



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 9T3O / pdb_00009t3o
BMRB ID : 35025
Title : Solution structure of thanatin in complex with LptDm
Authors : Schuster, M.; Zerbe, O.
Deposited on : 2025-10-28

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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

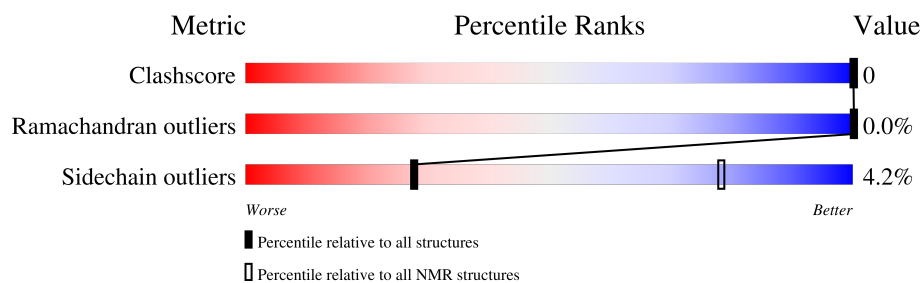
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR



The overall completeness of chemical shifts assignment is 89%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	181	
2	B	21	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:51-A:90, A:101-A:224, B:8-B:21 (178)	0.63	11

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3045 atoms, of which 1518 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms						Trace
1	A	181	Total	C	H	N	O	S	0
			2694	847	1335	229	281	2	

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	TRP	-	expression tag	UNP P31554
A	134	VAL	-	expression tag	UNP P31554
A	135	PHE	-	expression tag	UNP P31554
A	136	TYR	-	expression tag	UNP P31554
A	137	ASP	-	expression tag	UNP P31554
A	138	ALA	-	expression tag	UNP P31554
A	139	SER	-	expression tag	UNP P31554
A	140	ILE	-	expression tag	UNP P31554
A	141	GLU	-	expression tag	UNP P31554
A	142	THR	-	expression tag	UNP P31554
A	143	VAL	-	expression tag	UNP P31554
A	144	GLY	-	expression tag	UNP P31554
A	145	ALA	-	expression tag	UNP P31554
A	146	PRO	-	expression tag	UNP P31554
A	147	GLY	-	expression tag	UNP P31554
A	148	SER	-	expression tag	UNP P31554
A	149	ALA	-	expression tag	UNP P31554
A	150	SER	-	expression tag	UNP P31554
A	151	ALA	-	expression tag	UNP P31554
A	152	LYS	-	expression tag	UNP P31554
A	153	VAL	-	expression tag	UNP P31554
A	154	ILE	-	expression tag	UNP P31554
A	155	LYS	-	expression tag	UNP P31554
A	156	SER	-	expression tag	UNP P31554
A	157	LEU	-	expression tag	UNP P31554
A	158	ASP	-	expression tag	UNP P31554
A	159	ASN	-	expression tag	UNP P31554
A	160	GLY	-	expression tag	UNP P31554
A	161	LYS	-	expression tag	UNP P31554
A	162	THR	-	expression tag	UNP P31554
A	163	LEU	-	expression tag	UNP P31554

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Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLU	-	expression tag	UNP P31554
A	165	PHE	-	expression tag	UNP P31554
A	166	ASP	-	expression tag	UNP P31554
A	167	ASP	-	expression tag	UNP P31554
A	168	ALA	-	expression tag	UNP P31554
A	169	THR	-	expression tag	UNP P31554
A	170	PHE	-	expression tag	UNP P31554
A	171	ASP	-	expression tag	UNP P31554
A	172	SER	-	expression tag	UNP P31554
A	173	TYR	-	expression tag	UNP P31554
A	174	GLU	-	expression tag	UNP P31554
A	175	ASN	-	expression tag	UNP P31554
A	176	ALA	-	expression tag	UNP P31554
A	177	GLU	-	expression tag	UNP P31554
A	178	ALA	-	expression tag	UNP P31554
A	179	LEU	-	expression tag	UNP P31554
A	180	ILE	-	expression tag	UNP P31554
A	181	GLU	-	expression tag	UNP P31554
A	182	HIS	-	expression tag	UNP P31554
A	183	ALA	-	expression tag	UNP P31554
A	184	ILE	-	expression tag	UNP P31554
A	185	LYS	-	expression tag	UNP P31554
A	186	THR	-	expression tag	UNP P31554
A	187	MET	-	expression tag	UNP P31554
A	188	GLY	-	expression tag	UNP P31554
A	189	VAL	-	expression tag	UNP P31554
A	190	LYS	-	expression tag	UNP P31554
A	191	THR	-	expression tag	UNP P31554
A	192	ILE	-	expression tag	UNP P31554
A	193	THR	-	expression tag	UNP P31554
A	194	ILE	-	expression tag	UNP P31554
A	195	ASN	-	expression tag	UNP P31554
A	196	ASN	-	expression tag	UNP P31554
A	197	ALA	-	expression tag	UNP P31554
A	198	THR	-	expression tag	UNP P31554
A	199	GLY	-	expression tag	UNP P31554
A	200	ALA	-	expression tag	UNP P31554
A	201	ILE	-	expression tag	UNP P31554
A	202	THR	-	expression tag	UNP P31554
A	203	ALA	-	expression tag	UNP P31554
A	204	GLU	-	expression tag	UNP P31554
A	205	LYS	-	expression tag	UNP P31554

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Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ALA	-	expression tag	UNP P31554
A	207	THR	-	expression tag	UNP P31554
A	208	LYS	-	expression tag	UNP P31554
A	209	LEU	-	expression tag	UNP P31554
A	210	LYS	-	expression tag	UNP P31554
A	211	ALA	-	expression tag	UNP P31554
A	212	LYS	-	expression tag	UNP P31554
A	213	ALA	-	expression tag	UNP P31554
A	214	ALA	-	expression tag	UNP P31554
A	215	GLU	-	expression tag	UNP P31554
A	216	LEU	-	expression tag	UNP P31554
A	217	GLY	-	expression tag	UNP P31554
A	218	ALA	-	expression tag	UNP P31554
A	219	THR	-	expression tag	UNP P31554
A	220	LEU	-	expression tag	UNP P31554
A	221	THR	-	expression tag	UNP P31554
A	222	ILE	-	expression tag	UNP P31554
A	223	THR	-	expression tag	UNP P31554
A	224	LEU	-	expression tag	UNP P31554
A	225	LYS	-	expression tag	UNP P31554

- Molecule 2 is a protein called Thanatin.

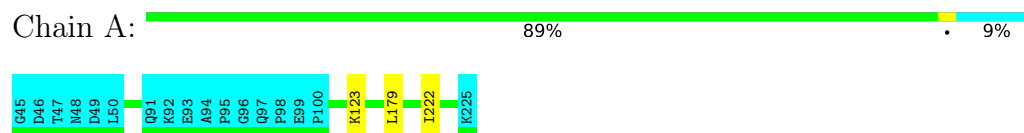
Mol	Chain	Residues	Atoms						Trace
2	B	21	Total	C	H	N	O	S	0
			351	103	183	35	27	3	

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: LPS-assembly protein LptD



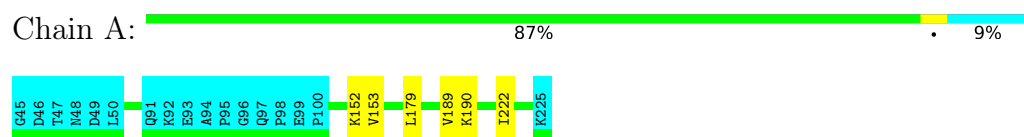
- Molecule 2: Thanatin



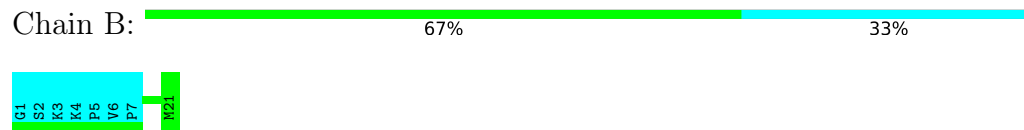
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 11. Colouring as in section 4.1 above.

- Molecule 1: LPS-assembly protein LptD



- Molecule 2: Thanatin



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
Amber	refinement	Amber19
CYANA	structure calculation	3.98

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	2278
Number of shifts mapped to atoms	2278
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.84±0.00	0±0/1251 (0.0± 0.0%)	1.37±0.01	0±0/1702 (0.0± 0.0%)
2	B	0.92±0.01	0±0/119 (0.0± 0.0%)	1.33±0.05	0±0/154 (0.0± 0.0%)
All	All	0.85	0/27400 (0.0%)	1.37	1/37120 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	2

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	132	ASP	CA-CB-CG	5.02	117.62	112.60	2	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	102	ARG	Sidechain	2

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
All	All	27000	26780	26780	-

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 -.

There are no clashes.

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	164/181 (91%)	158±2 (96±1%)	6±2 (4±1%)	0±0 (0±0%)	100	100
2	B	13/21 (62%)	13±0 (100±2%)	0±0 (0±2%)	0±0 (0±0%)	100	100
All	All	3540/4040 (88%)	3421 (97%)	118 (3%)	1 (0%)	100	100

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	72	SER	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/144 (90%)	125±2 (96±1%)	5±2 (4±1%)	29	79
2	B	13/19 (68%)	12±1 (93±4%)	1±1 (7±4%)	17	66
All	All	2860/3260 (88%)	2740 (96%)	120 (4%)	28	78

5 of 22 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	222	ILE	20
1	A	179	LEU	18
2	B	8	ILE	13
1	A	123	LYS	11
1	A	173	TYR	8

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *LptDm-Than*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	2278
Number of shifts mapped to atoms	2278
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	179	-0.21 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	166	-0.33 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	179	0.28 ± 0.08	None needed (< 0.5 ppm)
^{15}N	168	-0.15 ± 0.25	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 2073 atoms were assigned a chemical shift out of a possible 2320. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	846/895 (95%)	361/365 (99%)	328/356 (92%)	157/174 (90%)
Sidechain	1135/1288 (88%)	800/839 (95%)	321/404 (79%)	14/45 (31%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	92/137 (67%)	57/68 (84%)	35/63 (56%)	0/6 (0%)
Overall	2073/2320 (89%)	1218/1272 (96%)	684/823 (83%)	171/225 (76%)

7.1.4 Statistically unusual chemical shifts [i](#)

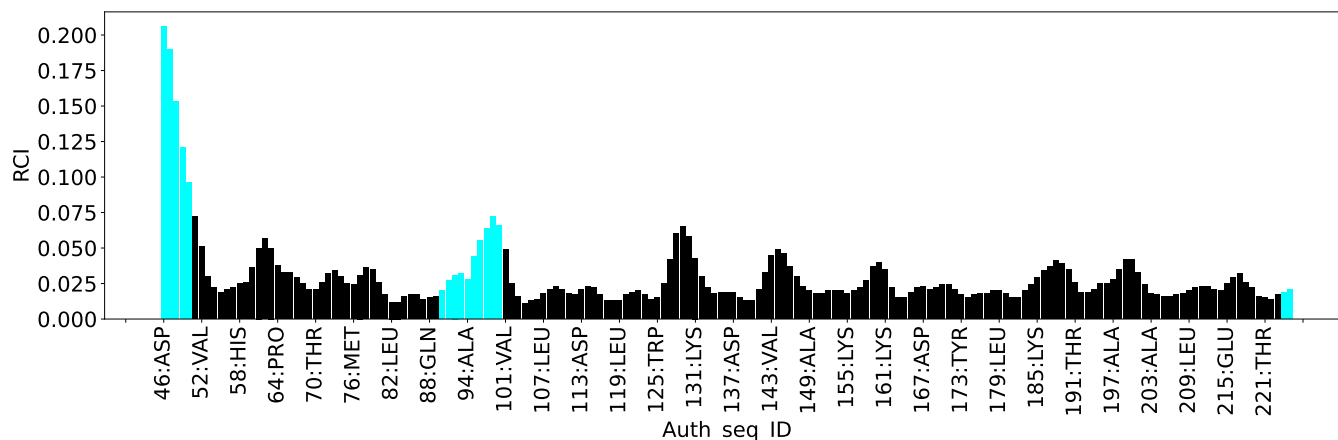
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	156	SER	HB2	1.73	2.61 – 5.13	-8.5
1	A	156	SER	HB3	1.56	2.49 – 5.20	-8.4

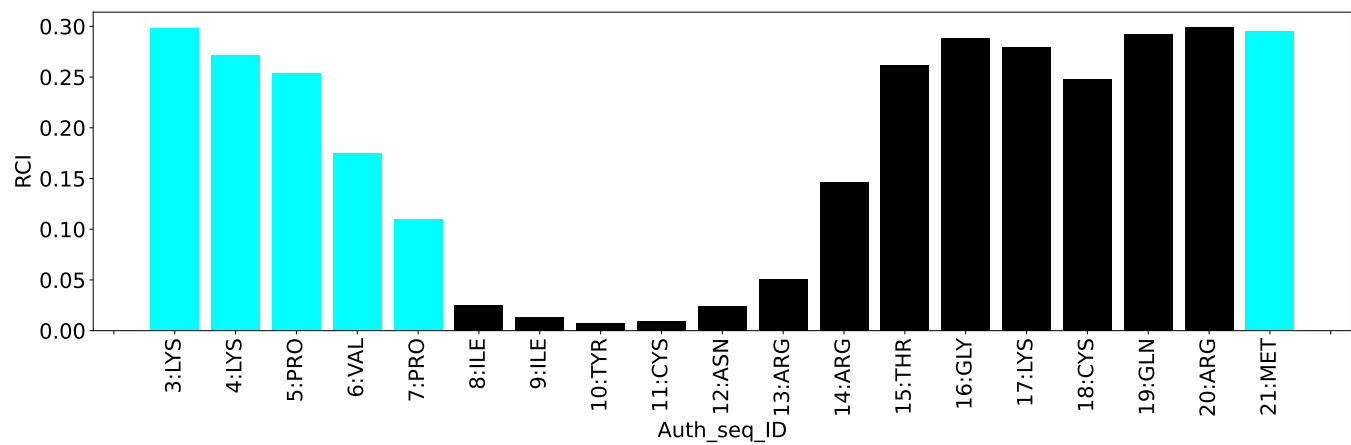
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	4051
Intra-residue ($ i-j =0$)	810
Sequential ($ i-j =1$)	1113
Medium range ($ i-j >1$ and $ i-j <5$)	540
Long range ($ i-j \geq 5$)	1469
Inter-chain	119
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	20.1
Number of long range restraints per residue ¹	7.3

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)	119.1	0.2
0.2-0.5 (Medium)	213.8	0.5
>0.5 (Large)	232.7	4.9

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 ⓘ

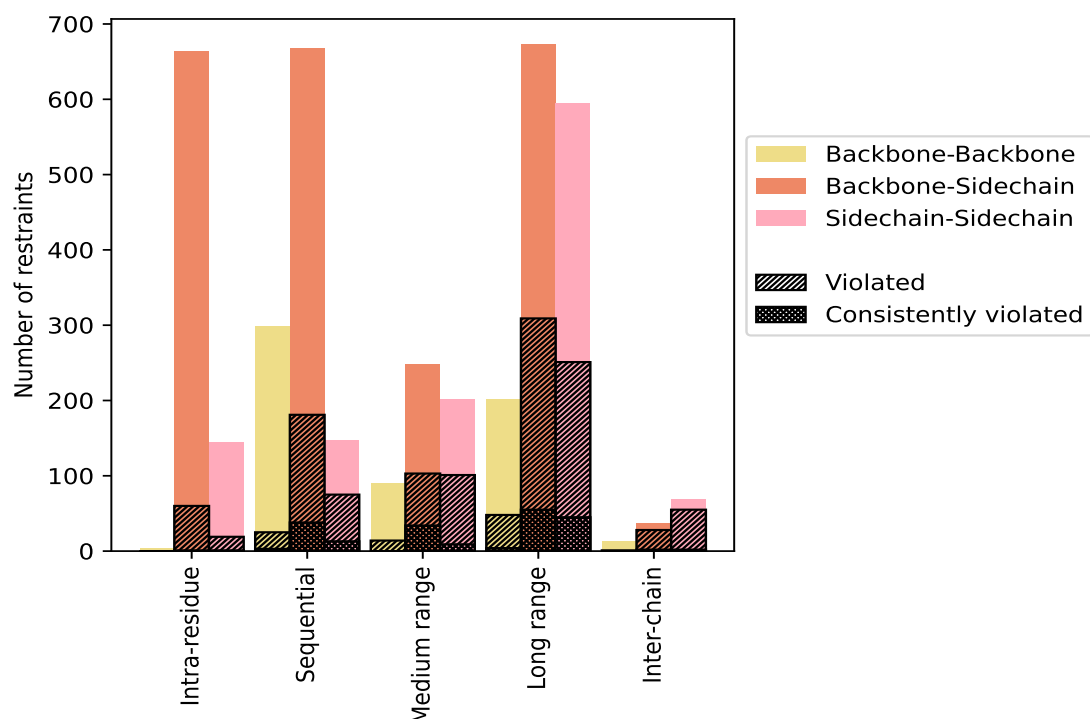
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	810	20.0	79	9.8	2.0	2	0.2	0.0
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	663	16.4	60	9.0	1.5	1	0.2	0.0
Sidechain-Sidechain	144	3.6	19	13.2	0.5	1	0.7	0.0
Sequential ($i-j =1$)	1113	27.5	281	25.2	6.9	54	4.9	1.3
Backbone-Backbone	299	7.4	25	8.4	0.6	3	1.0	0.1
Backbone-Sidechain	667	16.5	181	27.1	4.5	38	5.7	0.9
Sidechain-Sidechain	147	3.6	75	51.0	1.9	13	8.8	0.3
Medium range ($i-j >1$ & $i-j <5$)	540	13.3	218	40.4	5.4	43	8.0	1.1
Backbone-Backbone	90	2.2	14	15.6	0.3	0	0.0	0.0
Backbone-Sidechain	248	6.1	103	41.5	2.5	34	13.7	0.8
Sidechain-Sidechain	202	5.0	101	50.0	2.5	9	4.5	0.2
Long range ($i-j \geq 5$)	1469	36.3	608	41.4	15.0	104	7.1	2.6
Backbone-Backbone	202	5.0	48	23.8	1.2	4	2.0	0.1
Backbone-Sidechain	673	16.6	309	45.9	7.6	55	8.2	1.4
Sidechain-Sidechain	594	14.7	251	42.3	6.2	45	7.6	1.1
Inter-chain	119	2.9	84	70.6	2.1	4	3.4	0.1
Backbone-Backbone	13	0.3	1	7.7	0.0	0	0.0	0.0
Backbone-Sidechain	37	0.9	28	75.7	0.7	2	5.4	0.0
Sidechain-Sidechain	69	1.7	55	79.7	1.4	2	2.9	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	4051	100.0	1270	31.4	31.4	207	5.1	5.1
Backbone-Backbone	607	15.0	88	14.5	2.2	7	1.2	0.2
Backbone-Sidechain	2288	56.5	681	29.8	16.8	130	5.7	3.2
Sidechain-Sidechain	1156	28.5	501	43.3	12.4	70	6.1	1.7

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 disulfide 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	18	139	98	267	37	559	0.55	3.42	0.46	0.4
2	18	134	104	279	32	567	0.63	4.9	0.64	0.41
3	20	150	106	267	43	586	0.51	3.1	0.42	0.37
4	24	138	109	272	32	575	0.55	3.03	0.45	0.41
5	19	134	98	297	40	588	0.58	2.38	0.45	0.45
6	23	130	108	279	28	568	0.63	4.48	0.64	0.43
7	26	137	114	283	33	593	0.59	3.64	0.51	0.42
8	22	140	116	273	26	577	0.57	3.45	0.46	0.42
9	19	137	101	291	29	577	0.56	3.33	0.53	0.38
10	22	133	107	271	31	564	0.57	3.37	0.5	0.41

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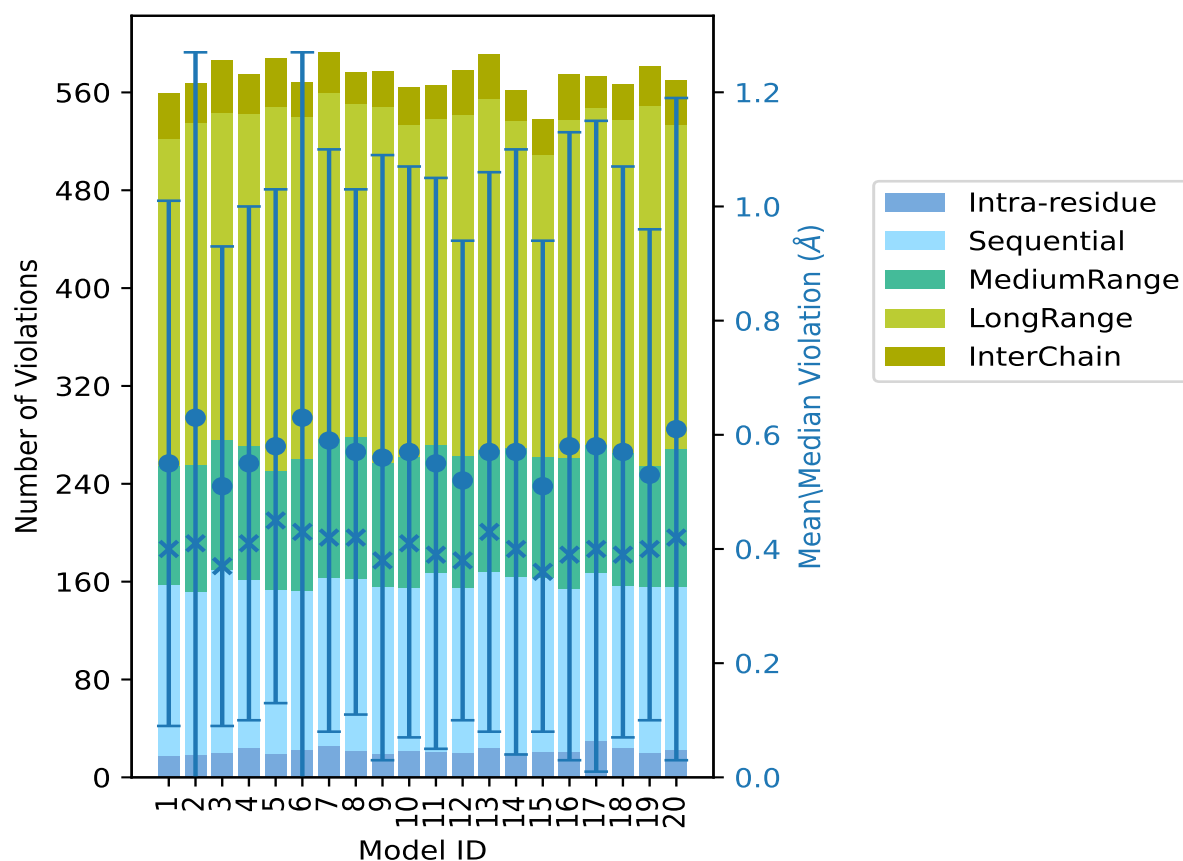
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	21	146	105	267	27	566	0.55	4.19	0.5	0.39
12	20	135	108	279	36	578	0.52	2.66	0.42	0.38
13	24	144	100	287	36	591	0.57	3.92	0.49	0.43
14	20	144	105	268	25	562	0.57	4.63	0.53	0.4
15	21	142	99	247	29	538	0.51	3.3	0.43	0.36
16	21	133	107	277	37	575	0.58	4.18	0.55	0.39
17	30	137	105	275	26	573	0.58	4.38	0.57	0.4
18	24	133	108	273	29	567	0.57	3.42	0.5	0.39
19	20	136	99	294	32	581	0.53	3.39	0.43	0.4
20	22	134	113	265	36	570	0.61	4.86	0.58	0.42

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

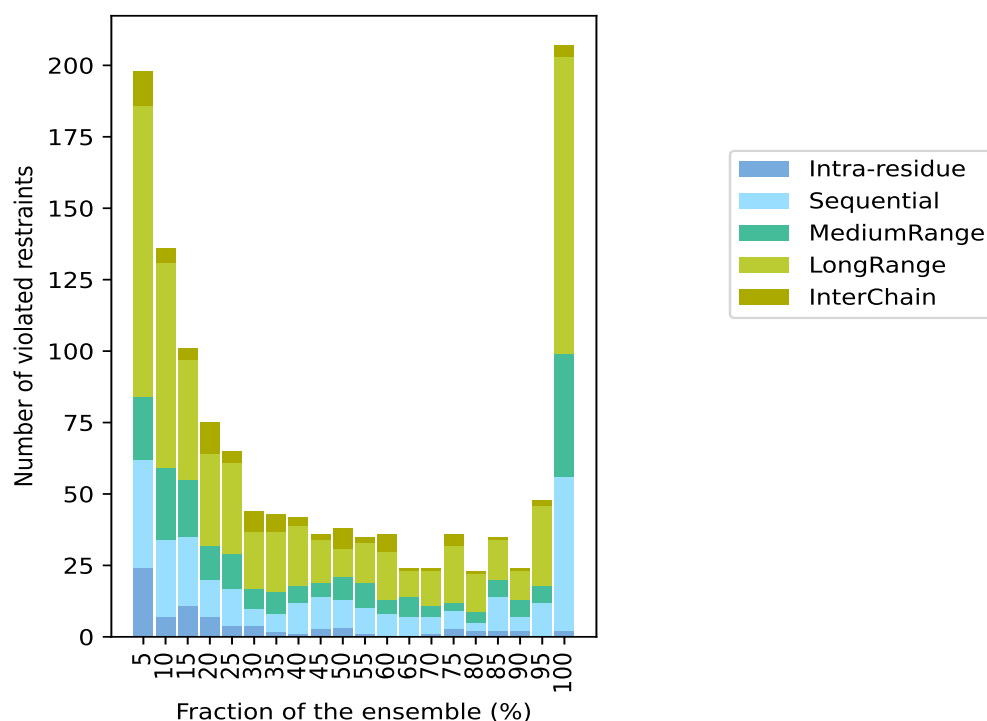
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2781(IR:731, SQ:832, MR:322, LR:861, IC:35) restraints are 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	%
24	38	22	102	12	198	1	5.0
7	27	25	72	5	136	2	10.0
11	24	20	42	4	101	3	15.0
7	13	12	32	11	75	4	20.0
4	13	12	32	4	65	5	25.0
4	6	7	20	7	44	6	30.0
2	6	8	21	6	43	7	35.0
1	11	6	21	3	42	8	40.0
3	11	5	15	2	36	9	45.0
3	10	8	10	7	38	10	50.0
1	9	9	14	2	35	11	55.0
0	8	5	17	6	36	12	60.0
0	7	7	9	1	24	13	65.0
1	6	4	12	1	24	14	70.0
3	6	3	20	4	36	15	75.0
2	3	4	13	1	23	16	80.0
2	12	6	14	1	35	17	85.0
2	5	6	10	1	24	18	90.0
0	12	6	28	2	48	19	95.0
2	54	43	104	4	207	20	100.0

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

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

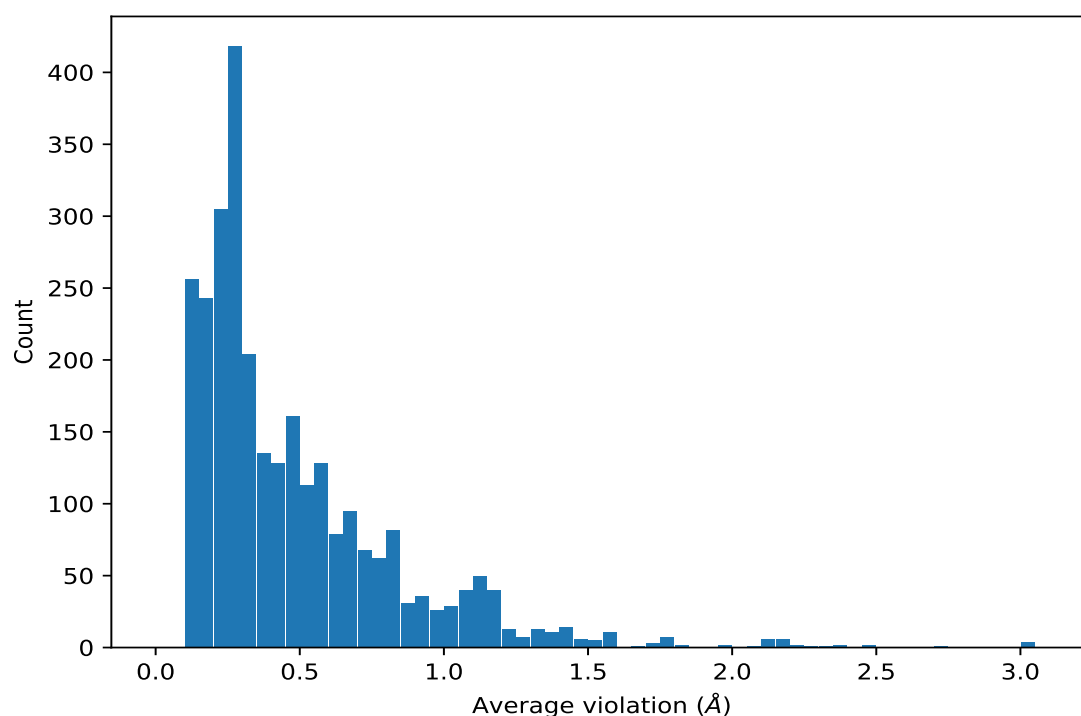
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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.

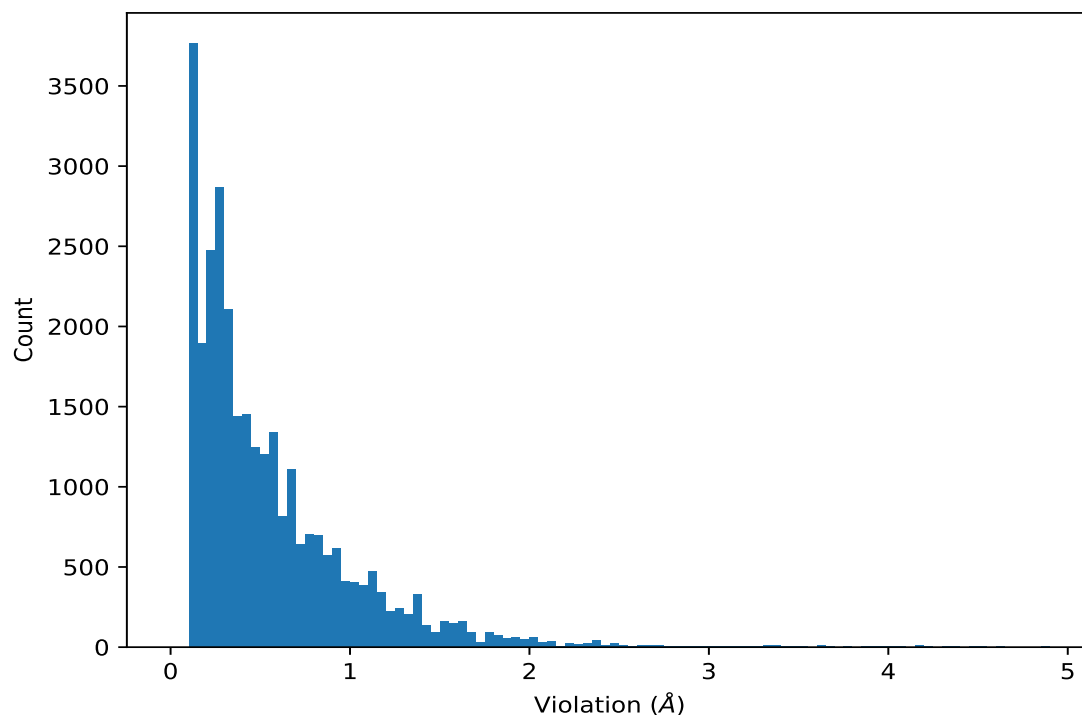
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3347)	2:10:B:TYR:HE1	2:21:B:MET:HB2	20	3.02	1.27	2.87
(1,3347)	2:10:B:TYR:HE2	2:21:B:MET:HB2	20	3.02	1.27	2.87
(1,3459)	2:10:B:TYR:HE1	2:21:B:MET:H	20	3.01	0.92	2.93
(1,3459)	2:10:B:TYR:HE2	2:21:B:MET:H	20	3.01	0.92	2.93
(1,3076)	1:196:A:ASN:HD22	1:225:A:LYS:H	20	2.71	0.51	2.75
(1,3476)	2:10:B:TYR:HE1	2:21:B:MET:HB3	20	2.49	1.25	2.34
(1,3476)	2:10:B:TYR:HE2	2:21:B:MET:HB3	20	2.49	1.25	2.34
(1,3346)	2:10:B:TYR:HD1	2:21:B:MET:HB2	20	2.39	1.19	2.24
(1,3346)	2:10:B:TYR:HD2	2:21:B:MET:HB2	20	2.39	1.19	2.24
(1,329)	1:196:A:ASN:HD22	1:225:A:LYS:HA	20	2.33	1.29	3.14
(1,3046)	1:196:A:ASN:HD21	1:225:A:LYS:H	20	2.27	0.47	2.3
(1,2888)	1:116:A:GLN:HE21	1:188:A:GLY:H	20	2.09	0.36	1.99
(1,2090)	1:196:A:ASN:HD22	1:225:A:LYS:HG2	20	1.8	0.31	1.8
(1,2090)	1:196:A:ASN:HD22	1:225:A:LYS:HG3	20	1.8	0.31	1.8
(1,3265)	1:58:A:HIS:HE1	1:60:A:LYS:HG2	20	1.78	0.51	1.8

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 provides the 10 worst performing restraints, sorted by the violation 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)
(1,3347)	2:10:B:TYR:HE1	2:21:B:MET:HB2	2	4.9
(1,3347)	2:10:B:TYR:HE2	2:21:B:MET:HB2	2	4.9
(1,3347)	2:10:B:TYR:HE1	2:21:B:MET:HB2	20	4.86
(1,3347)	2:10:B:TYR:HE2	2:21:B:MET:HB2	20	4.86
(1,3347)	2:10:B:TYR:HE1	2:21:B:MET:HB2	14	4.63
(1,3347)	2:10:B:TYR:HE2	2:21:B:MET:HB2	14	4.63
(1,3476)	2:10:B:TYR:HE1	2:21:B:MET:HB3	2	4.5
(1,3476)	2:10:B:TYR:HE2	2:21:B:MET:HB3	2	4.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3347)	2:10:B:TYR:HE1	2:21:B:MET:HB2	6	4.48
(1,3347)	2:10:B:TYR:HE2	2:21:B:MET:HB2	6	4.48
(1,3459)	2:10:B:TYR:HE1	2:21:B:MET:H	17	4.38
(1,3459)	2:10:B:TYR:HE2	2:21:B:MET:H	17	4.38
(1,3459)	2:10:B:TYR:HE1	2:21:B:MET:H	20	4.33
(1,3459)	2:10:B:TYR:HE2	2:21:B:MET:H	20	4.33
(1,3347)	2:10:B:TYR:HE1	2:21:B:MET:HB2	17	4.32
(1,3347)	2:10:B:TYR:HE2	2:21:B:MET:HB2	17	4.32
(1,3476)	2:10:B:TYR:HE1	2:21:B:MET:HB3	20	4.24
(1,3476)	2:10:B:TYR:HE2	2:21:B:MET:HB3	20	4.24
(1,3476)	2:10:B:TYR:HE1	2:21:B:MET:HB3	14	4.22

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found