Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 02:37 pm BST

PDB ID	:	5M8I
BMRB ID	:	34057
Title	:	Solution structure of CUG-BP2 RRM3 in complex with 5'-UUUAA-3' RNA
Authors	:	Diarra dit Konte, N.; Damberger, F.F.; Allain, F.H.T.
Deposited on	:	2016-10-28

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 (i) 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 (1)) were used in the production of this report:

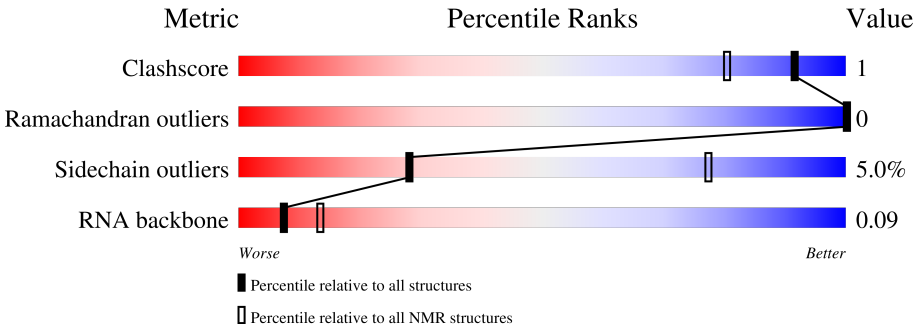
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428
RNA backbone	4643	676

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	114	68% · 28%
2	B	5	20% 40% 40%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:24-A:105 (82)	0.35	1

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1935 atoms, of which 933 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CUGBP Elav-like family member 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	114	1782	571	881	164	159	7	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O95319
A	2	GLY	-	expression tag	UNP O95319
A	3	SER	-	expression tag	UNP O95319
A	4	SER	-	expression tag	UNP O95319
A	5	HIS	-	expression tag	UNP O95319
A	6	HIS	-	expression tag	UNP O95319
A	7	HIS	-	expression tag	UNP O95319
A	8	HIS	-	expression tag	UNP O95319
A	9	HIS	-	expression tag	UNP O95319
A	10	HIS	-	expression tag	UNP O95319
A	11	SER	-	expression tag	UNP O95319
A	12	SER	-	expression tag	UNP O95319
A	13	GLY	-	expression tag	UNP O95319
A	14	LEU	-	expression tag	UNP O95319
A	15	VAL	-	expression tag	UNP O95319
A	16	PRO	-	expression tag	UNP O95319
A	17	ARG	-	expression tag	UNP O95319
A	18	GLY	-	expression tag	UNP O95319
A	19	SER	-	expression tag	UNP O95319
A	20	HIS	-	expression tag	UNP O95319
A	21	MET	-	expression tag	UNP O95319
A	114	TRP	TYR	engineered mutation	UNP O95319

- Molecule 2 is a RNA chain called RNA (5'-R(*UP*UP*UP*AP*A)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	5	153	47	52	16	34	4	0

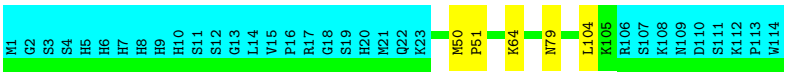
4 Residue-property plots (i)

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.

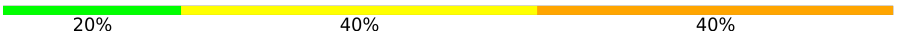
• Molecule 1: CUGBP Elav-like family member 2

Chain A:



• Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B:



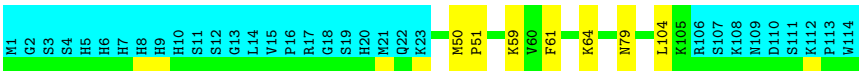
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

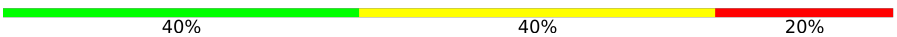
• Molecule 1: CUGBP Elav-like family member 2

Chain A:



• Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

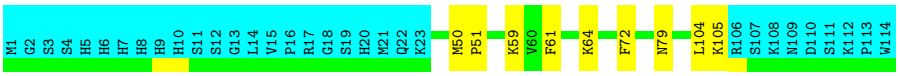
Chain B:



4.2.2 Score per residue for model 2

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 64% 8% 28%



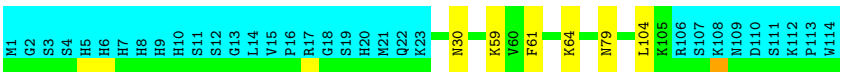
- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 80% 20%

4.2.3 Score per residue for model 3

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 67% 5% 28%



- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 40% 40% 20%

4.2.4 Score per residue for model 4

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 68% 28%

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 40% 40% 20%

4.2.5 Score per residue for model 5

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 68% • 28%

M1 G2 S3 S4 H5 H6 H7 H8 H9 H10 S11 S12 G13 L14 V15 P16 R17 G18 S19 H20 M21 Q22 K23 M50 P51 K64 N79 L104 K105 R106 S107 K108 N109 D110 S111 K112 P113 W114

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 40% 40% 20%

U115 U116 U117 A118 A119

4.2.6 Score per residue for model 6

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 67% 5% 28%

M1 G2 S3 S4 H5 H6 H7 H8 H9 H10 S11 S12 G13 L14 V15 P16 R17 G18 S19 H20 M21 Q22 K23 N30 M50 P51 F74 N79 L104 K105 R106 S107 K108 N109 D110 S111 K112 P113 W114

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 20% 40% 20% 20%

U115 U116 U117 A118 A119

4.2.7 Score per residue for model 7

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 66% 6% 28%

M1 G2 S3 S4 H5 H6 H7 H8 H9 H10 S11 S12 G13 L14 V15 P16 R17 G18 S19 H20 M21 Q22 K23 N30 M50 P51 K64 Q65 T66 N79 L104 K105 R106 S107 K108 N109 D110 S111 K112 P113 W114

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 20% 80%

U115 U116 U117 A118 A119

4.2.8 Score per residue for model 8

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 67% 5% 28%

M1 G2 S3 S4 H5 H6 H7 H8 H9 H10 S11 S12 G13 L14 V15 P16 R17 G18 S19 H20 M21 Q22 K23 M50 P51 K59 K64 N79 L104 K105 R106 S107 K108 N109 D110 S111 K112 P113 W114

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 40% 20% 20% 20%

U115 U116 U117 A118 A119

4.2.9 Score per residue for model 9

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 65% 7% 28%

M1 G2 S3 S4 H5 H6 H7 H8 H9 H10 S11 S12 G13 L14 V15 P16 R17 G18 S19 H20 M21 Q22 K23 N30 H35 M50 P51 K64 N79 K98 L104 K105 R106 S107 K108 N109 D110 S111 K112 P113 W114

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 60% 20% 20%

U115 A118 A119

4.2.10 Score per residue for model 10

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 66% 6% 28%

M1 G2 S3 S4 H5 H6 H7 H8 H9 H10 S11 S12 G13 L14 V15 P16 R17 G18 S19 H20 M21 Q22 K23 M50 P51 K59 V60 F61 K64 F72 N79 R106 S107 K108 N109 D110 S111 K112 P113 W114

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 60% 20% 20%

U115 A118 A119

4.2.11 Score per residue for model 11

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 64% 7% • 28%

M1 G2 S3 S4 H5 H6 H7 H8 H9 H10 S11 S12 G13 L14 V15 P16 R17 G18 S19 H20 M21 Q22 K23 N30 M50 P51 K59 V60 F61 F72 G73 F74 N79 L104 K105 R106 S107 K108 N109 D110 S111 K112 P113 W114

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 20% 20% 40% 20%

U115 U116 U117 A118 A119

4.2.12 Score per residue for model 12

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 65% 7% 28%

M1 G2 S3 S4 H5 H6 H7 H8 H9 H10 S11 S12 G13 L14 V15 P16 R17 G18 S19 H20 M21 Q22 K23 N30 M50 P51 V55 F61 F72 N79 L104 K105 R106 S107 K108 N109 D110 S111 K112 P113 W114

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 20% 40% 40%

U115 U116 U117 A118 A119

4.2.13 Score per residue for model 13

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 64% 8% 28%

M1 G2 S3 S4 H5 H6 H7 H8 H9 H10 S11 S12 G13 L14 V15 P16 R17 G18 S19 H20 M21 Q22 K23 N30 M50 P51 K59 V60 F61 K64 N79 M97 L104 K105 R106 S107 K108 N109 D110 S111 K112 P113 W114

- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

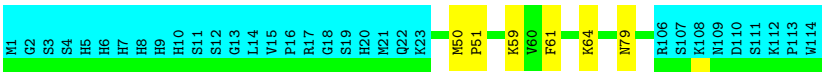
Chain B: 20% 40% 40%

U115 U116 U117 A118 A119

4.2.14 Score per residue for model 14

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 67% 5% 28%



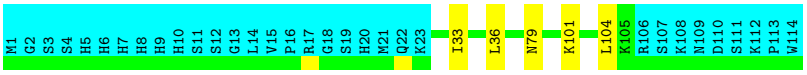
- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 40% 40% 20%

4.2.15 Score per residue for model 15

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 68% • 28%



- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 20% 40% 40%

4.2.16 Score per residue for model 16

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 67% 5% 28%

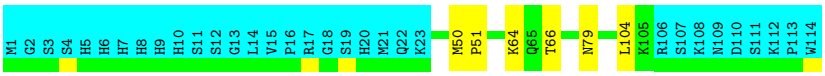
- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 60% 40%

4.2.17 Score per residue for model 17

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 67% 5% 28%



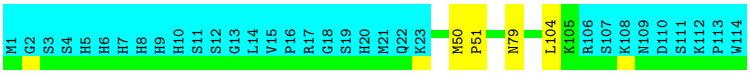
- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 20% 60% 20%

4.2.18 Score per residue for model 18

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 68% • 28%



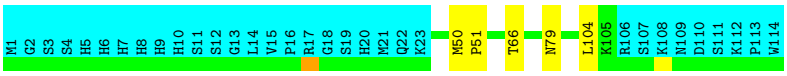
- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 40% 40% 20%

4.2.19 Score per residue for model 19

- Molecule 1: CUGBP Elav-like family member 2

Chain A: 68% • 28%



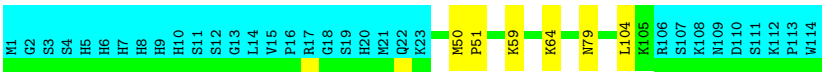
- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B: 20% 60% 20%

4.2.20 Score per residue for model 20

- Molecule 1: CUGBP Elav-like family member 2

Chain A:



- Molecule 2: RNA (5'-R(*UP*UP*UP*AP*A)-3')

Chain B:

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy and least restraints violation*.

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

Software name	**Classification**	**Version**
CYANA	structure calculation	
Amber	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	1222
Number of shifts mapped to atoms	1222
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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	0.53±0.00	0±0/659 (0.0± 0.0%)	0.70±0.01	0±0/887 (0.0± 0.0%)
2	B	1.07±0.02	0±0/112 (0.0± 0.0%)	1.67±0.07	2±1/172 (1.2± 0.6%)
All	All	0.64	0/15420 (0.0%)	0.93	43/21180 (0.2%)

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
2	B	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. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	119	A	O4'-C1'-N9	7.27	114.02	108.20	2	13
2	B	118	A	O4'-C1'-N9	6.47	113.38	108.20	20	16
2	B	118	A	C5'-C4'-C3'	-5.69	106.89	116.00	13	1
2	B	117	U	O4'-C1'-N1	5.57	112.65	108.20	12	2
2	B	118	A	C3'-C2'-C1'	5.40	105.82	101.50	18	10
2	B	115	U	O4'-C1'-N1	5.03	112.22	108.20	2	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	118	A	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
1	A	644	641	640	2±1
2	B	101	52	54	0±1
All	All	14900	13860	13880	42

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:HE3	1:A:61:PHE:CE1	0.50	2.41	3	1
1:A:59:LYS:HE3	1:A:61:PHE:CZ	0.46	2.45	1	1
1:A:61:PHE:CE1	1:A:72:PHE:CE1	0.45	3.05	11	1
1:A:50:MET:N	1:A:51:PRO:HD2	0.45	2.27	11	17
1:A:59:LYS:HE3	1:A:61:PHE:CD2	0.44	2.47	11	1
1:A:61:PHE:CD2	1:A:72:PHE:CZ	0.44	3.05	2	3
2:B:115:U:C6	2:B:115:U:H5"	0.44	2.47	13	1
1:A:33:ILE:HG22	1:A:36:LEU:HD21	0.44	1.88	15	1
1:A:101:LYS:HE3	2:B:116:U:C4	0.43	2.49	15	1
2:B:118:A:C8	2:B:118:A:H5"	0.43	2.49	10	3
1:A:74:PHE:CE1	2:B:118:A:N1	0.42	2.87	11	2
1:A:59:LYS:HE3	1:A:61:PHE:CE2	0.42	2.49	14	3
1:A:35:HIS:CE1	1:A:98:LYS:HE3	0.41	2.50	9	1
2:B:118:A:H5"	2:B:118:A:C8	0.41	2.51	8	1
1:A:50:MET:N	1:A:51:PRO:CD	0.40	2.84	6	4
1:A:59:LYS:CE	1:A:61:PHE:CZ	0.40	3.05	11	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	82/114 (72%)	81±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	100	100
All	All	1640/2280 (72%)	1611 (98%)	29 (2%)	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	A	69/98 (70%)	66±1 (95±1%)	3±1 (5±1%)	28	77
All	All	1380/1960 (70%)	1311 (95%)	69 (5%)	28	77

All 8 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	79	ASN	20
1	A	104	LEU	18
1	A	64	LYS	13
1	A	30	ASN	8
1	A	59	LYS	5
1	A	66	THR	3
1	A	55	VAL	1
1	A	97	MET	1

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	4/5 (80%)	2±1 (59±18%)	0±0 (8±11%)	0.09±0.05
All	All	86/100 (86%)	47 (55%)	6 (7%)	0.09

The overall RNA backbone suiteness is 0.09.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	119	A	20
2	B	116	U	10
2	B	117	U	10
2	B	118	A	7

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	115	U	6

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 monosaccharides 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 83% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starCH_chemical_shift_NMR_star_281016.txt*

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	1222
Number of shifts mapped to atoms	1222
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	100	-0.20 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	92	-0.07 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	96	0.25 ± 0.27	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 83%, i.e. 1005 atoms were assigned a chemical shift out of a possible 1212. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	324/409 (79%)	166/167 (99%)	80/164 (49%)	78/78 (100%)
Sidechain	569/608 (94%)	390/396 (98%)	165/190 (87%)	14/22 (64%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	76/106 (72%)	48/52 (92%)	28/52 (54%)	0/2 (0%)
Sugar	29/55 (53%)	29/30 (97%)	0/25 (0%)	0/0 (—%)
Base	7/34 (21%)	7/19 (37%)	0/10 (0%)	0/5 (0%)
Overall	1005/1212 (83%)	640/664 (96%)	273/441 (62%)	92/107 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 1219 atoms were assigned a chemical shift out of a possible 1634. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	402/568 (71%)	206/232 (89%)	100/228 (44%)	96/108 (89%)
Sidechain	693/810 (86%)	474/526 (90%)	202/251 (80%)	17/33 (52%)
Aromatic	88/167 (53%)	54/86 (63%)	33/71 (46%)	1/10 (10%)
Sugar	29/55 (53%)	29/30 (97%)	0/25 (0%)	0/0 (—%)
Base	7/34 (21%)	7/19 (37%)	0/10 (0%)	0/5 (0%)
Overall	1219/1634 (75%)	770/893 (86%)	335/585 (57%)	114/156 (73%)

7.1.4 Statistically unusual chemical shifts (i)

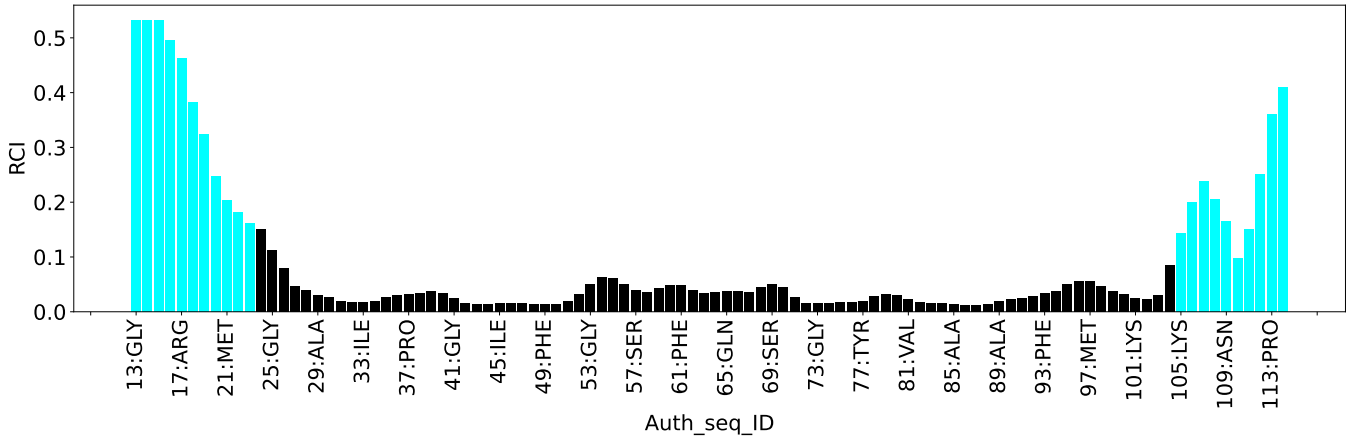
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	44	ASP	HB2	1.12	1.41 – 4.01	-6.1
1	A	51	PRO	HB2	0.12	0.37 – 3.78	-5.7

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:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
13:GLY
17:ARG
21:MET
25:GLY
29:ALA
33:ILE
37:PRO
41:GLY
45:ILE
49:PHE
53:GLY
57:SER
61:PHE
65:GLN
69:SER
73:GLY
77:TYR
81:VAL
85:ALA
89:ALA
93:PHE
97:MET
101:LYS
105:LYS
109:ASN
113:PRO
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	2373
Intra-residue (|i-j|=0)	481
Sequential (|i-j|=1)	655
Medium range (|i-j|>1 and |i-j|<5)	393
Long range (|i-j|≥5)	751
Inter-chain	49
Hydrogen bond restraints	44
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	19.9
Number of long range restraints per residue[1]	6.5

[1]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 (i)

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 (i)

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)	18.9	0.2
0.2-0.5 (Medium)	4.5	0.46
>0.5 (Large)	None	None

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 (i)

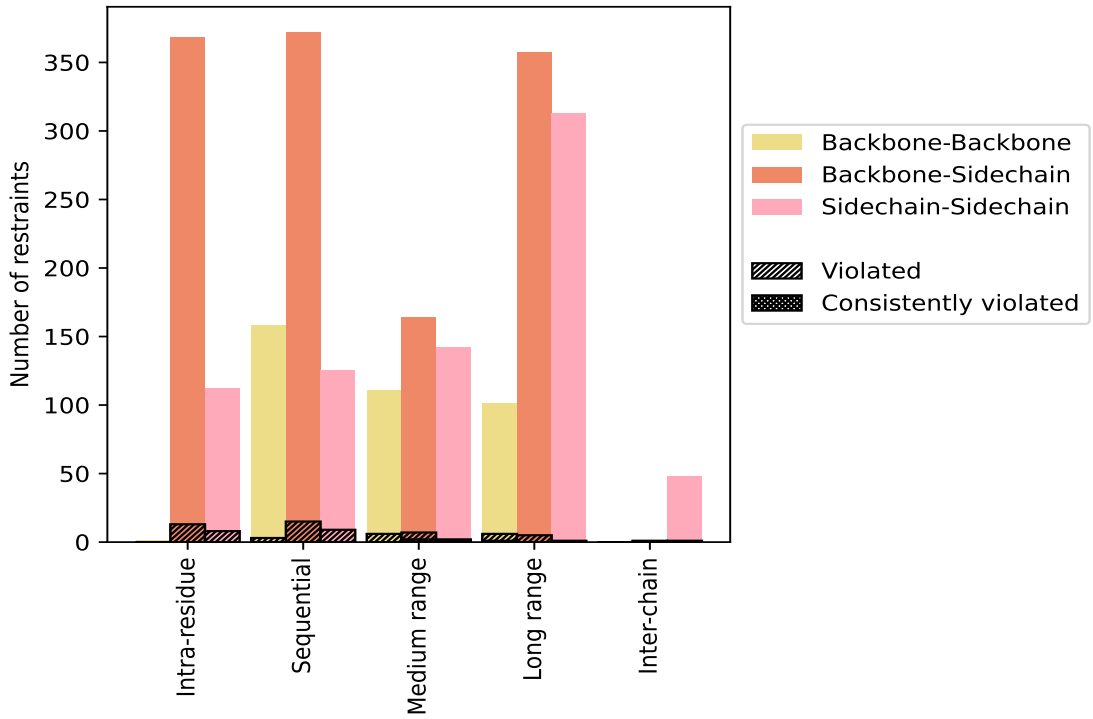
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	481	20.3	21	4.4	0.9	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	368	15.5	13	3.5	0.5	0	0.0	0.0
Sidechain-Sidechain	112	4.7	8	7.1	0.3	0	0.0	0.0
Sequential (|i-j|=1)	655	27.6	27	4.1	1.1	0	0.0	0.0
Backbone-Backbone	158	6.7	3	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	372	15.7	15	4.0	0.6	0	0.0	0.0
Sidechain-Sidechain	125	5.3	9	7.2	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	393	16.6	12	3.1	0.5	3	0.8	0.1
Backbone-Backbone	87	3.7	3	3.4	0.1	0	0.0	0.0
Backbone-Sidechain	164	6.9	7	4.3	0.3	2	1.2	0.1
Sidechain-Sidechain	142	6.0	2	1.4	0.1	1	0.7	0.0
Long range (|i-j|≥5)	751	31.6	12	1.6	0.5	1	0.1	0.0
Backbone-Backbone	81	3.4	6	7.4	0.3	1	1.2	0.0
Backbone-Sidechain	357	15.0	5	1.4	0.2	0	0.0	0.0
Sidechain-Sidechain	313	13.2	1	0.3	0.0	0	0.0	0.0
Inter-chain	49	2.1	2	4.1	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.0	1	100.0	0.0	0	0.0	0.0
Sidechain-Sidechain	48	2.0	1	2.1	0.0	0	0.0	0.0
Hydrogen bond	44	1.9	3	6.8	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2373	100.0	77	3.2	3.2	4	0.2	0.2
Backbone-Backbone	371	15.6	15	4.0	0.6	1	0.3	0.0
Backbone-Sidechain	1262	53.2	41	3.2	1.7	2	0.2	0.1
Sidechain-Sidechain	740	31.2	21	2.8	0.9	1	0.1	0.0

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and 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	5	7	5	5	1	23	0.16	0.35	0.06	0.15
2	6	5	7	4	0	22	0.15	0.26	0.04	0.14
3	4	10	5	4	1	24	0.17	0.34	0.06	0.15
4	7	10	6	5	1	29	0.15	0.33	0.05	0.14
5	3	7	6	4	1	21	0.17	0.34	0.06	0.15
6	3	8	5	3	0	19	0.16	0.29	0.05	0.14
7	5	8	5	6	1	25	0.16	0.4	0.06	0.13
8	5	3	8	3	1	20	0.15	0.22	0.03	0.14
9	3	9	8	4	1	25	0.18	0.36	0.07	0.14
10	2	8	4	6	0	20	0.19	0.46	0.09	0.16
11	6	7	6	6	0	25	0.16	0.27	0.05	0.15

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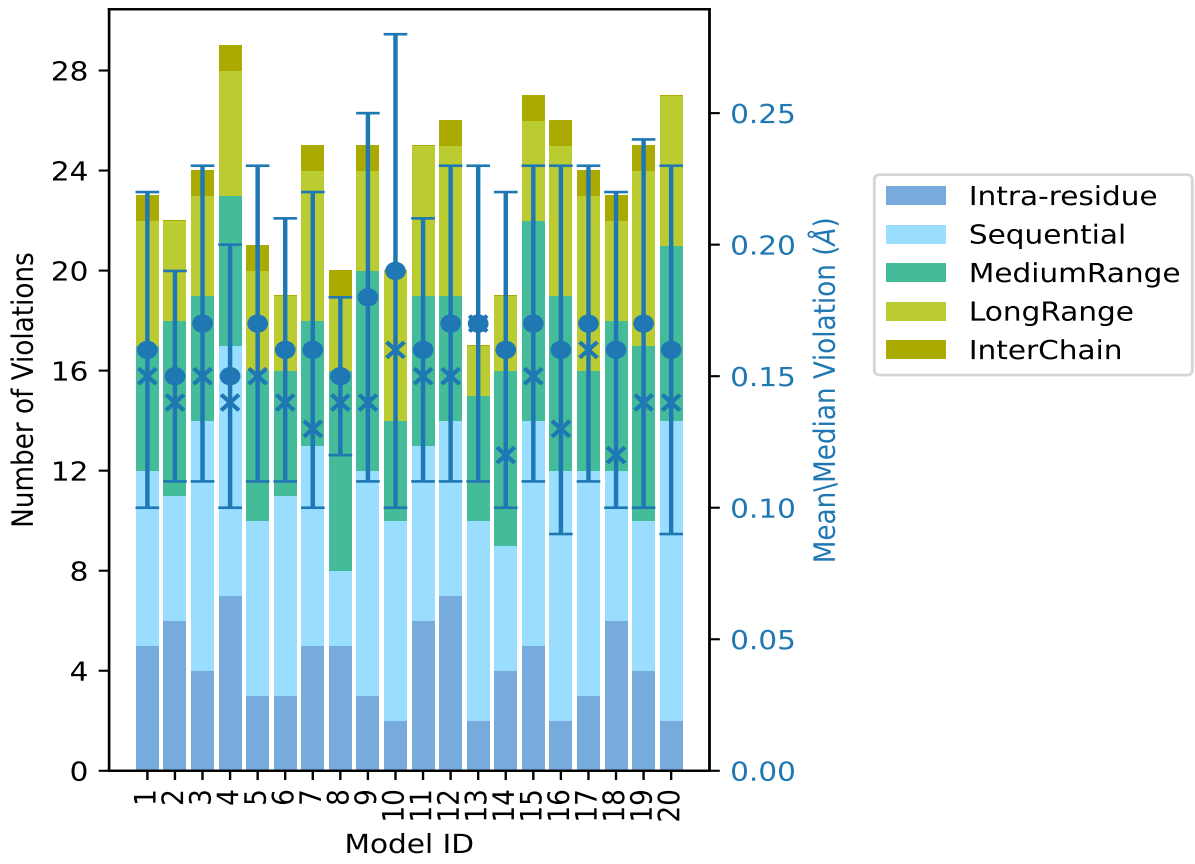
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	7	7	5	6	1	26	0.17	0.38	0.06	0.15
13	2	8	5	2	0	17	0.17	0.3	0.06	0.17
14	4	5	7	3	0	19	0.16	0.34	0.06	0.12
15	5	9	8	4	1	27	0.17	0.3	0.06	0.15
16	2	10	7	6	1	26	0.16	0.34	0.07	0.13
17	3	9	4	7	1	24	0.17	0.33	0.06	0.16
18	6	6	6	4	1	23	0.16	0.31	0.06	0.12
19	4	6	7	7	1	25	0.17	0.36	0.07	0.14
20	2	12	7	6	0	27	0.16	0.44	0.07	0.14

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard 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

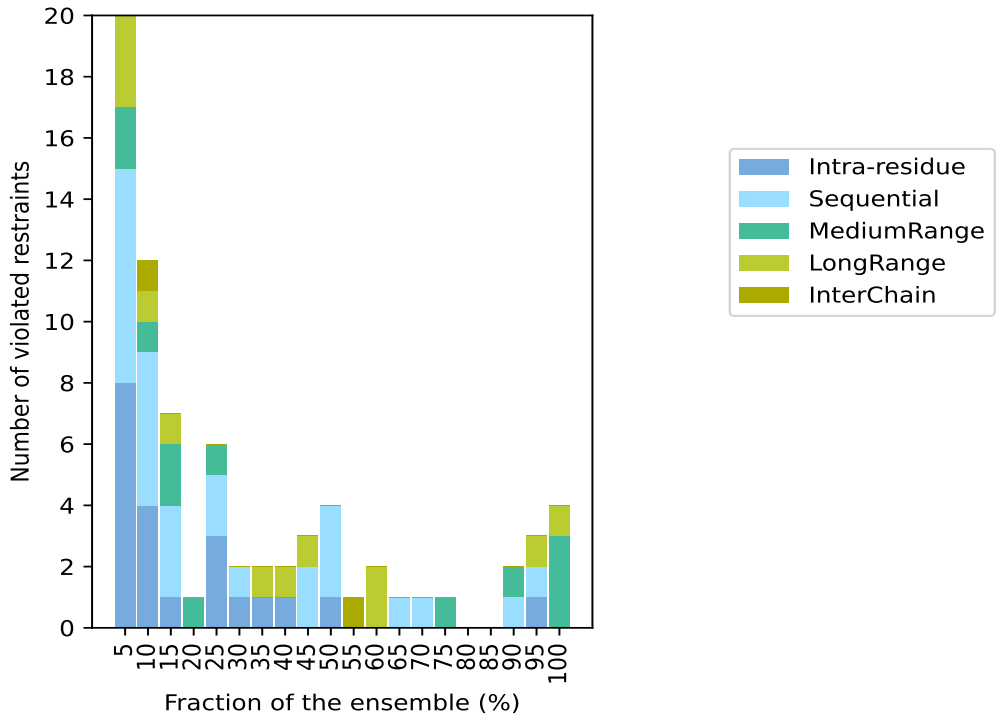
9.3 Distance violation statistics for the ensemble (i)

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, 2255(IR:460, SQ:628, MR:381, LR:739, IC:47) 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]	%
8	7	2	3	0	20	1	5.0
4	5	1	1	1	12	2	10.0
1	3	2	1	0	7	3	15.0
0	0	1	0	0	1	4	20.0
3	2	1	0	0	6	5	25.0
1	1	0	0	0	2	6	30.0
1	0	0	1	0	2	7	35.0
1	0	0	1	0	2	8	40.0
0	2	0	1	0	3	9	45.0
1	3	0	0	0	4	10	50.0
0	0	0	0	1	1	11	55.0
0	0	0	2	0	2	12	60.0
0	1	0	0	0	1	13	65.0
0	1	0	0	0	1	14	70.0
0	0	1	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	1	1	0	0	2	18	90.0
1	1	0	1	0	3	19	95.0
0	0	3	1	0	4	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

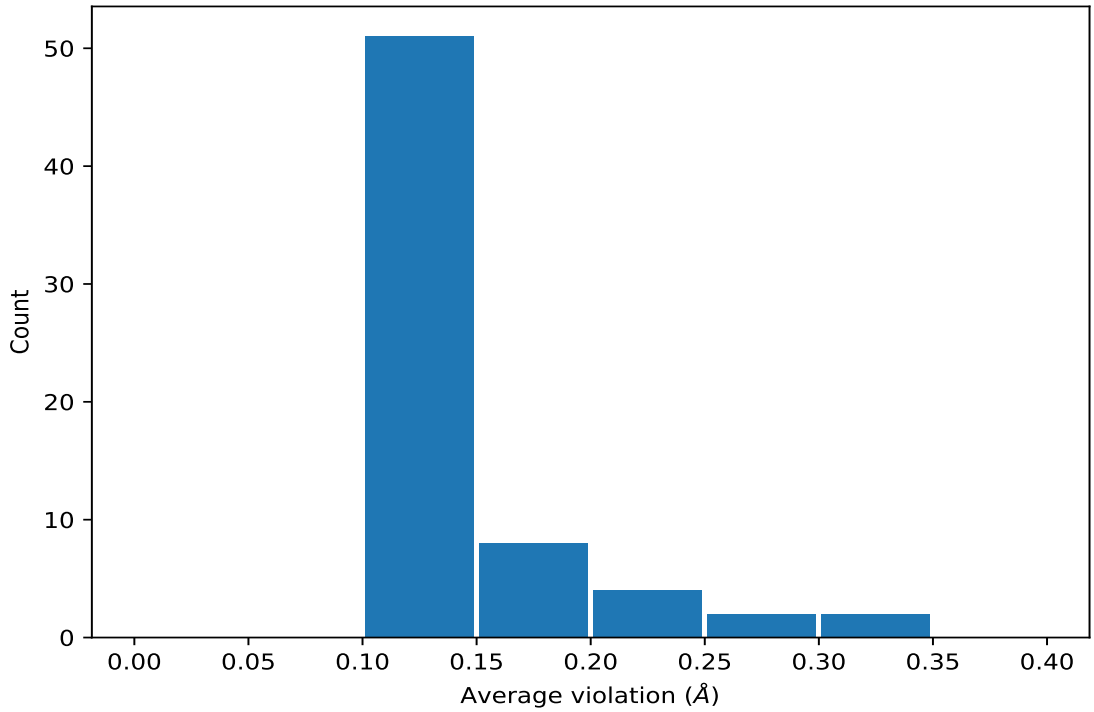
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	20	0.21	0.02	0.2
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	20	0.17	0.03	0.16
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	20	0.15	0.03	0.15
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	20	0.13	0.01	0.12
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	19	0.31	0.07	0.33
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	19	0.18	0.05	0.17
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	19	0.13	0.01	0.13
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	18	0.23	0.06	0.24
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	18	0.13	0.01	0.13
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	15	0.14	0.02	0.14
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	14	0.19	0.04	0.18
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	13	0.12	0.01	0.12
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	12	0.18	0.04	0.19
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	12	0.12	0.01	0.12
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	11	0.18	0.05	0.17
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	10	0.27	0.0	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	10	0.14	0.02	0.15
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	10	0.14	0.02	0.15
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	10	0.14	0.02	0.15
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	10	0.14	0.02	0.15
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	10	0.14	0.02	0.15
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	10	0.14	0.02	0.15
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	10	0.12	0.01	0.12
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	10	0.11	0.0	0.11
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	9	0.27	0.1	0.24
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	9	0.17	0.05	0.16
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	9	0.15	0.03	0.15
(1,2237)	2:B:116:U:H3'	2:B:116:U:H6	8	0.15	0.04	0.14
(1,1601)	1:A:54:ASN:H	1:A:79:ASN:HD22	8	0.13	0.02	0.12
(1,2235)	2:B:116:U:H2'	2:B:116:U:H5	7	0.14	0.03	0.15
(1,1317)	1:A:34:TYR:H	1:A:103:GLN:H	7	0.12	0.02	0.11
(1,2272)	2:B:118:A:H2'	2:B:119:A:H1'	6	0.2	0.05	0.19
(1,2244)	2:B:117:U:H3'	2:B:117:U:H6	6	0.13	0.02	0.12
(1,1399)	1:A:24:GLU:H	1:A:24:GLU:HG2	5	0.13	0.02	0.13
(1,501)	1:A:46:LEU:HG	1:A:47:GLN:HA	5	0.13	0.01	0.12
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD2	5	0.13	0.02	0.11
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD3	5	0.13	0.02	0.11
(1,481)	1:A:23:LYS:HA	1:A:24:GLU:HB3	5	0.12	0.01	0.12
(2,12)	1:A:46:LEU:H	1:A:42:ASP:O	5	0.12	0.01	0.12
(1,1606)	1:A:79:ASN:HD22	1:A:81:VAL:HB	5	0.12	0.01	0.12
(1,1637)	1:A:54:ASN:H	1:A:54:ASN:HD22	5	0.12	0.01	0.12
(1,335)	1:A:45:ILE:HA	1:A:48:MET:HB3	4	0.14	0.01	0.14
(1,338)	1:A:23:LYS:HA	1:A:24:GLU:HG2	3	0.23	0.03	0.24
(1,1289)	1:A:103:GLN:H	1:A:103:GLN:HG2	3	0.16	0.0	0.16
(1,1674)	1:A:28:GLY:H	1:A:30:ASN:HD22	3	0.14	0.02	0.15
(1,2230)	2:B:115:U:H3'	2:B:116:U:H5	3	0.14	0.01	0.13
(2,17)	1:A:85:ALA:H	1:A:81:VAL:O	3	0.13	0.01	0.13
(1,666)	1:A:22:GLN:HA	1:A:57:SER:HA	3	0.12	0.02	0.11
(1,406)	1:A:65:GLN:HB2	1:A:66:THR:HA	3	0.12	0.0	0.12
(1,1264)	1:A:108:LYS:HA	1:A:112:LYS:H	3	0.11	0.0	0.11
(1,480)	1:A:24:GLU:HB3	1:A:25:GLY:HA3	2	0.32	0.03	0.32
(1,1235)	1:A:114:TRP:H	1:A:114:TRP:HD1	2	0.16	0.0	0.16
(1,1308)	1:A:15:VAL:H	1:A:16:PRO:HD2	2	0.14	0.03	0.14
(1,1711)	1:A:13:GLY:H	1:A:14:LEU:HA	2	0.14	0.01	0.14
(1,1164)	1:A:93:PHE:H	1:A:94:GLN:H	2	0.13	0.0	0.13
(1,2268)	2:B:115:U:H4'	2:B:116:U:H5	2	0.13	0.02	0.13
(1,878)	1:A:29:ALA:HA	1:A:80:PRO:HD2	2	0.12	0.02	0.12
(1,2243)	2:B:117:U:H4'	2:B:117:U:H6	2	0.12	0.02	0.12

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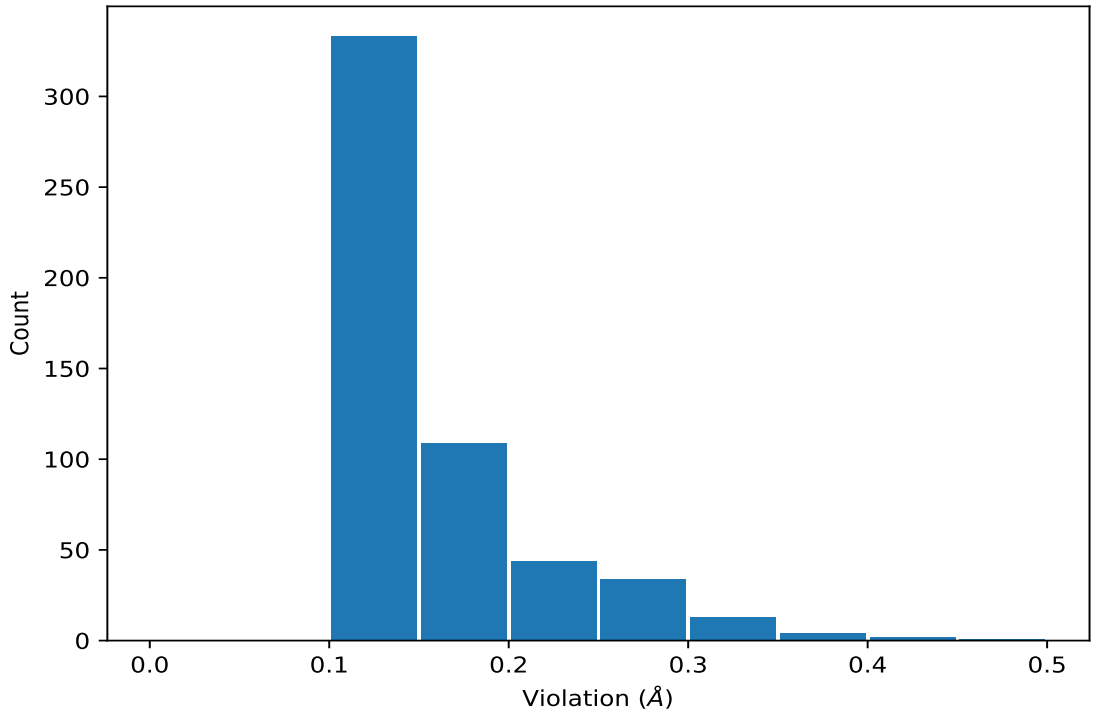
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2283)	1:A:35:HIS:HD2	2:B:116:U:H5	2	0.12	0.01	0.12
(1,1344)	1:A:15:VAL:HG11	1:A:17:ARG:H	2	0.12	0.01	0.12
(1,1344)	1:A:15:VAL:HG12	1:A:17:ARG:H	2	0.12	0.01	0.12
(1,1344)	1:A:15:VAL:HG13	1:A:17:ARG:H	2	0.12	0.01	0.12
(1,1344)	1:A:15:VAL:HG21	1:A:17:ARG:H	2	0.12	0.01	0.12
(1,1344)	1:A:15:VAL:HG22	1:A:17:ARG:H	2	0.12	0.01	0.12
(1,1344)	1:A:15:VAL:HG23	1:A:17:ARG:H	2	0.12	0.01	0.12
(1,599)	1:A:33:ILE:H	1:A:33:ILE:HG12	2	0.12	0.0	0.12
(1,513)	1:A:114:TRP:HA	1:A:114:TRP:HD1	2	0.11	0.0	0.11

[1]Number of violated models, [2]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)
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	10	0.46
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	20	0.44
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	7	0.4
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	10	0.38
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	12	0.38
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	9	0.36
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	19	0.36
(1,2227)	2:B:115:U:H4'	2:B:115:U:H6	1	0.35
(1,480)	1:A:24:GLU:HB3	1:A:25:GLY:HA3	9	0.34
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	3	0.34
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	5	0.34
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	14	0.34
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	16	0.34
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	16	0.34
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	19	0.34
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	4	0.33
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	17	0.33
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	19	0.32
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	18	0.31
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	16	0.31
(1,699)	1:A:35:HIS:H	1:A:36:LEU:HG	15	0.3
(1,2272)	2:B:118:A:H2'	2:B:119:A:H1'	9	0.3
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	13	0.3
(1,480)	1:A:24:GLU:HB3	1:A:25:GLY:HA3	3	0.29
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	6	0.29
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	5	0.28
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	11	0.27
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	11	0.27
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	9	0.27
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	17	0.27
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	1	0.27
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	3	0.27
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	4	0.27
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	6	0.27
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	13	0.27
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	15	0.27
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	16	0.27
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	18	0.27
(1,338)	1:A:23:LYS:HA	1:A:24:GLU:HG2	5	0.26
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	12	0.26
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	7	0.26
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	13	0.26
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	4	0.26
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	2	0.26
(1,1694)	1:A:65:GLN:HA	1:A:65:GLN:HE21	14	0.26
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	15	0.26
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	19	0.25
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	12	0.25
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	15	0.25
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	18	0.25
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	1	0.25
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	9	0.25
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	10	0.25
(1,623)	1:A:59:LYS:HD2	1:A:60:VAL:H	10	0.24
(1,338)	1:A:23:LYS:HA	1:A:24:GLU:HG2	15	0.24
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	2	0.24
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	14	0.24
(1,2247)	2:B:117:U:H2'	2:B:118:A:H8	10	0.24
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	9	0.24
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	11	0.24
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	7	0.24
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	19	0.24
(1,1127)	1:A:114:TRP:HA	1:A:114:TRP:HE3	17	0.24
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	3	0.23
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	5	0.23
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	9	0.23
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	15	0.23
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	18	0.23
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	12	0.23
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	9	0.23
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	12	0.23
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	16	0.23
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	18	0.23
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	5	0.22
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	12	0.22
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	19	0.22
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	14	0.22
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	1	0.22
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	6	0.22
(1,2237)	2:B:116:U:H3'	2:B:116:U:H6	2	0.22
(1,2225)	2:B:115:U:H2'	2:B:115:U:H5	8	0.22
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	7	0.21
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	5	0.21
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	20	0.21
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	12	0.21
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	17	0.21
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	20	0.21
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	10	0.2
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	16	0.2
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	17	0.2
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	9	0.2
(1,2272)	2:B:118:A:H2'	2:B:119:A:H1'	10	0.2
(1,2272)	2:B:118:A:H2'	2:B:119:A:H1'	11	0.2
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	11	0.2
(1,2226)	2:B:115:U:H2'	2:B:115:U:H6	8	0.2
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	5	0.2
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	8	0.19
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	11	0.19
(1,338)	1:A:23:LYS:HA	1:A:24:GLU:HG2	17	0.19
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	4	0.19
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	6	0.19
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	8	0.19
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	11	0.19
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	13	0.19
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	20	0.19
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	9	0.19
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	10	0.19
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	17	0.19
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	7	0.19
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	13	0.19
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	4	0.19
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	17	0.19
(1,2237)	2:B:116:U:H3'	2:B:116:U:H6	15	0.19
(1,2235)	2:B:116:U:H2'	2:B:116:U:H5	19	0.19
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	3	0.19
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	10	0.19
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	11	0.19
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	19	0.19
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	4	0.19
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	3	0.19
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	17	0.19
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	17	0.18
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	17	0.18
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	17	0.18
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	17	0.18
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	17	0.18
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	13	0.18
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	15	0.18
(1,296)	1:A:49:PHE:HB3	1:A:52:PHE:HB3	12	0.18
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	3	0.18
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	8	0.18
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	13	0.18
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	3	0.18
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	20	0.18
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	17	0.18
(1,2272)	2:B:118:A:H2'	2:B:119:A:H1'	1	0.18
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	15	0.18
(1,1397)	1:A:24:GLU:H	1:A:24:GLU:HB2	9	0.18
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	5	0.17
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	16	0.17
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	18	0.17
(1,2272)	2:B:118:A:H2'	2:B:119:A:H1'	15	0.17
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	1	0.17
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	3	0.17
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	20	0.17
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	14	0.17
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	15	0.17
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	18	0.17
(1,2244)	2:B:117:U:H3'	2:B:117:U:H6	2	0.17
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	20	0.17
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	4	0.17
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	12	0.17
(1,1399)	1:A:24:GLU:H	1:A:24:GLU:HG2	17	0.17
(1,1308)	1:A:15:VAL:H	1:A:16:PRO:HD2	13	0.17
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	1	0.17
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	11	0.17
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	13	0.17
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	1	0.16
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	1	0.16
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	1	0.16
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	1	0.16
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	1	0.16
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	1	0.16
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	4	0.16
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	4	0.16
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	4	0.16
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	4	0.16
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	4	0.16
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	12	0.16
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	12	0.16
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	12	0.16
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	12	0.16
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	12	0.16
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	12	0.16
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	1	0.16
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	7	0.16
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	9	0.16
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	14	0.16
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	16	0.16
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	6	0.16
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	11	0.16
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	7	0.16
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	15	0.16
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	8	0.16
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	6	0.16
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	7	0.16
(1,2235)	2:B:116:U:H2'	2:B:116:U:H5	2	0.16
(1,1674)	1:A:28:GLY:H	1:A:30:ASN:HD22	5	0.16
(1,1601)	1:A:54:ASN:H	1:A:79:ASN:HD22	19	0.16
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	7	0.16
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	12	0.16
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	17	0.16
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	20	0.16
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	11	0.16
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	17	0.16
(1,1289)	1:A:103:GLN:H	1:A:103:GLN:HG2	3	0.16
(1,1289)	1:A:103:GLN:H	1:A:103:GLN:HG2	15	0.16
(1,1235)	1:A:114:TRP:H	1:A:114:TRP:HD1	14	0.16
(1,1235)	1:A:114:TRP:H	1:A:114:TRP:HD1	18	0.16
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD2	10	0.16
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD3	10	0.16
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	6	0.16
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	8	0.16
(2,12)	1:A:46:LEU:H	1:A:42:ASP:O	16	0.15
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	3	0.15
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	3	0.15
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	3	0.15
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	3	0.15
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	3	0.15
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	6	0.15
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	6	0.15
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	6	0.15
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	6	0.15
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	6	0.15
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	6	0.15
(1,666)	1:A:22:GLN:HA	1:A:57:SER:HA	16	0.15
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	8	0.15
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	11	0.15
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	3	0.15
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	4	0.15
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	17	0.15
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	18	0.15
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	20	0.15
(1,501)	1:A:46:LEU:HG	1:A:47:GLN:HA	2	0.15
(1,335)	1:A:45:ILE:HA	1:A:48:MET:HB3	2	0.15
(1,335)	1:A:45:ILE:HA	1:A:48:MET:HB3	15	0.15
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	2	0.15
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	4	0.15
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	14	0.15
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	3	0.15
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	5	0.15
(1,2268)	2:B:115:U:H4'	2:B:116:U:H5	7	0.15
(1,2258)	2:B:118:A:H2'	2:B:119:A:H8	4	0.15
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	19	0.15
(1,2237)	2:B:116:U:H3'	2:B:116:U:H6	4	0.15
(1,2235)	2:B:116:U:H2'	2:B:116:U:H5	11	0.15
(1,2235)	2:B:116:U:H2'	2:B:116:U:H5	12	0.15
(1,2230)	2:B:115:U:H3'	2:B:116:U:H5	16	0.15
(1,1711)	1:A:13:GLY:H	1:A:14:LEU:HA	15	0.15
(1,1674)	1:A:28:GLY:H	1:A:30:ASN:HD22	16	0.15
(1,1601)	1:A:54:ASN:H	1:A:79:ASN:HD22	1	0.15
(1,1601)	1:A:54:ASN:H	1:A:79:ASN:HD22	2	0.15
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	1	0.15
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	10	0.15
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	11	0.15
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	5	0.15
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	10	0.15
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	8	0.15
(1,1317)	1:A:34:TYR:H	1:A:103:GLN:H	12	0.15
(1,1317)	1:A:34:TYR:H	1:A:103:GLN:H	20	0.15
(1,1289)	1:A:103:GLN:H	1:A:103:GLN:HG2	1	0.15
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	4	0.15
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	12	0.15
(2,17)	1:A:85:ALA:H	1:A:81:VAL:O	19	0.14
(1,878)	1:A:29:ALA:HA	1:A:80:PRO:HD2	4	0.14
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	5	0.14
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	10	0.14
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	12	0.14
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	19	0.14
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	20	0.14
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	6	0.14
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	10	0.14
(1,501)	1:A:46:LEU:HG	1:A:47:GLN:HA	4	0.14
(1,481)	1:A:23:LYS:HA	1:A:24:GLU:HB3	12	0.14
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	1	0.14
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	12	0.14
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	15	0.14
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	20	0.14
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	5	0.14
(1,2243)	2:B:117:U:H4'	2:B:117:U:H6	3	0.14
(1,2237)	2:B:116:U:H3'	2:B:116:U:H6	7	0.14
(1,1606)	1:A:79:ASN:HD22	1:A:81:VAL:HB	19	0.14
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	9	0.14
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	5	0.14
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	6	0.14
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	15	0.14
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	2	0.14
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	8	0.14
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	13	0.14
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	3	0.14
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	4	0.14
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	19	0.14
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	18	0.14
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD2	20	0.14
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD3	20	0.14
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	14	0.14
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1111)	1:A:32:PHE:HZ	1:A:105:LYS:HA	10	0.14
(2,17)	1:A:85:ALA:H	1:A:81:VAL:O	8	0.13
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	3	0.13
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	6	0.13
(1,481)	1:A:23:LYS:HA	1:A:24:GLU:HB3	6	0.13
(1,335)	1:A:45:ILE:HA	1:A:48:MET:HB3	5	0.13
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	7	0.13
(1,2283)	1:A:35:HIS:HD2	2:B:116:U:H5	1	0.13
(1,2272)	2:B:118:A:H2'	2:B:119:A:H1'	3	0.13
(1,2244)	2:B:117:U:H3'	2:B:117:U:H6	7	0.13
(1,2237)	2:B:116:U:H3'	2:B:116:U:H6	12	0.13
(1,2237)	2:B:116:U:H3'	2:B:116:U:H6	19	0.13
(1,2230)	2:B:115:U:H3'	2:B:116:U:H5	9	0.13
(1,2230)	2:B:115:U:H3'	2:B:116:U:H5	15	0.13
(1,2229)	2:B:115:U:H2'	2:B:116:U:H6	5	0.13
(1,1711)	1:A:13:GLY:H	1:A:14:LEU:HA	7	0.13
(1,1637)	1:A:54:ASN:H	1:A:54:ASN:HD22	5	0.13
(1,1601)	1:A:54:ASN:H	1:A:79:ASN:HD22	16	0.13
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	16	0.13
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	9	0.13
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	10	0.13
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	13	0.13
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	2	0.13
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	4	0.13
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	9	0.13
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	11	0.13
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	16	0.13
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	6	0.13
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	7	0.13
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	16	0.13
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	7	0.13
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	9	0.13
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	12	0.13
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	17	0.13
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	20	0.13
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	4	0.13
(1,1441)	1:A:96:GLY:HA2	1:A:98:LYS:H	4	0.13
(1,1399)	1:A:24:GLU:H	1:A:24:GLU:HG2	6	0.13
(1,1399)	1:A:24:GLU:H	1:A:24:GLU:HG2	12	0.13
(1,1344)	1:A:15:VAL:HG11	1:A:17:ARG:H	9	0.13
(1,1344)	1:A:15:VAL:HG12	1:A:17:ARG:H	9	0.13
(1,1344)	1:A:15:VAL:HG13	1:A:17:ARG:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	1:A:15:VAL:HG21	1:A:17:ARG:H	9	0.13
(1,1344)	1:A:15:VAL:HG22	1:A:17:ARG:H	9	0.13
(1,1344)	1:A:15:VAL:HG23	1:A:17:ARG:H	9	0.13
(1,1317)	1:A:34:TYR:H	1:A:103:GLN:H	2	0.13
(1,1164)	1:A:93:PHE:H	1:A:94:GLN:H	10	0.13
(1,1164)	1:A:93:PHE:H	1:A:94:GLN:H	17	0.13
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	5	0.13
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	9	0.13
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	20	0.13
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	19	0.13
(2,12)	1:A:46:LEU:H	1:A:42:ASP:O	11	0.12
(2,12)	1:A:46:LEU:H	1:A:42:ASP:O	14	0.12
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	11	0.12
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	11	0.12
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	11	0.12
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	11	0.12
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	11	0.12
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	11	0.12
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	18	0.12
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	18	0.12
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	18	0.12
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	18	0.12
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	18	0.12
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	18	0.12
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	20	0.12
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	20	0.12
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	20	0.12
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	20	0.12
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	20	0.12
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	20	0.12
(1,599)	1:A:33:ILE:H	1:A:33:ILE:HG12	4	0.12
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	2	0.12
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	4	0.12
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	7	0.12
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	9	0.12
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	15	0.12
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	16	0.12
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	18	0.12
(1,550)	1:A:40:PHE:HA	1:A:44:ASP:H	8	0.12
(1,535)	1:A:52:PHE:HA	1:A:86:ALA:H	2	0.12
(1,501)	1:A:46:LEU:HG	1:A:47:GLN:HA	3	0.12
(1,501)	1:A:46:LEU:HG	1:A:47:GLN:HA	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:A:23:LYS:HA	1:A:24:GLU:HB3	20	0.12
(1,406)	1:A:65:GLN:HB2	1:A:66:THR:HA	6	0.12
(1,406)	1:A:65:GLN:HB2	1:A:66:THR:HA	16	0.12
(1,335)	1:A:45:ILE:HA	1:A:48:MET:HB3	9	0.12
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	18	0.12
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	13	0.12
(1,2283)	1:A:35:HIS:HD2	2:B:116:U:H5	8	0.12
(1,2262)	2:B:119:A:H3'	2:B:119:A:H8	2	0.12
(1,2256)	2:B:118:A:H2	2:B:119:A:H1'	16	0.12
(1,2249)	2:B:117:U:H3'	2:B:118:A:H8	13	0.12
(1,2244)	2:B:117:U:H3'	2:B:117:U:H6	15	0.12
(1,2244)	2:B:117:U:H3'	2:B:117:U:H6	19	0.12
(1,2237)	2:B:116:U:H3'	2:B:116:U:H6	8	0.12
(1,2235)	2:B:116:U:H2'	2:B:116:U:H5	4	0.12
(1,2235)	2:B:116:U:H2'	2:B:116:U:H5	8	0.12
(1,1674)	1:A:28:GLY:H	1:A:30:ASN:HD22	9	0.12
(1,1637)	1:A:54:ASN:H	1:A:54:ASN:HD22	4	0.12
(1,1637)	1:A:54:ASN:H	1:A:54:ASN:HD22	12	0.12
(1,1606)	1:A:79:ASN:HD22	1:A:81:VAL:HB	1	0.12
(1,1606)	1:A:79:ASN:HD22	1:A:81:VAL:HB	2	0.12
(1,1601)	1:A:54:ASN:H	1:A:79:ASN:HD22	3	0.12
(1,1595)	1:A:30:ASN:H	1:A:31:LEU:H	1	0.12
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	7	0.12
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	12	0.12
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	17	0.12
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	18	0.12
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	20	0.12
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	4	0.12
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	7	0.12
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	18	0.12
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	3	0.12
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	13	0.12
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	14	0.12
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	18	0.12
(1,155)	1:A:17:ARG:HD2	1:A:18:GLY:H	13	0.12
(1,155)	1:A:17:ARG:HD3	1:A:18:GLY:H	13	0.12
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	1	0.12
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	16	0.12
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	18	0.12
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	2	0.12
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	3	0.12
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	7	0.12
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	11	0.12
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	12	0.12
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	15	0.12
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	20	0.12
(1,1399)	1:A:24:GLU:H	1:A:24:GLU:HG2	11	0.12
(1,1264)	1:A:108:LYS:HA	1:A:112:LYS:H	8	0.12
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	4	0.12
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	14	0.12
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	15	0.12
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	16	0.12
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	19	0.12
(2,17)	1:A:85:ALA:H	1:A:81:VAL:O	20	0.11
(2,14)	1:A:49:PHE:H	1:A:45:ILE:O	15	0.11
(2,12)	1:A:46:LEU:H	1:A:42:ASP:O	15	0.11
(2,12)	1:A:46:LEU:H	1:A:42:ASP:O	18	0.11
(1,899)	1:A:55:VAL:H	1:A:55:VAL:HG11	12	0.11
(1,899)	1:A:55:VAL:H	1:A:55:VAL:HG12	12	0.11
(1,899)	1:A:55:VAL:H	1:A:55:VAL:HG13	12	0.11
(1,878)	1:A:29:ALA:HA	1:A:80:PRO:HD2	17	0.11
(1,842)	1:A:104:LEU:HD13	1:A:105:LYS:H	16	0.11
(1,842)	1:A:104:LEU:HD21	1:A:105:LYS:H	16	0.11
(1,842)	1:A:104:LEU:HD22	1:A:105:LYS:H	16	0.11
(1,842)	1:A:104:LEU:HD23	1:A:105:LYS:H	16	0.11
(1,842)	1:A:104:LEU:HD11	1:A:105:LYS:H	16	0.11
(1,842)	1:A:104:LEU:HD12	1:A:105:LYS:H	16	0.11
(1,809)	1:A:30:ASN:HA	1:A:30:ASN:HD21	18	0.11
(1,682)	1:A:26:PRO:HG2	1:A:80:PRO:HG2	5	0.11
(1,666)	1:A:22:GLN:HA	1:A:57:SER:HA	11	0.11
(1,666)	1:A:22:GLN:HA	1:A:57:SER:HA	17	0.11
(1,599)	1:A:33:ILE:H	1:A:33:ILE:HG12	14	0.11
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	1	0.11
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	13	0.11
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	14	0.11
(1,557)	1:A:65:GLN:HB3	1:A:67:ASN:H	17	0.11
(1,513)	1:A:114:TRP:HA	1:A:114:TRP:HD1	2	0.11
(1,513)	1:A:114:TRP:HA	1:A:114:TRP:HD1	7	0.11
(1,501)	1:A:46:LEU:HG	1:A:47:GLN:HA	17	0.11
(1,481)	1:A:23:LYS:HA	1:A:24:GLU:HB3	16	0.11
(1,481)	1:A:23:LYS:HA	1:A:24:GLU:HB3	19	0.11
(1,406)	1:A:65:GLN:HB2	1:A:66:THR:HA	4	0.11
(1,342)	1:A:23:LYS:HA	1:A:24:GLU:HG3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	14	0.11
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	16	0.11
(1,286)	1:A:87:ILE:HB	1:A:90:MET:H	19	0.11
(1,2326)	2:B:116:U:H2'	2:B:117:U:H6	2	0.11
(1,2312)	1:A:61:PHE:HA	2:B:119:A:H2	4	0.11
(1,2268)	2:B:115:U:H4'	2:B:116:U:H5	2	0.11
(1,2244)	2:B:117:U:H3'	2:B:117:U:H6	4	0.11
(1,2244)	2:B:117:U:H3'	2:B:117:U:H6	11	0.11
(1,2243)	2:B:117:U:H4'	2:B:117:U:H6	1	0.11
(1,2237)	2:B:116:U:H3'	2:B:116:U:H6	11	0.11
(1,2235)	2:B:116:U:H2'	2:B:116:U:H5	7	0.11
(1,1973)	1:A:55:VAL:H	1:A:55:VAL:HG22	12	0.11
(1,1973)	1:A:55:VAL:H	1:A:55:VAL:HG23	12	0.11
(1,1973)	1:A:55:VAL:H	1:A:55:VAL:HG11	12	0.11
(1,1973)	1:A:55:VAL:H	1:A:55:VAL:HG12	12	0.11
(1,1973)	1:A:55:VAL:H	1:A:55:VAL:HG13	12	0.11
(1,1973)	1:A:55:VAL:H	1:A:55:VAL:HG21	12	0.11
(1,1637)	1:A:54:ASN:H	1:A:54:ASN:HD22	11	0.11
(1,1637)	1:A:54:ASN:H	1:A:54:ASN:HD22	18	0.11
(1,1606)	1:A:79:ASN:HD22	1:A:81:VAL:HB	18	0.11
(1,1606)	1:A:79:ASN:HD22	1:A:81:VAL:HB	20	0.11
(1,1601)	1:A:54:ASN:H	1:A:79:ASN:HD22	6	0.11
(1,1601)	1:A:54:ASN:H	1:A:79:ASN:HD22	7	0.11
(1,1601)	1:A:54:ASN:H	1:A:79:ASN:HD22	10	0.11
(1,1574)	1:A:43:GLN:H	1:A:60:VAL:H	15	0.11
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	2	0.11
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	3	0.11
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	4	0.11
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	6	0.11
(1,1567)	1:A:87:ILE:HG12	1:A:88:GLN:H	19	0.11
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	1	0.11
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	10	0.11
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	11	0.11
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	14	0.11
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	16	0.11
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	17	0.11
(1,1559)	1:A:44:ASP:HB3	1:A:45:ILE:H	20	0.11
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	1	0.11
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	8	0.11
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	19	0.11
(1,1550)	1:A:65:GLN:HB2	1:A:67:ASN:H	20	0.11
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	9	0.11
(1,1549)	1:A:63:ASP:HB2	1:A:67:ASN:H	14	0.11
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	6	0.11
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	8	0.11
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	11	0.11
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	13	0.11
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	15	0.11
(1,148)	1:A:40:PHE:HB2	1:A:41:GLY:HA2	20	0.11
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	14	0.11
(1,1460)	1:A:49:PHE:HZ	1:A:91:ASN:H	19	0.11
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	9	0.11
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	17	0.11
(1,1459)	1:A:91:ASN:H	1:A:102:VAL:H	19	0.11
(1,1399)	1:A:24:GLU:H	1:A:24:GLU:HG2	18	0.11
(1,1386)	1:A:31:LEU:H	1:A:77:TYR:H	16	0.11
(1,1344)	1:A:15:VAL:HG11	1:A:17:ARG:H	14	0.11
(1,1344)	1:A:15:VAL:HG12	1:A:17:ARG:H	14	0.11
(1,1344)	1:A:15:VAL:HG13	1:A:17:ARG:H	14	0.11
(1,1344)	1:A:15:VAL:HG21	1:A:17:ARG:H	14	0.11
(1,1344)	1:A:15:VAL:HG22	1:A:17:ARG:H	14	0.11
(1,1344)	1:A:15:VAL:HG23	1:A:17:ARG:H	14	0.11
(1,1317)	1:A:34:TYR:H	1:A:103:GLN:H	1	0.11
(1,1317)	1:A:34:TYR:H	1:A:103:GLN:H	7	0.11
(1,1317)	1:A:34:TYR:H	1:A:103:GLN:H	10	0.11
(1,1317)	1:A:34:TYR:H	1:A:103:GLN:H	19	0.11
(1,1308)	1:A:15:VAL:H	1:A:16:PRO:HD2	20	0.11
(1,1264)	1:A:108:LYS:HA	1:A:112:LYS:H	12	0.11
(1,1264)	1:A:108:LYS:HA	1:A:112:LYS:H	15	0.11
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD2	5	0.11
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD3	5	0.11
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD2	8	0.11
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD3	8	0.11
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD2	9	0.11
(1,1190)	1:A:64:LYS:H	1:A:64:LYS:HD3	9	0.11
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	6	0.11
(1,1158)	1:A:66:THR:H	1:A:67:ASN:HB2	8	0.11
(1,1129)	1:A:35:HIS:HD2	1:A:101:LYS:H	7	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value