(1,45)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	18	0.17
(1,45)	1:1:1:A1J2X:H1	1:3:1:TPO:HB	29	0.17
(1,43)	1:1:1:A1J2X:H1	1:4:1:PRO:HD2	17	0.16
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	4	0.15
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	4	0.15
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	4	0.15
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	5	0.15
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	5	0.15
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	5	0.15
(1,58)	1:3:1:TPO:HG21	1:4:1:PRO:HD3	20	0.15
(1,58)	1:3:1:TPO:HG22	1:4:1:PRO:HD3	20	0.15
(1,58)	1:3:1:TPO:HG23	1:4:1:PRO:HD3	20	0.15
(1,34)	1:1:1:A1J2X:H1	1:4:1:PRO:HG2	17	0.12
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	8	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	9	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	10	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	11	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	12	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	13	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	14	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	15	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	16	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	23	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	24	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	25	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	26	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	27	0.1
(1,35)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	28	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	9	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	10	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	11	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	12	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	13	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	14	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	15	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	16	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	23	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	24	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	25	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	26	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	27	0.1
(1,15)	1:1:1:A1J2X:H1	1:4:1:PRO:HG3	28	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found