



Full wwPDB NMR Structure Validation Report ⓘ

Jun 23, 2024 – 02:32 AM EDT

PDB ID : 6I4N
BMRB ID : 34327
Title : Dodecamer DNA containing the synthetic base pair P-Z in complex with a pyrrole-imidazole polyamide
Authors : Padroni, G.; Parkison, J.; Burley, G.A.
Deposited on : 2018-11-10

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 : 2022.3.0, CSD as543be (2022)
buster-report : 1.1.7 (2018)
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) : 2.37.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


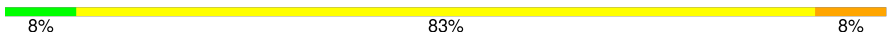
The overall completeness of chemical shifts assignment is 52%.

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

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	12	 92%8%
1	B	12	 8%83%8%

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

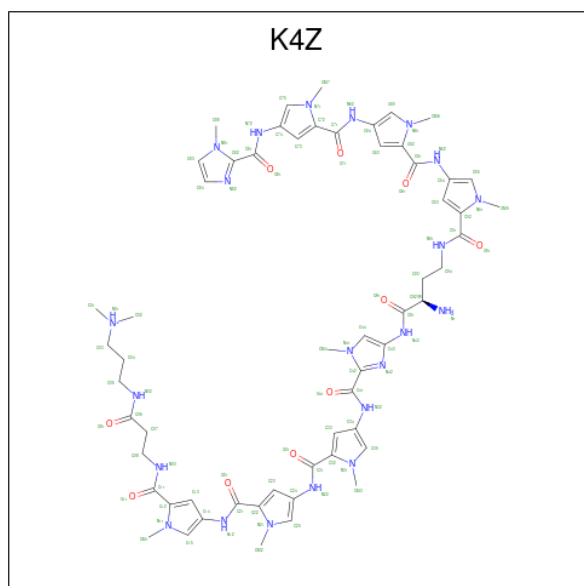
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 930 atoms, of which 348 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*A P*TP*CP*G)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	12	383	118	137	45	72	11	0
1	B	12	383	118	137	45	72	11	0

- Molecule 2 is 3-[3-[[4-[[4-[[4-[[2 {R}))-2-azaniumyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[(1-methylimidazol-2-yl)carbonylamino]pyrrol-2-yl]carbonylamino]pyrrol-2-yl]carbonylamino]pyrrol-2-yl]carbonylamino]butanoyl]amino]-1-methyl-imidazol-2-yl]carbonylamino]-1-methyl-pyrrol-2-yl]carbonylamino]-1-methyl-pyrrol-2-yl]carbonylamino]propanoylamino]propyl-dimethyl-azanium (three-letter code: K4Z) (formula: C₅₈H₇₄N₂₂O₁₀).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	B	1	164	58	74	22	10

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: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A: 

C1 G2 A3 T4 DP5 T6 A7 DZ8 A9 T10 C11 G12

- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain B: 

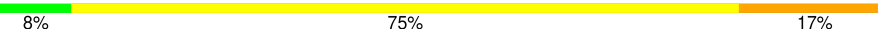
C13 G14 A15 T16 DP17 T18 A19 DZ20 A21 T22 C23 G24

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: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A: 

C1 G2 A3 T4 DP5 T6 A7 DZ8 A9 T10 C11 G12

- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain B: 

C13 G14 A15 T16 DP17 T18 A19 DZ20 A21 T22 C23 G24

4.2.2 Score per residue for model 2

- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A:  92% 8%



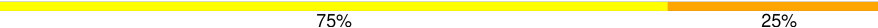
- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

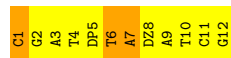
Chain B:  17% 75% 8%



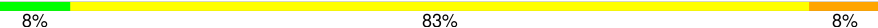
4.2.3 Score per residue for model 3

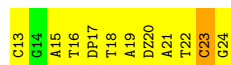
- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A:  75% 25%



- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

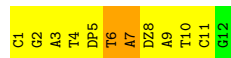
Chain B:  8% 83% 8%



4.2.4 Score per residue for model 4

- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A:  8% 75% 17%



- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain B:  8% 83% 8%



4.2.5 Score per residue for model 5

- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A:  92% 8%



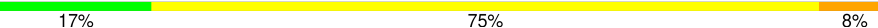
- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain B:  17% 75% 8%




4.2.6 Score per residue for model 6

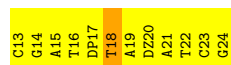
- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A:  17% 75% 8%



- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain B:  92% 8%



4.2.7 Score per residue for model 7

- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A:  8% 75% 17%



- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain B:  17% 67% 17%




4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A:  17% 67% 17%



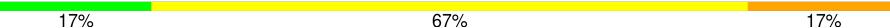
- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

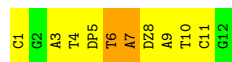
Chain B:  75% 25%



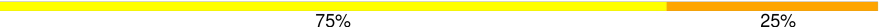
4.2.9 Score per residue for model 9

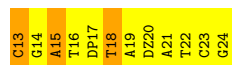
- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A:  17% 67% 17%



- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain B:  75% 25%



4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain A:  75% 25%



- Molecule 1: DNA (5'-D(*CP*GP*AP*TP*(DP)P*TP*AP*(DZ)P*AP*TP*CP*G)-3')

Chain B:  8% 75% 17%



5 Refinement protocol and experimental data overview

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

Of the 5000 calculated structures, 10 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
Amber	refinement	
Amber	structure calculation	
MARDIGRAS	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	370
Number of shifts mapped to atoms	273
Number of unparsed shifts	0
Number of shifts with mapping errors	97
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	52%

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: DZ, DP, K4Z

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	1.57±0.01	0±0/224 (0.0± 0.0%)	2.49±0.05	23±2/339 (6.8± 0.7%)
1	B	1.59±0.02	0±0/224 (0.0± 0.0%)	2.50±0.04	22±1/339 (6.4± 0.4%)
All	All	1.58	0/4480 (0.0%)	2.49	449/6780 (6.6%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.4±0.9
1	B	0.0±0.0	2.3±1.0
All	All	0	47

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	23	DC	O4'-C1'-N1	12.98	117.09	108.00	3	10
1	B	15	DA	N1-C6-N6	-9.10	113.14	118.60	5	10
1	A	9	DA	N1-C6-N6	-8.94	113.24	118.60	1	10
1	A	12	DG	O4'-C1'-N9	8.76	114.13	108.00	7	3
1	B	21	DA	N1-C6-N6	-8.38	113.57	118.60	6	10
1	B	14	DG	O4'-C1'-N9	8.32	113.83	108.00	10	4
1	A	7	DA	C5-C6-N1	8.30	121.85	117.70	7	10
1	A	3	DA	N1-C6-N6	-8.17	113.70	118.60	4	10
1	B	19	DA	C5-C6-N1	8.13	121.76	117.70	4	10
1	A	3	DA	C5-C6-N1	8.00	121.70	117.70	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	DC	N3-C2-O2	-7.95	116.33	121.90	9	10
1	A	11	DC	O4'-C1'-N1	7.94	113.56	108.00	10	8
1	A	4	DT	C6-C5-C7	-7.57	118.36	122.90	2	10
1	B	13	DC	N3-C2-O2	-7.54	116.62	121.90	8	10
1	A	10	DT	O4'-C1'-N1	7.45	113.22	108.00	2	8
1	B	23	DC	N3-C2-O2	-7.42	116.70	121.90	5	10
1	B	15	DA	C5-C6-N1	7.41	121.40	117.70	1	10
1	A	1	DC	N3-C2-O2	-7.38	116.73	121.90	3	10
1	B	21	DA	C5-C6-N1	7.37	121.39	117.70	10	10
1	A	9	DA	C5-C6-N1	7.22	121.31	117.70	4	10
1	B	15	DA	C4-C5-C6	-7.11	113.45	117.00	5	10
1	B	16	DT	C6-C5-C7	-7.03	118.68	122.90	3	10
1	B	22	DT	C6-C5-C7	-7.01	118.70	122.90	4	10
1	A	1	DC	O4'-C1'-N1	7.00	112.90	108.00	3	7
1	A	7	DA	N1-C6-N6	-6.86	114.48	118.60	9	10
1	B	22	DT	O4'-C1'-C2'	-6.84	100.42	105.90	8	8
1	B	18	DT	C6-C5-C7	-6.77	118.84	122.90	6	10
1	A	3	DA	C4-C5-C6	-6.76	113.62	117.00	5	10
1	B	13	DC	O4'-C1'-N1	6.73	112.71	108.00	10	2
1	B	19	DA	N1-C6-N6	-6.60	114.64	118.60	9	10
1	B	16	DT	O4'-C1'-N1	6.57	112.60	108.00	7	5
1	B	22	DT	O4'-C1'-N1	6.56	112.59	108.00	8	5
1	A	4	DT	O4'-C1'-N1	6.54	112.58	108.00	5	7
1	A	11	DC	N1-C2-O2	6.49	122.80	118.90	7	7
1	B	22	DT	N3-C2-O2	-6.46	118.42	122.30	8	10
1	B	16	DT	N3-C2-O2	-6.46	118.43	122.30	6	10
1	A	9	DA	C4-C5-C6	-6.32	113.84	117.00	3	10
1	B	13	DC	N1-C2-O2	6.23	122.64	118.90	6	10
1	A	3	DA	P-O3'-C3'	6.18	127.12	119.70	10	2
1	A	1	DC	N1-C2-O2	6.14	122.58	118.90	6	10
1	A	10	DT	C6-C5-C7	-6.14	119.22	122.90	6	10
1	B	23	DC	O4'-C1'-C2'	-6.05	101.06	105.90	3	4
1	A	6	DT	N3-C2-O2	-6.04	118.67	122.30	9	10
1	A	6	DT	C6-C5-C7	-6.03	119.28	122.90	5	10
1	A	10	DT	N3-C2-O2	-5.98	118.71	122.30	3	10
1	B	21	DA	C4-C5-C6	-5.95	114.02	117.00	6	10
1	A	7	DA	C4-C5-C6	-5.94	114.03	117.00	2	10
1	B	19	DA	C4-C5-C6	-5.93	114.03	117.00	9	10
1	A	4	DT	N3-C2-O2	-5.84	118.79	122.30	3	10
1	A	12	DG	N1-C6-O6	-5.62	116.53	119.90	7	5
1	B	18	DT	N3-C2-O2	-5.34	119.09	122.30	5	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	4	DT	O4'-C1'-C2'	-5.23	101.72	105.90	2	1
1	A	10	DT	O4'-C1'-C2'	-5.23	101.72	105.90	9	3
1	A	2	DG	O4'-C1'-N9	5.09	111.57	108.00	4	1
1	B	14	DG	N3-C2-N2	-5.09	116.34	119.90	6	1
1	B	23	DC	N1-C2-O2	5.03	121.92	118.90	5	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	6	DT	Sidechain	10
1	B	18	DT	Sidechain	8
1	B	24	DG	Sidechain	6
1	A	2	DG	Sidechain	5
1	B	23	DC	Sidechain	4
1	A	7	DA	Sidechain	4
1	A	1	DC	Sidechain	2
1	B	19	DA	Sidechain	2
1	A	4	DT	Sidechain	1
1	B	13	DC	Sidechain	1
1	B	15	DA	Sidechain	1
1	A	11	DC	Sidechain	1
1	A	12	DG	Sidechain	1
1	B	14	DG	Sidechain	1

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
All	All	5820	3480	2300	-

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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
1	DP	A	5	1	19,24,25	1.23±0.01	2±0 (10±0%)
1	DZ	A	8	1	18,23,24	1.13±0.02	1±0 (6±1%)
1	DZ	B	20	1	18,23,24	1.09±0.02	1±0 (5±0%)
1	DP	B	17	1	19,24,25	1.17±0.01	2±0 (10±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	Bond angles		
					Counts	RMSZ	#Z>2
1	DP	A	5	1	22,35,38	1.32±0.04	3±0 (15±2%)
1	DZ	A	8	1	17,33,36	1.07±0.03	0±0 (1±2%)
1	DZ	B	20	1	17,33,36	1.06±0.05	0±1 (1±3%)
1	DP	B	17	1	22,35,38	1.09±0.08	2±1 (10±3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DZ	A	8	1	-	0±0,7,25,26	0±0,2,2,2
1	DP	A	5	1	-	0±0,7,21,22	0±0,3,3,3
1	DP	B	17	1	-	0±0,7,21,22	0±0,3,3,3
1	DZ	B	20	1	-	0±0,7,25,26	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
1	A	5	DP	C4-N3	3.55	1.36	1.31	10	10
1	A	8	DZ	C6-C1	3.39	1.41	1.35	3	10
1	B	20	DZ	C6-C1	3.38	1.41	1.35	6	10
1	B	17	DP	C4-N3	3.09	1.35	1.31	2	10
1	B	17	DP	C7-C8	2.45	1.38	1.34	9	10
1	A	5	DP	C7-C8	2.23	1.38	1.34	6	10
1	A	8	DZ	ON1-N	2.08	1.21	1.35	10	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
1	A	5	DP	N5-C4-N3	2.88	123.84	126.21	1	10
1	A	5	DP	C7-N5-C4	2.62	109.15	105.99	10	10
1	B	17	DP	N5-C4-N3	2.49	124.15	126.21	2	4
1	A	5	DP	N2-C2-N1	2.49	113.25	117.09	3	7
1	B	17	DP	C7-N5-C4	2.27	108.73	105.99	7	8
1	B	17	DP	O6-C6-N1	2.26	118.76	122.33	1	10
1	A	8	DZ	C6-C5-N	2.24	121.26	116.10	10	3
1	A	5	DP	O6-C6-N1	2.21	118.84	122.33	6	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	20	DZ	C5-C4-N4	2.15	122.50	125.13	3	2
1	A	5	DP	O3'-C3'-C2'	2.07	118.08	110.88	8	1
1	B	20	DZ	C6-C5-N	2.06	120.84	116.10	3	1

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	20	DZ	C4-C5-N-ON2	1

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	K4Z	B	101	-	80,97,97	1.27±0.02	10±0 (12±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
2	K4Z	B	101	-	90,139,139	2.02±0.04	18±1 (19±1%)

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
2	K4Z	B	101	-	-	0±0,44,83,83	0±0,8,8,8

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	101	K4Z	C23-C24	3.80	1.42	1.39	1	10
2	B	101	K4Z	C73-C74	3.47	1.42	1.39	5	10
2	B	101	K4Z	C63-C64	3.46	1.42	1.39	9	10
2	B	101	K4Z	C13-C14	3.25	1.42	1.39	5	10
2	B	101	K4Z	C33-C34	3.20	1.42	1.39	2	10
2	B	101	K4Z	C82-C81	3.11	1.50	1.53	6	10
2	B	101	K4Z	C42-C41	3.06	1.50	1.53	4	10
2	B	101	K4Z	C53-C54	2.58	1.41	1.39	7	10
2	B	101	K4Z	C01-N01	2.50	1.53	1.46	8	10
2	B	101	K4Z	C02-N01	2.39	1.53	1.46	1	10
2	B	101	K4Z	C03-N01	2.03	1.53	1.46	8	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
2	B	101	K4Z	C35-C34-C33	6.57	109.26	106.05	3	10
2	B	101	K4Z	C55-C54-C53	6.22	109.09	106.05	10	10
2	B	101	K4Z	C75-C74-C73	6.21	109.09	106.05	7	10
2	B	101	K4Z	C13-C14-C15	5.90	108.93	106.05	8	10
2	B	101	K4Z	C65-C64-C63	5.27	108.63	106.05	10	10
2	B	101	K4Z	C13-C14-N12	5.03	124.18	131.11	2	10
2	B	101	K4Z	C53-C54-N52	4.98	124.25	131.11	5	10
2	B	101	K4Z	C44-C43-N43	4.89	124.36	131.11	2	10
2	B	101	K4Z	C25-C24-C23	4.77	108.39	106.05	8	10
2	B	101	K4Z	C63-C64-N62	4.45	124.98	131.11	3	10

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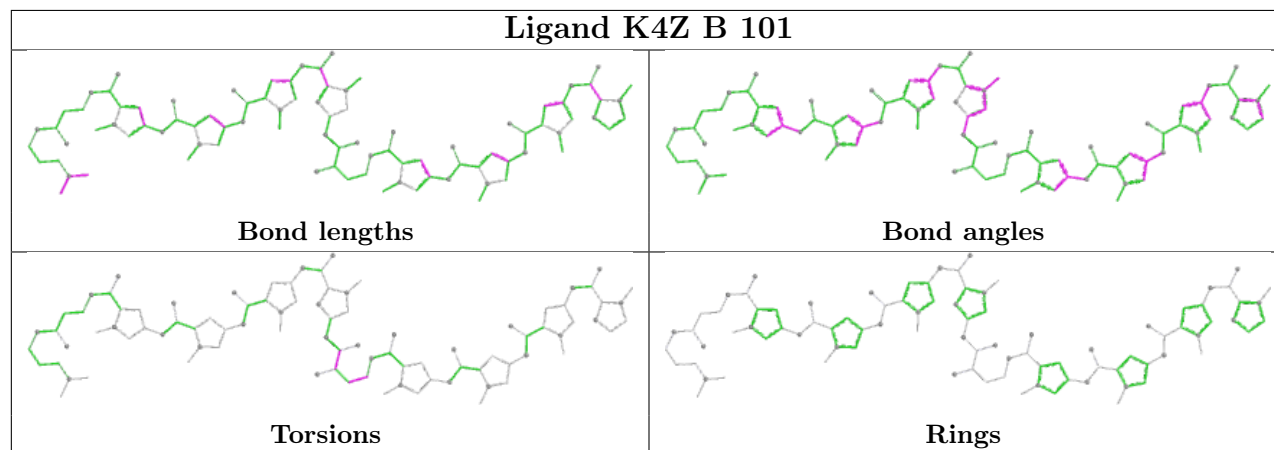
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	101	K4Z	C33-C34-N32	4.00	125.59	131.11	1	10
2	B	101	K4Z	C73-C74-N72	4.00	125.60	131.11	7	10
2	B	101	K4Z	C23-C24-N22	3.95	125.66	131.11	8	10
2	B	101	K4Z	C88-N81-C82	3.53	131.39	126.39	10	7
2	B	101	K4Z	CM4-N41-C42	2.70	130.22	126.39	8	10
2	B	101	K4Z	C44-N41-C42	2.69	105.69	108.60	6	10
2	B	101	K4Z	C93-C92-C91	2.63	116.14	110.76	2	2
2	B	101	K4Z	C83-N81-C82	2.53	105.68	108.56	10	10
2	B	101	K4Z	C42-C41-N32	2.48	116.38	113.11	7	5
2	B	101	K4Z	O81-C81-C82	2.05	124.17	121.66	10	1
2	B	101	K4Z	CM3-N31-C35	2.02	121.10	124.90	2	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 52% for the well-defined parts and 52% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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	370
Number of shifts mapped to atoms	273
Number of unparsed shifts	0
Number of shifts with mapping errors	97
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

- No matching atom found in the structure. All 97 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	DCZ	H1'	5.746	0.001	.
1	A	1	DCZ	H2'1	1.957	0.001	.
1	A	1	DCZ	H2'2	2.429	0.001	.
1	A	1	DCZ	H3'	4.719	0.001	.
1	A	1	DCZ	H5	5.893	0.001	.
1	A	1	DCZ	H6	7.637	0.001	.
1	A	1	DCZ	C1'	85.228	0.000	.
1	A	1	DCZ	C2'	37.27	0.000	.
1	A	1	DCZ	C3'	75.093	0.000	.
1	A	1	DCZ	C4'	85.679	0.000	.
1	A	1	DCZ	C5	96.826	0.000	.
1	A	1	DCZ	C6	140.43	0.000	.
1	A	1	DCZ	H4'	4.065	0.000	.
1	A	1	DCZ	H5'1	3.71	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	DT	H7	1.525	0.001	.
1	A	6	DT	H7	1.55	0.001	.
1	A	8	DZ	H4	7.611	0.001	.
1	A	10	DT	H7	1.363	0.001	.
1	B	13	DCZ	H1'	5.768	0.000	.
1	B	13	DCZ	H2'1	1.87	0.001	.
1	B	13	DCZ	H2'2	2.383	0.001	.
1	B	13	DCZ	H3'	4.707	0.001	.
1	B	13	DCZ	H5	5.869	0.001	.
1	B	13	DCZ	H6	7.586	0.001	.
1	B	13	DCZ	C1'	85.228	0.000	.
1	B	13	DCZ	C2'	37.158	0.000	.
1	B	13	DCZ	C3'	75.66	0.000	.
1	B	13	DCZ	C4'	85.54	0.000	.
1	B	13	DCZ	C5	96.969	0.000	.
1	B	13	DCZ	C5'	61.037	0.065	.
1	B	13	DCZ	C6	140.407	0.000	.
1	B	13	DCZ	H4'	4.071	0.000	.
1	B	13	DCZ	H5'1	3.737	0.000	.
1	B	16	DT	H7	1.552	0.001	.
1	B	18	DT	H7	1.445	0.001	.
1	B	20	DZ	H4	7.57	0.001	.
1	B	22	DT	H7	1.41	0.001	.
1	C	25	K4Z	C111	36.222	0.000	.
1	C	25	K4Z	C13	106.088	0.000	.
1	C	25	K4Z	C15	119.634	0.000	.
1	C	25	K4Z	C222	37.019	0.000	.
1	C	25	K4Z	C23	102.484	0.000	.
1	C	25	K4Z	C25	121.9	0.000	.
1	C	25	K4Z	C33	104.117	0.000	.
1	C	25	K4Z	C333	37.983	0.000	.
1	C	25	K4Z	C35	122.602	0.000	.
1	C	25	K4Z	C444	35.753	0.000	.
1	C	25	K4Z	C53	105.056	0.000	.
1	C	25	K4Z	C55	119.539	0.000	.
1	C	25	K4Z	C555	36.303	0.000	.
1	C	25	K4Z	C63	102.996	0.000	.
1	C	25	K4Z	C65	121.844	0.000	.
1	C	25	K4Z	C666	37.14	0.000	.
1	C	25	K4Z	C73	104.0	0.000	.
1	C	25	K4Z	C75	121.025	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	25	K4Z	C777	37.68	0.000	.
1	C	25	K4Z	C84	129.524	0.000	.
1	C	25	K4Z	C85	125.003	0.000	.
1	C	25	K4Z	C888	36.822	0.000	.
1	C	25	K4Z	H13	6.256	0.001	.
1	C	25	K4Z	H15	7.132	0.001	.
1	C	25	K4Z	H23	6.235	0.001	.
1	C	25	K4Z	H25	7.536	0.001	.
1	C	25	K4Z	H33	6.178	0.001	.
1	C	25	K4Z	H35	7.627	0.001	.
1	C	25	K4Z	H53	6.282	0.001	.
1	C	25	K4Z	H55	7.178	0.001	.
1	C	25	K4Z	H63	6.046	0.001	.
1	C	25	K4Z	H65	7.645	0.000	.
1	C	25	K4Z	H73	5.93	0.001	.
1	C	25	K4Z	H75	7.596	0.001	.
1	C	25	K4Z	H84	7.057	0.001	.
1	C	25	K4Z	H85	7.127	0.001	.
1	C	25	K4Z	HN09	8.132	0.000	.
1	C	25	K4Z	HN3	9.673	0.000	.
1	C	25	K4Z	M11	3.573	0.001	.
1	C	25	K4Z	M22	3.69	0.001	.
1	C	25	K4Z	M33	3.856	0.001	.
1	C	25	K4Z	M44	3.979	0.000	.
1	C	25	K4Z	M55	3.545	0.001	.
1	C	25	K4Z	M66	3.827	0.001	.
1	C	25	K4Z	M77	3.92	0.001	.
1	C	25	K4Z	M88	3.981	0.001	.
1	C	25	K4Z	bH2'	1.773	0.001	.
1	C	25	K4Z	bH2''	2.246	0.001	.
1	C	25	K4Z	bH3'	2.942	0.001	.
1	C	25	K4Z	bH3''	3.827	0.000	.
1	C	25	K4Z	dHpH2'	3.165	0.000	.
1	C	25	K4Z	dpC3	24.153	0.000	.
1	C	25	K4Z	dpH3'	1.954	0.001	.
1	C	25	K4Z	dpH3''	2.149	0.001	.
1	C	25	K4Z	dpH4'	2.984	0.000	.
1	C	25	K4Z	dpH4''	3.638	0.001	.
1	C	25	K4Z	t-H4'	2.878	0.001	.
1	C	25	K4Z	t-H4''	3.992	0.001	.
1	C	25	K4Z	t-H3'	1.526	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	25	K4Z	t-H3''	2.354	0.001	.

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

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 52%, i.e. 203 atoms were assigned a chemical shift out of a possible 392. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	150/240 (62%)	94/140 (67%)	56/100 (56%)	0/0 (—%)
Base	53/152 (35%)	27/92 (29%)	26/36 (72%)	0/24 (0%)
Overall	203/392 (52%)	121/232 (52%)	82/136 (60%)	0/24 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 203 atoms were assigned a chemical shift out of a possible 392. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	150/240 (62%)	94/140 (67%)	56/100 (56%)	0/0 (—%)
Base	53/152 (35%)	27/92 (29%)	26/36 (72%)	0/24 (0%)
Overall	203/392 (52%)	121/232 (52%)	82/136 (60%)	0/24 (0%)

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	6	DT	H4'	1.98	2.69 – 5.59	-7.5
1	B	18	DT	H4'	2.01	2.69 – 5.59	-7.4
1	A	7	DA	H4'	2.50	2.85 – 5.81	-6.2
1	B	19	DA	H4'	2.65	2.85 – 5.81	-5.7
1	B	21	DA	H4'	2.65	2.85 – 5.81	-5.7

7.1.5 Random Coil Index (RCI) plots

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins