Preliminary Full wwPDB NMR Structure Validation Report (i)

Sep 14, 2019 – 03:57 PM JST

Deposition ID : D_1300011914
PDB ID : *(not yet assigned)*

This is a Preliminary Full wwPDB NMR Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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

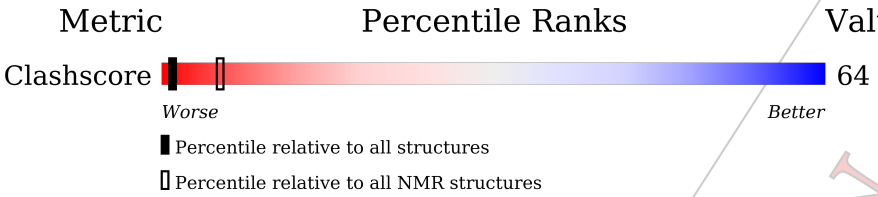
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.4
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 43%.

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	136327	12091

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	20	25% 70% 5%

2 Ensemble composition and analysis

This entry contains 20 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.

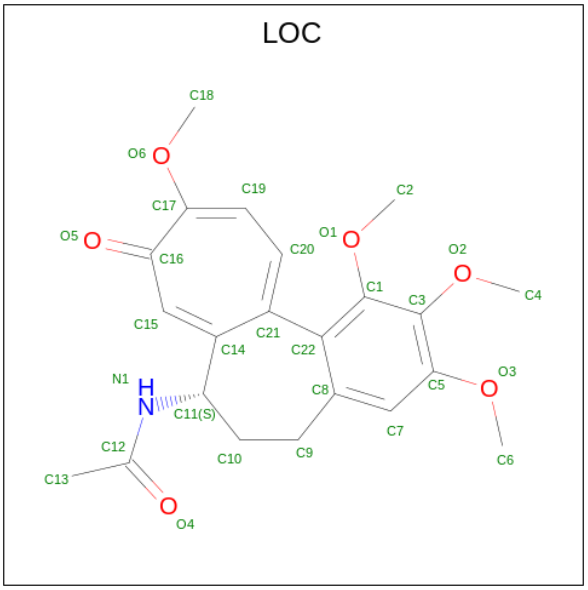
3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 703 atoms, of which 248 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	20	649	197	223	91	119	19	0

- Molecule 2 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]eth anamide (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	54	22	25	1	6

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

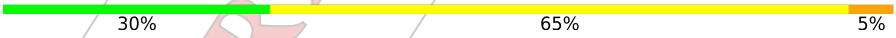
Chain A: 

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

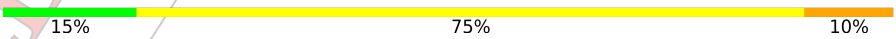
4.2.1 Score per residue for model 1

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 

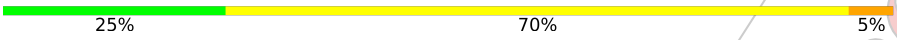
4.2.2 Score per residue for model 2

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 

4.2.3 Score per residue for model 3

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 

4.2.4 Score per residue for model 4

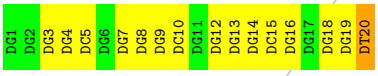
• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 

4.2.5 Score per residue for model 5

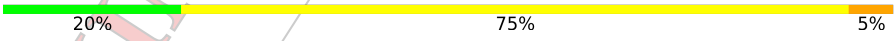
• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 



4.2.6 Score per residue for model 6

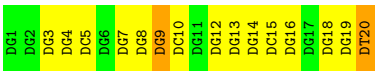
• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 

4.2.7 Score per residue for model 7

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 65% 10%



4.2.8 Score per residue for model 8

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 70% 5%

4.2.9 Score per residue for model 9

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 70% 5%

4.2.10 Score per residue for model 10

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 70% 5%

4.2.11 Score per residue for model 11

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 20% 70% 10%

4.2.12 Score per residue for model 12

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 70% 5%

4.2.13 Score per residue for model 13

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 70% 5%

4.2.14 Score per residue for model 14

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 70% 5%

4.2.15 Score per residue for model 15

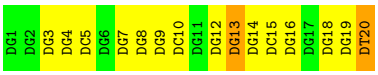
• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 70% 5%

4.2.16 Score per residue for model 16

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

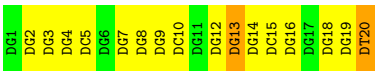
Chain A: 25% 65% 10%



4.2.17 Score per residue for model 17

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 20% 70% 10%



4.2.18 Score per residue for model 18

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 70% 5%

4.2.19 Score per residue for model 19

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 25% 70% 5%

4.2.20 Score per residue for model 20

• Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*T)-3')

Chain A: 30% 65% 5%

5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	D_1300011914_cs_P1.cif.V20
Number of chemical shift lists	1
Total number of shifts	205
Number of shifts mapped to atoms	205
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	43%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	455	248	248	45±4
All	All	9100	4960	4960	900

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 64.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:DG:H1'	1:A:15:DC:O2	0.94	1.61	3	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:DG:H5"	1:A:15:DC:O4'	0.83	1.74	7	8
1:A:101:LOC:C20	1:A:101:LOC:O1	0.76	2.31	4	10
1:A:101:LOC:O1	1:A:101:LOC:C20	0.76	2.30	1	10
1:A:9:DG:H4'	1:A:10:DC:O1P	0.72	1.84	2	15
1:A:16:DG:N9	1:A:18:DG:O2P	0.69	2.26	17	17
1:A:14:DG:H4'	1:A:15:DC:O4'	0.69	1.88	4	4
1:A:20:DT:N3	1:A:101:LOC:H6	0.67	2.04	10	20
1:A:13:DG:N2	1:A:16:DG:C2	0.67	2.62	2	14
1:A:14:DG:H5'	1:A:15:DC:O4'	0.66	1.90	3	5
1:A:13:DG:N2	1:A:16:DG:N2	0.65	2.44	5	20
1:A:14:DG:O1P	1:A:14:DG:H3'	0.65	1.90	2	2
1:A:19:DG:C8	1:A:20:DT:C4	0.64	2.86	20	20
1:A:7:DG:P	1:A:7:DG:H21	0.63	2.16	6	7
1:A:7:DG:H21	1:A:7:DG:P	0.62	2.16	2	13
1:A:19:DG:C8	1:A:20:DT:N3	0.62	2.68	10	20
1:A:20:DT:O2	1:A:101:LOC:H4A	0.61	1.95	16	20
1:A:15:DC:C2	1:A:16:DG:C8	0.61	2.88	6	2
1:A:13:DG:C2	1:A:16:DG:N2	0.61	2.69	11	20
1:A:15:DC:C4	1:A:16:DG:C6	0.61	2.88	16	7
1:A:13:DG:C6	1:A:101:LOC:C7	0.60	2.84	10	20
1:A:10:DC:O5'	1:A:10:DC:C6	0.60	2.55	9	7
1:A:15:DC:O2	1:A:16:DG:C5	0.59	2.56	19	1
1:A:16:DG:C4	1:A:18:DG:O2P	0.59	2.55	9	6
1:A:13:DG:N7	1:A:101:LOC:C10	0.58	2.66	10	20
1:A:15:DC:N3	1:A:16:DG:C6	0.58	2.71	20	8
1:A:14:DG:H4'	1:A:15:DC:O5'	0.58	1.97	3	1
1:A:15:DC:H6	1:A:15:DC:O5'	0.58	1.82	13	4
1:A:15:DC:C6	1:A:15:DC:O5'	0.58	2.56	13	3
1:A:10:DC:O5'	1:A:10:DC:H6	0.57	1.82	9	7
1:A:10:DC:C6	1:A:10:DC:O5'	0.57	2.58	13	5
1:A:13:DG:N2	1:A:16:DG:H22	0.56	1.98	16	12
1:A:16:DG:C8	1:A:18:DG:O2P	0.56	2.59	19	16
1:A:4:DG:O5'	1:A:4:DG:C8	0.56	2.59	4	9
1:A:19:DG:N7	1:A:20:DT:N3	0.56	2.53	20	20
1:A:4:DG:C8	1:A:4:DG:O5'	0.55	2.60	8	11
1:A:101:LOC:O3	1:A:101:LOC:H4A	0.55	2.00	10	10
1:A:13:DG:N1	1:A:101:LOC:C7	0.55	2.69	2	16
1:A:13:DG:C2	1:A:16:DG:C2	0.55	2.95	6	2
1:A:101:LOC:H4A	1:A:101:LOC:O3	0.54	2.00	2	10
1:A:13:DG:C5	1:A:101:LOC:H9	0.54	2.36	16	20
1:A:14:DG:C5'	1:A:15:DC:O4'	0.54	2.55	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:DC:C2	1:A:12:DG:O2P	0.54	2.61	3	17
1:A:10:DC:C1'	1:A:12:DG:O2P	0.54	2.56	13	17
1:A:10:DC:O2	1:A:12:DG:C8	0.54	2.60	17	3
1:A:13:DG:C8	1:A:101:LOC:H10A	0.54	2.38	12	20
1:A:15:DC:C2	1:A:16:DG:C5	0.54	2.96	20	6
1:A:15:DC:O5'	1:A:15:DC:H6	0.53	1.86	1	3
1:A:3:DG:O4'	1:A:5:DC:C5	0.53	2.62	1	20
1:A:10:DC:N1	1:A:12:DG:O2P	0.53	2.41	5	15
1:A:13:DG:N7	1:A:101:LOC:H10	0.53	2.18	8	17
1:A:13:DG:C4	1:A:101:LOC:H9	0.53	2.39	2	20
1:A:15:DC:C4	1:A:16:DG:O6	0.52	2.63	1	4
1:A:8:DG:N2	1:A:10:DC:O2	0.52	2.43	1	5
1:A:8:DG:H21	1:A:10:DC:C1'	0.52	2.18	17	3
1:A:15:DC:C2'	1:A:16:DG:C8	0.52	2.93	13	1
1:A:13:DG:C8	1:A:101:LOC:C10	0.52	2.93	9	18
1:A:10:DC:H6	1:A:10:DC:O5'	0.52	1.88	10	5
1:A:15:DC:O2	1:A:16:DG:C6	0.51	2.64	19	1
1:A:13:DG:N2	1:A:16:DG:N1	0.51	2.58	2	7
1:A:9:DG:O4'	1:A:10:DC:H5'	0.51	2.05	17	6
1:A:14:DG:C4'	1:A:15:DC:O4'	0.51	2.58	17	4
1:A:16:DG:C2'	1:A:18:DG:O2P	0.51	2.59	4	16
1:A:10:DC:C2'	1:A:12:DG:O2P	0.51	2.59	1	15
1:A:15:DC:O5'	1:A:15:DC:C6	0.50	2.64	1	2
1:A:5:DC:C2	1:A:7:DG:O1P	0.50	2.63	9	2
1:A:16:DG:C1'	1:A:18:DG:O2P	0.50	2.59	13	6
1:A:13:DG:N3	1:A:15:DC:O2	0.50	2.44	1	4
1:A:2:DG:H21	1:A:5:DC:N4	0.50	2.05	2	4
1:A:15:DC:N3	1:A:16:DG:O6	0.50	2.45	19	1
1:A:14:DG:H3'	1:A:15:DC:H5'	0.49	1.84	14	7
1:A:20:DT:C7	1:A:20:DT:O2P	0.49	2.60	2	8
1:A:13:DG:C2	1:A:101:LOC:H7	0.49	2.42	2	6
1:A:20:DT:O2P	1:A:20:DT:C7	0.48	2.61	10	7
1:A:8:DG:C2'	1:A:9:DG:O4'	0.48	2.61	5	20
1:A:16:DG:N2	1:A:18:DG:N7	0.48	2.61	2	6
1:A:15:DC:C2	1:A:16:DG:C6	0.48	3.02	19	1
1:A:13:DG:C6	1:A:101:LOC:C8	0.47	2.96	2	14
1:A:20:DT:C2	1:A:101:LOC:H6	0.47	2.44	12	17
1:A:8:DG:H21	1:A:10:DC:C2'	0.47	2.23	2	3
1:A:15:DC:N4	1:A:20:DT:O4	0.47	2.47	11	5
1:A:10:DC:O2	1:A:12:DG:H8	0.47	1.92	17	1
1:A:13:DG:C5	1:A:101:LOC:C9	0.46	2.98	2	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:DT:O2	1:A:101:LOC:C4	0.46	2.64	4	4
1:A:5:DC:O2	1:A:7:DG:O1P	0.45	2.34	14	20
1:A:20:DT:N3	1:A:101:LOC:C6	0.44	2.78	10	12
1:A:15:DC:C2	1:A:16:DG:N7	0.44	2.85	6	2
1:A:14:DG:O1P	1:A:14:DG:C3'	0.43	2.64	2	2
1:A:7:DG:O2P	1:A:7:DG:N2	0.43	2.52	6	1
1:A:13:DG:C1'	1:A:15:DC:O2	0.43	2.64	12	5
1:A:14:DG:H3'	1:A:14:DG:O1P	0.43	2.14	12	2
1:A:8:DG:H21	1:A:10:DC:C4'	0.43	2.25	2	3
1:A:7:DG:N2	1:A:7:DG:P	0.43	2.91	17	1
1:A:7:DG:N2	1:A:7:DG:O2P	0.43	2.52	2	5
1:A:16:DG:O6	1:A:19:DG:O2P	0.43	2.37	19	5
1:A:14:DG:H4'	1:A:15:DC:C5'	0.42	2.44	11	4
1:A:16:DG:N2	1:A:18:DG:C8	0.42	2.87	14	3
1:A:15:DC:O2	1:A:16:DG:C8	0.42	2.72	6	1
1:A:15:DC:H2"	1:A:16:DG:C8	0.42	2.50	13	1
1:A:8:DG:N2	1:A:10:DC:C1'	0.42	2.83	17	2
1:A:9:DG:N2	1:A:101:LOC:H10	0.41	2.30	16	1
1:A:14:DG:O1P	1:A:15:DC:H5'	0.41	2.15	14	1
1:A:13:DG:C2	1:A:101:LOC:C7	0.41	3.03	2	2

5.2 Torsion angles (i)

5.2.1 Protein backbone (i)

There are no protein molecules in this entry.

5.2.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.2.3 RNA (i)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains (i)

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

5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

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5.5 Other polymers (i)

There are no such molecules in this entry.

5.6 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 43% for the well-defined parts and 43% for the entire structure.

6.1 Chemical shift list 1

File name: D_1300011914_cs_P1.cif.V20

Chemical shift list name: *starch_ output*

6.1.1 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	205
Number of shifts mapped to atoms	205
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

6.1.2 Chemical shift referencing

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

6.1.3 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 43%, i.e. 177 atoms were assigned a chemical shift out of a possible 414. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	177/414 (43%)	177/254 (70%)	0/124 (0%)	0/36 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 177 atoms were assigned a chemical shift out of a possible 414. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	177/414 (43%)	177/254 (70%)	0/124 (0%)	0/36 (0%)

6.1.4 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.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	16	DG	H3'	5.90	5.66 – 4.16	6.6
1	A	15	DC	H5"	2.75	5.15 – 2.85	-5.4
1	A	14	DG	H2'	1.46	3.71 – 1.51	-5.2
1	A	5	DC	H6	6.32	8.72 – 6.32	-5.0

6.1.5 Random Coil Index (RCI) plots (i)

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