



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2KQL
Title : Maurocalcine in D configuration from Scorpio maurus palmatus
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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 ⓘ 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

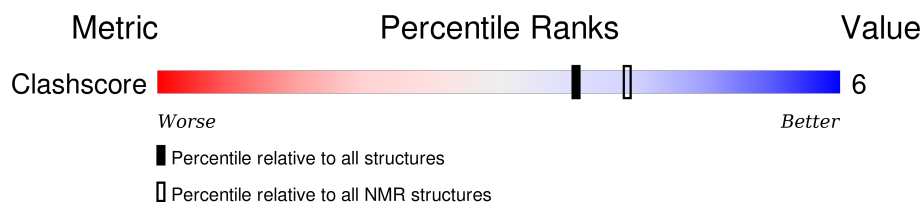
1 Overall quality at a glance

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

WHATHAPPENED 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	DIL	28	20	-
1	A	DTH	26	20	-

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. This entry does not contain protein, 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 is only 1 type of molecule in this entry. The entry contains 542 atoms, of which 278 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein (with D amino acids) called D-MAUROCALCINE.

Mol	Chain	Residues	Atoms						Trace
1	A	33	Total	C	H	N	O	S	0
			542	156	278	56	46	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.

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

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.2 Score per residue for model 2

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.3 Score per residue for model 3

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.4 Score per residue for model 4

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.5 Score per residue for model 5

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.6 Score per residue for model 6

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.7 Score per residue for model 7

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.8 Score per residue for model 8

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.9 Score per residue for model 9

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.10 Score per residue for model 10

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.11 Score per residue for model 11

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.12 Score per residue for model 12

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.13 Score per residue for model 13

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.14 Score per residue for model 14

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.15 Score per residue for model 15

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.16 Score per residue for model 16

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.17 Score per residue for model 17

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.18 Score per residue for model 18

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.19 Score per residue for model 19

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

4.2.20 Score per residue for model 20

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
X-PLOR NIH	refinement	2.21

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 16605
Number of chemical shift lists	1
Total number of shifts	254
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	254
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 [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DIL, DLE, DTH, DPR, DHI, DCY, DGL, DSN, DAR, DAS, DSG, DLY

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	40	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	26	DTH	CB	20
1	A	28	DIL	CB	20

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
1	A	264	278	245	3±2
All	All	5280	5560	4909	57

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:DCY:HB3	1:A:32:DCY:SG	0.76	2.20	2	2
1:A:10:DCY:SG	1:A:32:DCY:HB2	0.74	2.22	20	1
1:A:13:DSG:O	1:A:19:DLY:HA	0.63	1.92	10	18
1:A:4:DLE:HB2	1:A:16:DCY:SG	0.59	2.38	5	1
1:A:3:DCY:HA	1:A:15:DAS:O	0.59	1.98	10	1
1:A:20:DLY:O	1:A:32:DCY:HA	0.55	2.01	2	4
1:A:13:DSG:HA	1:A:21:DCY:SG	0.55	2.41	14	3
1:A:10:DCY:HA	1:A:32:DCY:SG	0.52	2.45	5	3
1:A:23:DAR:HA	1:A:29:DGL:O	0.49	2.08	2	2
1:A:7:DLE:C	1:A:8:DLY:HD2	0.48	2.38	20	4
1:A:14:DLY:O	1:A:14:DLY:HD3	0.48	2.08	10	2
1:A:21:DCY:SG	1:A:30:DLY:HE3	0.48	2.49	16	1
1:A:21:DCY:SG	1:A:32:DCY:SG	0.47	3.12	5	1
1:A:21:DCY:SG	1:A:30:DLY:HE2	0.46	2.51	8	1
1:A:8:DLY:O	1:A:31:DAR:HB3	0.45	2.12	7	1
1:A:10:DCY:SG	1:A:30:DLY:HG3	0.44	2.53	10	1
1:A:13:DSG:OD1	1:A:21:DCY:HB3	0.43	2.13	19	2
1:A:23:DAR:HB2	1:A:28:DIL:O	0.43	2.14	8	1
1:A:16:DCY:SG	1:A:21:DCY:HB2	0.43	2.54	8	1
1:A:16:DCY:SG	1:A:21:DCY:SG	0.42	3.18	15	1
1:A:5:DPR:O	1:A:8:DLY:HB2	0.42	2.14	16	1
1:A:4:DLE:HD13	1:A:9:DLE:O	0.41	2.15	4	1
1:A:6:DHI:HB2	1:A:33:DAR:O	0.41	2.16	12	1
1:A:21:DCY:SG	1:A:30:DLY:HD2	0.40	2.56	2	1
1:A:22:DLY:HB2	1:A:33:DAR:NH2	0.40	2.32	4	1
1:A:4:DLE:HD23	1:A:10:DCY:HA	0.40	1.94	14	1

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 ⓘ

31 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	DCY	A	10	1	3,5,6	0.88±0.25	0±0 (0±0%)
1	DLY	A	11	1	6,8,9	0.49±0.13	0±0 (0±0%)
1	DGL	A	12	1	3,8,9	0.78±0.22	0±0 (0±0%)
1	DSG	A	13	1	5,7,8	0.58±0.15	0±0 (0±0%)
1	DLY	A	14	1	6,8,9	0.55±0.16	0±0 (0±0%)
1	DAS	A	15	1	2,7,8	0.45±0.17	0±0 (0±0%)
1	DCY	A	16	1	3,5,6	0.87±0.41	0±0 (0±0%)
1	DCY	A	17	1	3,5,6	0.93±0.21	0±0 (0±0%)
1	DSN	A	18	1	3,5,6	0.56±0.10	0±0 (0±0%)
1	DLY	A	19	1	6,8,9	0.54±0.15	0±0 (0±0%)
1	DAS	A	2	1	2,7,8	0.74±0.17	0±0 (0±0%)
1	DLY	A	20	1	6,8,9	0.47±0.09	0±0 (0±0%)
1	DCY	A	21	1	3,5,6	0.81±0.20	0±0 (0±0%)
1	DLY	A	22	1	6,8,9	0.47±0.15	0±0 (0±0%)
1	DAR	A	23	1	8,10,11	0.63±0.11	0±0 (0±0%)
1	DAR	A	24	1	8,10,11	0.70±0.16	0±0 (0±0%)
1	DTH	A	26	1	5,6,7	0.79±0.10	0±0 (0±0%)
1	DSG	A	27	1	5,7,8	0.65±0.14	0±0 (0±0%)
1	DIL	A	28	1	6,7,8	0.74±0.14	0±0 (0±0%)
1	DGL	A	29	1	3,8,9	0.81±0.19	0±0 (0±0%)
1	DCY	A	3	1	3,5,6	1.33±0.28	0±0 (0±0%)
1	DLY	A	30	1	6,8,9	0.58±0.14	0±0 (0±0%)
1	DAR	A	31	1	8,10,11	0.67±0.17	0±0 (0±0%)
1	DCY	A	32	1	3,5,6	0.79±0.25	0±0 (0±0%)
1	DAR	A	33	1	8,11,11	0.54±0.12	0±0 (0±0%)
1	DLE	A	4	1	5,7,8	0.54±0.13	0±0 (0±0%)
1	DPR	A	5	1	5,7,8	0.56±0.04	0±0 (0±0%)
1	DHI	A	6	1	3,10,11	0.81±0.17	0±0 (0±0%)
1	DLE	A	7	1	5,7,8	0.51±0.09	0±0 (0±0%)
1	DLY	A	8	1	6,8,9	0.58±0.19	0±0 (0±0%)
1	DLE	A	9	1	5,7,8	0.81±0.15	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	DCY	A	10	1	3,5,7	1.38±0.14	0±0 (0±0%)
1	DLY	A	11	1	6,8,10	0.78±0.09	0±0 (0±0%)
1	DGL	A	12	1	4,9,11	1.12±0.11	0±0 (0±0%)
1	DSG	A	13	1	6,8,10	0.94±0.09	0±0 (0±0%)
1	DLY	A	14	1	6,8,10	0.82±0.06	0±0 (0±0%)
1	DAS	A	15	1	2,8,10	1.16±0.12	0±0 (0±0%)
1	DCY	A	16	1	3,5,7	1.32±0.19	0±0 (0±0%)
1	DCY	A	17	1	3,5,7	1.07±0.17	0±0 (0±0%)
1	DSN	A	18	1	3,5,7	1.25±0.14	0±0 (0±0%)
1	DLY	A	19	1	6,8,10	0.88±0.07	0±0 (0±0%)
1	DAS	A	2	1	2,8,10	1.31±0.19	0±0 (0±0%)
1	DLY	A	20	1	6,8,10	0.80±0.06	0±0 (0±0%)
1	DCY	A	21	1	3,5,7	1.20±0.09	0±0 (0±0%)
1	DLY	A	22	1	6,8,10	0.91±0.08	0±0 (0±0%)
1	DAR	A	23	1	9,11,13	0.77±0.10	0±0 (0±0%)
1	DAR	A	24	1	9,11,13	0.76±0.12	0±0 (0±0%)
1	DTH	A	26	1	5,7,9	0.90±0.18	0±0 (0±0%)
1	DSG	A	27	1	6,8,10	1.04±0.12	0±0 (0±0%)
1	DIL	A	28	1	7,8,10	0.82±0.22	0±0 (0±0%)
1	DGL	A	29	1	4,9,11	1.06±0.16	0±0 (0±0%)
1	DCY	A	3	1	3,5,7	1.30±0.14	0±0 (0±0%)
1	DLY	A	30	1	6,8,10	0.92±0.12	0±0 (0±0%)
1	DAR	A	31	1	9,11,13	0.71±0.08	0±0 (0±0%)
1	DCY	A	32	1	3,5,7	1.43±0.18	0±0 (0±0%)
1	DAR	A	33	1	7,13,13	0.39±0.14	0±0 (0±0%)
1	DLE	A	4	1	6,8,10	1.07±0.14	0±0 (0±0%)
1	DPR	A	5	1	7,8,10	1.21±0.06	0±0 (0±0%)
1	DHI	A	6	1	2,12,14	1.56±0.13	0±0 (0±0%)
1	DLE	A	7	1	6,8,10	0.97±0.19	0±0 (0±0%)
1	DLY	A	8	1	6,8,10	1.05±0.06	0±0 (0±0%)
1	DLE	A	9	1	6,8,10	1.37±0.28	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	DCY	A	10	1	-	0±0,1,4,6	0±0,0,0,0
1	DLY	A	11	1	-	0±0,5,7,9	0±0,0,0,0
1	DGL	A	12	1	-	0±0,3,7,9	0±0,0,0,0
1	DSG	A	13	1	-	0±0,4,6,8	0±0,0,0,0
1	DLY	A	14	1	-	0±0,5,7,9	0±0,0,0,0
1	DAS	A	15	1	-	0±0,2,6,8	0±0,0,0,0
1	DCY	A	16	1	-	0±0,1,4,6	0±0,0,0,0
1	DCY	A	17	1	-	0±0,1,4,6	0±0,0,0,0
1	DSN	A	18	1	-	0±0,2,4,6	0±0,0,0,0
1	DLY	A	19	1	-	0±0,5,7,9	0±0,0,0,0
1	DAS	A	2	1	-	0±0,2,6,8	0±0,0,0,0
1	DLY	A	20	1	-	0±0,5,7,9	0±0,0,0,0
1	DCY	A	21	1	-	0±0,1,4,6	0±0,0,0,0
1	DLY	A	22	1	-	0±0,5,7,9	0±0,0,0,0
1	DAR	A	23	1	-	0±0,7,9,11	0±0,0,0,0
1	DAR	A	24	1	-	0±0,7,9,11	0±0,0,0,0
1	DTH	A	26	1	1±0,1,2,3	0±0,4,6,8	0±0,0,0,0
1	DSG	A	27	1	-	0±0,4,6,8	0±0,0,0,0
1	DIL	A	28	1	1±0,1,2,3	0±0,6,8,10	0±0,0,0,0
1	DGL	A	29	1	-	0±0,3,7,9	0±0,0,0,0
1	DCY	A	3	1	-	0±0,1,4,6	0±0,0,0,0
1	DLY	A	30	1	-	0±0,5,7,9	0±0,0,0,0
1	DAR	A	31	1	-	0±0,7,9,11	0±0,0,0,0
1	DCY	A	32	1	-	0±0,1,4,6	0±0,0,0,0
1	DAR	A	33	1	-	0±0,7,11,11	0±0,0,0,0
1	DLE	A	4	1	-	0±0,4,6,8	0±0,0,0,0
1	DPR	A	5	1	-	0±0,0,9,11	0±0,1,1,1
1	DHI	A	6	1	-	0±0,3,6,8	0±0,1,1,1
1	DLE	A	7	1	-	0±0,4,6,8	0±0,0,0,0
1	DLY	A	8	1	-	0±0,5,7,9	0±0,0,0,0
1	DLE	A	9	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. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	28	DIL	CB	20
1	A	26	DTH	CB	20

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

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 16605

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	254
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	254
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 254 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	13	ASN	H	8.964	0.025	1
UNMAPPED	30	LYS	HB2	1.736	0.025	1
UNMAPPED	24	ARG	HD3	3.04	0.025	1
UNMAPPED	19	LYS	HB3	1.835	0.025	1
UNMAPPED	15	ASP	HB2	2.885	0.025	1
UNMAPPED	4	LEU	HA	4.716	0.025	1
UNMAPPED	28	ILE	HG23	0.838	0.025	1
UNMAPPED	24	ARG	HB2	1.669	0.025	1
UNMAPPED	24	ARG	HG2	1.446	0.025	1
UNMAPPED	20	LYS	H	7.3	0.025	1
UNMAPPED	4	LEU	HD23	0.859	0.025	1
UNMAPPED	11	LYS	HE3	2.885	0.025	1
UNMAPPED	20	LYS	HG3	1.107	0.025	1
UNMAPPED	33	ARG	HA	4.33	0.025	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	27	ASN	H	7.895	0.025	1
UNMAPPED	27	ASN	HA	4.557	0.025	1
UNMAPPED	8	LYS	HG3	1.344	0.025	1
UNMAPPED	26	THR	HG22	1.094	0.025	1
UNMAPPED	4	LEU	HD12	1.239	0.025	1
UNMAPPED	19	LYS	HZ1	7.434	0.025	1
UNMAPPED	8	LYS	HD2	1.624	0.025	1
UNMAPPED	12	GLU	HG2	2.208	0.025	1
UNMAPPED	21	CYS	H	8.879	0.025	1
UNMAPPED	16	CYS	HB2	3.385	0.025	1
UNMAPPED	16	CYS	HA	4.878	0.025	1
UNMAPPED	14	LYS	HG3	1.211	0.025	1
UNMAPPED	29	GLU	HB3	1.729	0.025	1
UNMAPPED	19	LYS	HA	4.057	0.025	1
UNMAPPED	29	GLU	HG3	2.295	0.025	1
UNMAPPED	13	ASN	HD21	7.636	0.025	1
UNMAPPED	29	GLU	HA	4.083	0.025	1
UNMAPPED	31	ARG	HA	5.138	0.025	1
UNMAPPED	15	ASP	H	7.674	0.025	1
UNMAPPED	13	ASN	HD22	6.764	0.025	1
UNMAPPED	17	CYS	HA	4.402	0.025	1
UNMAPPED	30	LYS	HZ1	7.389	0.025	1
UNMAPPED	22	LYS	HB3	1.514	0.025	1
UNMAPPED	5	PRO	HA	4.484	0.025	1
UNMAPPED	7	LEU	HD11	0.623	0.025	1
UNMAPPED	30	LYS	HZ3	7.389	0.025	1
UNMAPPED	11	LYS	H	8.598	0.025	1
UNMAPPED	8	LYS	HZ3	7.519	0.025	1
UNMAPPED	14	LYS	HD3	1.514	0.025	1
UNMAPPED	32	CYS	H	8.518	0.025	1
UNMAPPED	22	LYS	HE3	2.883	0.025	1
UNMAPPED	11	LYS	HD3	1.34	0.025	1
UNMAPPED	8	LYS	HA	4.213	0.025	1
UNMAPPED	9	LEU	HG	1.587	0.025	1
UNMAPPED	24	ARG	HD2	3.04	0.025	1
UNMAPPED	27	ASN	HB2	2.84	0.025	1
UNMAPPED	30	LYS	HD2	1.467	0.025	1
UNMAPPED	33	ARG	HE	6.629	0.025	1
UNMAPPED	18	SER	HB3	3.762	0.025	1
UNMAPPED	5	PRO	HB3	2.122	0.025	1
UNMAPPED	3	CYS	HB3	2.821	0.025	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	27	ASN	HD22	6.882	0.025	1
UNMAPPED	4	LEU	HB3	2.096	0.025	1
UNMAPPED	33	ARG	HG3	1.617	0.025	1
UNMAPPED	26	THR	HG23	1.094	0.025	1
UNMAPPED	12	GLU	H	7.741	0.025	1
UNMAPPED	24	ARG	HE	7.126	0.025	1
UNMAPPED	33	ARG	HG2	1.552	0.025	1
UNMAPPED	9	LEU	HB3	1.362	0.025	1
UNMAPPED	11	LYS	HZ2	7.399	0.025	1
UNMAPPED	3	CYS	H	8.165	0.025	1
UNMAPPED	20	LYS	HE2	2.845	0.025	1
UNMAPPED	13	ASN	HA	3.874	0.025	1
UNMAPPED	11	LYS	HZ1	7.399	0.025	1
UNMAPPED	33	ARG	HB3	1.753	0.025	1
UNMAPPED	10	CYS	H	7.879	0.025	1
UNMAPPED	31	ARG	HE	7.199	0.025	1
UNMAPPED	7	LEU	HB3	1.478	0.025	1
UNMAPPED	7	LEU	HD21	0.519	0.025	1
UNMAPPED	22	LYS	HG2	1.25	0.025	1
UNMAPPED	7	LEU	HD22	0.519	0.025	1
UNMAPPED	19	LYS	H	7.52	0.025	1
UNMAPPED	28	ILE	HG12	1.259	0.025	1
UNMAPPED	4	LEU	HD13	1.239	0.025	1
UNMAPPED	13	ASN	HB3	2.722	0.025	1
UNMAPPED	23	ARG	HA	4.516	0.025	1
UNMAPPED	20	LYS	HD2	1.416	0.025	1
UNMAPPED	23	ARG	H	9.0	0.025	1
UNMAPPED	8	LYS	HB2	1.802	0.025	1
UNMAPPED	10	CYS	HB3	2.951	0.025	1
UNMAPPED	21	CYS	HA	4.836	0.025	1
UNMAPPED	6	HIS	HA	4.071	0.025	1
UNMAPPED	19	LYS	HE3	2.906	0.025	1
UNMAPPED	22	LYS	HG3	1.25	0.025	1
UNMAPPED	9	LEU	HD21	0.745	0.025	1
UNMAPPED	19	LYS	HB2	2.006	0.025	1
UNMAPPED	26	THR	H	8.424	0.025	1
UNMAPPED	28	ILE	HG22	0.838	0.025	1
UNMAPPED	29	GLU	HB2	1.854	0.025	1
UNMAPPED	24	ARG	HG3	1.446	0.025	1
UNMAPPED	4	LEU	HG	1.781	0.025	1
UNMAPPED	4	LEU	HD22	0.859	0.025	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	5	PRO	HG3	1.721	0.025	1
UNMAPPED	25	GLY	H	8.649	0.025	1
UNMAPPED	4	LEU	HD21	0.859	0.025	1
UNMAPPED	30	LYS	H	8.389	0.025	1
UNMAPPED	33	ARG	HB2	2.002	0.025	1
UNMAPPED	5	PRO	HD2	3.938	0.025	1
UNMAPPED	8	LYS	HG2	1.454	0.025	1
UNMAPPED	17	CYS	HB2	3.109	0.025	1
UNMAPPED	8	LYS	HB3	1.714	0.025	1
UNMAPPED	8	LYS	HD3	1.624	0.025	1
UNMAPPED	11	LYS	HA	4.314	0.025	1
UNMAPPED	31	ARG	HB3	1.122	0.025	1
UNMAPPED	14	LYS	HA	3.927	0.025	1
UNMAPPED	14	LYS	HG2	1.211	0.025	1
UNMAPPED	23	ARG	HG3	1.38	0.025	1
UNMAPPED	31	ARG	H	7.588	0.025	1
UNMAPPED	11	LYS	HG2	1.249	0.025	1
UNMAPPED	11	LYS	HB3	1.528	0.025	1
UNMAPPED	29	GLU	HG2	2.327	0.025	1
UNMAPPED	22	LYS	HD2	1.609	0.025	1
UNMAPPED	19	LYS	HG2	1.275	0.025	1
UNMAPPED	30	LYS	HZ2	7.389	0.025	1
UNMAPPED	30	LYS	HE2	2.771	0.025	1
UNMAPPED	18	SER	HA	4.095	0.025	1
UNMAPPED	28	ILE	HG21	0.838	0.025	1
UNMAPPED	19	LYS	HD3	1.455	0.025	1
UNMAPPED	31	ARG	HG2	1.23	0.025	1
UNMAPPED	30	LYS	HE3	2.771	0.025	1
UNMAPPED	7	LEU	HD13	0.623	0.025	1
UNMAPPED	16	CYS	H	7.679	0.025	1
UNMAPPED	8	LYS	HZ1	7.519	0.025	1
UNMAPPED	9	LEU	HD13	0.835	0.025	1
UNMAPPED	11	LYS	HD2	1.34	0.025	1
UNMAPPED	31	ARG	HH12	6.904	0.025	1
UNMAPPED	18	SER	HB2	3.981	0.025	1
UNMAPPED	7	LEU	HG	0.227	0.025	1
UNMAPPED	27	ASN	HB3	2.84	0.025	1
UNMAPPED	23	ARG	HD3	3.067	0.025	1
UNMAPPED	20	LYS	HB3	1.575	0.025	1
UNMAPPED	26	THR	HB	4.302	0.025	1
UNMAPPED	6	HIS	HE1	8.629	0.025	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	23	ARG	HB3	1.49	0.025	1
UNMAPPED	2	ASP	HB2	2.823	0.025	1
UNMAPPED	25	GLY	HA3	3.702	0.025	1
UNMAPPED	24	ARG	HA	4.384	0.025	1
UNMAPPED	33	ARG	HD3	2.836	0.025	1
UNMAPPED	11	LYS	HG3	1.249	0.025	1
UNMAPPED	30	LYS	HB3	1.736	0.025	1
UNMAPPED	9	LEU	HB2	1.507	0.025	1
UNMAPPED	6	HIS	HB2	3.132	0.025	1
UNMAPPED	6	HIS	HD1	7.3	0.025	1
UNMAPPED	4	LEU	H	9.114	0.025	1
UNMAPPED	20	LYS	HE3	2.845	0.025	1
UNMAPPED	32	CYS	HA	5.165	0.025	1
UNMAPPED	20	LYS	HA	4.311	0.025	1
UNMAPPED	14	LYS	H	8.361	0.025	1
UNMAPPED	28	ILE	H	8.241	0.025	1
UNMAPPED	8	LYS	HE3	2.857	0.025	1
UNMAPPED	7	LEU	HB2	1.862	0.025	1
UNMAPPED	23	ARG	HD2	3.067	0.025	1
UNMAPPED	22	LYS	HZ3	7.584	0.025	1
UNMAPPED	7	LEU	HD23	0.519	0.025	1
UNMAPPED	29	GLU	H	8.105	0.025	1
UNMAPPED	28	ILE	HG13	1.182	0.025	1
UNMAPPED	1	GLY	HA2	3.775	0.025	1
UNMAPPED	22	LYS	HZ1	7.584	0.025	1
UNMAPPED	13	ASN	HB2	2.722	0.025	1
UNMAPPED	28	ILE	HD12	0.76	0.025	1
UNMAPPED	3	CYS	HA	4.646	0.025	1
UNMAPPED	6	HIS	H	8.013	0.025	1
UNMAPPED	32	CYS	HB3	2.798	0.025	1
UNMAPPED	10	CYS	HB2	3.017	0.025	1
UNMAPPED	19	LYS	HZ2	7.434	0.025	1
UNMAPPED	14	LYS	HB2	1.826	0.025	1
UNMAPPED	19	LYS	HG3	1.17	0.025	1
UNMAPPED	26	THR	HG21	1.094	0.025	1
UNMAPPED	28	ILE	HA	3.866	0.025	1
UNMAPPED	9	LEU	HD22	0.745	0.025	1
UNMAPPED	28	ILE	HB	1.866	0.025	1
UNMAPPED	2	ASP	H	8.687	0.025	1
UNMAPPED	22	LYS	HD3	1.609	0.025	1
UNMAPPED	15	ASP	HB3	2.885	0.025	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	14	LYS	HE2	2.83	0.025	1
UNMAPPED	5	PRO	HG2	2.062	0.025	1
UNMAPPED	30	LYS	HD3	1.467	0.025	1
UNMAPPED	31	ARG	HD3	2.762	0.025	1
UNMAPPED	11	LYS	HE2	2.885	0.025	1
UNMAPPED	31	ARG	HH21	6.427	0.025	1
UNMAPPED	20	LYS	HG2	1.269	0.025	1
UNMAPPED	5	PRO	HD3	3.532	0.025	1
UNMAPPED	17	CYS	HB3	2.748	0.025	1
UNMAPPED	4	LEU	HD11	1.239	0.025	1
UNMAPPED	31	ARG	HH22	6.427	0.025	1
UNMAPPED	31	ARG	HB2	1.045	0.025	1
UNMAPPED	12	GLU	HA	4.579	0.025	1
UNMAPPED	22	LYS	HB2	1.872	0.025	1
UNMAPPED	12	GLU	HG3	2.208	0.025	1
UNMAPPED	28	ILE	HD11	0.76	0.025	1
UNMAPPED	16	CYS	HB3	2.502	0.025	1
UNMAPPED	23	ARG	HG2	1.38	0.025	1
UNMAPPED	33	ARG	H	9.049	0.025	1
UNMAPPED	10	CYS	HA	4.805	0.025	1
UNMAPPED	11	LYS	HB2	1.755	0.025	1
UNMAPPED	7	LEU	H	9.271	0.025	1
UNMAPPED	19	LYS	HZ3	7.434	0.025	1
UNMAPPED	31	ARG	HD2	3.013	0.025	1
UNMAPPED	28	ILE	HD13	0.76	0.025	1
UNMAPPED	19	LYS	HD2	1.705	0.025	1
UNMAPPED	31	ARG	HG3	1.23	0.025	1
UNMAPPED	22	LYS	HA	4.848	0.025	1
UNMAPPED	7	LEU	HD12	0.623	0.025	1
UNMAPPED	8	LYS	HZ2	7.519	0.025	1
UNMAPPED	12	GLU	HB3	1.748	0.025	1
UNMAPPED	14	LYS	HD2	1.514	0.025	1
UNMAPPED	22	LYS	HE2	2.883	0.025	1
UNMAPPED	9	LEU	HA	4.504	0.025	1
UNMAPPED	9	LEU	H	8.147	0.025	1
UNMAPPED	24	ARG	HB3	1.635	0.025	1
UNMAPPED	7	LEU	HA	3.454	0.025	1
UNMAPPED	20	LYS	HB2	1.575	0.025	1
UNMAPPED	21	CYS	HB3	2.6	0.025	1
UNMAPPED	5	PRO	HB2	2.262	0.025	1
UNMAPPED	9	LEU	HD12	0.835	0.025	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	30	LYS	HA	3.923	0.025	1
UNMAPPED	2	ASP	HB3	2.72	0.025	1
UNMAPPED	3	CYS	HB2	3.088	0.025	1
UNMAPPED	9	LEU	HD11	0.835	0.025	1
UNMAPPED	25	GLY	HA2	3.998	0.025	1
UNMAPPED	15	ASP	HA	4.306	0.025	1
UNMAPPED	4	LEU	HB2	2.096	0.025	1
UNMAPPED	33	ARG	HD2	2.987	0.025	1
UNMAPPED	31	ARG	HH11	6.904	0.025	1
UNMAPPED	6	HIS	HB3	2.984	0.025	1
UNMAPPED	6	HIS	HD2	7.3	0.025	1
UNMAPPED	26	THR	HA	4.06	0.025	1
UNMAPPED	8	LYS	H	7.358	0.025	1
UNMAPPED	11	LYS	HZ3	7.399	0.025	1
UNMAPPED	24	ARG	H	8.786	0.025	1
UNMAPPED	2	ASP	HA	4.737	0.025	1
UNMAPPED	8	LYS	HE2	2.935	0.025	1
UNMAPPED	12	GLU	HB2	1.748	0.025	1
UNMAPPED	17	CYS	H	9.984	0.025	1
UNMAPPED	22	LYS	HZ2	7.584	0.025	1
UNMAPPED	1	GLY	HA3	3.775	0.025	1
UNMAPPED	22	LYS	H	8.242	0.025	1
UNMAPPED	27	ASN	HD21	7.592	0.025	1
UNMAPPED	30	LYS	HG2	0.964	0.025	1
UNMAPPED	14	LYS	HE3	2.83	0.025	1
UNMAPPED	20	LYS	HD3	1.416	0.025	1
UNMAPPED	32	CYS	HB2	3.258	0.025	1
UNMAPPED	23	ARG	HE	6.736	0.025	1
UNMAPPED	19	LYS	HE2	2.906	0.025	1
UNMAPPED	21	CYS	HB2	2.854	0.025	1
UNMAPPED	14	LYS	HB3	1.723	0.025	1
UNMAPPED	23	ARG	HB2	1.629	0.025	1
UNMAPPED	30	LYS	HG3	0.964	0.025	1
UNMAPPED	18	SER	H	9.223	0.025	1
UNMAPPED	9	LEU	HD23	0.745	0.025	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 10. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/10 (0%)	0/4 (0%)	0/4 (0%)	0/2 (0%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/10 (0%)	0/4 (0%)	0/4 (0%)	0/2 (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 10. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/10 (0%)	0/4 (0%)	0/4 (0%)	0/2 (0%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/10 (0%)	0/4 (0%)	0/4 (0%)	0/2 (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.