



Full wwPDB NMR Structure Validation Report ⓘ

Apr 20, 2024 – 09:04 PM EDT

PDB ID : 2KY8
BMRB ID : 16936
Title : Solution structure and dynamic analysis of chicken MBD2 methyl binding domain bound to a target methylated DNA sequence
Authors : Williams Jr., D.C.; Scarsdale Jr., J.N.
Deposited on : 2010-05-18

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

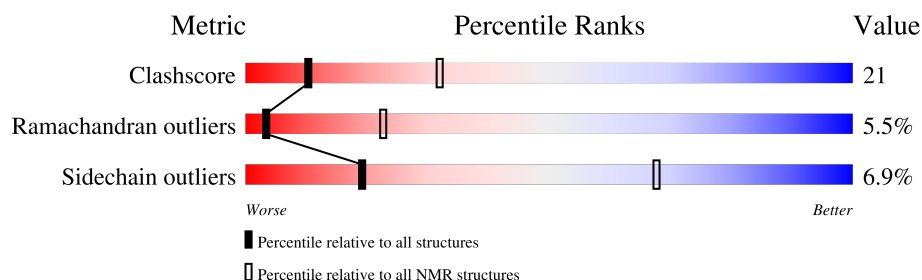
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR




The overall completeness of chemical shifts assignment is 64%.

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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	72	 65% 24% • 6% •
2	B	11	 64% 36%
3	C	11	 45% 55%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:71 (66)	0.82	13

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

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2081 atoms, of which 923 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Methyl-CpG-binding domain protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1104	349	555	98	98	4	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q5EFL0
A	2	SER	-	expression tag	UNP Q5EFL0

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3').

Mol	Chain	Residues	Atoms						Trace
2	B	11	Total	C	H	N	O	P	0
			487	150	184	55	88	10	

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3').

Mol	Chain	Residues	Atoms						Trace
3	C	11	Total	C	H	N	O	P	0
			484	149	184	53	88	10	

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

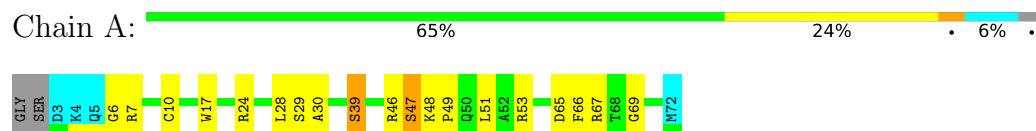
Mol	Chain	Residues	Atoms	
4	B	1	Total	Mn
			3	3
4	C	1	Total	Mn
			3	3

4 Residue-property plots [i](#)

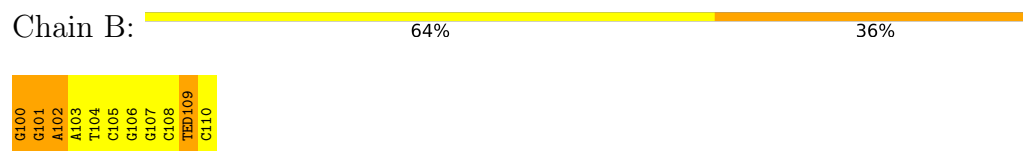
4.1 Average score per residue in the NMR ensemble

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: Methyl-CpG-binding domain protein 2



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

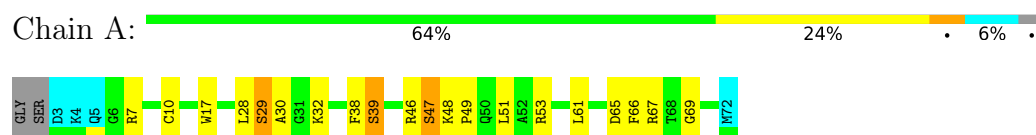


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Methyl-CpG-binding domain protein 2



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B: 



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C: 



4.2.2 Score per residue for model 2

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A: 



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B: 



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C: 



4.2.3 Score per residue for model 3

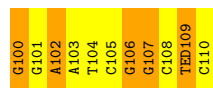
- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A: 



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B: 



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C: 



4.2.4 Score per residue for model 4

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A: 



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B: 



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C: 



4.2.5 Score per residue for model 5

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A: 



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  64% 36%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:  64% 36%



4.2.6 Score per residue for model 6

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  60% 26% 6% 6%




- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  73% 27%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

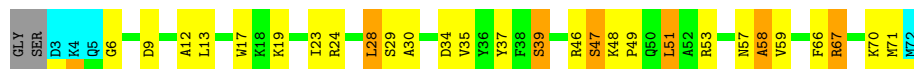
Chain C:  45% 55%



4.2.7 Score per residue for model 7

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  53% 31% 8% 6%



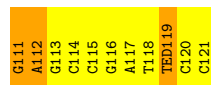
- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  64% 36%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

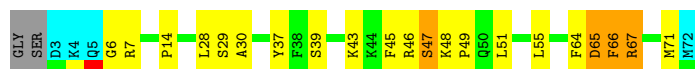
Chain C:  73% 27%



4.2.8 Score per residue for model 8

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  62% 24% 6% 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  55% 45%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

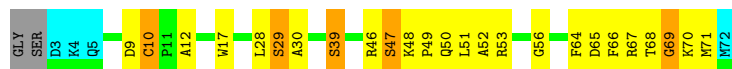
Chain C:  45% 55%



4.2.9 Score per residue for model 9

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  57% 28% 7% 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  55% 45%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

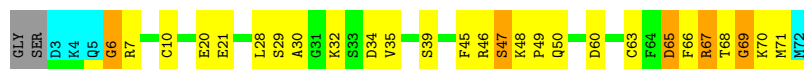
Chain C:  36% 64%



4.2.10 Score per residue for model 10

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  54% 31% 7% 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  64% 36%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:  55% 45%



4.2.11 Score per residue for model 11

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  58% 28% . . 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  64% 36%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

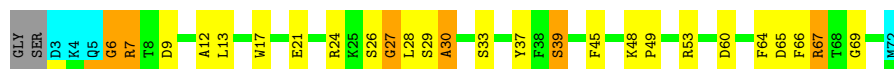
Chain C:  45% 55%



4.2.12 Score per residue for model 12

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  56% 28% 8% 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  64% 36%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:  55% 45%



4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  53% 35% . 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  64% 36%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

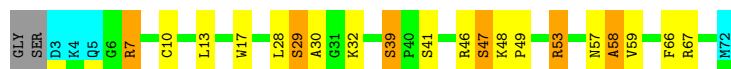
Chain C:  45% 55%



4.2.14 Score per residue for model 14

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  64% 19% 8% 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  64% 36%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

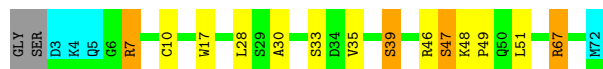
Chain C:  36% 64%



4.2.15 Score per residue for model 15

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  72% 14% 6% 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  73% 27%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:  64% 36%



4.2.16 Score per residue for model 16

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  62% 24% 6% 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  55% 45%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:  45% 55%



4.2.17 Score per residue for model 17

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  56% 28% 8% 6% .



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  73% 27%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

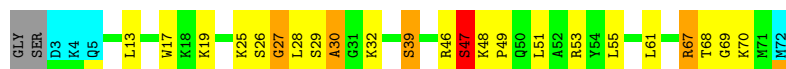
Chain C:  45% 55%



4.2.18 Score per residue for model 18

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  60% 25% 6% 6%



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  64% 36%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:  45% 55%



4.2.19 Score per residue for model 19

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  53% 35% 6%



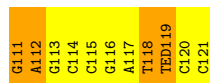
- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  64% 36%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:  64% 36%



4.2.20 Score per residue for model 20

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:  56% 28% 7% 6%



- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:  55% 45%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:  36% 64%



5 Refinement protocol and experimental data overview

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

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
X-PLOR NIH	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	959
Number of shifts mapped to atoms	852
Number of unparsed shifts	0
Number of shifts with mapping errors	107
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TED, MN, 5CM

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	1.02±0.00	0±0/530 (0.0± 0.0%)	0.89±0.00	0±0/711 (0.0± 0.0%)
2	B	1.51±0.04	7±1/206 (3.5± 0.4%)	2.13±0.01	11±0/312 (3.6± 0.1%)
3	C	1.52±0.03	7±1/202 (3.5± 0.5%)	2.13±0.01	11±0/305 (3.6± 0.1%)
All	All	1.26	287/18760 (1.5%)	1.59	442/26560 (1.7%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	110	DC	O4'-C1'	7.45	1.51	1.42	15	20
3	C	118	DT	O4'-C1'	7.19	1.50	1.42	8	20
3	C	120	DC	O4'-C1'	6.93	1.50	1.42	8	20
2	B	100	DG	O4'-C1'	6.90	1.50	1.42	6	15
3	C	111	DG	O4'-C1'	6.83	1.50	1.42	12	20
2	B	103	DA	O4'-C1'	6.76	1.50	1.42	15	20
2	B	104	DT	O4'-C1'	6.66	1.50	1.42	15	20
3	C	113	DG	O4'-C1'	6.45	1.50	1.42	15	17
3	C	117	DA	O4'-C1'	6.30	1.49	1.42	15	19
2	B	107	DG	O4'-C1'	6.20	1.49	1.42	15	20
3	C	114	DC	O4'-C1'	5.99	1.49	1.42	15	17
2	B	106	DG	O4'-C1'	5.98	1.49	1.42	15	19
2	B	108	DC	O4'-C1'	5.73	1.49	1.42	20	19
2	B	101	DG	O4'-C1'	5.66	1.49	1.42	15	4
2	B	102	DA	O4'-C1'	5.60	1.49	1.42	3	6
3	C	112	DA	O4'-C1'	5.52	1.48	1.42	15	15
3	C	116	DG	O4'-C1'	5.50	1.48	1.42	15	14
2	B	104	DT	C5-C7	5.04	1.53	1.50	8	1
3	C	118	DT	C5-C7	5.04	1.53	1.50	16	1

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

occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	120	DC	C4'-C3'-C2'	8.81	111.03	103.10	12	20
3	C	117	DA	C4'-C3'-C2'	8.79	111.01	103.10	18	20
3	C	111	DG	C4'-C3'-C2'	8.79	111.01	103.10	17	20
2	B	100	DG	C4'-C3'-C2'	8.78	111.00	103.10	2	20
2	B	107	DG	C4'-C3'-C2'	8.78	111.00	103.10	19	20
2	B	104	DT	C4'-C3'-C2'	8.78	111.00	103.10	19	20
3	C	114	DC	C4'-C3'-C2'	8.77	111.00	103.10	14	20
3	C	112	DA	C4'-C3'-C2'	8.77	110.99	103.10	5	20
3	C	118	DT	C4'-C3'-C2'	8.77	110.99	103.10	1	20
2	B	106	DG	C4'-C3'-C2'	8.77	110.99	103.10	3	20
3	C	113	DG	C4'-C3'-C2'	8.77	110.99	103.10	6	20
3	C	116	DG	C4'-C3'-C2'	8.77	110.99	103.10	5	20
2	B	103	DA	C4'-C3'-C2'	8.76	110.98	103.10	1	20
2	B	101	DG	C4'-C3'-C2'	8.75	110.98	103.10	17	20
2	B	102	DA	C4'-C3'-C2'	8.75	110.98	103.10	1	20
2	B	108	DC	C4'-C3'-C2'	8.74	110.97	103.10	20	20
3	C	121	DC	C4'-C3'-C2'	8.41	110.67	103.10	20	20
2	B	110	DC	C4'-C3'-C2'	8.40	110.66	103.10	8	20
2	B	104	DT	C6-C5-C7	-5.81	119.42	122.90	8	20
3	C	118	DT	C6-C5-C7	-5.79	119.43	122.90	16	20
2	B	101	DG	O4'-C1'-C2'	5.26	110.11	105.90	9	3
3	C	118	DT	C4-C5-C6	5.25	121.15	118.00	19	18
2	B	104	DT	C4-C5-C6	5.24	121.14	118.00	8	20
2	B	104	DT	O4'-C1'-N1	5.22	111.66	108.00	16	1

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	516	521	521	27±5
2	B	303	184	175	9±3
3	C	300	184	175	10±3
All	All	22500	17780	17420	849

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:111:DG:HO5'	3:C:111:DG:H8	0.96	0.99	18	20
2:B:100:DG:HO5'	2:B:100:DG:H8	0.95	0.95	11	20
1:A:28:LEU:O	1:A:28:LEU:HD13	0.83	1.73	7	2
1:A:26:SER:O	1:A:27:GLY:O	0.81	1.99	18	2
1:A:48:LYS:N	1:A:49:PRO:HD2	0.80	1.92	8	20
1:A:13:LEU:HD23	1:A:17:TRP:CD2	0.79	2.11	19	3
1:A:17:TRP:CH2	1:A:51:LEU:HD11	0.79	2.12	5	1
1:A:65:ASP:O	1:A:69:GLY:N	0.78	2.17	5	5
1:A:46:ARG:O	1:A:47:SER:CB	0.78	2.32	9	19
1:A:61:LEU:N	1:A:61:LEU:HD12	0.77	1.94	4	4
1:A:28:LEU:C	1:A:28:LEU:HD13	0.77	2.00	13	1
1:A:46:ARG:O	1:A:47:SER:OG	0.73	2.06	9	13
1:A:26:SER:O	1:A:27:GLY:C	0.73	2.25	18	2
1:A:66:PHE:CG	1:A:67:ARG:N	0.73	2.57	16	6
1:A:51:LEU:C	1:A:51:LEU:HD23	0.72	2.03	16	2
2:B:100:DG:H8	2:B:100:DG:O5'	0.72	1.68	13	19
3:C:111:DG:H8	3:C:111:DG:O5'	0.71	1.68	6	20
1:A:13:LEU:HD23	1:A:17:TRP:CE3	0.71	2.20	19	1
1:A:13:LEU:HD21	1:A:51:LEU:HD21	0.71	1.60	11	2
1:A:45:PHE:CD1	1:A:51:LEU:HD21	0.69	2.21	4	1
1:A:28:LEU:HD13	1:A:28:LEU:O	0.69	1.88	13	1
1:A:19:LYS:HZ3	1:A:35:VAL:HG13	0.68	1.45	6	1
1:A:64:PHE:CD1	1:A:65:ASP:N	0.68	2.61	2	1
1:A:66:PHE:CZ	1:A:67:ARG:NH1	0.68	2.61	14	1
1:A:48:LYS:N	1:A:49:PRO:CD	0.67	2.57	11	20
1:A:7:ARG:CG	1:A:7:ARG:HH11	0.67	2.03	15	2
1:A:32:LYS:NZ	3:C:114:DC:N4	0.66	2.44	14	6
1:A:50:GLN:NE2	1:A:53:ARG:HH21	0.66	1.88	9	1
1:A:7:ARG:NH2	1:A:9:ASP:N	0.65	2.44	12	1
1:A:64:PHE:CE1	1:A:70:LYS:O	0.65	2.49	2	1
1:A:17:TRP:CH2	1:A:39:SER:OG	0.65	2.48	1	4
2:B:109[B]:TED:CY7	2:B:109[B]:TED:CY6	0.65	2.73	15	5
1:A:51:LEU:HD23	1:A:51:LEU:O	0.65	1.90	9	4
1:A:45:PHE:CD1	1:A:50:GLN:OE1	0.65	2.50	10	2
2:B:109[C]:TED:CY7	2:B:109[C]:TED:CY6	0.64	2.75	12	10
2:B:109[A]:TED:CY6	2:B:109[A]:TED:CY7	0.64	2.75	7	6
2:B:109[C]:TED:CY5	2:B:109[C]:TED:CY8	0.64	2.75	20	5
1:A:66:PHE:CD2	1:A:67:ARG:N	0.64	2.65	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ARG:CG	1:A:53:ARG:HH11	0.64	2.05	5	3
1:A:37:TYR:CD1	1:A:66:PHE:CE2	0.64	2.86	12	1
1:A:28:LEU:O	1:A:30:ALA:N	0.64	2.30	6	17
1:A:32:LYS:NZ	3:C:114:DC:H41	0.64	1.90	1	4
1:A:48:LYS:NZ	1:A:61:LEU:HD12	0.64	2.07	2	1
1:A:13:LEU:N	1:A:13:LEU:HD22	0.64	2.08	14	2
2:B:109[B]:TED:CY8	2:B:109[B]:TED:CY5	0.63	2.75	10	6
1:A:65:ASP:OD1	1:A:70:LYS:N	0.63	2.31	9	1
2:B:109[A]:TED:CY5	2:B:109[A]:TED:CY8	0.63	2.77	9	6
1:A:67:ARG:CG	1:A:67:ARG:HH11	0.63	2.05	17	4
1:A:17:TRP:CZ2	1:A:39:SER:OG	0.63	2.51	19	4
1:A:50:GLN:NE2	1:A:53:ARG:NH2	0.63	2.45	13	2
3:C:119[C]:TED:CY5	3:C:119[C]:TED:CY8	0.63	2.76	18	7
3:C:119[B]:TED:CY7	3:C:119[B]:TED:CY6	0.63	2.77	19	5
1:A:13:LEU:N	1:A:13:LEU:CD2	0.63	2.62	14	2
3:C:119[C]:TED:CY7	3:C:119[C]:TED:CY6	0.62	2.77	19	12
1:A:19:LYS:NZ	1:A:35:VAL:HG13	0.62	2.09	6	1
1:A:64:PHE:CZ	1:A:70:LYS:O	0.62	2.52	2	1
3:C:119[A]:TED:CY5	3:C:119[A]:TED:CY8	0.62	2.78	13	11
1:A:61:LEU:N	1:A:61:LEU:CD1	0.61	2.63	4	3
1:A:68:THR:O	1:A:70:LYS:N	0.61	2.34	9	3
3:C:119[B]:TED:CY5	3:C:119[B]:TED:CY8	0.61	2.79	12	10
1:A:37:TYR:CE1	1:A:66:PHE:CD2	0.61	2.88	12	1
1:A:9:ASP:OD1	1:A:10:CYS:N	0.61	2.33	9	2
1:A:49:PRO:O	1:A:53:ARG:NH1	0.61	2.33	13	3
1:A:67:ARG:HH11	1:A:67:ARG:HG2	0.61	1.55	14	3
3:C:119[A]:TED:CY7	3:C:119[A]:TED:CY6	0.61	2.79	14	3
1:A:20:GLU:OE1	1:A:21:GLU:N	0.61	2.32	10	2
1:A:28:LEU:C	1:A:30:ALA:H	0.60	1.99	6	19
1:A:68:THR:O	1:A:69:GLY:C	0.60	2.39	18	6
1:A:67:ARG:CG	1:A:67:ARG:NH1	0.60	2.64	18	5
1:A:7:ARG:CG	1:A:7:ARG:NH1	0.60	2.62	15	2
1:A:34:ASP:OD1	1:A:35:VAL:N	0.60	2.34	10	5
1:A:67:ARG:NH1	1:A:67:ARG:CG	0.59	2.64	14	1
1:A:12:ALA:C	1:A:13:LEU:HD12	0.59	2.18	13	4
1:A:53:ARG:CG	1:A:53:ARG:NH1	0.59	2.65	18	5
1:A:7:ARG:NH2	1:A:9:ASP:OD1	0.59	2.36	20	1
3:C:111:DG:O5'	3:C:111:DG:C8	0.58	2.56	3	15
1:A:65:ASP:OD1	1:A:69:GLY:N	0.58	2.36	9	1
1:A:48:LYS:NZ	1:A:61:LEU:O	0.58	2.36	1	2
1:A:65:ASP:CB	1:A:68:THR:OG1	0.58	2.51	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLU:CD	1:A:21:GLU:N	0.58	2.57	20	2
1:A:17:TRP:CH2	1:A:51:LEU:CD1	0.58	2.87	1	4
1:A:66:PHE:O	1:A:67:ARG:C	0.57	2.43	10	6
1:A:66:PHE:O	1:A:68:THR:N	0.57	2.38	10	1
2:B:106:DG:C2	3:C:116:DG:N2	0.57	2.73	8	5
1:A:34:ASP:OD2	1:A:36:TYR:CZ	0.57	2.58	2	1
1:A:45:PHE:CG	1:A:50:GLN:OE1	0.57	2.58	11	2
1:A:12:ALA:CB	1:A:64:PHE:CD1	0.57	2.88	12	2
2:B:106:DG:N2	3:C:116:DG:C2	0.56	2.73	16	8
1:A:19:LYS:NZ	1:A:69:GLY:O	0.56	2.37	2	1
2:B:100:DG:H2'	2:B:101:DG:N7	0.56	2.16	11	4
1:A:34:ASP:OD2	1:A:36:TYR:CE2	0.56	2.58	2	1
1:A:32:LYS:HZ3	3:C:114:DC:N4	0.56	1.98	14	3
2:B:100:DG:O5'	2:B:100:DG:C8	0.55	2.54	20	7
1:A:12:ALA:CB	1:A:71:MET:SD	0.55	2.94	2	2
1:A:24:ARG:HH11	1:A:24:ARG:HG2	0.55	1.61	5	3
1:A:28:LEU:C	1:A:28:LEU:CD1	0.55	2.74	13	3
1:A:17:TRP:CH2	1:A:51:LEU:CD2	0.55	2.89	18	1
1:A:9:ASP:OD1	1:A:17:TRP:O	0.55	2.25	3	1
1:A:33:SER:O	1:A:67:ARG:NH1	0.55	2.39	15	2
2:B:102:DA:N6	3:C:118:DT:O4	0.55	2.40	9	17
1:A:53:ARG:HH11	1:A:53:ARG:HG2	0.55	1.61	19	6
1:A:63:CYS:O	1:A:70:LYS:O	0.55	2.25	5	2
1:A:47:SER:OG	3:C:115:5CM:P	0.55	2.65	18	2
1:A:66:PHE:CD1	1:A:66:PHE:N	0.55	2.75	19	4
1:A:28:LEU:C	1:A:30:ALA:N	0.54	2.61	18	16
1:A:52:ALA:O	1:A:56:GLY:N	0.54	2.40	9	1
1:A:53:ARG:HH11	1:A:53:ARG:CG	0.54	2.16	19	3
1:A:57:ASN:O	1:A:59:VAL:N	0.54	2.41	16	5
1:A:37:TYR:OH	1:A:66:PHE:O	0.54	2.26	4	5
1:A:55:LEU:HD12	1:A:56:GLY:O	0.54	2.02	5	1
1:A:67:ARG:CB	1:A:67:ARG:HH11	0.54	2.15	8	1
1:A:65:ASP:OD1	1:A:69:GLY:CA	0.54	2.55	9	1
1:A:37:TYR:CD1	1:A:66:PHE:CD2	0.54	2.96	12	1
1:A:10:CYS:SG	1:A:17:TRP:O	0.54	2.66	4	1
1:A:65:ASP:C	1:A:68:THR:HG1	0.53	2.05	10	1
1:A:46:ARG:O	1:A:47:SER:HB3	0.53	2.03	8	4
1:A:64:PHE:CE2	1:A:65:ASP:O	0.53	2.62	6	2
1:A:9:ASP:O	1:A:19:LYS:NZ	0.53	2.42	13	1
1:A:67:ARG:CZ	3:C:114:DC:OP2	0.53	2.57	18	1
1:A:67:ARG:HH11	1:A:67:ARG:CG	0.52	2.17	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:C	1:A:51:LEU:CD2	0.52	2.77	16	1
1:A:60:ASP:O	1:A:60:ASP:OD1	0.52	2.27	20	5
1:A:67:ARG:NE	3:C:114:DC:OP2	0.52	2.42	18	1
1:A:51:LEU:O	1:A:51:LEU:HD13	0.52	2.05	7	1
1:A:28:LEU:HD13	1:A:28:LEU:C	0.52	2.24	20	2
1:A:67:ARG:HE	1:A:67:ARG:CA	0.52	2.17	7	1
1:A:50:GLN:OE1	1:A:50:GLN:C	0.52	2.48	11	2
1:A:17:TRP:CH2	1:A:39:SER:CB	0.52	2.93	7	6
1:A:51:LEU:HD23	1:A:51:LEU:C	0.52	2.24	9	1
1:A:33:SER:C	1:A:67:ARG:NH2	0.52	2.62	13	1
1:A:7:ARG:HH11	1:A:7:ARG:HG2	0.52	1.65	15	2
1:A:45:PHE:CG	1:A:51:LEU:HD21	0.52	2.40	20	1
1:A:24:ARG:CG	1:A:24:ARG:HH11	0.52	2.17	3	1
2:B:100:DG:H2''	2:B:101:DG:C8	0.51	2.40	9	11
1:A:47:SER:OG	3:C:115:5CM:OP1	0.51	2.25	5	4
1:A:32:LYS:NZ	3:C:113:DG:C8	0.51	2.78	13	1
1:A:29:SER:O	1:A:30:ALA:O	0.51	2.27	20	1
1:A:6:GLY:O	1:A:20:GLU:OE1	0.51	2.29	19	1
2:B:109[B]:TED:CY8	2:B:109[B]:TED:CYB	0.51	2.88	8	1
1:A:45:PHE:CD1	1:A:50:GLN:CD	0.51	2.84	11	2
1:A:67:ARG:NH2	3:C:114:DC:OP2	0.51	2.44	18	1
1:A:17:TRP:CE2	1:A:39:SER:OG	0.51	2.64	17	1
1:A:24:ARG:CG	1:A:24:ARG:NH1	0.51	2.72	3	2
1:A:67:ARG:HG2	1:A:67:ARG:HH11	0.51	1.65	6	1
1:A:65:ASP:OD2	1:A:68:THR:OG1	0.51	2.29	9	1
1:A:33:SER:O	1:A:67:ARG:NH2	0.51	2.44	12	1
1:A:30:ALA:C	1:A:32:LYS:H	0.50	2.10	18	1
1:A:17:TRP:CE3	1:A:38:PHE:O	0.50	2.63	1	1
1:A:32:LYS:HZ3	3:C:114:DC:H41	0.50	1.48	1	2
1:A:65:ASP:O	1:A:66:PHE:CB	0.50	2.57	4	1
1:A:35:VAL:CG2	1:A:67:ARG:NH2	0.50	2.74	15	1
2:B:109[B]:TED:CYA	2:B:109[B]:TED:CY6	0.50	2.88	8	6
1:A:20:GLU:OE2	1:A:21:GLU:O	0.50	2.29	4	1
1:A:46:ARG:C	1:A:47:SER:OG	0.50	2.49	5	6
2:B:100:DG:C2'	2:B:101:DG:C8	0.50	2.94	9	8
1:A:19:LYS:HZ1	1:A:35:VAL:CG2	0.50	2.18	6	1
1:A:64:PHE:CD1	1:A:70:LYS:O	0.50	2.65	2	1
1:A:24:ARG:NH1	1:A:24:ARG:CG	0.50	2.74	5	1
1:A:24:ARG:HH11	1:A:24:ARG:CG	0.50	2.19	5	3
1:A:68:THR:C	1:A:70:LYS:N	0.50	2.65	9	2
1:A:32:LYS:NZ	3:C:113:DG:N7	0.50	2.60	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:N	1:A:51:LEU:HD12	0.50	2.22	19	1
1:A:6:GLY:O	1:A:20:GLU:OE2	0.49	2.30	10	1
1:A:65:ASP:OD1	1:A:66:PHE:N	0.49	2.45	20	1
1:A:29:SER:O	1:A:30:ALA:C	0.49	2.51	16	8
1:A:28:LEU:O	1:A:28:LEU:CD1	0.49	2.55	7	1
1:A:50:GLN:CD	1:A:53:ARG:HH22	0.49	2.10	13	1
2:B:109[C]:TED:CYA	2:B:109[C]:TED:CY6	0.49	2.91	1	3
1:A:64:PHE:CG	1:A:65:ASP:N	0.48	2.81	8	2
1:A:19:LYS:HZ1	1:A:35:VAL:HG22	0.48	1.69	6	1
2:B:109[A]:TED:CY6	2:B:109[A]:TED:CYA	0.48	2.91	13	5
1:A:57:ASN:OD1	1:A:58:ALA:N	0.48	2.47	20	1
1:A:43:LYS:CG	1:A:45:PHE:CZ	0.48	2.97	8	1
1:A:66:PHE:O	1:A:69:GLY:N	0.48	2.46	10	1
1:A:6:GLY:C	1:A:20:GLU:OE1	0.48	2.52	19	1
1:A:19:LYS:NZ	1:A:35:VAL:CG1	0.48	2.77	6	1
1:A:12:ALA:HB1	1:A:71:MET:SD	0.48	2.48	9	1
1:A:33:SER:CB	1:A:67:ARG:HH22	0.48	2.21	13	1
1:A:48:LYS:HZ2	1:A:61:LEU:HD12	0.47	1.68	2	1
1:A:60:ASP:C	1:A:61:LEU:HD22	0.47	2.30	2	1
1:A:20:GLU:OE1	1:A:22:VAL:HG23	0.47	2.08	4	2
1:A:65:ASP:OD2	1:A:70:LYS:NZ	0.47	2.47	5	1
1:A:53:ARG:NH1	1:A:53:ARG:CG	0.47	2.77	14	2
1:A:65:ASP:CG	1:A:66:PHE:H	0.47	2.12	16	1
1:A:9:ASP:O	1:A:9:ASP:OD1	0.47	2.32	16	3
1:A:57:ASN:C	1:A:59:VAL:N	0.47	2.68	14	4
3:C:112:DA:H2''	3:C:113:DG:C8	0.47	2.45	20	9
1:A:50:GLN:C	1:A:50:GLN:CD	0.47	2.73	11	2
1:A:17:TRP:CZ3	1:A:51:LEU:HD13	0.47	2.44	11	1
2:B:101:DG:H2'	2:B:102:DA:N7	0.47	2.25	9	3
2:B:101:DG:H2''	2:B:102:DA:C8	0.47	2.45	8	14
1:A:46:ARG:O	1:A:47:SER:HB2	0.47	2.08	5	3
1:A:32:LYS:NZ	2:B:107:DG:O6	0.46	2.48	3	1
1:A:67:ARG:HG3	1:A:67:ARG:NH1	0.46	2.25	9	2
1:A:53:ARG:HG3	1:A:53:ARG:HH11	0.46	1.70	3	1
1:A:48:LYS:NZ	1:A:64:PHE:O	0.46	2.48	19	1
1:A:57:ASN:O	1:A:58:ALA:C	0.46	2.53	16	6
3:C:111:DG:C2'	3:C:112:DA:C8	0.46	2.98	14	5
1:A:61:LEU:O	1:A:64:PHE:O	0.46	2.33	2	1
1:A:65:ASP:CB	1:A:68:THR:HG1	0.46	2.24	10	1
1:A:61:LEU:N	1:A:61:LEU:CD2	0.46	2.79	2	1
2:B:109[C]:TED:O9	2:B:109[C]:TED:C12	0.46	2.64	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:TRP:CH2	1:A:51:LEU:HD13	0.46	2.45	1	2
2:B:101:DG:C2'	2:B:102:DA:C8	0.46	2.99	9	4
3:C:119[A]:TED:O9	3:C:119[A]:TED:C12	0.45	2.64	2	1
1:A:65:ASP:O	1:A:66:PHE:HB2	0.45	2.09	4	1
1:A:55:LEU:HD12	1:A:61:LEU:HD11	0.45	1.88	11	2
1:A:21:GLU:OE1	1:A:21:GLU:C	0.45	2.54	12	1
1:A:7:ARG:N	1:A:7:ARG:HD3	0.45	2.27	14	1
3:C:111:DG:H2'	3:C:112:DA:N7	0.45	2.27	20	3
3:C:113:DG:H2''	3:C:114:DC:C6	0.45	2.46	20	6
1:A:48:LYS:HB3	1:A:49:PRO:HD3	0.45	1.89	2	1
1:A:23:ILE:O	1:A:24:ARG:C	0.45	2.54	4	5
1:A:66:PHE:CD2	3:C:114:DC:OP1	0.45	2.70	5	1
1:A:21:GLU:CB	1:A:67:ARG:HH21	0.45	2.25	10	1
1:A:10:CYS:SG	1:A:13:LEU:CD1	0.45	3.05	16	1
1:A:67:ARG:HH11	1:A:67:ARG:HG3	0.45	1.72	1	1
1:A:24:ARG:HB2	1:A:30:ALA:HB1	0.45	1.87	12	1
1:A:51:LEU:HD21	1:A:55:LEU:CD1	0.44	2.42	8	1
1:A:64:PHE:CE2	1:A:70:LYS:O	0.44	2.71	2	1
1:A:32:LYS:HZ1	3:C:114:DC:H41	0.44	1.56	6	1
1:A:9:ASP:OD1	1:A:9:ASP:C	0.44	2.56	16	1
1:A:13:LEU:HD12	1:A:13:LEU:N	0.44	2.27	2	3
1:A:19:LYS:NZ	1:A:68:THR:O	0.44	2.50	18	1
1:A:17:TRP:CZ2	1:A:39:SER:HB2	0.44	2.48	12	1
1:A:53:ARG:NH1	1:A:53:ARG:HG3	0.44	2.28	17	1
1:A:17:TRP:CZ3	1:A:51:LEU:HD21	0.44	2.47	7	2
1:A:55:LEU:HD12	1:A:55:LEU:N	0.44	2.27	20	1
1:A:19:LYS:NZ	1:A:69:GLY:C	0.44	2.71	2	1
1:A:13:LEU:N	1:A:13:LEU:CD1	0.44	2.81	2	1
3:C:111:DG:H2''	3:C:112:DA:C8	0.43	2.49	14	8
1:A:64:PHE:CD2	1:A:65:ASP:O	0.43	2.71	16	2
1:A:17:TRP:CH2	1:A:39:SER:HB2	0.43	2.48	18	2
1:A:60:ASP:N	1:A:60:ASP:OD1	0.43	2.51	10	1
1:A:50:GLN:OE1	1:A:50:GLN:O	0.43	2.36	11	1
1:A:53:ARG:NH1	1:A:53:ARG:HG2	0.43	2.28	14	1
1:A:10:CYS:SG	1:A:64:PHE:CZ	0.43	3.12	16	1
1:A:17:TRP:CZ3	1:A:51:LEU:CD2	0.43	3.01	18	1
1:A:43:LYS:CG	1:A:45:PHE:CE1	0.43	3.02	8	1
1:A:34:ASP:OD2	1:A:36:TYR:OH	0.43	2.30	2	1
1:A:60:ASP:C	1:A:61:LEU:HD12	0.43	2.34	17	1
1:A:12:ALA:C	1:A:13:LEU:HD22	0.43	2.35	6	1
1:A:67:ARG:CA	1:A:67:ARG:HE	0.43	2.27	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:PHE:CD1	1:A:67:ARG:N	0.43	2.87	3	1
1:A:10:CYS:SG	1:A:13:LEU:HD13	0.43	2.54	16	1
1:A:61:LEU:HD22	1:A:61:LEU:N	0.42	2.29	2	1
3:C:119[C]:TED:CYB	3:C:119[C]:TED:CY8	0.42	2.97	11	1
1:A:43:LYS:O	1:A:45:PHE:CE1	0.42	2.73	13	2
1:A:7:ARG:N	1:A:7:ARG:CD	0.42	2.81	14	1
1:A:10:CYS:SG	1:A:17:TRP:CB	0.42	3.08	2	1
1:A:34:ASP:OD1	1:A:34:ASP:N	0.42	2.53	2	1
1:A:65:ASP:O	1:A:69:GLY:CA	0.42	2.67	5	1
1:A:67:ARG:NH1	1:A:67:ARG:HG3	0.42	2.30	13	1
1:A:13:LEU:CD2	1:A:17:TRP:CE3	0.42	2.98	19	1
1:A:60:ASP:OD1	1:A:60:ASP:O	0.42	2.37	10	1
1:A:47:SER:O	1:A:48:LYS:C	0.42	2.59	6	2
1:A:17:TRP:CZ3	1:A:39:SER:CB	0.41	3.03	17	1
1:A:30:ALA:C	1:A:32:LYS:N	0.41	2.73	18	1
1:A:51:LEU:N	1:A:51:LEU:CD1	0.41	2.83	19	1
1:A:61:LEU:HD12	1:A:61:LEU:N	0.41	2.31	17	1
1:A:46:ARG:NH2	3:C:115:5CM:C6	0.41	2.83	6	1
1:A:48:LYS:HZ1	1:A:51:LEU:HD22	0.41	1.74	16	1
1:A:32:LYS:HZ1	3:C:114:DC:N4	0.41	2.13	1	1
1:A:47:SER:OG	3:C:115:5CM:OP2	0.41	2.39	18	1
1:A:48:LYS:CB	1:A:49:PRO:CD	0.41	2.99	18	1
1:A:45:PHE:CD1	1:A:45:PHE:N	0.41	2.87	4	2
1:A:48:LYS:CB	1:A:48:LYS:NZ	0.41	2.84	11	1
1:A:60:ASP:OD1	1:A:60:ASP:N	0.41	2.52	12	1
1:A:48:LYS:O	1:A:52:ALA:N	0.41	2.52	17	1
1:A:39:SER:OG	1:A:45:PHE:CE1	0.40	2.73	6	1
1:A:66:PHE:C	1:A:68:THR:N	0.40	2.74	10	1
1:A:50:GLN:CD	1:A:50:GLN:O	0.40	2.60	11	1
1:A:68:THR:O	1:A:69:GLY:O	0.40	2.39	10	1
1:A:17:TRP:CH2	1:A:55:LEU:HD21	0.40	2.51	4	1
1:A:20:GLU:OE1	1:A:20:GLU:C	0.40	2.59	20	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	66/72 (92%)	58±2 (88±2%)	4±2 (7±3%)	4±1 (5±2%)	3	23
All	All	1320/1440 (92%)	1161 (88%)	87 (7%)	72 (5%)	3	23

All 12 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	47	SER	19
1	A	29	SER	18
1	A	6	GLY	9
1	A	14	PRO	5
1	A	58	ALA	4
1	A	69	GLY	4
1	A	66	PHE	3
1	A	65	ASP	3
1	A	30	ALA	3
1	A	27	GLY	2
1	A	71	MET	1
1	A	67	ARG	1

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	55/60 (92%)	51±1 (93±2%)	4±1 (7±2%)	19	68
All	All	1100/1200 (92%)	1024 (93%)	76 (7%)	19	68

All 19 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	39	SER	17
1	A	10	CYS	9
1	A	47	SER	7
1	A	67	ARG	7
1	A	48	LYS	6
1	A	24	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	25	LYS	4
1	A	7	ARG	3
1	A	71	MET	2
1	A	51	LEU	2
1	A	53	ARG	2
1	A	41	SER	2
1	A	19	LYS	2
1	A	28	LEU	2
1	A	32	LYS	2
1	A	45	PHE	1
1	A	46	ARG	1
1	A	63	CYS	1
1	A	65	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	TED	C	119[C]	4	44,47,48	0.96±0.02	4±0 (9±0%)
3	TED	C	119[B]	4	44,47,48	0.96±0.02	4±0 (9±0%)
2	TED	B	109[B]	4	44,47,48	0.95±0.01	4±0 (9±0%)
3	TED	C	119[A]	4	44,47,48	0.96±0.02	4±0 (9±0%)
2	TED	B	109[A]	4	44,47,48	0.95±0.01	4±0 (9±0%)
3	5CM	C	115	2,3	17,21,22	0.75±0.03	1±0 (5±0%)
2	TED	B	109[C]	4	44,47,48	0.95±0.01	4±0 (9±0%)
2	5CM	B	105	2,3	17,21,22	0.79±0.03	1±0 (5±0%)

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

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	TED	C	119[C]	4	56,63,66	1.44±0.02	11±1 (19±0%)
3	TED	C	119[B]	4	56,63,66	1.42±0.01	10±0 (18±0%)
2	TED	B	109[B]	4	56,63,66	1.42±0.01	10±1 (18±1%)
3	TED	C	119[A]	4	56,63,66	1.43±0.02	10±1 (18±1%)
2	TED	B	109[A]	4	56,63,66	1.41±0.01	10±1 (17±1%)
3	5CM	C	115	2,3	24,30,33	1.14±0.01	2±0 (8±0%)
2	TED	B	109[C]	4	56,63,66	1.42±0.02	10±1 (18±0%)
2	5CM	B	105	2,3	24,30,33	1.14±0.01	2±0 (8±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5CM	C	115	2,3	-	0±0,7,21,22	0±0,2,2,2
2	TED	B	109[B]	4	-	0±0,40,54,55	0±0,2,2,2
3	TED	C	119[B]	4	-	0±0,40,54,55	0±0,2,2,2
2	TED	B	109[C]	4	-	0±0,40,54,55	0±0,2,2,2
3	TED	C	119[C]	4	-	0±0,40,54,55	0±0,2,2,2
2	5CM	B	105	2,3	-	0±0,7,21,22	0±0,2,2,2
2	TED	B	109[A]	4	-	0±0,40,54,55	0±0,2,2,2
3	TED	C	119[A]	4	-	0±0,40,54,55	0±0,2,2,2

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	119[A]	TED	O4'-C1'	3.27	1.49	1.42	14	20
3	C	119[B]	TED	O4'-C1'	3.27	1.49	1.42	14	20
3	C	119[C]	TED	O4'-C1'	3.27	1.49	1.42	14	20
2	B	109[A]	TED	O4'-C1'	3.13	1.49	1.42	15	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	109[B]	TED	O4'-C1'	3.13	1.49	1.42	15	20
2	B	109[C]	TED	O4'-C1'	3.13	1.49	1.42	15	20
2	B	105	5CM	O4'-C1'	3.04	1.49	1.42	15	20
3	C	115	5CM	O4'-C1'	2.87	1.48	1.42	15	20
2	B	109[A]	TED	OY6-CY6	2.81	1.21	1.30	15	20
2	B	109[B]	TED	OY6-CY6	2.81	1.21	1.30	13	20
3	C	119[C]	TED	OY7-CY7	2.79	1.21	1.30	9	20
2	B	109[B]	TED	OY7-CY7	2.79	1.21	1.30	1	20
3	C	119[A]	TED	OY6-CY6	2.79	1.21	1.30	15	20
3	C	119[B]	TED	OY7-CY7	2.79	1.21	1.30	11	20
3	C	119[A]	TED	OY7-CY7	2.79	1.21	1.30	16	20
3	C	119[B]	TED	OY6-CY6	2.79	1.21	1.30	6	20
2	B	109[A]	TED	OY7-CY7	2.78	1.21	1.30	18	20
2	B	109[C]	TED	OY6-CY6	2.78	1.21	1.30	5	20
2	B	109[C]	TED	OY7-CY7	2.78	1.21	1.30	8	20
3	C	119[C]	TED	OY6-CY6	2.78	1.21	1.30	3	20
3	C	119[A]	TED	C7-C5	2.18	1.51	1.46	11	20
3	C	119[B]	TED	C7-C5	2.18	1.51	1.46	11	20
3	C	119[C]	TED	C7-C5	2.18	1.51	1.46	11	20
2	B	109[A]	TED	C7-C5	2.14	1.51	1.46	7	20
2	B	109[B]	TED	C7-C5	2.14	1.51	1.46	7	20
2	B	109[C]	TED	C7-C5	2.14	1.51	1.46	7	20

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	105	5CM	C2'-C3'-C4'	3.95	110.99	102.76	15	20
3	C	115	5CM	C2'-C3'-C4'	3.95	110.98	102.76	18	20
2	B	109[A]	TED	C2'-C3'-C4'	3.94	110.97	102.76	6	20
2	B	109[B]	TED	C2'-C3'-C4'	3.94	110.97	102.76	6	20
2	B	109[C]	TED	C2'-C3'-C4'	3.94	110.97	102.76	6	20
3	C	119[A]	TED	C2'-C3'-C4'	3.94	110.97	102.76	18	20
3	C	119[B]	TED	C2'-C3'-C4'	3.94	110.97	102.76	18	20
3	C	119[C]	TED	C2'-C3'-C4'	3.94	110.97	102.76	18	20
3	C	119[C]	TED	CY1-CY5-N13	3.37	123.20	115.52	15	18
2	B	109[B]	TED	CY5-CY1-NYA	3.18	105.98	113.36	19	15
3	C	119[C]	TED	CY5-CY1-NYA	3.17	106.00	113.36	11	15
3	C	119[A]	TED	CY1-CY5-N13	3.10	122.59	115.52	18	15
2	B	109[C]	TED	C8-C7-C5	3.06	119.64	127.32	1	20
3	C	119[A]	TED	CY5-CY1-NYA	3.04	106.30	113.36	17	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	109[B]	TED	C8-C7-C5	3.01	119.78	127.32	8	20
2	B	109[C]	TED	CY5-CY1-NYA	3.00	106.39	113.36	8	15
3	C	119[B]	TED	C8-C7-C5	3.00	119.81	127.32	17	20
2	B	109[A]	TED	C8-C7-C5	2.98	119.86	127.32	7	20
3	C	119[C]	TED	C8-C7-C5	2.97	119.87	127.32	17	20
3	C	119[A]	TED	C8-C7-C5	2.94	119.96	127.32	8	20
2	B	109[A]	TED	CY5-CY1-NYA	2.88	106.67	113.36	10	14
2	B	105	5CM	C5-C6-N1	2.75	120.50	123.34	14	20
3	C	115	5CM	C5-C6-N1	2.72	120.53	123.34	3	20
2	B	109[B]	TED	C8-C9-N10	2.72	120.10	114.97	1	20
2	B	109[A]	TED	C8-C9-N10	2.72	120.09	114.97	11	20
3	C	119[B]	TED	C8-C9-N10	2.72	120.09	114.97	15	20
2	B	109[C]	TED	C8-C9-N10	2.71	120.07	114.97	2	20
3	C	119[A]	TED	C8-C9-N10	2.70	120.05	114.97	10	20
3	C	119[C]	TED	C8-C9-N10	2.69	120.04	114.97	6	20
3	C	119[B]	TED	CY5-CY1-NYA	2.61	107.29	113.36	2	9
3	C	119[B]	TED	CY1-CY5-N13	2.48	121.17	115.52	20	19
3	C	119[C]	TED	OY1-CY5-CY1	2.43	116.82	121.08	15	1
2	B	109[C]	TED	CY1-CY5-N13	2.37	120.93	115.52	20	9
2	B	109[B]	TED	CY1-CY5-N13	2.36	120.90	115.52	13	13
2	B	109[C]	TED	CY1-NYA-CYA	2.20	106.58	111.94	15	20
3	C	119[C]	TED	CY3-NYB-CYB	2.20	106.59	111.94	6	20
3	C	119[A]	TED	CY3-NYB-CYB	2.20	106.59	111.94	11	20
3	C	119[B]	TED	CY3-NYB-CY2	2.20	106.57	111.54	5	20
2	B	109[B]	TED	CY4-NYA-CYA	2.20	106.60	111.94	9	20
3	C	119[A]	TED	CY3-NYB-CY2	2.20	106.58	111.54	4	20
3	C	119[C]	TED	CY4-NYA-CY1	2.20	106.57	111.54	7	20
2	B	109[A]	TED	CY4-NYA-CYA	2.19	106.61	111.94	6	20
3	C	119[C]	TED	CY2-NYB-CYB	2.19	106.61	111.94	8	20
3	C	119[A]	TED	CY2-NYB-CYB	2.19	106.61	111.94	6	20
2	B	109[B]	TED	CY1-NYA-CYA	2.19	106.61	111.94	3	20
2	B	109[B]	TED	CY2-NYB-CYB	2.19	106.61	111.94	4	20
2	B	109[C]	TED	CY3-NYB-CYB	2.19	106.62	111.94	5	20
3	C	119[B]	TED	CY4-NYA-CYA	2.19	106.62	111.94	6	20
3	C	119[C]	TED	CY1-NYA-CYA	2.19	106.62	111.94	20	20
2	B	109[C]	TED	CY4-NYA-CY1	2.19	106.60	111.54	4	20
2	B	109[C]	TED	CY4-NYA-CYA	2.19	106.63	111.94	17	20
3	C	119[A]	TED	CY4-NYA-CYA	2.19	106.63	111.94	8	20
2	B	109[A]	TED	CY3-NYB-CYB	2.18	106.63	111.94	9	20
2	B	109[C]	TED	CY2-NYB-CYB	2.18	106.63	111.94	12	20
3	C	119[B]	TED	CY2-NYB-CYB	2.18	106.63	111.94	19	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	109[A]	TED	CY2-NYB-CYB	2.18	106.64	111.94	18	20
2	B	109[C]	TED	CY3-NYB-CY2	2.18	106.61	111.54	1	20
3	C	119[B]	TED	CY3-NYB-CYB	2.18	106.64	111.94	7	20
3	C	119[C]	TED	CY3-NYB-CY2	2.18	106.61	111.54	5	20
3	C	119[B]	TED	CY1-NYA-CYA	2.18	106.64	111.94	20	20
2	B	109[A]	TED	CY1-NYA-CYA	2.18	106.64	111.94	7	20
2	B	109[B]	TED	CY4-NYA-CY1	2.18	106.62	111.54	3	20
3	C	119[A]	TED	CY1-NYA-CYA	2.18	106.65	111.94	6	20
3	C	119[B]	TED	CY4-NYA-CY1	2.18	106.62	111.54	1	20
3	C	119[C]	TED	CY4-NYA-CYA	2.18	106.65	111.94	17	20
2	B	109[A]	TED	CY4-NYA-CY1	2.17	106.63	111.54	18	20
2	B	109[B]	TED	CY3-NYB-CY2	2.17	106.63	111.54	12	20
3	C	119[A]	TED	CY4-NYA-CY1	2.17	106.63	111.54	7	20
2	B	109[B]	TED	CY3-NYB-CYB	2.17	106.67	111.94	11	20
2	B	109[A]	TED	CY3-NYB-CY2	2.17	106.64	111.54	8	20
2	B	109[A]	TED	CY1-CY5-N13	2.16	120.44	115.52	4	6
3	C	119[A]	TED	OY1-CY5-CY1	2.10	117.39	121.08	18	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	10-C	3
3	8-C	3
3	13-C	3
3	17-C	3
3	11-C	3
3	6-C	3
3	14-C	3
3	18-C	3
3	16-C	3
3	4-C	3
3	15-C	3
3	12-C	3
2	17-B	3
2	13-B	3
3	7-C	3
3	5-C	3
3	3-C	3
2	3-B	3
2	2-B	3
3	20-C	3
3	1-C	3
2	8-B	3
3	19-C	3
3	2-C	3
2	18-B	3
2	10-B	3
2	9-B	3
2	11-B	3
2	1-B	3
2	6-B	3
3	9-C	3
2	4-B	3
2	19-B	3
2	7-B	3
2	5-B	3
2	20-B	3
2	12-B	3
2	16-B	3
2	14-B	3
2	15-B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
10	C	119[C]:TED	OY6	120:DC	P	20.80
8	C	119[B]:TED	OY4	120:DC	P	19.91
13	C	119[C]:TED	OY6	120:DC	P	19.06
17	C	119[B]:TED	OY6	120:DC	P	18.52
11	C	119[C]:TED	OY6	120:DC	P	18.51
6	C	119[C]:TED	OY4	120:DC	P	18.49
14	C	119[C]:TED	OY6	120:DC	P	18.44
18	C	119[C]:TED	OY6	120:DC	P	18.43
16	C	119[B]:TED	OY4	120:DC	P	17.88
4	C	119[C]:TED	OY6	120:DC	P	17.71
14	C	119[B]:TED	OY6	120:DC	P	17.53
6	C	119[A]:TED	OY4	120:DC	P	17.33
8	C	119[C]:TED	OY4	120:DC	P	17.15
15	C	119[C]:TED	OY4	120:DC	P	16.83
12	C	119[B]:TED	OY4	120:DC	P	16.78
17	C	119[C]:TED	OY6	120:DC	P	16.73
11	C	119[B]:TED	OY6	120:DC	P	16.50
17	B	109[B]:TED	OY6	110:DC	P	16.42
4	C	119[A]:TED	OY6	120:DC	P	16.40
12	C	119[A]:TED	OY4	120:DC	P	16.29
13	B	109[C]:TED	OY7	110:DC	P	16.28
7	C	119[A]:TED	OY6	120:DC	P	16.27
5	C	119[C]:TED	OY4	120:DC	P	16.23
3	C	119[B]:TED	OY4	120:DC	P	16.21
3	B	109[B]:TED	OY6	110:DC	P	16.20
2	B	109[B]:TED	OY6	110:DC	P	16.16
2	B	109[C]:TED	OY6	110:DC	P	16.15
20	C	119[C]:TED	OY4	120:DC	P	16.14
1	C	119[B]:TED	OY4	120:DC	P	16.13
13	B	109[B]:TED	OY7	110:DC	P	15.93
16	C	119[C]:TED	OY4	120:DC	P	15.92
8	B	109[A]:TED	OY4	110:DC	P	15.69
18	C	119[B]:TED	OY6	120:DC	P	15.65
19	C	119[A]:TED	OY4	120:DC	P	15.60
2	C	119[C]:TED	OY4	120:DC	P	15.56
10	C	119[A]:TED	OY6	120:DC	P	15.48
18	B	109[B]:TED	OY6	110:DC	P	15.33
10	B	109[A]:TED	OY6	110:DC	P	15.31
18	B	109[C]:TED	OY6	110:DC	P	15.29
9	B	109[C]:TED	OY4	110:DC	P	15.13
11	B	109[C]:TED	OY4	110:DC	P	15.10
13	C	119[A]:TED	OY6	120:DC	P	14.85
1	B	109[C]:TED	OY6	110:DC	P	14.78

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
6	B	109[A]:TED	OY6	110:DC	P	14.73
17	B	109[C]:TED	OY6	110:DC	P	14.60
2	C	119[A]:TED	OY4	120:DC	P	14.55
3	C	119[A]:TED	OY4	120:DC	P	14.43
17	C	119[A]:TED	OY6	120:DC	P	14.41
5	C	119[B]:TED	OY4	120:DC	P	14.39
9	C	119[C]:TED	OY4	120:DC	P	14.32
4	B	109[A]:TED	OY4	110:DC	P	14.15
19	B	109[C]:TED	OY6	110:DC	P	14.08
15	C	119[B]:TED	OY4	120:DC	P	14.02
7	C	119[C]:TED	OY6	120:DC	P	13.98
7	B	109[C]:TED	OY6	110:DC	P	13.95
20	C	119[B]:TED	OY4	120:DC	P	13.81
20	C	119[A]:TED	OY4	120:DC	P	13.78
5	B	109[C]:TED	OY6	110:DC	P	13.69
10	B	109[B]:TED	OY6	110:DC	P	13.68
6	C	119[B]:TED	OY4	120:DC	P	13.53
20	B	109[B]:TED	OY4	110:DC	P	13.38
19	C	119[B]:TED	OY4	120:DC	P	13.30
9	B	109[A]:TED	OY4	110:DC	P	13.27
2	C	119[B]:TED	OY4	120:DC	P	13.26
20	B	109[A]:TED	OY4	110:DC	P	13.24
19	B	109[B]:TED	OY6	110:DC	P	13.23
12	B	109[B]:TED	OY6	110:DC	P	13.21
16	C	119[A]:TED	OY4	120:DC	P	13.19
5	C	119[A]:TED	OY4	120:DC	P	13.18
3	C	119[C]:TED	OY4	120:DC	P	13.15
9	C	119[B]:TED	OY4	120:DC	P	13.14
5	B	109[A]:TED	OY6	110:DC	P	13.10
16	B	109[A]:TED	OY4	110:DC	P	13.07
1	C	119[A]:TED	OY4	120:DC	P	13.00
7	C	119[B]:TED	OY6	120:DC	P	12.95
1	C	119[C]:TED	OY4	120:DC	P	12.86
1	B	109[A]:TED	OY6	110:DC	P	12.70
14	B	109[A]:TED	OY4	110:DC	P	12.68
4	B	109[B]:TED	OY4	110:DC	P	12.66
16	B	109[B]:TED	OY4	110:DC	P	12.56
9	C	119[A]:TED	OY4	120:DC	P	12.54
8	C	119[A]:TED	OY4	120:DC	P	12.40
11	B	109[B]:TED	OY4	110:DC	P	12.18
8	B	109[B]:TED	OY4	110:DC	P	11.99
15	B	109[A]:TED	OY6	110:DC	P	11.98

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
8	B	109[C]:TED	OY4	110:DC	P	11.95
14	C	119[A]:TED	OY6	120:DC	P	11.94
19	C	119[C]:TED	OY4	120:DC	P	11.88
11	C	119[A]:TED	OY6	120:DC	P	11.84
14	B	109[B]:TED	OY4	110:DC	P	11.73
12	C	119[C]:TED	OY4	120:DC	P	11.72
15	B	109[B]:TED	OY6	110:DC	P	11.72
15	C	119[A]:TED	OY4	120:DC	P	11.54
16	B	109[C]:TED	OY4	110:DC	P	11.50
11	B	109[A]:TED	OY4	110:DC	P	11.49
1	B	109[B]:TED	OY6	110:DC	P	11.36
4	C	119[B]:TED	OY6	120:DC	P	11.24
2	B	109[A]:TED	OY6	110:DC	P	11.02
18	B	109[A]:TED	OY6	110:DC	P	11.01
13	C	119[B]:TED	OY6	120:DC	P	10.99
10	C	119[B]:TED	OY6	120:DC	P	10.97
14	B	109[C]:TED	OY4	110:DC	P	10.96
15	B	109[C]:TED	OY6	110:DC	P	10.96
7	B	109[A]:TED	OY6	110:DC	P	10.20
20	B	109[C]:TED	OY4	110:DC	P	9.97
9	B	109[B]:TED	OY4	110:DC	P	9.92
10	B	109[C]:TED	OY6	110:DC	P	9.80
3	B	109[C]:TED	OY6	110:DC	P	9.45
4	B	109[C]:TED	OY4	110:DC	P	9.43
7	B	109[B]:TED	OY6	110:DC	P	9.29
17	B	109[A]:TED	OY6	110:DC	P	9.25
12	B	109[C]:TED	OY6	110:DC	P	9.23
6	B	109[B]:TED	OY6	110:DC	P	8.80
12	B	109[A]:TED	OY6	110:DC	P	8.02
18	C	119[A]:TED	OY6	120:DC	P	8.00
19	B	109[A]:TED	OY6	110:DC	P	7.80
3	B	109[A]:TED	OY6	110:DC	P	7.65
6	B	109[C]:TED	OY6	110:DC	P	6.97
13	B	109[A]:TED	OY7	110:DC	P	6.79
5	B	109[B]:TED	OY6	110:DC	P	5.26

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	959
Number of shifts mapped to atoms	852
Number of unparsed shifts	0
Number of shifts with mapping errors	107
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- No matching atom found in the structure. All 107 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	SER	HA	4.5403	.	1
1	A	2	SER	HB2	3.8951	.	2
1	A	2	SER	HB3	3.8951	.	2
1	A	2	SER	C	174.2497	.	1
1	A	2	SER	CA	58.3359	.	1
1	A	2	SER	CB	63.9052	.	1
1	UNMAPPED	4	DA	H2	7.826	.	1
1	UNMAPPED	4	DA	H2'	2.887	.	2
1	UNMAPPED	4	DA	H2''	2.555	.	2
1	UNMAPPED	4	DA	H8	7.883	.	1
1	UNMAPPED	4	DA	H62	6.472	.	2
1	UNMAPPED	5	DT	H1'	5.913	.	1
1	UNMAPPED	5	DT	H2'	2.054	.	2
1	UNMAPPED	5	DT	H2''	2.536	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	UNMAPPED	5	DT	H3	13.984	.	1
1	UNMAPPED	5	DT	H5'	4.196	.	2
1	UNMAPPED	5	DT	H5''	4.196	.	2
1	UNMAPPED	5	DT	H6	7.264	.	1
1	UNMAPPED	5	DT	H71	1.206	.	1
1	UNMAPPED	5	DT	H72	1.206	.	1
1	UNMAPPED	5	DT	H73	1.206	.	1
1	UNMAPPED	6	5CM	H5A1	1.585	.	1
1	UNMAPPED	6	5CM	H5A2	1.585	.	1
1	UNMAPPED	6	5CM	H5A3	1.585	.	1
1	UNMAPPED	6	5CM	H6	7.208	.	1
1	UNMAPPED	6	5CM	H2'	2.09	.	2
1	UNMAPPED	6	5CM	H2''	2.602	.	2
1	UNMAPPED	6	5CM	HN41	6.759	.	2
1	UNMAPPED	6	5CM	HN42	9.212	.	2
1	UNMAPPED	7	DG	H1	13.024	.	1
1	UNMAPPED	7	DG	H8	7.82	.	1
1	UNMAPPED	8	DG	H1	12.694	.	1
1	UNMAPPED	8	DG	H2'	2.612	.	2
1	UNMAPPED	8	DG	H2''	2.531	.	2
1	UNMAPPED	9	DC	H2'	2.528	.	2
1	UNMAPPED	9	DC	H2''	2.226	.	2
1	UNMAPPED	9	DC	H5	5.425	.	1
1	UNMAPPED	9	DC	H6	7.562	.	1
1	UNMAPPED	9	DC	H41	7.888	.	2
1	UNMAPPED	9	DC	H42	6.456	.	2
1	UNMAPPED	10	THY	H6	7.542	.	1
1	UNMAPPED	10	THY	H71	1.755	.	1
1	UNMAPPED	10	THY	H72	1.755	.	1
1	UNMAPPED	10	THY	H73	1.755	.	1
1	UNMAPPED	10	THY	H3	13.883	.	1
1	UNMAPPED	10	THY	H1'	6.152	.	1
1	UNMAPPED	10	THY	H2'	2.226	.	2
1	UNMAPPED	10	THY	H2''	2.528	.	2
1	UNMAPPED	10	THY	H3'	4.888	.	1
1	UNMAPPED	11	DC	H2'	2.287	.	2
1	UNMAPPED	11	DC	H2''	2.623	.	2
1	UNMAPPED	11	DC	H5	5.889	.	1
1	UNMAPPED	11	DC	H5'	4.181	.	2
1	UNMAPPED	11	DC	H5''	4.054	.	2
1	UNMAPPED	11	DC	H6	7.692	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	UNMAPPED	1	DG	H1'	5.966	.	1
1	UNMAPPED	2	DA	H1'	5.565	.	1
1	UNMAPPED	2	DA	H2	7.875	.	1
1	UNMAPPED	2	DA	H2'	2.79	.	2
1	UNMAPPED	2	DA	H2''	2.459	.	2
1	UNMAPPED	2	DA	H8	8.228	.	1
1	UNMAPPED	3	DG	H1	12.901	.	1
1	UNMAPPED	3	DG	H1'	5.938	.	1
1	UNMAPPED	3	DG	H2'	2.457	.	1
1	UNMAPPED	3	DG	H5'	3.66	.	1
1	UNMAPPED	3	DG	H8	7.844	.	1
1	UNMAPPED	4	DC	H1'	5.428	.	1
1	UNMAPPED	4	DC	H2'	2.772	.	2
1	UNMAPPED	4	DC	H2''	2.478	.	2
1	UNMAPPED	4	DC	H3'	4.792	.	1
1	UNMAPPED	4	DC	H5	5.412	.	1
1	UNMAPPED	4	DC	H5'	4.094	.	2
1	UNMAPPED	4	DC	H5''	4.094	.	2
1	UNMAPPED	4	DC	H6	7.367	.	1
1	UNMAPPED	4	DC	H41	6.957	.	2
1	UNMAPPED	4	DC	H42	8.171	.	2
1	UNMAPPED	5	5CM	H5A1	1.637	.	1
1	UNMAPPED	5	5CM	H5A2	1.637	.	1
1	UNMAPPED	5	5CM	H5A3	1.637	.	1
1	UNMAPPED	5	5CM	H6	7.382	.	1
1	UNMAPPED	5	5CM	H1'	5.586	.	1
1	UNMAPPED	5	5CM	H2'	2.342	.	2
1	UNMAPPED	5	5CM	H2''	2.611	.	2
1	UNMAPPED	5	5CM	H3'	4.86	.	1
1	UNMAPPED	5	5CM	H5'	4.094	.	2
1	UNMAPPED	5	5CM	H5''	4.094	.	2
1	UNMAPPED	5	5CM	H41	6.814	.	2
1	UNMAPPED	5	5CM	H42	8.686	.	2
1	UNMAPPED	6	DG	H1	12.681	.	1
1	UNMAPPED	6	DG	H1'	5.83	.	1
1	UNMAPPED	6	DG	H2'	2.464	.	2
1	UNMAPPED	6	DG	H2''	2.668	.	2
1	UNMAPPED	6	DG	H8	7.855	.	1
1	UNMAPPED	7	DA	H1'	6.229	.	1
1	UNMAPPED	7	DA	H2	7.897	.	1
1	UNMAPPED	7	DA	H2'	2.625	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	UNMAPPED	7	DA	H2''	2.928	.	2
1	UNMAPPED	7	DA	H3'	5.056	.	1
1	UNMAPPED	7	DA	H8	8.255	.	1
1	UNMAPPED	7	DA	H62	7.902	.	2
1	UNMAPPED	9	THY	H6	7.248	.	1
1	UNMAPPED	9	THY	H71	1.248	.	1
1	UNMAPPED	9	THY	H72	1.248	.	1
1	UNMAPPED	9	THY	H73	1.248	.	1
1	UNMAPPED	9	THY	H3	13.445	.	1
1	UNMAPPED	9	THY	H2'	2.115	.	2
1	UNMAPPED	9	THY	H2''	2.468	.	2

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	71	-0.28 ± 0.28	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	62	-0.42 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	61	-0.12 ± 0.34	None needed (< 0.5 ppm)
^{15}N	61	-0.40 ± 0.37	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 64%, i.e. 799 atoms were assigned a chemical shift out of a possible 1252. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	309/327 (94%)	129/134 (96%)	123/132 (93%)	57/61 (93%)
Sidechain	424/483 (88%)	285/311 (92%)	132/147 (90%)	7/25 (28%)
Aromatic	66/79 (84%)	33/38 (87%)	32/40 (80%)	1/1 (100%)
Sugar	0/216 (0%)	0/126 (0%)	0/90 (0%)	0/0 (—%)
Base	0/147 (0%)	0/93 (0%)	0/29 (0%)	0/25 (0%)
Overall	799/1252 (64%)	447/702 (64%)	287/438 (66%)	65/112 (58%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 65%, i.e. 852 atoms were assigned a chemical shift out of a possible 1309. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	328/347 (95%)	137/142 (96%)	130/140 (93%)	61/65 (94%)
Sidechain	458/520 (88%)	308/334 (92%)	142/159 (89%)	8/27 (30%)
Aromatic	66/79 (84%)	33/38 (87%)	32/40 (80%)	1/1 (100%)
Sugar	0/216 (0%)	0/126 (0%)	0/90 (0%)	0/0 (—%)
Base	0/147 (0%)	0/93 (0%)	0/29 (0%)	0/25 (0%)
Overall	852/1309 (65%)	478/733 (65%)	304/458 (66%)	70/118 (59%)

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	39	SER	HA	2.00	2.50 – 6.44	-6.2
1	A	40	PRO	HD2	1.63	1.93 – 5.38	-5.8

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:

