



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 01:58 PM BST

PDB ID : 1BFW
Title : RETRO-INVERSO ANALOGUE OF THE G-H LOOP OF VP1 IN FOOT-AND-MOUTH-DISEASE (FMD) VIRUS, NMR, 10 STRUCTURES
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Deposited on : 1998-05-22

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

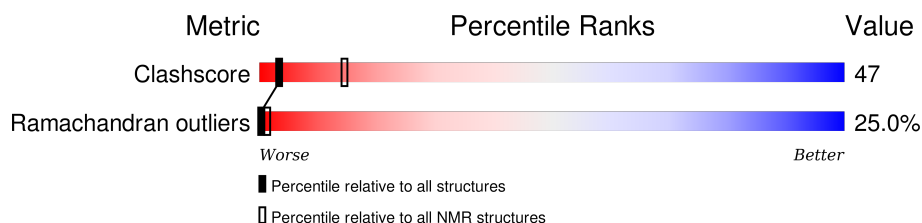
1 Overall quality at a glance

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	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975

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	20	

2 Ensemble composition and analysis ⓘ

This entry contains 10 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (3) was below the domain threshold value (8).

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 277 atoms, of which 138 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called VP1 PROTEIN.

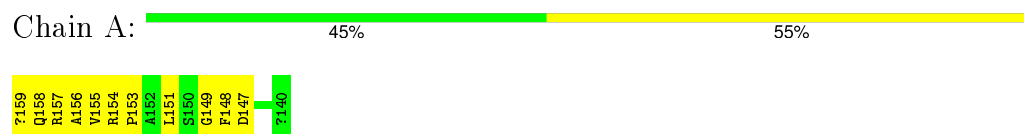
Mol	Chain	Residues	Atoms					Trace
1	A	20	Total	C	H	N	O	1
			277	84	138	29	26	

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: VP1 PROTEIN

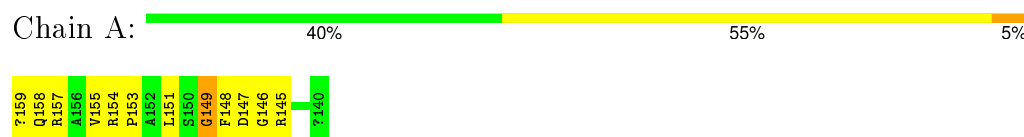


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

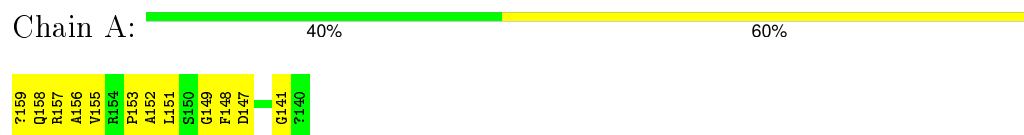
4.2.1 Score per residue for model 1

- Molecule 1: VP1 PROTEIN



4.2.2 Score per residue for model 2

- Molecule 1: VP1 PROTEIN



4.2.3 Score per residue for model 3

- Molecule 1: VP1 PROTEIN

Chain A:  55% 40% 5%



4.2.4 Score per residue for model 4

- Molecule 1: VP1 PROTEIN

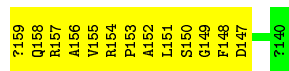
Chain A:  35% 65%



4.2.5 Score per residue for model 5

- Molecule 1: VP1 PROTEIN

Chain A:  35% 65%



4.2.6 Score per residue for model 6

- Molecule 1: VP1 PROTEIN

Chain A:  55% 45%



4.2.7 Score per residue for model 7

- Molecule 1: VP1 PROTEIN

Chain A:  20% 75% 5%



4.2.8 Score per residue for model 8

- Molecule 1: VP1 PROTEIN



4.2.9 Score per residue for model 9

- Molecule 1: VP1 PROTEIN



4.2.10 Score per residue for model 10

- Molecule 1: VP1 PROTEIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS, ANNEALING, MINIMIZATION*.

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *LEAST RESTRAINTS VIOLATIONS, TARGET FUNCTION*.

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

Software name	Classification	Version
DYANA	refinement	1.4
DYANA	structure solution	1.4

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 4213
Number of chemical shift lists	1
Total number of shifts	102
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	102
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DPR, DLE, DAL, DGN, DAS, DVA, DSN, LML, DAR, NH2, DPN

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

There are no bond-length outliers.

There are no bond-angle outliers.

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	139	138	130	13±5
All	All	1390	1380	1302	126

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 47.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:DPR:O	1:A:151:DLE:HD12	0.93	1.64	6	4
1:A:153:DPR:O	1:A:152:DAL:C	0.80	2.30	5	4
1:A:159:LML:HD23	1:A:151:DLE:HD13	0.70	1.62	6	1
1:A:155:DVA:HG12	1:A:153:DPR:HD2	0.68	1.65	5	5
1:A:157:DAR:CD	1:A:157:DAR:C	0.65	2.75	5	1
1:A:146:GLY:O	1:A:145:DAR:C	0.62	2.46	4	1
1:A:153:DPR:HG2	1:A:151:DLE:HD11	0.60	1.74	9	5
1:A:159:LML:C	1:A:158:DGN:CD	0.58	2.81	8	4
1:A:148:DPN:C	1:A:147:DAS:CG	0.56	2.82	6	10
1:A:156:DAL:C	1:A:155:DVA:CG2	0.56	2.84	6	7
1:A:149:GLY:O	1:A:148:DPN:CD1	0.55	2.54	5	4
1:A:149:GLY:C	1:A:148:DPN:CG	0.54	2.76	5	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:DLE:HD23	1:A:150:DSN:H	0.53	1.63	5	1
1:A:151:DLE:O	1:A:150:DSN:C	0.53	2.57	3	1
1:A:149:GLY:O	1:A:148:DPN:CD2	0.52	2.58	7	1
1:A:153:DPR:O	1:A:151:DLE:N	0.52	2.43	3	5
1:A:158:DGN:O	1:A:157:DAR:C	0.52	2.57	7	3
1:A:146:GLY:O	1:A:145:DAR:CZ	0.51	2.58	1	1
1:A:159:LML:HD21	1:A:151:DLE:HD12	0.51	1.82	5	1
1:A:155:DVA:HG13	1:A:153:DPR:HD2	0.51	1.82	3	1
1:A:159:LML:O	1:A:158:DGN:CD	0.50	2.60	8	4
1:A:149:GLY:O	1:A:148:DPN:C	0.50	2.60	4	1
1:A:154:DAR:N	1:A:154:DAR:NE	0.50	2.59	9	1
1:A:154:DAR:NE	1:A:154:DAR:N	0.49	2.59	5	1
1:A:148:DPN:O	1:A:147:DAS:CG	0.49	2.61	6	7
1:A:155:DVA:O	1:A:154:DAR:CD	0.49	2.60	4	2
1:A:149:GLY:O	1:A:148:DPN:CG	0.49	2.60	5	1
1:A:153:DPR:HD3	1:A:151:DLE:HD11	0.49	1.85	1	3
1:A:153:DPR:O	1:A:151:DLE:HB3	0.48	2.09	5	1
1:A:148:DPN:CD1	1:A:148:DPN:C	0.48	2.91	6	1
1:A:159:LML:C	1:A:158:DGN:OE1	0.47	2.63	4	1
1:A:155:DVA:O	1:A:154:DAR:NE	0.46	2.49	1	2
1:A:155:DVA:C	1:A:154:DAR:HG3	0.46	2.40	6	3
1:A:145:DAR:CG	1:A:145:DAR:O	0.45	2.64	4	1
1:A:155:DVA:C	1:A:154:DAR:HG2	0.45	2.42	1	2
1:A:158:DGN:CD	1:A:157:DAR:H	0.45	2.25	5	1
1:A:157:DAR:C	1:A:157:DAR:HD3	0.45	2.41	5	1
1:A:146:GLY:O	1:A:144:DVA:N	0.45	2.50	4	1
1:A:158:DGN:O	1:A:157:DAR:NE	0.44	2.50	2	1
1:A:153:DPR:CD	1:A:151:DLE:HD11	0.44	2.43	4	2
1:A:154:DAR:N	1:A:153:DPR:HD2	0.44	2.28	5	2
1:A:151:DLE:C	1:A:150:DSN:OG	0.44	2.65	5	1
1:A:154:DAR:C	1:A:151:DLE:HD22	0.43	2.43	5	1
1:A:153:DPR:HD3	1:A:151:DLE:CD1	0.43	2.44	6	4
1:A:145:DAR:HH11	1:A:144:DVA:CG2	0.42	2.28	7	1
1:A:145:DAR:O	1:A:143:GLY:N	0.42	2.53	7	1
1:A:155:DVA:C	1:A:154:DAR:CG	0.42	2.98	1	2
1:A:159:LML:HD13	1:A:159:LML:O1	0.41	2.14	7	2
1:A:155:DVA:C	1:A:154:DAR:HD3	0.41	2.45	7	1
1:A:158:DGN:C	1:A:157:DAR:HG2	0.41	2.46	2	2
1:A:157:DAR:C	1:A:157:DAR:HD2	0.41	2.46	5	1
1:A:145:DAR:N	1:A:145:DAR:NE	0.41	2.68	10	1
1:A:146:GLY:HA2	1:A:145:DAR:CZ	0.41	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:GLY:C	1:A:148:DPN:CD2	0.41	2.89	9	1
1:A:149:GLY:O	1:A:148:DPN:O	0.41	2.39	4	1
1:A:158:DGN:HG2	1:A:155:DVA:CG2	0.40	2.47	5	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4/20 (20%)	1±1 (22±13%)	2±1 (52±18%)	1±1 (25±22%)	0	1
All	All	40/200 (20%)	9 (22%)	21 (52%)	10 (25%)	0	1

All 3 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	149	GLY	6
1	A	141	GLY	3
1	A	146	GLY	1

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 ⓘ

There are no RNA molecules in this entry.

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

14 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	DSN	A	142	1	3,5,6	0.49±0.00	0±0 (0±0%)
1	DVA	A	144	1	5,6,7	0.53±0.00	0±0 (0±0%)
1	DAR	A	145	1	8,10,11	0.84±0.00	0±0 (0±0%)
1	DAS	A	147	1	5,7,8	0.63±0.01	0±0 (0±0%)
1	DPN	A	148	1	9,11,12	1.12±0.01	0±0 (0±0%)
1	DSN	A	150	1	3,5,6	0.48±0.00	0±0 (0±0%)
1	DLE	A	151	1	5,7,8	0.43±0.00	0±0 (0±0%)
1	DAL	A	152	1	1,4,5	0.80±0.01	0±0 (0±0%)
1	DPR	A	153	1	5,7,8	0.49±0.00	0±0 (0±0%)
1	DAR	A	154	1	8,10,11	0.83±0.00	0±0 (0±0%)
1	DVA	A	155	1	5,6,7	0.53±0.00	0±0 (0±0%)
1	DAL	A	156	1	1,4,5	0.80±0.01	0±0 (0±0%)
1	DAR	A	157	1	8,10,11	0.84±0.00	0±0 (0±0%)
1	DGN	A	158	1	6,8,9	0.46±0.01	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	DSN	A	142	1	3,5,7	1.19±0.01	0±0 (0±0%)
1	DVA	A	144	1	5,7,9	0.87±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	DAR	A	145	1	9,11,13	0.77±0.00	0±0 (0±0%)
1	DAS	A	147	1	6,8,10	0.88±0.00	0±0 (0±0%)
1	DPN	A	148	1	11,13,15	0.79±0.00	0±0 (0±0%)
1	DSN	A	150	1	3,5,7	1.19±0.00	0±0 (0±0%)
1	DLE	A	151	1	6,8,10	0.84±0.00	0±0 (0±0%)
1	DAL	A	152	1	1,4,6	0.58±0.00	0±0 (0±0%)
1	DPR	A	153	1	7,8,10	1.22±0.00	0±0 (0±0%)
1	DAR	A	154	1	9,11,13	0.77±0.00	0±0 (0±0%)
1	DVA	A	155	1	5,7,9	0.86±0.00	0±0 (0±0%)
1	DAL	A	156	1	1,4,6	0.58±0.00	0±0 (0±0%)
1	DAR	A	157	1	9,11,13	0.77±0.00	0±0 (0±0%)
1	DGN	A	158	1	7,9,11	0.99±0.00	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	DSN	A	142	1	-	0±0,2,4,6	0±0,0,0,0
1	DVA	A	144	1	-	0±0,4,6,8	0±0,0,0,0
1	DAR	A	145	1	-	0±0,7,9,11	0±0,0,0,0
1	DAS	A	147	1	-	0±0,4,6,8	0±0,0,0,0
1	DPN	A	148	1	-	0±0,4,6,8	0±0,1,1,1
1	DSN	A	150	1	-	0±0,2,4,6	0±0,0,0,0
1	DLE	A	151	1	-	0±0,4,6,8	0±0,0,0,0
1	DAL	A	152	1	-	0±0,0,2,4	0±0,0,0,0
1	DPR	A	153	1	-	0±0,0,9,11	0±0,1,1,1
1	DAR	A	154	1	-	0±0,7,9,11	0±0,0,0,0
1	DVA	A	155	1	-	0±0,4,6,8	0±0,0,0,0
1	DAL	A	156	1	-	0±0,0,2,4	0±0,0,0,0
1	DAR	A	157	1	-	0±0,7,9,11	0±0,0,0,0
1	DGN	A	158	1	-	0±0,5,7,9	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4213

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	102
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	102
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 102 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	6	DAR	HA	4.643	0.007	1
UNMAPPED	6	DAR	H	8.551	0.006	1
UNMAPPED	12	DPN	H	8.306	0.006	1
UNMAPPED	3	DAR	HE	7.831	0.005	1
UNMAPPED	17	GLY	H	8.693	0.006	1
UNMAPPED	6	DAR	HD3	3.208	0.007	1
UNMAPPED	6	DAR	HB3	1.841	0.008	1
UNMAPPED	3	DAR	HB3	1.802	0.007	2
UNMAPPED	9	DLE	HG	1.635	0.005	1
UNMAPPED	7	DPR	HG2	2.018	0.008	1
UNMAPPED	10	DSN	HB2	3.949	0.017	2
UNMAPPED	7	DPR	HB3	1.885	0.008	2
UNMAPPED	7	DPR	HD3	3.639	0.009	2
UNMAPPED	4	DAL	HB	1.373	0.004	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	9	DLE	HB3	1.676	0.015	1
UNMAPPED	2	DGN	HB2	2.395	0.005	2
UNMAPPED	18	DSN	HB2	3.929	0.001	2
UNMAPPED	12	DPN	HB2	3.114	0.013	2
UNMAPPED	14	GLY	H	7.954	0.007	1
UNMAPPED	15	DAR	HB3	1.83	0.008	1
UNMAPPED	19	GLY	HA2	3.923	0.012	1
UNMAPPED	3	DAR	H	8.84	0.006	1
UNMAPPED	11	GLY	H	8.539	0.006	1
UNMAPPED	15	DAR	HG2	1.605	0.007	1
UNMAPPED	12	DPN	HE2	7.359	0.003	1
UNMAPPED	12	DPN	HE1	7.359	0.003	1
UNMAPPED	10	DSN	H	8.442	0.014	1
UNMAPPED	9	DLE	HD1	0.926	0.005	1
UNMAPPED	15	DAR	HE	7.412	0.006	1
UNMAPPED	9	DLE	HD2	0.873	0.008	1
UNMAPPED	6	DAR	HG2	1.729	0.005	2
UNMAPPED	6	DAR	HE	7.256	0.005	1
UNMAPPED	16	DVA	H	8.358	0.006	1
UNMAPPED	19	GLY	H	8.67	0.006	1
UNMAPPED	15	DAR	H	8.128	0.003	1
UNMAPPED	5	DVA	H	8.135	0.006	1
UNMAPPED	6	DAR	HD2	3.208	0.007	1
UNMAPPED	6	DAR	HB2	1.841	0.008	1
UNMAPPED	8	DAL	H	8.573	0.004	1
UNMAPPED	9	DLE	HA	4.38	0.005	1
UNMAPPED	1	LML	HD1	0.896	0.005	1
UNMAPPED	7	DPR	HA	4.382	0.005	1
UNMAPPED	7	DPR	HG3	2.018	0.008	1
UNMAPPED	7	DPR	HB2	2.307	0.015	2
UNMAPPED	13	DAS	HB3	2.672	0.003	1
UNMAPPED	7	DPR	HD2	3.838	0.008	2
UNMAPPED	1	LML	HB2	1.851	0.008	2
UNMAPPED	3	DAR	HG3	1.666	0.008	1
UNMAPPED	3	DAR	HD2	3.187	0.006	1
UNMAPPED	12	DPN	HB3	3.049	0.008	2
UNMAPPED	19	GLY	HA3	3.923	0.012	1
UNMAPPED	14	GLY	HA3	3.837	0.001	2
UNMAPPED	12	DPN	HA	4.604	0.007	1
UNMAPPED	2	DGN	HG3	1.938	0.007	1
UNMAPPED	13	DAS	H	8.396	0.006	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	15	DAR	HD2	3.179	0.009	1
UNMAPPED	2	DGN	HG2	1.938	0.007	1
UNMAPPED	5	DVA	HB	2.04	0.012	1
UNMAPPED	5	DVA	HA	4.052	0.007	1
UNMAPPED	15	DAR	HA	4.334	0.007	1
UNMAPPED	12	DPN	HD1	7.259	0.003	1
UNMAPPED	6	DAR	HG3	1.666	0.005	2
UNMAPPED	12	DPN	HD2	7.259	0.003	1
UNMAPPED	16	DVA	HG2	0.961	0.01	1
UNMAPPED	9	DLE	H	8.448	0.005	1
UNMAPPED	8	DAL	HA	4.281	0.002	1
UNMAPPED	16	DVA	HA	4.102	0.004	1
UNMAPPED	16	DVA	HB	2.086	0.014	1
UNMAPPED	18	DSN	H	8.453	0.005	1
UNMAPPED	2	DGN	H	8.766	0.006	1
UNMAPPED	2	DGN	HA	4.384	0.008	1
UNMAPPED	10	DSN	HG	1.454	0.0	1
UNMAPPED	3	DAR	HA	4.209	0.007	1
UNMAPPED	10	DSN	HA	4.429	0.012	1
UNMAPPED	3	DAR	HB2	1.872	0.01	2
UNMAPPED	1	LML	HD2	0.896	0.005	1
UNMAPPED	13	DAS	HB2	2.672	0.003	1
UNMAPPED	10	DSN	HB3	3.868	0.012	2
UNMAPPED	13	DAS	HA	4.529	0.008	1
UNMAPPED	4	DAL	HA	4.281	0.001	1
UNMAPPED	9	DLE	HB2	1.676	0.015	1
UNMAPPED	1	LML	HB3	1.585	0.007	2
UNMAPPED	3	DAR	HG2	1.666	0.008	1
UNMAPPED	3	DAR	HD3	3.187	0.006	1
UNMAPPED	2	DGN	HB3	2.26	0.011	2
UNMAPPED	18	DSN	HB3	3.875	0.006	2
UNMAPPED	4	DAL	H	8.221	0.004	1
UNMAPPED	15	DAR	HG3	1.605	0.007	1
UNMAPPED	15	DAR	HB2	1.83	0.008	1
UNMAPPED	16	DVA	HG1	0.983	0.001	1
UNMAPPED	11	GLY	HA2	3.933	0.002	1
UNMAPPED	18	DSN	HA	4.415	0.01	1
UNMAPPED	14	GLY	HA2	3.906	0.0	2
UNMAPPED	15	DAR	HD3	3.179	0.009	1
UNMAPPED	5	DVA	HG2	0.918	0.014	1
UNMAPPED	1	LML	HG	1.444	0.008	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	5	DVA	HG1	0.955	0.005	1
UNMAPPED	17	GLY	HA2	4.049	0.012	2
UNMAPPED	17	GLY	HA3	3.978	0.002	2
UNMAPPED	1	LML	HA	3.398	0.005	1
UNMAPPED	11	GLY	HA3	3.933	0.002	1
UNMAPPED	8	DAL	HB	1.389	0.006	1

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 20. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/20 (0%)	0/8 (0%)	0/8 (0%)	0/4 (0%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/20 (0%)	0/8 (0%)	0/8 (0%)	0/4 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 20. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/20 (0%)	0/8 (0%)	0/8 (0%)	0/4 (0%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/20 (0%)	0/8 (0%)	0/8 (0%)	0/4 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

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.