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Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1R9V
Title	:	NMR Structure of a D,L-Alternating Dodecamer of Norleucine
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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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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 was not calculated.

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	Percentile Ranks	Value
Clashscore		0
	Worse *Better*	

▌ Percentile relative to all structures
▐ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133

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	13	92% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
1	A	DNE	5	5	-

2 Ensemble composition and analysis (i)

This entry contains 5 models.

Cyrange was unable to find well-defined residues.

Error message: No amino acid residues in sequence.

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 234 atoms, of which 136 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BOC-(D-NLE-L-NLE)4-D-NLE(METHYL)-L-NLE-D-NLE-L -NLE METHYL ESTER.

Mol	Chain	Residues	Atoms					Trace
1	A	12	Total	C	H	N	O	0
			234	73	136	12	13	

4   Residue-property plots (i)

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: BOC-(D-NLE-L-NLE)4-D-NLE(METHYL)-L-NLE-D-NLE-L-NLE METHYL ESTER

Chain A: 92%   8%

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: BOC-(D-NLE-L-NLE)4-D-NLE(METHYL)-L-NLE-D-NLE-L-NLE METHYL ESTER

Chain A: 92%   8%

4.2.2   Score per residue for model 2

• Molecule 1: BOC-(D-NLE-L-NLE)4-D-NLE(METHYL)-L-NLE-D-NLE-L-NLE METHYL ESTER

Chain A: 92%   8%

4.2.3 Score per residue for model 3

• Molecule 1: BOC-(D-NLE-L-NLE)4-D-NLE(METHYL)-L-NLE-D-NLE-L-NLE METHYL ESTER

Chain A:

92%   8%

4.2.4 Score per residue for model 4

• Molecule 1: BOC-(D-NLE-L-NLE)4-D-NLE(METHYL)-L-NLE-D-NLE-L-NLE METHYL ESTER

Chain A:

92%   8%

4.2.5 Score per residue for model 5

• Molecule 1: BOC-(D-NLE-L-NLE)4-D-NLE(METHYL)-L-NLE-D-NLE-L-NLE METHYL ESTER

Chain A:

92%   8%

5   Refinement protocol and experimental data overview (i)

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

Of the 25 calculated structures, 5 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
DISCOVER	structure solution	2.9.7
DISCOVER	refinement	2.9.7

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)	BMRB entry 6039
Number of chemical shift lists	1
Total number of shifts	84
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	84
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	—

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

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: DNE, DNM, NLE, NLO

There are no covalent bond-length or bond-angle outliers.

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	2.0±0.0	0.0±0.0
All	All	10	0

There are no bond-length outliers.

There are no bond-angle outliers.

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	5	DNE	CA	5
1	A	9	DNM	CA	5

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	490	680	628	-

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)

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	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

11 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	DNE	A	1	1	5,7,8	0.47±0.02	0±0 (0±0%)
1	NLE	A	10	1	5,7,8	0.51±0.01	0±0 (0±0%)
1	DNE	A	11	1	5,7,8	0.46±0.01	0±0 (0±0%)
1	NLO	A	12	1	5,8,9	0.39±0.01	0±0 (0±0%)
1	NLE	A	2	1	5,7,8	0.49±0.00	0±0 (0±0%)
1	DNE	A	3	1	5,7,8	0.48±0.02	0±0 (0±0%)
1	NLE	A	4	1	5,7,8	0.48±0.01	0±0 (0±0%)
1	DNE	A	5	1	5,7,8	0.50±0.00	0±0 (0±0%)
1	NLE	A	6	1	5,7,8	0.53±0.03	0±0 (0±0%)
1	DNE	A	7	1	5,7,8	0.47±0.01	0±0 (0±0%)
1	NLE	A	8	1	5,7,8	0.48±0.00	0±0 (0±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	DNE	A	1	1	5,7,9	1.05±0.04	0±0 (0±0%)
1	NLE	A	10	1	5,7,9	0.77±0.12	0±0 (0±0%)
1	DNE	A	11	1	5,7,9	0.95±0.02	0±0 (0±0%)
1	NLO	A	12	1	3,9,10	0.38±0.02	0±0 (0±0%)
1	NLE	A	2	1	5,7,9	1.10±0.01	0±0 (0±0%)
1	DNE	A	3	1	5,7,9	0.86±0.06	0±0 (0±0%)
1	NLE	A	4	1	5,7,9	0.98±0.01	0±0 (0±0%)
1	DNE	A	5	1	5,7,9	1.06±0.02	0±0 (0±0%)
1	NLE	A	6	1	5,7,9	0.76±0.04	0±0 (0±0%)
1	DNE	A	7	1	5,7,9	0.95±0.04	0±0 (0±0%)
1	NLE	A	8	1	5,7,9	1.28±0.05	0±0 (0±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
1	DNE	A	1	1	-	0±0,4,6,8	0±0,0,0,0
1	NLE	A	10	1	-	0±0,4,6,8	0±0,0,0,0
1	DNE	A	11	1	-	0±0,4,6,8	0±0,0,0,0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NLO	A	12	1	-	0±0,4,8,10	0±0,0,0,0
1	NLE	A	2	1	-	0±0,4,6,8	0±0,0,0,0
1	DNE	A	3	1	-	0±0,4,6,8	0±0,0,0,0
1	NLE	A	4	1	-	0±0,4,6,8	0±0,0,0,0
1	DNE	A	5	1	1±0,1,1,2	0±0,4,6,8	0±0,0,0,0
1	NLE	A	6	1	-	0±0,4,6,8	0±0,0,0,0
1	DNE	A	7	1	-	0±0,4,6,8	0±0,0,0,0
1	NLE	A	8	1	-	0±0,4,6,8	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	5	DNE	CA	5

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

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

7.1 Chemical shift list 1

File name: BMRB entry 6039

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	84
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	84
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 84 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	11	DNE	HA	4.58	-1.0	1
UNMAPPED	12	NLE	CA	51.536	-1.0	1
UNMAPPED	4	NLE	HD2	1.26	-1.0	1
UNMAPPED	5	DNE	H	8.43	-1.0	1
UNMAPPED	11	DNE	CA	52.435	-1.0	1
UNMAPPED	6	NLE	HG2	1.75	-1.0	1
UNMAPPED	4	NLE	HB2	1.56	-1.0	1
UNMAPPED	8	NLE	H	8.44	-1.0	1
UNMAPPED	9	DNM	HB2	1.61	-1.0	1
UNMAPPED	9	DNM	HC3	3.01	-1.0	1
UNMAPPED	6	NLE	H	7.98	-1.0	1
UNMAPPED	8	NLE	CA	48.722	-1.0	1
UNMAPPED	9	DNM	HA	5.21	-1.0	1
UNMAPPED	2	NLE	CA	51.951	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	10	NLE	H	8.21	-1.0	1
UNMAPPED	3	DNE	HD2	1.34	-1.0	1
UNMAPPED	11	DNE	HD2	1.31	-1.0	1
UNMAPPED	6	NLE	CA	53.032	-1.0	1
UNMAPPED	10	NLE	HE1	0.86	-1.0	1
UNMAPPED	1	DNE	HA	4.2	-1.0	1
UNMAPPED	1	DNE	H	6.35	-1.0	1
UNMAPPED	10	NLE	HA	4.37	-1.0	1
UNMAPPED	2	NLE	HE1	0.88	-1.0	1
UNMAPPED	3	DNE	HB2	1.68	-1.0	1
UNMAPPED	4	NLE	HA	4.5	-1.0	1
UNMAPPED	10	NLE	HD2	1.26	-1.0	1
UNMAPPED	10	NLE	HG2	1.86	-1.0	1
UNMAPPED	9	DNM	HG2	1.84	-1.0	1
UNMAPPED	11	DNE	H	6.99	-1.0	1
UNMAPPED	7	DNE	CA	51.712	-1.0	1
UNMAPPED	12	NLE	HG2	1.82	-1.0	1
UNMAPPED	10	NLE	HB2	1.64	-1.0	1
UNMAPPED	11	DNE	HE1	0.88	-1.0	1
UNMAPPED	5	DNE	CA	51.204	-1.0	1
UNMAPPED	7	DNE	HD2	1.26	-1.0	1
UNMAPPED	7	DNE	HB2	1.59	-1.0	1
UNMAPPED	5	DNE	HG2	1.67	-1.0	1
UNMAPPED	1	DNE	HE1	0.9	-1.0	1
UNMAPPED	10	NLE	CA	53.028	-1.0	1
UNMAPPED	8	NLE	HA	4.64	-1.0	1
UNMAPPED	6	NLE	HD2	1.35	-1.0	1
UNMAPPED	2	NLE	HG2	1.64	-1.0	1
UNMAPPED	7	DNE	HG2	1.72	-1.0	1
UNMAPPED	8	NLE	HD2	1.26	-1.0	1
UNMAPPED	9	DNM	HE1	0.86	-1.0	1
UNMAPPED	4	NLE	HE1	0.85	-1.0	1
UNMAPPED	11	DNE	HB2	1.73	-1.0	1
UNMAPPED	3	DNE	HG2	1.95	-1.0	1
UNMAPPED	12	NLE	HE1	0.88	-1.0	1
UNMAPPED	4	NLE	H	6.64	-1.0	1
UNMAPPED	7	DNE	HE1	0.86	-1.0	1
UNMAPPED	7	DNE	H	7.72	-1.0	1
UNMAPPED	12	NLE	HB2	1.68	-1.0	1
UNMAPPED	4	NLE	CA	51.992	-1.0	1
UNMAPPED	4	NLE	HG2	1.72	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	12	NLE	HD2	1.3	-1.0	1
UNMAPPED	6	NLE	HA	4.35	-1.0	1
UNMAPPED	5	DNE	HE1	0.9	-1.0	1
UNMAPPED	6	NLE	HB2	1.83	-1.0	1
UNMAPPED	3	DNE	HE1	0.9	-1.0	1
UNMAPPED	8	NLE	HB2	1.79	-1.0	1
UNMAPPED	6	NLE	HE1	0.89	-1.0	1
UNMAPPED	11	DNE	HG2	1.86	-1.0	1
UNMAPPED	12	NLE	H	7.45	-1.0	1
UNMAPPED	3	DNE	CA	50.7	-1.0	1
UNMAPPED	2	NLE	HD2	1.35	-1.0	1
UNMAPPED	1	DNE	HD2	1.36	-1.0	1
UNMAPPED	3	DNE	H	8.24	-1.0	1
UNMAPPED	3	DNE	HA	4.48	-1.0	1
UNMAPPED	12	NLE	HA	4.45	-1.0	1
UNMAPPED	5	DNE	HA	4.35	-1.0	1
UNMAPPED	2	NLE	HB2	1.74	-1.0	1
UNMAPPED	5	DNE	HB2	1.7	-1.0	1
UNMAPPED	2	NLE	H	6.94	-1.0	1
UNMAPPED	2	NLE	HA	4.54	-1.0	1
UNMAPPED	5	DNE	HD2	1.22	-1.0	1
UNMAPPED	7	DNE	HA	4.41	-1.0	1
UNMAPPED	8	NLE	HG2	1.57	-1.0	1
UNMAPPED	1	DNE	CA	52.988	-1.0	1
UNMAPPED	9	DNM	HD2	1.2	-1.0	1
UNMAPPED	9	DNM	CA	54.873	-1.0	1
UNMAPPED	1	DNE	HB2	1.63	-1.0	1
UNMAPPED	8	NLE	HE1	0.84	-1.0	1
UNMAPPED	1	DNE	HG2	2.04	-1.0	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	12	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_\beta$	0	—	—
$^{13}C'$	0	—	—
^{15}N	0	—	—

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 —%, i.e. 0 atoms were assigned a chemical shift out of a possible 0. 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	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is —%, i.e. 0 atoms were assigned a chemical shift out of a possible 0. 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	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.