



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 01:06 AM UTC

PDB ID : 9RKL / pdb\_00009rkl  
BMRB ID : 35000  
Title : Staphylokinase THR174  
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Deposited on : 2025-06-13

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

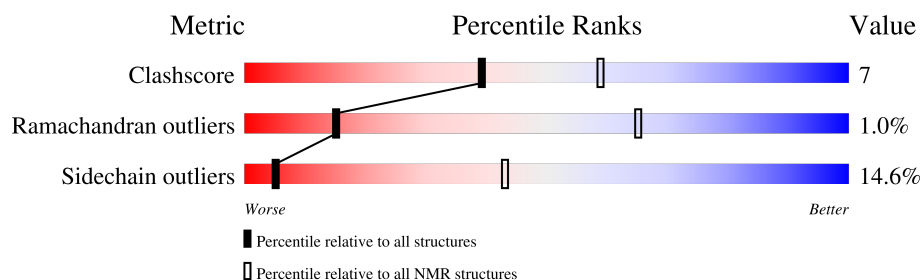
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 94%.

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  $\geq 3$ , 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	136	<div> <div></div> <div>67%</div> <div>18%</div> <div>15%</div> </div>

## 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:22-A:136 (115)	1.07	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	1, 2, 6, 8, 11, 12, 14, 16, 18
2	7, 9, 15, 17, 19, 20
3	3, 5, 13
Single-model clusters	4; 10

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2176 atoms, of which 1083 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Staphylokinase.

Mol	Chain	Residues	Atoms						Trace
1	A	136	Total	C	H	N	O	S	0
			2176	710	1083	168	214	1	

There are 8 discrepancies between the modelled and reference sequences:

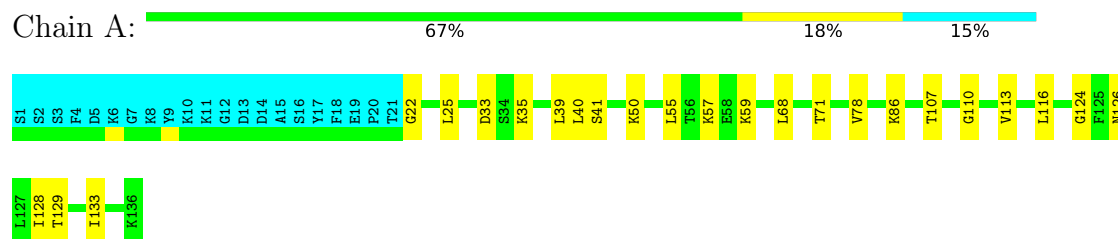
Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ASP	GLU	conflict	UNP Q99SU7
A	74	GLN	LYS	conflict	UNP Q99SU7
A	77	GLU	ARG	conflict	UNP Q99SU7
A	80	SER	GLU	conflict	UNP Q99SU7
A	82	SER	ASP	conflict	UNP Q99SU7
A	112	THR	VAL	conflict	UNP Q99SU7
A	130	TYR	LYS	conflict	UNP Q99SU7
A	134	ARG	GLU	conflict	UNP Q99SU7

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Staphylokinase

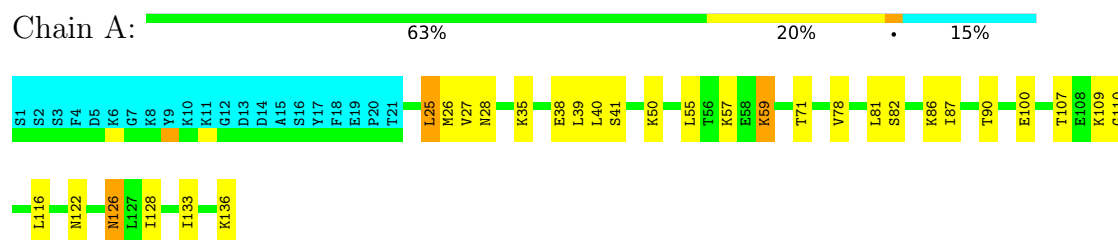


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

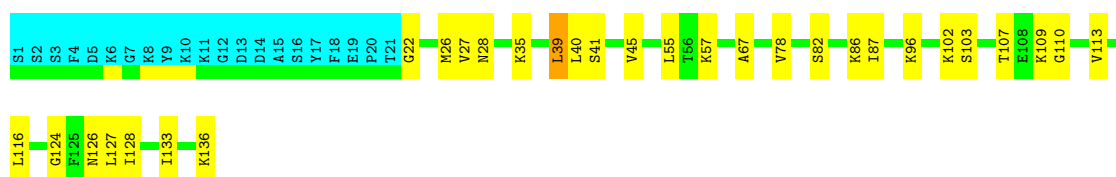
- Molecule 1: Staphylokinase



#### 4.2.2 Score per residue for model 2

- Molecule 1: Staphylokinase

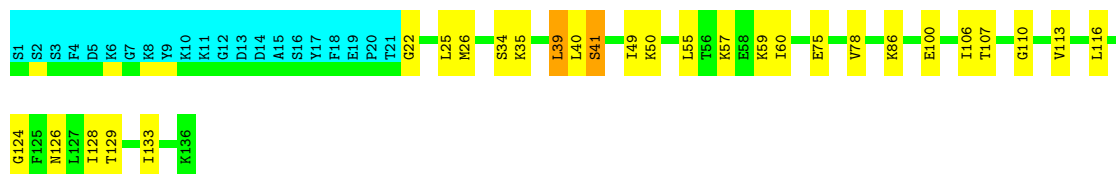




#### 4.2.3 Score per residue for model 3

- Molecule 1: Staphylokinase

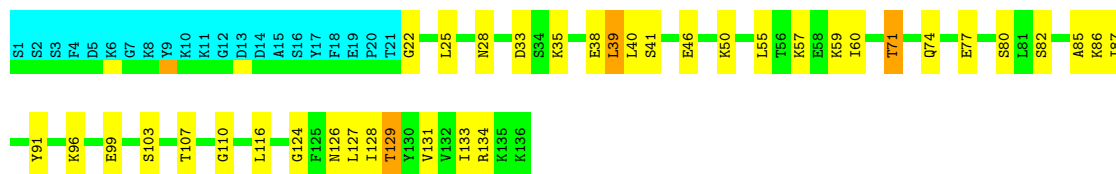
Chain A: 64% 19% 15%



#### 4.2.4 Score per residue for model 4

- Molecule 1: Staphylokinase

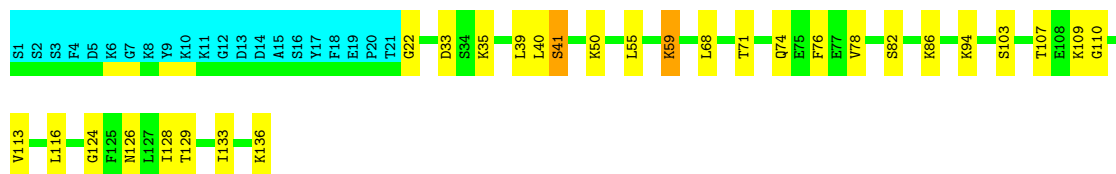
Chain A: 57% 26% 15%



#### 4.2.5 Score per residue for model 5

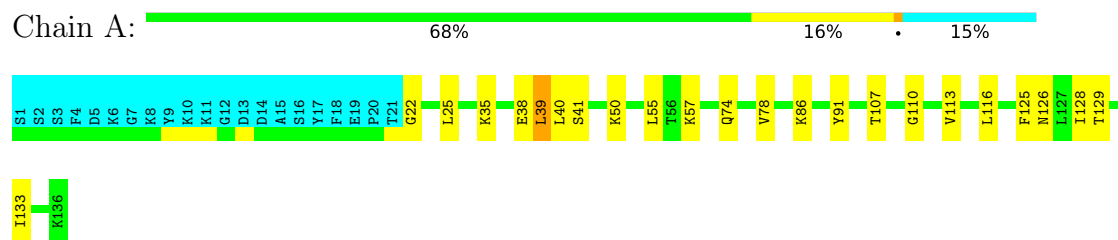
- Molecule 1: Staphylokinase

Chain A: 63% 20% 15%



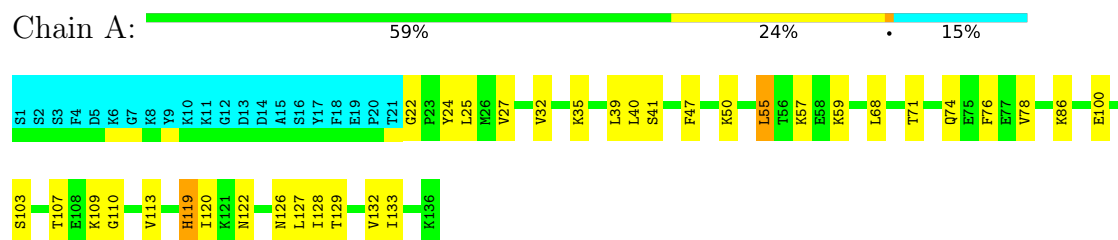
#### 4.2.6 Score per residue for model 6

- Molecule 1: Staphylokinase



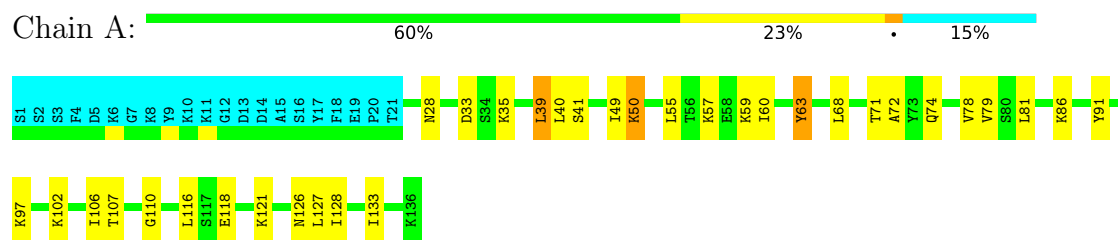
#### 4.2.7 Score per residue for model 7

- Molecule 1: Staphylokinase



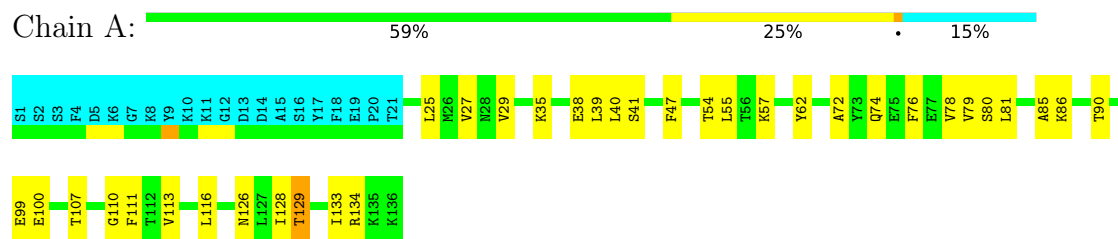
#### 4.2.8 Score per residue for model 8

- Molecule 1: Staphylokinase



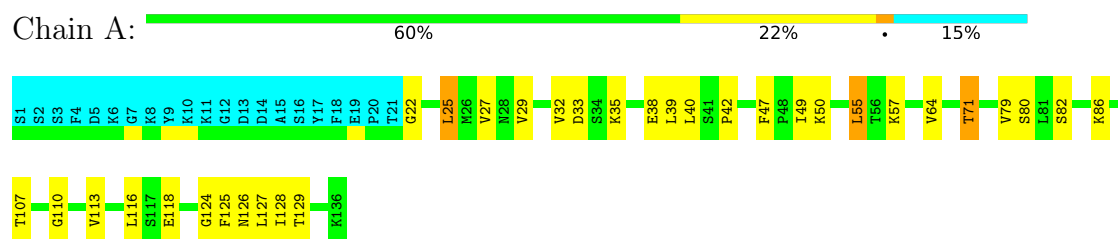
#### 4.2.9 Score per residue for model 9

- Molecule 1: Staphylokinase



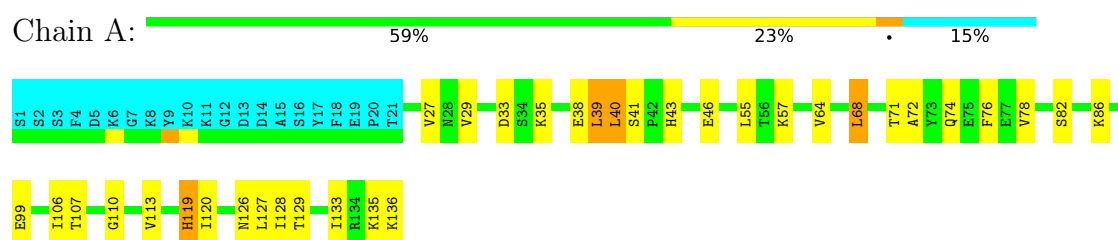
### 4.2.10 Score per residue for model 10

- Molecule 1: Staphylokinase



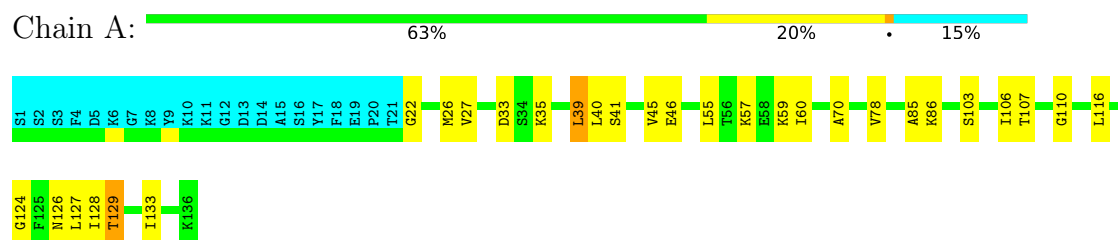
### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Staphylokinase



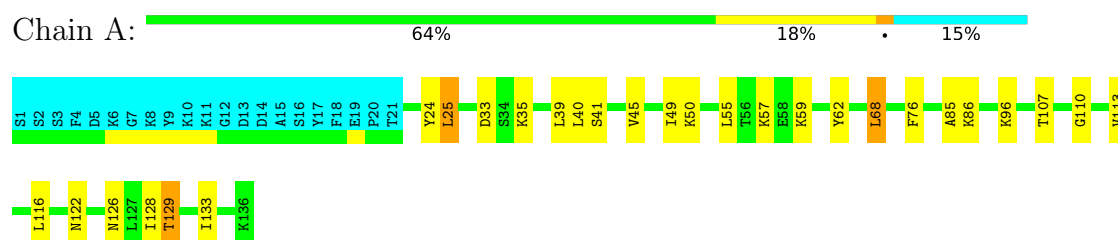
### 4.2.12 Score per residue for model 12

- Molecule 1: Staphylokinase



### 4.2.13 Score per residue for model 13

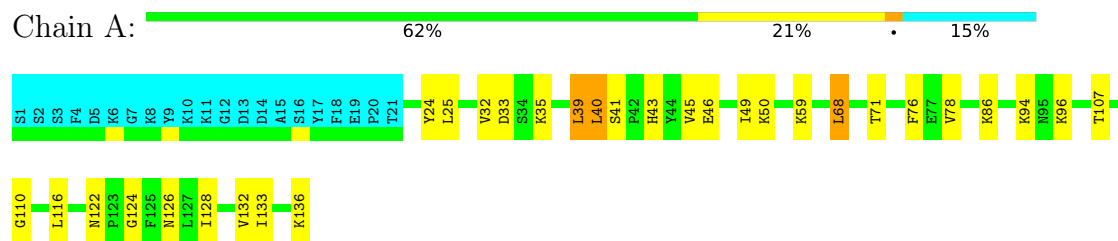
- Molecule 1: Staphylokinase





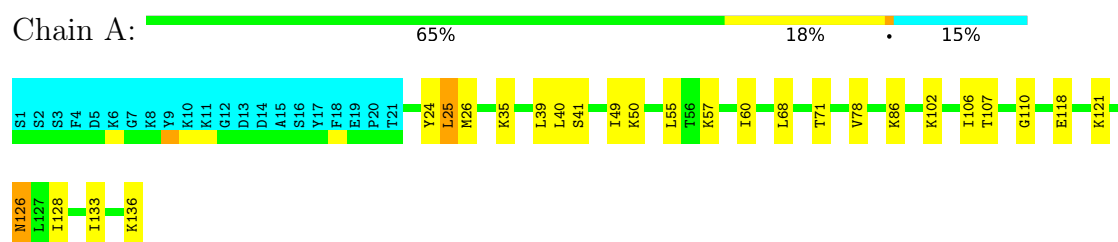
#### 4.2.14 Score per residue for model 14

- Molecule 1: Staphylokinase



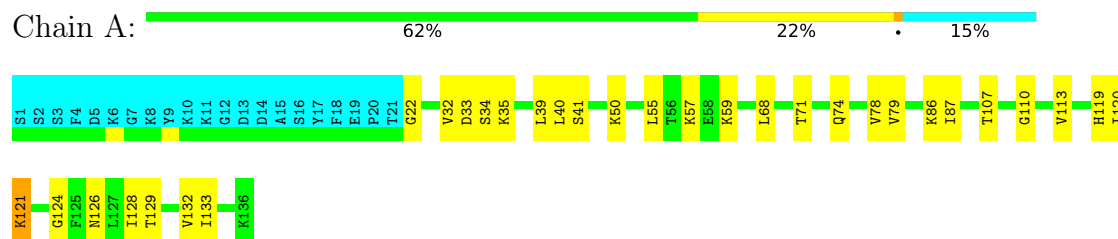
#### 4.2.15 Score per residue for model 15

- Molecule 1: Staphylokinase



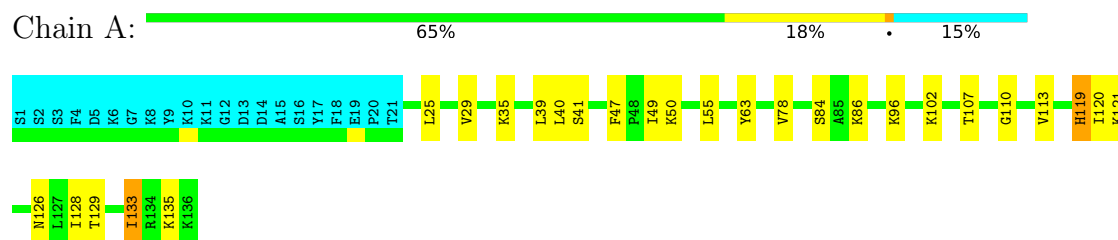
#### 4.2.16 Score per residue for model 16

- Molecule 1: Staphylokinase



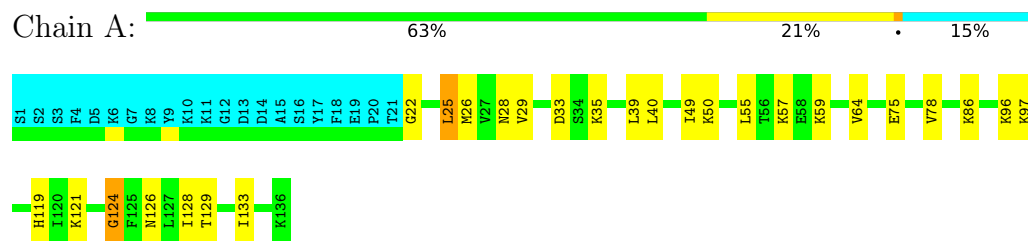
#### 4.2.17 Score per residue for model 17

- Molecule 1: Staphylokinase



### 4.2.18 Score per residue for model 18

- Molecule 1: Staphylokinase



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 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 calculation	
ARTINA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1718
Number of shifts mapped to atoms	1718
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

## 6 Model quality

### 6.1 Standard geometry

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

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	927	932	932	13±3
All	All	18540	18640	18640	268

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:VAL:HG13	1:A:127:LEU:HD21	0.84	1.49	10	1
1:A:55:LEU:HD12	1:A:60:ILE:HD11	0.81	1.53	12	4
1:A:33:ASP:CG	1:A:39:LEU:HD23	0.68	2.14	19	6
1:A:29:VAL:HG12	1:A:64:VAL:HG23	0.64	1.68	10	1
1:A:29:VAL:CG1	1:A:64:VAL:HG23	0.64	2.23	10	1
1:A:33:ASP:OD2	1:A:39:LEU:HD23	0.63	1.94	4	5
1:A:55:LEU:HD21	1:A:113:VAL:HG22	0.62	1.70	17	7
1:A:40:LEU:HD21	1:A:71:THR:CG2	0.61	2.25	8	1
1:A:40:LEU:HD13	1:A:41:SER:N	0.61	2.11	17	7
1:A:78:VAL:HG22	1:A:133:ILE:HG22	0.60	1.73	1	4
1:A:78:VAL:HA	1:A:133:ILE:HG22	0.60	1.74	8	13
1:A:68:LEU:HD21	1:A:76:PHE:CB	0.60	2.26	14	2
1:A:39:LEU:HD12	1:A:40:LEU:N	0.59	2.12	5	20
1:A:41:SER:HB3	1:A:71:THR:HG21	0.59	1.74	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LEU:HD21	1:A:113:VAL:CG2	0.59	2.27	7	7
1:A:27:VAL:HG21	1:A:47:PHE:CE2	0.58	2.34	9	2
1:A:55:LEU:CD1	1:A:60:ILE:HD11	0.58	2.29	4	2
1:A:29:VAL:HG11	1:A:64:VAL:HG23	0.58	1.75	11	1
1:A:72:ALA:HB1	1:A:76:PHE:CE1	0.58	2.34	19	3
1:A:41:SER:CB	1:A:71:THR:HG21	0.57	2.29	1	4
1:A:55:LEU:HD13	1:A:59:LYS:HD3	0.57	1.76	18	3
1:A:40:LEU:HB2	1:A:133:ILE:HD11	0.56	1.76	19	4
1:A:133:ILE:HD12	1:A:133:ILE:O	0.56	2.00	20	9
1:A:40:LEU:HD23	1:A:41:SER:O	0.56	2.01	8	1
1:A:85:ALA:HA	1:A:129:THR:HG21	0.56	1.76	4	4
1:A:55:LEU:HD11	1:A:113:VAL:HG22	0.55	1.76	9	4
1:A:40:LEU:HD11	1:A:71:THR:OG1	0.55	2.01	11	1
1:A:119:HIS:O	1:A:120:ILE:HD13	0.55	2.00	17	3
1:A:68:LEU:HD21	1:A:76:PHE:HB2	0.55	1.77	11	2
1:A:41:SER:OG	1:A:71:THR:HG21	0.54	2.02	5	2
1:A:27:VAL:HG13	1:A:127:LEU:HB3	0.54	1.79	2	2
1:A:40:LEU:HD21	1:A:71:THR:OG1	0.54	2.01	19	1
1:A:107:THR:HG23	1:A:110:GLY:H	0.54	1.61	5	20
1:A:25:LEU:HD22	1:A:47:PHE:CZ	0.54	2.37	10	1
1:A:40:LEU:HD12	1:A:72:ALA:CB	0.54	2.32	9	1
1:A:32:VAL:CG2	1:A:132:VAL:HG22	0.53	2.33	16	2
1:A:91:TYR:CZ	1:A:116:LEU:HD22	0.53	2.39	4	1
1:A:72:ALA:HB1	1:A:76:PHE:CD1	0.53	2.38	19	2
1:A:45:VAL:HG21	1:A:67:ALA:HA	0.53	1.79	2	1
1:A:40:LEU:HB3	1:A:133:ILE:HD11	0.52	1.81	9	1
1:A:102:LYS:NZ	1:A:116:LEU:HD11	0.52	2.19	20	1
1:A:116:LEU:HD12	1:A:125:PHE:CE1	0.52	2.40	10	1
1:A:87:ILE:HG13	1:A:127:LEU:HD12	0.52	1.81	4	1
1:A:25:LEU:HD13	1:A:47:PHE:CE2	0.52	2.40	20	1
1:A:55:LEU:HD12	1:A:87:ILE:HD11	0.51	1.81	1	1
1:A:40:LEU:HD12	1:A:72:ALA:HB3	0.51	1.81	9	1
1:A:40:LEU:CB	1:A:133:ILE:HD11	0.51	2.36	3	3
1:A:79:VAL:HG22	1:A:134:ARG:NE	0.51	2.20	9	1
1:A:25:LEU:HD13	1:A:47:PHE:CZ	0.51	2.41	17	1
1:A:40:LEU:CD1	1:A:72:ALA:HB2	0.50	2.36	8	1
1:A:78:VAL:HG13	1:A:133:ILE:HG22	0.49	1.84	19	1
1:A:55:LEU:HD12	1:A:87:ILE:HD13	0.49	1.85	16	3
1:A:42:PRO:HB2	1:A:71:THR:HG21	0.49	1.83	10	1
1:A:29:VAL:HG23	1:A:41:SER:CB	0.49	2.37	17	1
1:A:25:LEU:HD12	1:A:49:ILE:HG12	0.48	1.84	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LEU:HD13	1:A:76:PHE:HB2	0.48	1.84	5	1
1:A:78:VAL:HG22	1:A:133:ILE:CG2	0.47	2.39	1	2
1:A:32:VAL:HG12	1:A:38:GLU:HA	0.47	1.86	10	1
1:A:68:LEU:CD1	1:A:133:ILE:HG21	0.47	2.39	19	1
1:A:57:LYS:HG2	1:A:106:ILE:HG21	0.47	1.84	3	4
1:A:25:LEU:HD23	1:A:27:VAL:CG2	0.47	2.40	1	1
1:A:25:LEU:HD12	1:A:125:PHE:HB2	0.47	1.85	6	2
1:A:116:LEU:HD12	1:A:125:PHE:CZ	0.47	2.45	10	1
1:A:49:ILE:HD12	1:A:49:ILE:O	0.47	2.10	17	1
1:A:63:TYR:OH	1:A:127:LEU:HD13	0.46	2.10	8	1
1:A:40:LEU:HD13	1:A:40:LEU:C	0.46	2.35	1	5
1:A:91:TYR:CD2	1:A:116:LEU:HD13	0.46	2.45	8	2
1:A:27:VAL:HG13	1:A:127:LEU:CD2	0.46	2.40	7	1
1:A:40:LEU:HD12	1:A:72:ALA:HB2	0.46	1.88	8	1
1:A:29:VAL:HG11	1:A:64:VAL:HG13	0.46	1.88	18	1
1:A:55:LEU:HD23	1:A:113:VAL:CG2	0.45	2.41	5	2
1:A:57:LYS:CE	1:A:106:ILE:HD13	0.45	2.41	19	2
1:A:68:LEU:HD21	1:A:76:PHE:HB3	0.45	1.89	14	1
1:A:40:LEU:HD21	1:A:71:THR:HG23	0.45	1.88	8	1
1:A:26:MET:HE2	1:A:124:GLY:O	0.45	2.12	18	2
1:A:49:ILE:C	1:A:49:ILE:HD12	0.44	2.38	10	6
1:A:55:LEU:HD23	1:A:113:VAL:HG23	0.44	1.89	5	2
1:A:27:VAL:HG13	1:A:127:LEU:HD23	0.44	1.89	11	1
1:A:33:ASP:OD1	1:A:39:LEU:HD23	0.44	2.13	19	2
1:A:107:THR:HG23	1:A:110:GLY:N	0.44	2.27	5	1
1:A:81:LEU:HD12	1:A:82:SER:N	0.44	2.28	1	1
1:A:127:LEU:HD13	1:A:127:LEU:C	0.44	2.38	2	1
1:A:29:VAL:HG23	1:A:41:SER:OG	0.43	2.13	9	1
1:A:26:MET:HE3	1:A:126:ASN:HB3	0.43	1.89	1	2
1:A:32:VAL:HG22	1:A:132:VAL:HG22	0.43	1.88	16	2
1:A:90:THR:HG23	1:A:100:GLU:O	0.43	2.13	9	2
1:A:39:LEU:HD13	1:A:76:PHE:CE2	0.43	2.49	9	1
1:A:49:ILE:HD12	1:A:49:ILE:C	0.43	2.38	17	1
1:A:41:SER:HB2	1:A:71:THR:HG21	0.43	1.90	7	1
1:A:133:ILE:HD12	1:A:133:ILE:C	0.42	2.39	20	7
1:A:45:VAL:HG21	1:A:70:ALA:CB	0.42	2.45	12	1
1:A:40:LEU:CD2	1:A:72:ALA:HB2	0.42	2.43	11	1
1:A:79:VAL:HG21	1:A:132:VAL:HG12	0.42	1.91	16	1
1:A:39:LEU:HD11	1:A:133:ILE:HD13	0.42	1.91	17	1
1:A:55:LEU:HD11	1:A:113:VAL:CG2	0.42	2.44	10	1
1:A:40:LEU:HD23	1:A:41:SER:OG	0.42	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ILE:HD12	1:A:50:LYS:N	0.42	2.30	8	1
1:A:68:LEU:HD11	1:A:76:PHE:CG	0.41	2.50	13	1
1:A:32:VAL:HG22	1:A:132:VAL:HG13	0.41	1.92	7	1
1:A:25:LEU:HD12	1:A:49:ILE:HD11	0.41	1.90	13	1
1:A:79:VAL:HG23	1:A:133:ILE:HA	0.41	1.91	8	1
1:A:91:TYR:CG	1:A:116:LEU:HD13	0.41	2.50	6	1
1:A:32:VAL:CG2	1:A:132:VAL:HG13	0.41	2.45	7	1
1:A:133:ILE:C	1:A:133:ILE:HD12	0.41	2.40	1	2
1:A:80:SER:O	1:A:131:VAL:HG13	0.41	2.16	4	1
1:A:55:LEU:N	1:A:55:LEU:HD22	0.41	2.31	6	1
1:A:39:LEU:HD13	1:A:76:PHE:HE2	0.41	1.76	7	1
1:A:39:LEU:HD11	1:A:133:ILE:HD12	0.41	1.93	20	2
1:A:54:THR:HG23	1:A:111:PHE:O	0.41	2.15	9	1
1:A:120:ILE:HG22	1:A:121:LYS:N	0.40	2.31	16	1
1:A:40:LEU:HD11	1:A:71:THR:HB	0.40	1.93	16	1
1:A:43:HIS:CE1	1:A:71:THR:HG22	0.40	2.52	11	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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	114/136 (84%)	106±2 (93±1%)	7±2 (6±2%)	1±1 (1±1%)	15	65
All	All	2280/2720 (84%)	2110 (93%)	147 (6%)	23 (1%)	15	65

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	22	GLY	12
1	A	124	GLY	11

### 6.3.2 Protein sidechains ⓘ

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	105/123 (85%)	90±3 (85±3%)	15±3 (15±3%)	5	43
All	All	2100/2460 (85%)	1793 (85%)	307 (15%)	5	43

All 52 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	35	LYS	20
1	A	126	ASN	20
1	A	128	ILE	20
1	A	86	LYS	19
1	A	50	LYS	15
1	A	129	THR	15
1	A	57	LYS	12
1	A	25	LEU	11
1	A	59	LYS	11
1	A	74	GLN	10
1	A	116	LEU	9
1	A	39	LEU	8
1	A	68	LEU	8
1	A	136	LYS	7
1	A	82	SER	7
1	A	96	LYS	7
1	A	41	SER	6
1	A	103	SER	6
1	A	121	LYS	6
1	A	28	ASN	5
1	A	38	GLU	5
1	A	109	LYS	5
1	A	119	HIS	5
1	A	122	ASN	4
1	A	102	LYS	4
1	A	46	GLU	4
1	A	71	THR	4
1	A	24	TYR	4
1	A	118	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	26	MET	3
1	A	34	SER	3
1	A	99	GLU	3
1	A	97	LYS	3
1	A	80	SER	3
1	A	33	ASP	3
1	A	75	GLU	2
1	A	100	GLU	2
1	A	94	LYS	2
1	A	55	LEU	2
1	A	63	TYR	2
1	A	81	LEU	2
1	A	62	TYR	2
1	A	79	VAL	2
1	A	40	LEU	2
1	A	135	LYS	2
1	A	45	VAL	2
1	A	77	GLU	1
1	A	134	ARG	1
1	A	43	HIS	1
1	A	84	SER	1
1	A	133	ILE	1
1	A	127	LEU	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry ⓘ

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 94% for the well-defined parts and 93% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `starch_output`

#### 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	1718
Number of shifts mapped to atoms	1718
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

#### 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
$^{13}\text{C}_\alpha$	136	$2.79 \pm 0.13$	Should be applied
$^{13}\text{C}_\beta$	128	$2.65 \pm 0.14$	Should be applied
$^{13}\text{C}'$	122	$3.00 \pm 0.14$	Should be applied
$^{15}\text{N}$	126	$-0.29 \pm 0.25$	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 94%, i.e. 1486 atoms were assigned a chemical shift out of a possible 1587. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	553/565 (98%)	228/228 (100%)	218/230 (95%)	107/107 (100%)
Sidechain	830/874 (95%)	564/568 (99%)	260/283 (92%)	6/23 (26%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	103/148 (70%)	67/71 (94%)	35/74 (47%)	1/3 (33%)
Overall	1486/1587 (94%)	859/867 (99%)	513/587 (87%)	114/133 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1718 atoms were assigned a chemical shift out of a possible 1844. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	654/670 (98%)	270/271 (100%)	258/272 (95%)	126/127 (99%)
Sidechain	936/988 (95%)	635/639 (99%)	295/322 (92%)	6/27 (22%)
Aromatic	128/186 (69%)	85/89 (96%)	42/94 (45%)	1/3 (33%)
Overall	1718/1844 (93%)	990/999 (99%)	595/688 (86%)	133/157 (85%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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.

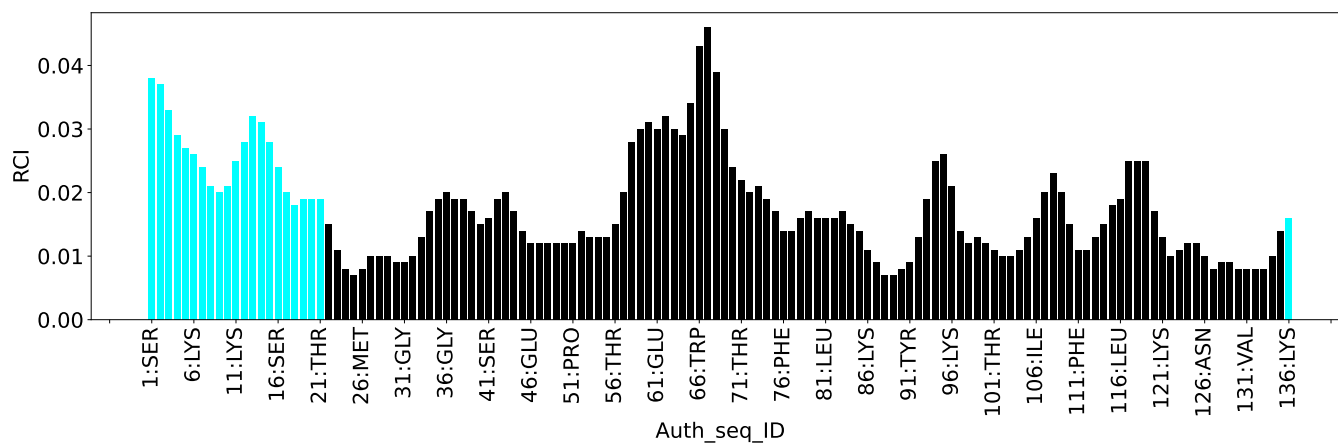
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	121	LYS	HE2	0.99	1.95 – 3.88	-9.9
1	A	17	TYR	HE1	4.61	5.59 – 7.82	-9.4
1	A	96	LYS	HE2	1.38	1.95 – 3.88	-7.9
1	A	86	LYS	HE2	1.44	1.95 – 3.88	-7.6
1	A	10	LYS	HE2	1.50	1.95 – 3.88	-7.3
1	A	130	TYR	HD2	8.89	5.48 – 8.39	6.7
1	A	121	LYS	HD2	0.29	0.58 – 2.64	-6.4
1	A	121	LYS	HE3	1.65	1.92 – 3.89	-6.4
1	A	123	PRO	HD2	1.54	1.93 – 5.38	-6.1
1	A	114	PRO	HD2	1.55	1.93 – 5.38	-6.1
1	A	94	LYS	HE2	1.77	1.95 – 3.88	-5.9
1	A	86	LYS	HE3	1.89	1.92 – 3.89	-5.2
1	A	100	GLU	HB2	0.97	1.00 – 3.05	-5.1

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

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	1649
Intra-residue ( $ i-j =0$ )	471
Sequential ( $ i-j =1$ )	547
Medium range ( $ i-j >1$ and $ i-j <5$ )	191
Long range ( $ i-j \geq 5$ )	440
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	12.1
Number of long range restraints per residue <sup>1</sup>	3.2

<sup>1</sup>Long 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)	5.1	0.2
0.2-0.5 (Medium)	1.4	0.48
>0.5 (Large)	1.3	2.04

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

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis [i](#)

### 9.1 Summary of distance violations [i](#)

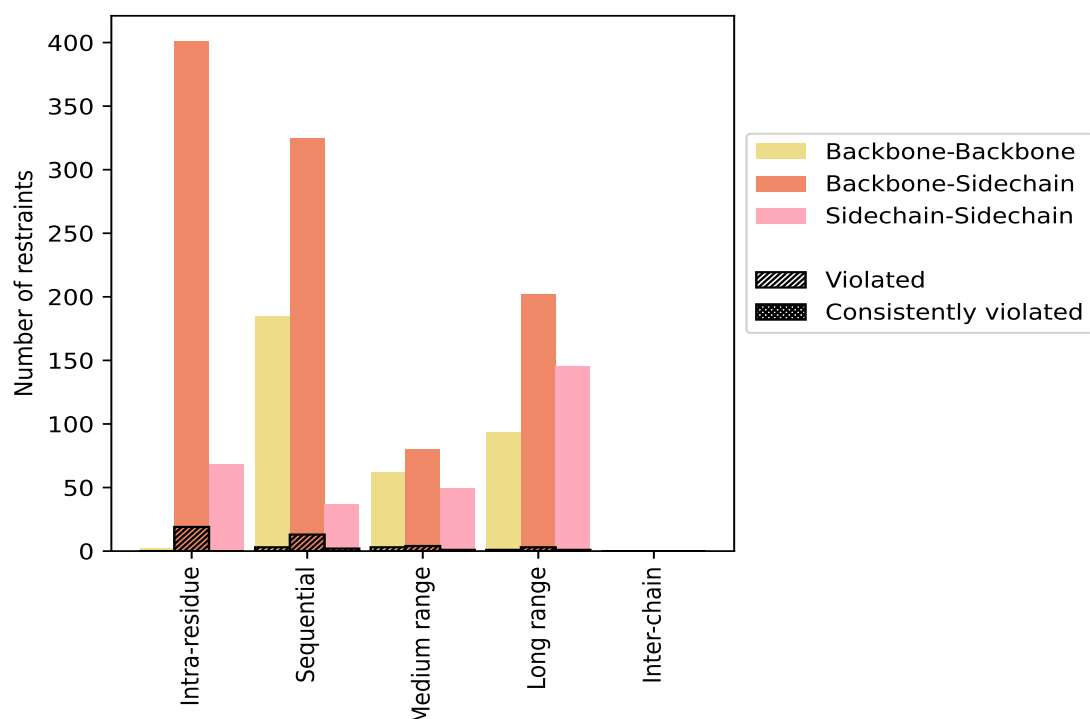
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">471</a>	<a href="#">28.6</a>	<a href="#">19</a>	<a href="#">4.0</a>	<a href="#">1.2</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	401	24.3	19	4.7	1.2	0	0.0	0.0
Sidechain-Sidechain	68	4.1	0	0.0	0.0	0	0.0	0.0
<a href="#">Sequential ( i-j =1)</a>	<a href="#">547</a>	<a href="#">33.2</a>	<a href="#">18</a>	<a href="#">3.3</a>	<a href="#">1.1</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	185	11.2	3	1.6	0.2	0	0.0	0.0
Backbone-Sidechain	325	19.7	13	4.0	0.8	0	0.0	0.0
Sidechain-Sidechain	37	2.2	2	5.4	0.1	0	0.0	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">191</a>	<a href="#">11.6</a>	<a href="#">8</a>	<a href="#">4.2</a>	<a href="#">0.5</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	62	3.8	3	4.8	0.2	0	0.0	0.0
Backbone-Sidechain	80	4.9	4	5.0	0.2	0	0.0	0.0
Sidechain-Sidechain	49	3.0	1	2.0	0.1	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">440</a>	<a href="#">26.7</a>	<a href="#">5</a>	<a href="#">1.1</a>	<a href="#">0.3</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	93	5.6	1	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	202	12.2	3	1.5	0.2	0	0.0	0.0
Sidechain-Sidechain	145	8.8	1	0.7	0.1	0	0.0	0.0
<a href="#">Inter-chain</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
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
<a href="#">Hydrogen bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">1649</a>	<a href="#">100.0</a>	<a href="#">50</a>	<a href="#">3.0</a>	<a href="#">3.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	342	20.7	7	2.0	0.4	0	0.0	0.0
Backbone-Sidechain	1008	61.1	39	3.9	2.4	0	0.0	0.0
Sidechain-Sidechain	299	18.1	4	1.3	0.2	0	0.0	0.0

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	1	1	0	0	2	0.17	0.2	0.03	0.17
2	2	3	2	0	0	7	0.17	0.25	0.05	0.14
3	3	3	2	0	0	8	0.15	0.24	0.04	0.14
4	3	4	2	0	0	9	0.26	1.1	0.3	0.15
5	3	0	3	0	0	6	0.32	0.98	0.3	0.2
6	5	2	1	2	0	10	0.23	0.93	0.24	0.15
7	4	2	0	0	0	6	0.32	0.68	0.22	0.2
8	3	3	2	0	0	8	0.53	1.68	0.62	0.18
9	5	2	2	0	0	9	0.48	2.04	0.59	0.13
10	5	6	3	2	0	16	0.25	1.68	0.37	0.14

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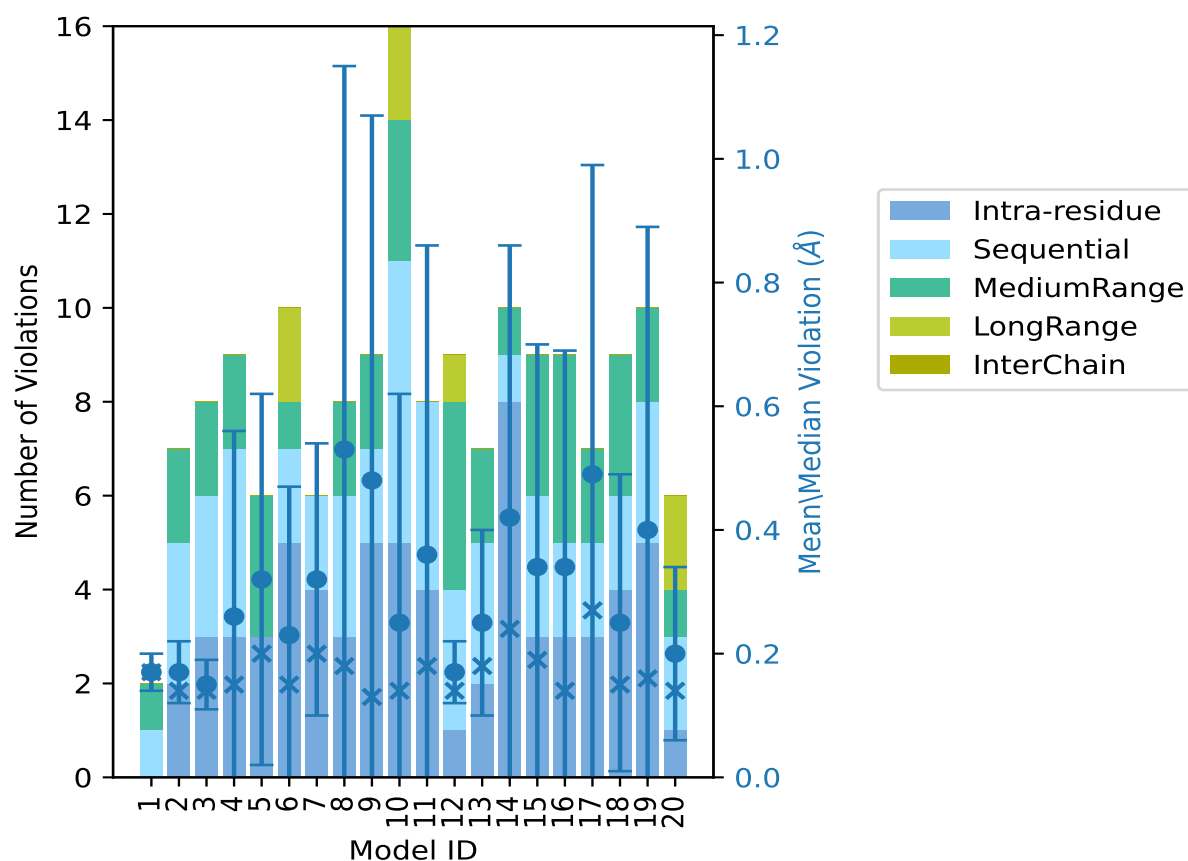
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	4	4	0	0	0	8	0.36	1.68	0.5	0.18
12	1	3	4	1	0	9	0.17	0.26	0.05	0.14
13	2	3	2	0	0	7	0.25	0.48	0.15	0.18
14	8	1	1	0	0	10	0.42	1.63	0.44	0.24
15	3	3	3	0	0	9	0.34	1.12	0.36	0.19
16	3	2	4	0	0	9	0.34	1.13	0.35	0.14
17	3	2	2	0	0	7	0.49	1.5	0.5	0.27
18	4	2	3	0	0	9	0.25	0.92	0.24	0.15
19	5	3	2	0	0	10	0.4	1.61	0.49	0.16
20	1	2	1	2	0	6	0.2	0.51	0.14	0.14

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard 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

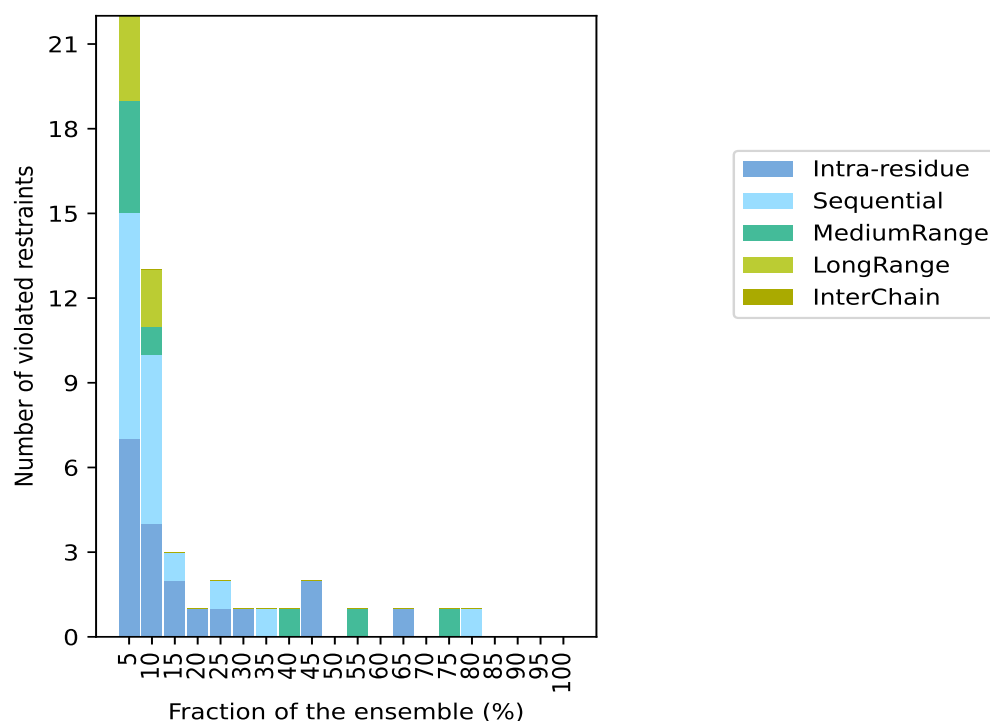
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1599(IR:452, SQ:529, MR:183, LR:435, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
7	8	4	3	0	22	1	5.0
4	6	1	2	0	13	2	10.0
2	1	0	0	0	3	3	15.0
1	0	0	0	0	1	4	20.0
1	1	0	0	0	2	5	25.0
1	0	0	0	0	1	6	30.0
0	1	0	0	0	1	7	35.0
0	0	1	0	0	1	8	40.0
2	0	0	0	0	2	9	45.0
0	0	0	0	0	0	10	50.0
0	0	1	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
1	0	0	0	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	1	0	0	1	15	75.0
0	1	0	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

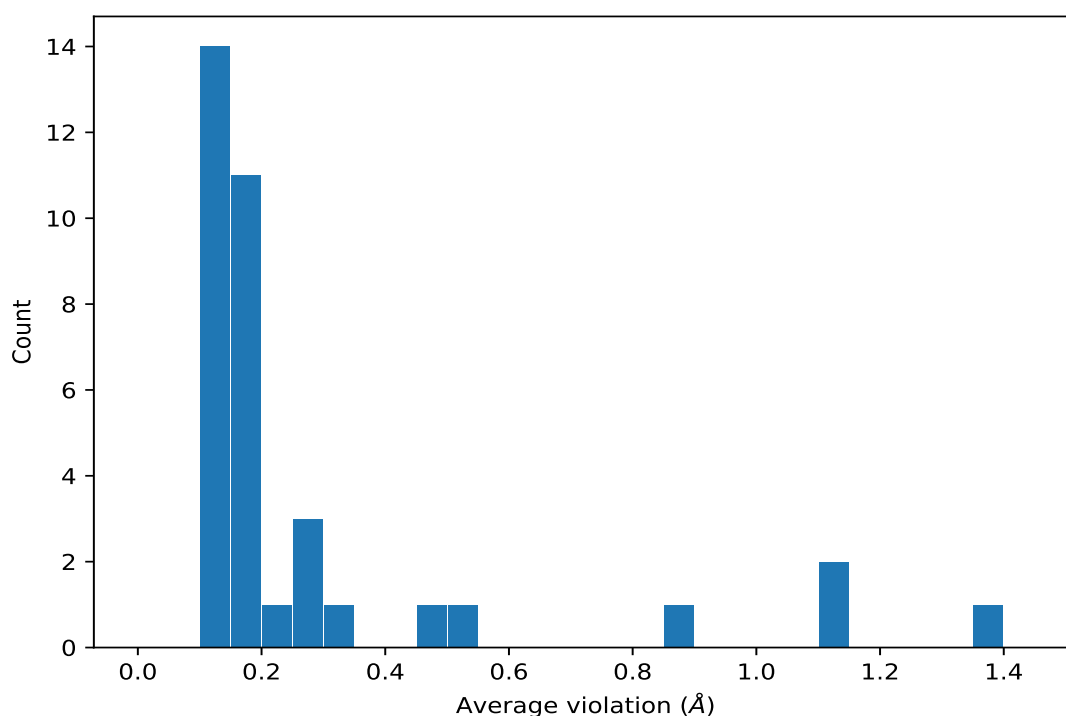
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	16	0.2	0.06	0.2
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	15	0.12	0.01	0.12
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	13	1.11	0.49	0.98
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	11	0.13	0.01	0.13
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	11	0.13	0.01	0.13
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	9	0.33	0.6	0.12
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	9	0.18	0.05	0.15
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	9	0.18	0.05	0.15
(1,802)	1:116:A:LEU:HA	1:119:A:HIS:H	8	0.13	0.02	0.14
(1,997)	1:9:A:TYR:HD2	1:10:A:LYS:H	7	0.19	0.0	0.19
(1,782)	1:47:A:PHE:H	1:47:A:PHE:HD2	6	0.49	0.19	0.51
(1,1182)	1:68:A:LEU:H	1:68:A:LEU:HG	5	0.18	0.01	0.18
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD2	5	0.15	0.06	0.13
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD3	5	0.15	0.06	0.13
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD1	4	0.25	0.02	0.24
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD2	4	0.25	0.02	0.24

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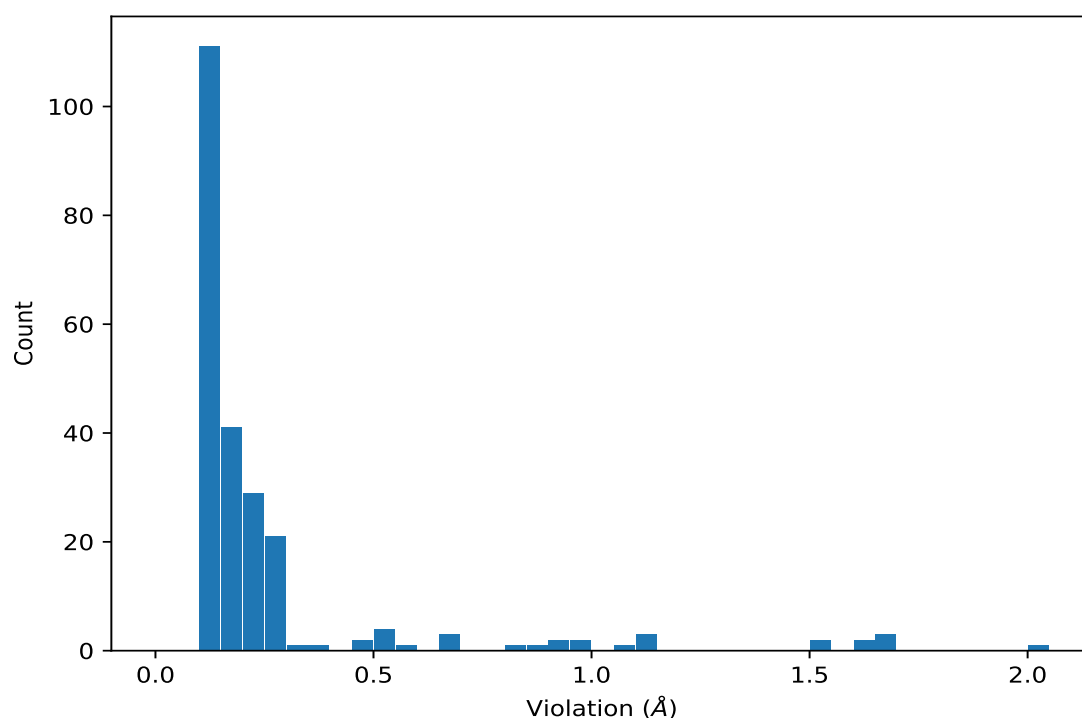
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1179)	1:63:A:TYR:H	1:63:A:TYR:HE2	3	1.37	0.21	1.5
(1,1193)	1:47:A:PHE:H	1:47:A:PHE:HE2	3	0.54	0.02	0.53
(1,1319)	1:19:A:GLU:HG2	1:20:A:PRO:HD2	3	0.14	0.0	0.14
(1,1319)	1:19:A:GLU:HG2	1:20:A:PRO:HD3	3	0.14	0.0	0.14
(1,1319)	1:19:A:GLU:HG3	1:20:A:PRO:HD2	3	0.14	0.0	0.14
(1,1319)	1:19:A:GLU:HG3	1:20:A:PRO:HD3	3	0.14	0.0	0.14
(1,821)	1:130:A:TYR:HD1	1:131:A:VAL:H	2	1.12	0.0	1.12
(1,567)	1:130:A:TYR:H	1:130:A:TYR:HD2	2	0.86	0.03	0.86
(1,1227)	1:6:A:LYS:HD2	1:7:A:GLY:H	2	0.27	0.0	0.27
(1,656)	1:10:A:LYS:H	1:10:A:LYS:HB3	2	0.18	0.0	0.18
(1,719)	1:8:A:LYS:H	1:8:A:LYS:HB3	2	0.18	0.0	0.18
(1,801)	1:57:A:LYS:HB3	1:58:A:GLU:H	2	0.17	0.01	0.17
(1,134)	1:6:A:LYS:HA	1:6:A:LYS:HD3	2	0.15	0.0	0.15
(1,1024)	1:40:A:LEU:HB2	1:41:A:SER:H	2	0.15	0.0	0.15
(1,927)	1:23:A:PRO:HB2	1:24:A:TYR:H	2	0.13	0.0	0.13
(1,927)	1:23:A:PRO:HB3	1:24:A:TYR:H	2	0.13	0.0	0.13
(1,660)	1:79:A:VAL:HB	1:80:A:SER:H	2	0.12	0.02	0.12
(1,287)	1:79:A:VAL:HB	1:132:A:VAL:HB	2	0.12	0.0	0.12
(1,59)	1:79:A:VAL:HA	1:133:A:ILE:HA	2	0.11	0.0	0.11
(1,1224)	1:129:A:THR:H	1:131:A:VAL:H	2	0.1	0.0	0.1

<sup>1</sup>Number of violated models, <sup>2</sup>Standard 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)
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	9	2.04
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	8	1.68
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	10	1.68
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	11	1.68
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	14	1.63
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	19	1.61
(1,1179)	1:63:A:TYR:H	1:63:A:TYR:HE2	8	1.53
(1,1179)	1:63:A:TYR:H	1:63:A:TYR:HE2	17	1.5
(1,821)	1:130:A:TYR:HD1	1:131:A:VAL:H	16	1.13
(1,821)	1:130:A:TYR:HD1	1:131:A:VAL:H	15	1.12
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	4	1.1
(1,1179)	1:63:A:TYR:H	1:63:A:TYR:HE2	19	1.08
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	5	0.98
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	17	0.97
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	6	0.93
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	18	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:130:A:TYR:H	1:130:A:TYR:HD2	15	0.88
(1,567)	1:130:A:TYR:H	1:130:A:TYR:HD2	16	0.83
(1,782)	1:47:A:PHE:H	1:47:A:PHE:HD2	7	0.68
(1,782)	1:47:A:PHE:H	1:47:A:PHE:HD2	14	0.68
(1,782)	1:47:A:PHE:H	1:47:A:PHE:HD2	9	0.66
(1,1193)	1:47:A:PHE:H	1:47:A:PHE:HE2	7	0.56
(1,1193)	1:47:A:PHE:H	1:47:A:PHE:HE2	14	0.53
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	9	0.53
(1,1193)	1:47:A:PHE:H	1:47:A:PHE:HE2	9	0.52
(1,392)	1:9:A:TYR:HA	1:10:A:LYS:H	20	0.51
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	13	0.48
(1,375)	1:11:A:LYS:HA	1:12:A:GLY:H	13	0.48
(1,782)	1:47:A:PHE:H	1:47:A:PHE:HD2	10	0.36
(1,782)	1:47:A:PHE:H	1:47:A:PHE:HD2	17	0.32
(1,1583)	1:107:A:THR:HG21	1:109:A:LYS:HB2	5	0.29
(1,1583)	1:107:A:THR:HG21	1:109:A:LYS:HB3	5	0.29
(1,1583)	1:107:A:THR:HG22	1:109:A:LYS:HB2	5	0.29
(1,1583)	1:107:A:THR:HG22	1:109:A:LYS:HB3	5	0.29
(1,1583)	1:107:A:THR:HG23	1:109:A:LYS:HB2	5	0.29
(1,1583)	1:107:A:THR:HG23	1:109:A:LYS:HB3	5	0.29
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD1	18	0.29
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD2	18	0.29
(1,1227)	1:6:A:LYS:HD2	1:7:A:GLY:H	10	0.27
(1,1227)	1:6:A:LYS:HD2	1:7:A:GLY:H	19	0.27
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	8	0.27
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	13	0.27
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	14	0.27
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	16	0.27
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	17	0.27
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD2	12	0.26
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD3	12	0.26
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	11	0.25
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	11	0.25
(1,610)	1:100:A:GLU:H	1:100:A:GLU:HG2	2	0.25
(1,610)	1:100:A:GLU:H	1:100:A:GLU:HG3	2	0.25
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	6	0.24
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	6	0.24
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	15	0.24
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	15	0.24
(1,303)	1:109:A:LYS:HA	1:109:A:LYS:HD2	5	0.24
(1,303)	1:109:A:LYS:HA	1:109:A:LYS:HD3	5	0.24
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD1	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD2	3	0.24
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD1	14	0.24
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD2	14	0.24
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD1	16	0.24
(1,233)	1:17:A:TYR:HA	1:17:A:TYR:HD2	16	0.24
(1,89)	1:60:A:ILE:HA	1:60:A:ILE:HD11	14	0.23
(1,89)	1:60:A:ILE:HA	1:60:A:ILE:HD12	14	0.23
(1,89)	1:60:A:ILE:HA	1:60:A:ILE:HD13	14	0.23
(1,1574)	1:100:A:GLU:HB2	1:101:A:THR:H	2	0.22
(1,1574)	1:100:A:GLU:HB3	1:101:A:THR:H	2	0.22
(1,1553)	1:93:A:ASP:HB2	1:98:A:LYS:H	12	0.22
(1,1553)	1:93:A:ASP:HB3	1:98:A:LYS:H	12	0.22
(1,1138)	1:73:A:TYR:H	1:73:A:TYR:HD2	7	0.21
(1,1103)	1:84:A:SER:H	1:85:A:ALA:HA	4	0.21
(1,841)	1:93:A:ASP:H	1:96:A:LYS:HB2	12	0.21
(1,782)	1:47:A:PHE:H	1:47:A:PHE:HD2	20	0.21
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	1	0.2
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	4	0.2
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	11	0.2
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	15	0.2
(1,997)	1:9:A:TYR:HD2	1:10:A:LYS:H	2	0.2
(1,997)	1:9:A:TYR:HD2	1:10:A:LYS:H	18	0.2
(1,1182)	1:68:A:LEU:H	1:68:A:LEU:HG	15	0.19
(1,997)	1:9:A:TYR:HD2	1:10:A:LYS:H	3	0.19
(1,997)	1:9:A:TYR:HD2	1:10:A:LYS:H	7	0.19
(1,997)	1:9:A:TYR:HD2	1:10:A:LYS:H	10	0.19
(1,997)	1:9:A:TYR:HD2	1:10:A:LYS:H	12	0.19
(1,997)	1:9:A:TYR:HD2	1:10:A:LYS:H	19	0.19
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	8	0.18
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	8	0.18
(1,1182)	1:68:A:LEU:H	1:68:A:LEU:HG	11	0.18
(1,1182)	1:68:A:LEU:H	1:68:A:LEU:HG	13	0.18
(1,801)	1:57:A:LYS:HB3	1:58:A:GLU:H	8	0.18
(1,719)	1:8:A:LYS:H	1:8:A:LYS:HB3	4	0.18
(1,719)	1:8:A:LYS:H	1:8:A:LYS:HB3	14	0.18
(1,656)	1:10:A:LYS:H	1:10:A:LYS:HB3	11	0.18
(1,656)	1:10:A:LYS:H	1:10:A:LYS:HB3	18	0.18
(1,454)	1:11:A:LYS:H	1:11:A:LYS:HB2	6	0.18
(1,401)	1:17:A:TYR:HB2	1:18:A:PHE:H	11	0.18
(1,401)	1:17:A:TYR:HB3	1:18:A:PHE:H	11	0.18
(1,1182)	1:68:A:LEU:H	1:68:A:LEU:HG	14	0.17
(1,1182)	1:68:A:LEU:H	1:68:A:LEU:HG	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:18:A:PHE:H	1:18:A:PHE:HD1	10	0.17
(1,737)	1:18:A:PHE:H	1:18:A:PHE:HD2	10	0.17
(1,155)	1:109:A:LYS:HA	1:109:A:LYS:HG2	5	0.17
(1,801)	1:57:A:LYS:HB3	1:58:A:GLU:H	15	0.16
(1,698)	1:22:A:GLY:H	1:122:A:ASN:HB2	6	0.16
(1,1515)	1:81:A:LEU:HD11	1:82:A:SER:H	4	0.15
(1,1515)	1:81:A:LEU:HD12	1:82:A:SER:H	4	0.15
(1,1515)	1:81:A:LEU:HD13	1:82:A:SER:H	4	0.15
(1,1515)	1:81:A:LEU:HD21	1:82:A:SER:H	4	0.15
(1,1515)	1:81:A:LEU:HD22	1:82:A:SER:H	4	0.15
(1,1515)	1:81:A:LEU:HD23	1:82:A:SER:H	4	0.15
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	3	0.15
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	3	0.15
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	14	0.15
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	14	0.15
(1,1024)	1:40:A:LEU:HB2	1:41:A:SER:H	6	0.15
(1,1024)	1:40:A:LEU:HB2	1:41:A:SER:H	11	0.15
(1,802)	1:116:A:LEU:HA	1:119:A:HIS:H	6	0.15
(1,802)	1:116:A:LEU:HA	1:119:A:HIS:H	18	0.15
(1,134)	1:6:A:LYS:HA	1:6:A:LYS:HD3	10	0.15
(1,134)	1:6:A:LYS:HA	1:6:A:LYS:HD3	19	0.15
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD2	4	0.14
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD3	4	0.14
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	10	0.14
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	10	0.14
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	20	0.14
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	20	0.14
(1,1319)	1:19:A:GLU:HG2	1:20:A:PRO:HD2	10	0.14
(1,1319)	1:19:A:GLU:HG2	1:20:A:PRO:HD3	10	0.14
(1,1319)	1:19:A:GLU:HG3	1:20:A:PRO:HD2	10	0.14
(1,1319)	1:19:A:GLU:HG3	1:20:A:PRO:HD3	10	0.14
(1,1319)	1:19:A:GLU:HG2	1:20:A:PRO:HD2	13	0.14
(1,1319)	1:19:A:GLU:HG2	1:20:A:PRO:HD3	13	0.14
(1,1319)	1:19:A:GLU:HG3	1:20:A:PRO:HD2	13	0.14
(1,1319)	1:19:A:GLU:HG3	1:20:A:PRO:HD3	13	0.14
(1,1319)	1:19:A:GLU:HG2	1:20:A:PRO:HD2	17	0.14
(1,1319)	1:19:A:GLU:HG2	1:20:A:PRO:HD3	17	0.14
(1,1319)	1:19:A:GLU:HG3	1:20:A:PRO:HD2	17	0.14
(1,1319)	1:19:A:GLU:HG3	1:20:A:PRO:HD3	17	0.14
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	2	0.14
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	3	0.14
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	10	0.14
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	12	0.14
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	18	0.14
(1,1126)	1:9:A:TYR:HD1	1:10:A:LYS:H	19	0.14
(1,802)	1:116:A:LEU:HA	1:119:A:HIS:H	1	0.14
(1,802)	1:116:A:LEU:HA	1:119:A:HIS:H	16	0.14
(1,660)	1:79:A:VAL:HB	1:80:A:SER:H	20	0.14
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	16	0.13
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	16	0.13
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD2	6	0.13
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD3	6	0.13
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD2	9	0.13
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD3	9	0.13
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	2	0.13
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	2	0.13
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	3	0.13
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	3	0.13
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	12	0.13
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	12	0.13
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	16	0.13
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	16	0.13
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	3	0.13
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	10	0.13
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	14	0.13
(1,927)	1:23:A:PRO:HB2	1:24:A:TYR:H	8	0.13
(1,927)	1:23:A:PRO:HB3	1:24:A:TYR:H	8	0.13
(1,927)	1:23:A:PRO:HB2	1:24:A:TYR:H	9	0.13
(1,927)	1:23:A:PRO:HB3	1:24:A:TYR:H	9	0.13
(1,802)	1:116:A:LEU:HA	1:119:A:HIS:H	8	0.13
(1,802)	1:116:A:LEU:HA	1:119:A:HIS:H	13	0.13
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	19	0.13
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	4	0.12
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	4	0.12
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD2	9	0.12
(1,1452)	1:59:A:LYS:H	1:59:A:LYS:HD3	9	0.12
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	4	0.12
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	4	0.12
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	5	0.12
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	5	0.12
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	18	0.12
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	18	0.12
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	19	0.12
(1,1313)	1:18:A:PHE:HB2	1:19:A:GLU:H	10	0.12
(1,1313)	1:18:A:PHE:HB3	1:19:A:GLU:H	10	0.12
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	4	0.12
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	5	0.12
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	8	0.12
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	12	0.12
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	16	0.12
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	17	0.12
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	18	0.12
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	19	0.12
(1,1108)	1:21:A:THR:HG21	1:122:A:ASN:H	6	0.12
(1,1108)	1:21:A:THR:HG22	1:122:A:ASN:H	6	0.12
(1,1108)	1:21:A:THR:HG23	1:122:A:ASN:H	6	0.12
(1,1094)	1:126:A:ASN:HB2	1:128:A:ILE:H	10	0.12
(1,802)	1:116:A:LEU:HA	1:119:A:HIS:H	9	0.12
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	2	0.12
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	3	0.12
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	6	0.12
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	7	0.12
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	10	0.12
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	12	0.12
(1,772)	1:9:A:TYR:H	1:9:A:TYR:HD2	18	0.12
(1,746)	1:94:A:LYS:HA	1:97:A:LYS:H	12	0.12
(1,287)	1:79:A:VAL:HB	1:132:A:VAL:HB	10	0.12
(1,1466)	1:64:A:VAL:HG11	1:65:A:ASP:H	3	0.11
(1,1466)	1:64:A:VAL:HG12	1:65:A:ASP:H	3	0.11
(1,1466)	1:64:A:VAL:HG13	1:65:A:ASP:H	3	0.11
(1,1466)	1:64:A:VAL:HG21	1:65:A:ASP:H	3	0.11
(1,1466)	1:64:A:VAL:HG22	1:65:A:ASP:H	3	0.11
(1,1466)	1:64:A:VAL:HG23	1:65:A:ASP:H	3	0.11
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD2	17	0.11
(1,1323)	1:21:A:THR:H	1:23:A:PRO:HD3	17	0.11
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	9	0.11
(1,660)	1:79:A:VAL:HB	1:80:A:SER:H	10	0.11
(1,287)	1:79:A:VAL:HB	1:132:A:VAL:HB	20	0.11
(1,59)	1:79:A:VAL:HA	1:133:A:ILE:HA	10	0.11
(1,59)	1:79:A:VAL:HA	1:133:A:ILE:HA	20	0.11
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD2	11	0.1
(1,1450)	1:58:A:GLU:HB2	1:59:A:LYS:HD3	11	0.1
(1,1288)	1:6:A:LYS:HA	1:6:A:LYS:HG2	6	0.1
(1,1288)	1:6:A:LYS:HA	1:6:A:LYS:HG3	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:129:A:THR:H	1:131:A:VAL:H	15	0.1
(1,1224)	1:129:A:THR:H	1:131:A:VAL:H	16	0.1
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	2	0.1
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	13	0.1
(1,1135)	1:35:A:LYS:H	1:37:A:ASN:HD22	15	0.1
(1,802)	1:116:A:LEU:HA	1:119:A:HIS:H	15	0.1

## 10 Dihedral-angle violation analysis

No dihedral-angle restraints found