



Full wwPDB NMR Structure Validation Report ⓘ

Feb 19, 2018 – 08:21 pm GMT

PDB ID : 1J2O
Title : Structure of FLIN2, a complex containing the N-terminal LIM domain of LMO2 and ldb1-LID
Authors : Deane, J.E.; Mackay, J.P.; Kwan, A.H.; Sum, E.Y.; Visvader, J.E.; Matthews, J.M.
Deposited on : 2003-01-08

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 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
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	:	trunk30686
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

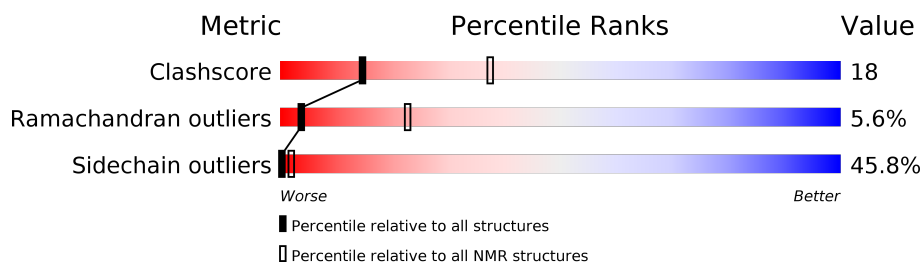
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	114	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:37, A:48-A:60, A:96-A:103 (56)	0.97	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 3, 6, 10, 12, 15
2	2, 7, 9, 11, 14
3	4, 5, 18
4	8, 13
Single-model clusters	16; 17; 19; 20

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1708 atoms, of which 829 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fusion of Rhombotin-2 and LIM domain-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1706	535	829	159	173	10	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P25801
A	64	GLY	-	LINKER	UNP P25801
A	65	GLY	-	LINKER	UNP P25801
A	66	SER	-	LINKER	UNP P25801
A	67	GLY	-	LINKER	UNP P25801
A	68	GLY	-	LINKER	UNP P25801
A	69	HIS	-	LINKER	UNP P25801
A	70	MET	-	LINKER	UNP P25801
A	71	GLY	-	LINKER	UNP P25801
A	72	SER	-	LINKER	UNP P25801
A	73	GLY	-	LINKER	UNP P25801
A	74	GLY	-	LINKER	UNP P25801

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

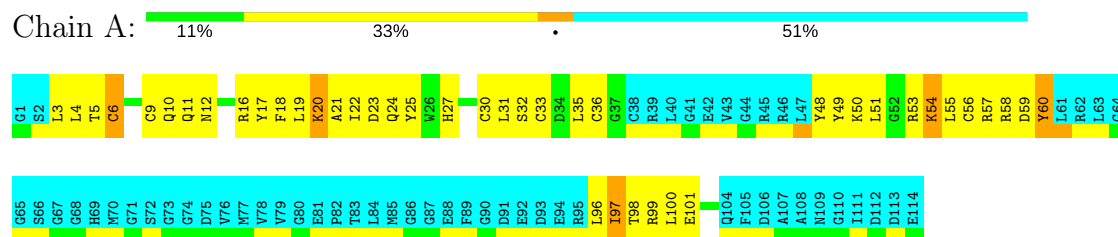
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

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: Fusion of Rhombotin-2 and LIM domain-binding protein 1

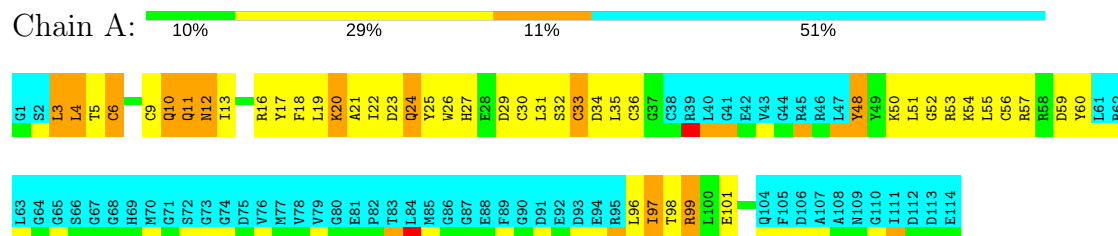


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

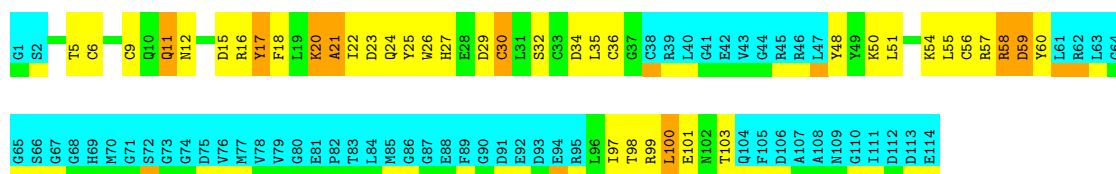
- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



4.2.2 Score per residue for model 2

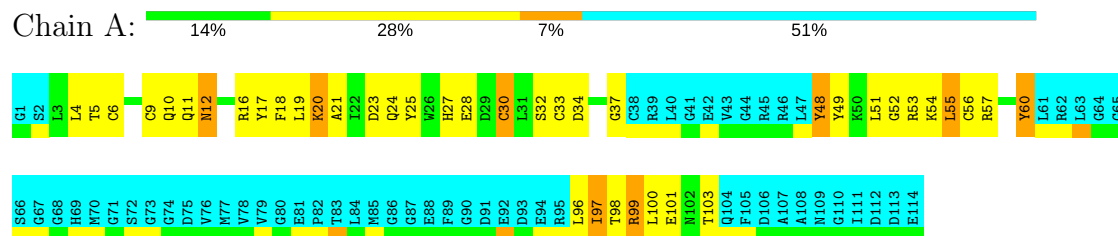
- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1





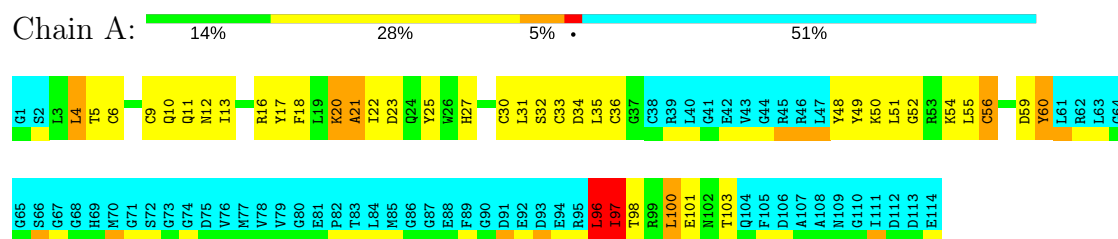
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



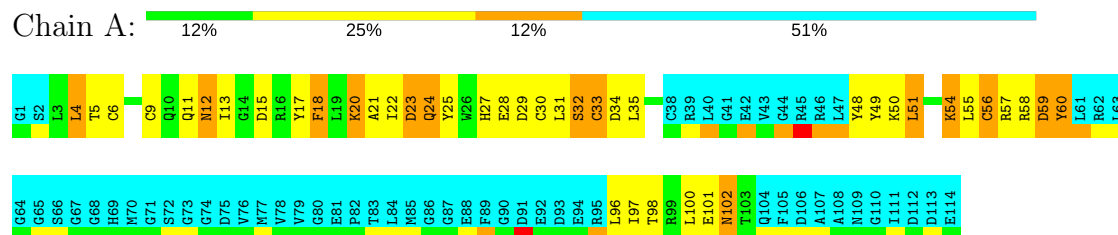
4.2.4 Score per residue for model 4

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



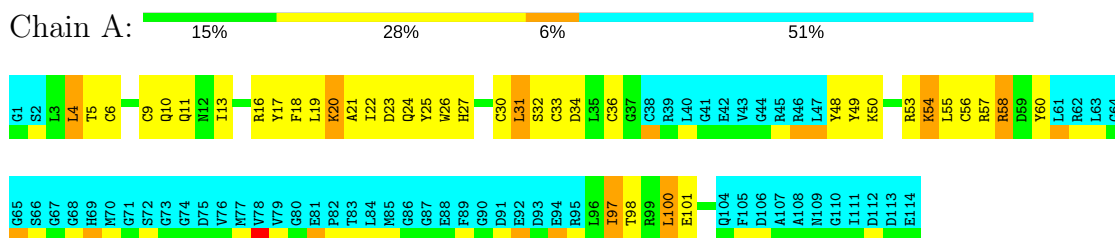
4.2.5 Score per residue for model 5

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



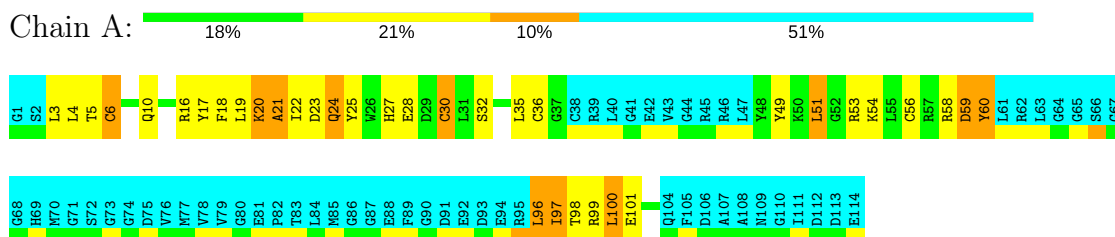
4.2.6 Score per residue for model 6

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



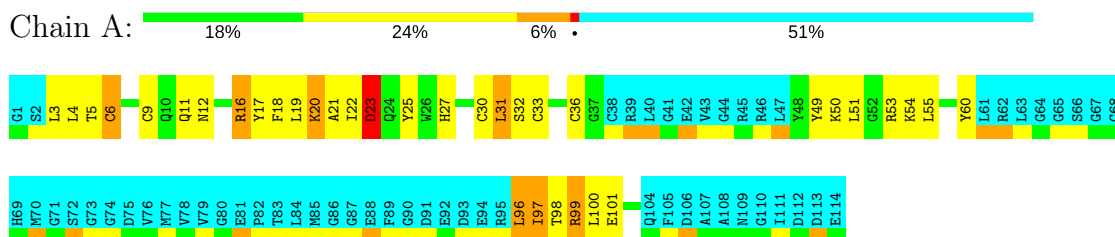
4.2.7 Score per residue for model 7

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



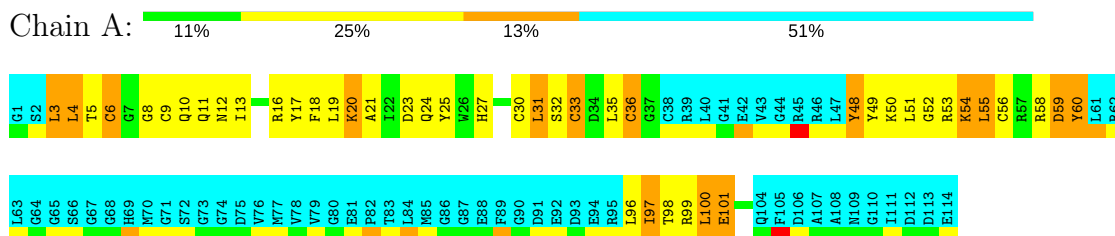
4.2.8 Score per residue for model 8

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



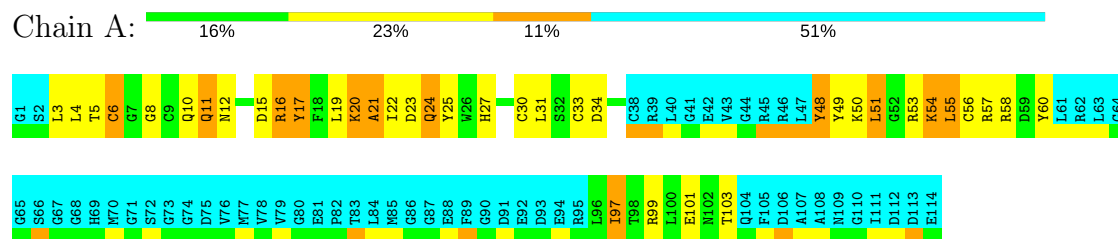
4.2.9 Score per residue for model 9

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



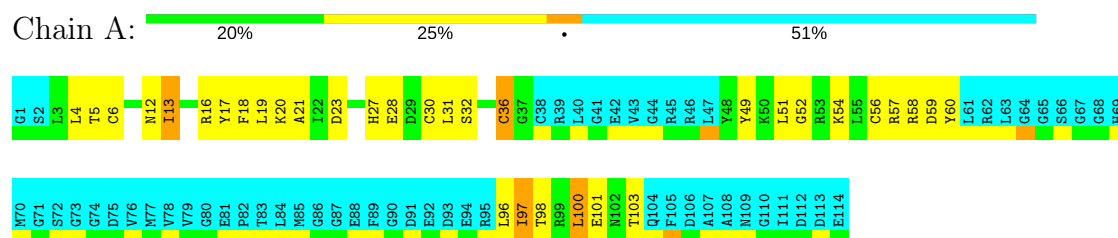
4.2.10 Score per residue for model 10

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



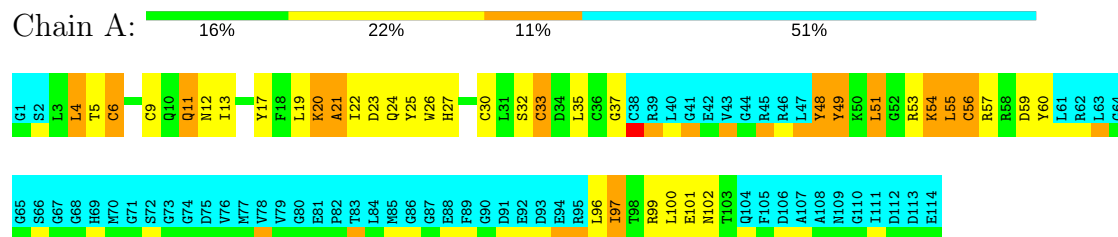
4.2.11 Score per residue for model 11

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



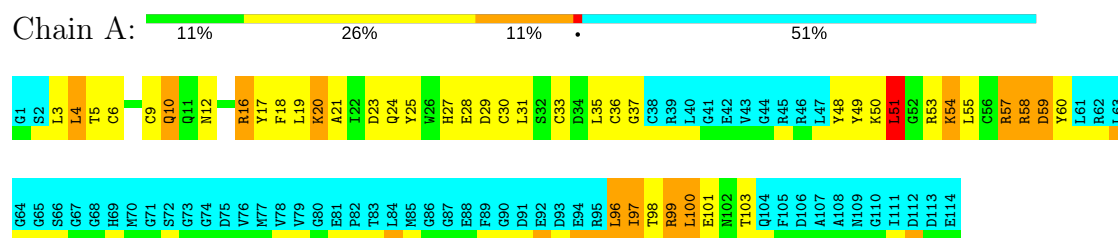
4.2.12 Score per residue for model 12

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



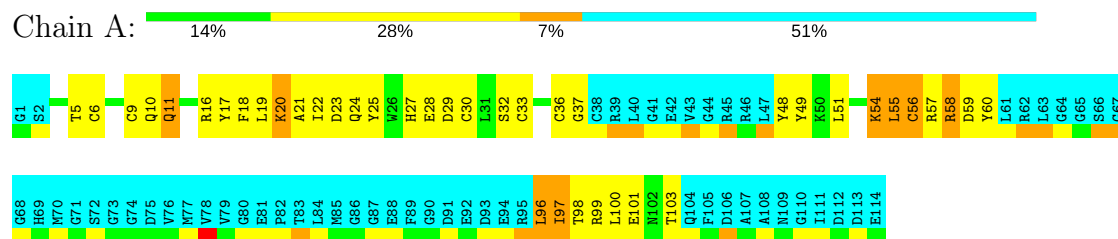
4.2.13 Score per residue for model 13

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1

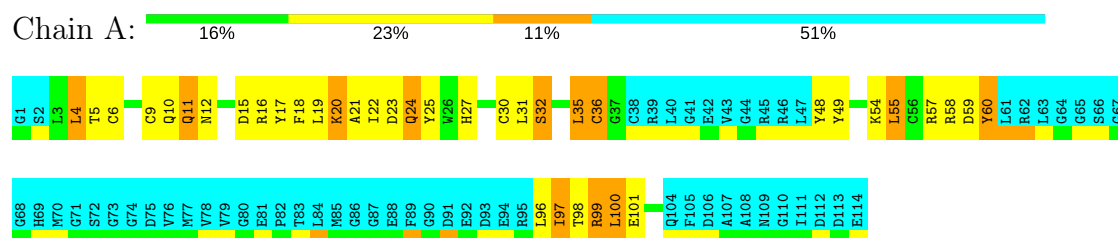


4.2.14 Score per residue for model 14

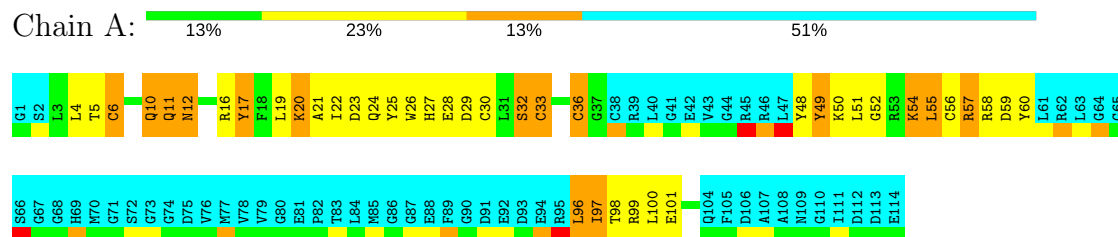
- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



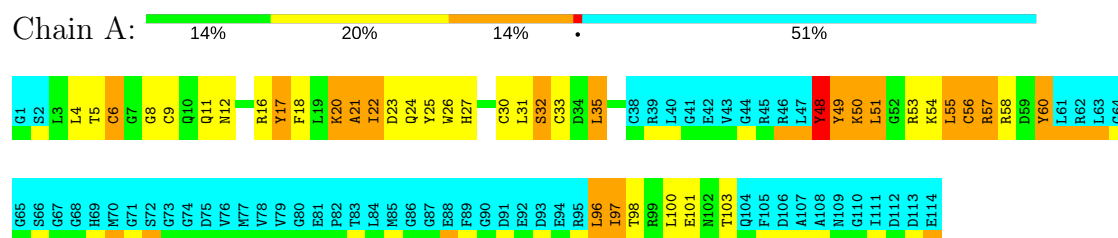
- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1

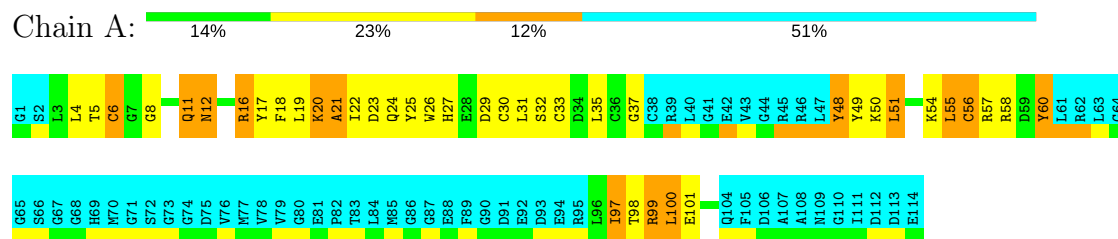


- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



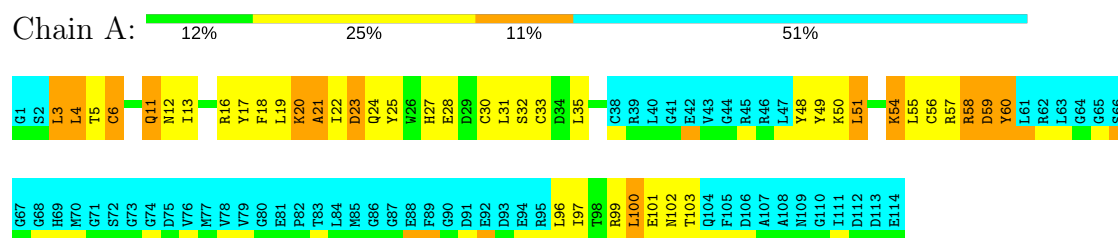
4.2.18 Score per residue for model 18

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



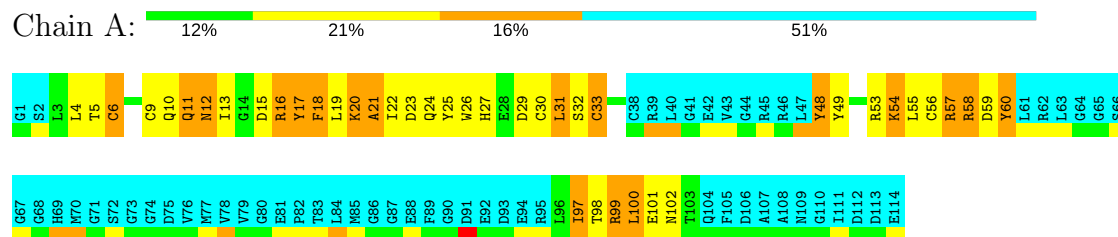
4.2.19 Score per residue for model 19

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



4.2.20 Score per residue for model 20

- Molecule 1: Fusion of Rhombotin-2 and LIM domain-binding protein 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, simulated annealing, molecular dynamics, automated noe assignment of ambiguous NOES*.

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *structures with favorable non-bond energy*.

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

Software name	Classification	Version
ARIA	structure solution	1.1.2
CNS	structure solution	1.1
CNS	refinement	1.1

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 5100
Number of chemical shift lists	2
Total number of shifts	1775
Number of shifts mapped to atoms	1775
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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:
ZN

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	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	48	TYR	Mainchain	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
1	A	462	445	445	17±4
All	All	9280	8900	8900	335

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:TYR:HB2	1:A:54:LYS:HA	0.94	1.39	12	13
1:A:33:CYS:HB3	1:A:55:LEU:HA	0.92	1.39	9	1
1:A:27:HIS:HB2	1:A:30:CYS:HB2	0.88	1.46	17	20
1:A:35:LEU:HB2	1:A:55:LEU:HB2	0.84	1.49	5	2
1:A:20:LYS:HB2	1:A:25:TYR:HA	0.83	1.47	8	17
1:A:19:LEU:HD22	1:A:97:ILE:HB	0.82	1.51	3	9
1:A:36:CYS:SG	1:A:59:ASP:HB3	0.80	2.16	2	5
1:A:19:LEU:HD12	1:A:97:ILE:HB	0.74	1.57	1	1
1:A:33:CYS:HB3	1:A:37:GLY:H	0.74	1.42	3	4
1:A:33:CYS:HB3	1:A:36:CYS:HB2	0.73	1.60	6	2
1:A:19:LEU:HD12	1:A:28:GLU:HA	0.72	1.62	11	2
1:A:9:CYS:HB3	1:A:11:GLN:HG2	0.72	1.62	8	3
1:A:49:TYR:CB	1:A:54:LYS:HA	0.71	2.15	18	4
1:A:17:TYR:CE1	1:A:101:GLU:HA	0.70	2.22	20	1
1:A:35:LEU:HD23	1:A:59:ASP:HB2	0.70	1.63	19	2
1:A:22:ILE:HA	1:A:96:LEU:HB3	0.69	1.64	7	1
1:A:56:CYS:SG	1:A:58:ARG:HG2	0.67	2.29	2	3
1:A:19:LEU:HD21	1:A:99:ARG:HD2	0.67	1.64	18	3
1:A:56:CYS:O	1:A:60:TYR:HB3	0.67	1.90	19	8
1:A:51:LEU:H	1:A:51:LEU:HD13	0.66	1.51	10	2
1:A:17:TYR:CD1	1:A:101:GLU:HA	0.66	2.26	20	1
1:A:22:ILE:HB	1:A:24:GLN:OE1	0.65	1.91	10	4
1:A:27:HIS:HB2	1:A:30:CYS:SG	0.65	2.31	8	3
1:A:8:GLY:HA2	1:A:54:LYS:HE2	0.64	1.68	9	1
1:A:17:TYR:HE2	1:A:99:ARG:HB3	0.64	1.52	10	3
1:A:35:LEU:HB3	1:A:55:LEU:HD13	0.63	1.69	15	1
1:A:9:CYS:SG	1:A:11:GLN:HG2	0.63	2.34	6	10
1:A:35:LEU:HB3	1:A:59:ASP:HB2	0.63	1.69	2	3
1:A:4:LEU:HB2	1:A:25:TYR:CD2	0.63	2.28	15	2
1:A:55:LEU:HD11	1:A:60:TYR:HB2	0.63	1.70	18	3
1:A:4:LEU:HB2	1:A:13:ILE:HD12	0.63	1.69	4	7
1:A:33:CYS:SG	1:A:55:LEU:HB2	0.62	2.34	19	2
1:A:31:LEU:HD12	1:A:97:ILE:HG21	0.62	1.71	20	1
1:A:56:CYS:SG	1:A:59:ASP:HB2	0.61	2.35	20	3
1:A:18:PHE:CE1	1:A:100:LEU:HB3	0.61	2.29	2	12
1:A:35:LEU:HB3	1:A:56:CYS:SG	0.61	2.35	4	4
1:A:49:TYR:HB3	1:A:96:LEU:H	0.61	1.55	16	1
1:A:18:PHE:HA	1:A:28:GLU:HG3	0.60	1.72	5	1
1:A:19:LEU:HD22	1:A:97:ILE:HD13	0.60	1.74	16	1
1:A:22:ILE:HG13	1:A:97:ILE:HD11	0.59	1.74	5	1
1:A:6:CYS:HA	1:A:25:TYR:O	0.58	1.98	16	11
1:A:36:CYS:SG	1:A:59:ASP:HB2	0.58	2.38	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ILE:HB	1:A:26:TRP:HE1	0.58	1.58	12	2
1:A:48:TYR:CD2	1:A:57:ARG:HD3	0.57	2.34	3	1
1:A:33:CYS:HB2	1:A:37:GLY:H	0.57	1.59	13	1
1:A:55:LEU:HD21	1:A:60:TYR:HB2	0.57	1.76	19	1
1:A:27:HIS:HB2	1:A:30:CYS:CB	0.57	2.28	14	14
1:A:27:HIS:CB	1:A:30:CYS:HB2	0.56	2.25	2	8
1:A:50:LYS:HE2	1:A:60:TYR:CE1	0.56	2.34	5	1
1:A:51:LEU:HG	1:A:52:GLY:N	0.56	2.16	16	6
1:A:21:ALA:HB3	1:A:97:ILE:HA	0.56	1.75	17	3
1:A:20:LYS:HE2	1:A:100:LEU:HD13	0.56	1.76	6	1
1:A:48:TYR:HD2	1:A:57:ARG:HD3	0.56	1.61	3	1
1:A:51:LEU:HD13	1:A:51:LEU:H	0.54	1.62	18	3
1:A:22:ILE:HD13	1:A:54:LYS:HG2	0.53	1.79	16	1
1:A:16:ARG:CD	1:A:102:ASN:HA	0.53	2.34	20	1
1:A:57:ARG:HD3	1:A:60:TYR:CD2	0.52	2.39	17	1
1:A:50:LYS:HB2	1:A:55:LEU:HD22	0.52	1.81	13	2
1:A:16:ARG:HD2	1:A:17:TYR:HB2	0.52	1.81	2	2
1:A:55:LEU:HG	1:A:56:CYS:N	0.51	2.20	14	1
1:A:3:LEU:HD13	1:A:102:ASN:HD21	0.51	1.65	19	1
1:A:48:TYR:CD2	1:A:57:ARG:HB2	0.50	2.41	15	1
1:A:55:LEU:HB2	1:A:59:ASP:OD1	0.50	2.07	13	1
1:A:19:LEU:HB3	1:A:31:LEU:HD12	0.50	1.83	6	1
1:A:22:ILE:HD11	1:A:31:LEU:HD11	0.50	1.84	20	1
1:A:33:CYS:SG	1:A:34:ASP:N	0.49	2.85	1	1
1:A:20:LYS:HE3	1:A:100:LEU:HD22	0.49	1.85	20	1
1:A:26:TRP:CG	1:A:31:LEU:HG	0.49	2.43	20	2
1:A:19:LEU:CD2	1:A:99:ARG:HA	0.49	2.37	1	2
1:A:21:ALA:HB3	1:A:96:LEU:C	0.49	2.28	7	1
1:A:11:GLN:HG3	1:A:12:ASN:N	0.48	2.22	18	1
1:A:16:ARG:HA	1:A:103:THR:HG22	0.48	1.84	13	1
1:A:19:LEU:HG	1:A:99:ARG:HG3	0.48	1.85	9	1
1:A:17:TYR:CE2	1:A:99:ARG:HB3	0.48	2.40	10	2
1:A:18:PHE:O	1:A:19:LEU:HD22	0.48	2.08	8	2
1:A:57:ARG:NE	1:A:57:ARG:HA	0.48	2.24	17	1
1:A:59:ASP:N	1:A:59:ASP:OD1	0.48	2.46	5	1
1:A:20:LYS:O	1:A:21:ALA:HB2	0.47	2.09	7	4
1:A:21:ALA:HB2	1:A:97:ILE:HA	0.47	1.86	18	2
1:A:35:LEU:HB3	1:A:59:ASP:CG	0.47	2.30	1	1
1:A:21:ALA:HB3	1:A:97:ILE:HG22	0.46	1.85	4	1
1:A:11:GLN:O	1:A:12:ASN:HB3	0.46	2.10	1	4
1:A:36:CYS:SG	1:A:59:ASP:CB	0.46	3.00	2	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ILE:O	1:A:23:ASP:HB2	0.46	2.09	19	2
1:A:4:LEU:HB3	1:A:25:TYR:CD2	0.46	2.46	1	4
1:A:31:LEU:HB3	1:A:48:TYR:CD1	0.46	2.45	17	1
1:A:51:LEU:HD22	1:A:51:LEU:H	0.46	1.71	5	1
1:A:22:ILE:HA	1:A:96:LEU:CB	0.46	2.40	7	1
1:A:22:ILE:HG23	1:A:49:TYR:CE2	0.45	2.46	10	2
1:A:27:HIS:H	1:A:30:CYS:HB2	0.45	1.71	8	1
1:A:15:ASP:O	1:A:102:ASN:HB3	0.45	2.11	5	1
1:A:22:ILE:HG21	1:A:54:LYS:HG2	0.45	1.88	16	1
1:A:4:LEU:CB	1:A:13:ILE:HD12	0.45	2.41	5	2
1:A:22:ILE:HD12	1:A:26:TRP:CZ2	0.45	2.46	1	2
1:A:56:CYS:SG	1:A:58:ARG:HB2	0.45	2.52	11	1
1:A:97:ILE:HG22	1:A:98:THR:N	0.45	2.26	5	1
1:A:49:TYR:HB3	1:A:97:ILE:HD11	0.44	1.88	19	1
1:A:19:LEU:HG	1:A:99:ARG:HD3	0.44	1.88	15	1
1:A:19:LEU:C	1:A:20:LYS:HG3	0.44	2.31	18	1
1:A:21:ALA:CB	1:A:97:ILE:HA	0.44	2.42	19	1
1:A:6:CYS:HB2	1:A:26:TRP:HA	0.44	1.88	16	1
1:A:11:GLN:O	1:A:12:ASN:CB	0.44	2.66	18	1
1:A:48:TYR:CD1	1:A:57:ARG:HD3	0.44	2.47	19	1
1:A:51:LEU:N	1:A:51:LEU:HD22	0.43	2.28	5	3
1:A:50:LYS:CD	1:A:53:ARG:HB2	0.43	2.43	17	1
1:A:17:TYR:HE1	1:A:101:GLU:HG2	0.43	1.73	17	1
1:A:51:LEU:HD22	1:A:51:LEU:N	0.43	2.28	7	2
1:A:22:ILE:HG12	1:A:96:LEU:O	0.43	2.13	17	1
1:A:9:CYS:O	1:A:10:GLN:HB2	0.43	2.13	13	1
1:A:50:LYS:HB2	1:A:55:LEU:CD2	0.43	2.44	13	1
1:A:34:ASP:HB3	1:A:55:LEU:HA	0.43	1.90	3	1
1:A:33:CYS:HB2	1:A:55:LEU:HA	0.43	1.90	20	1
1:A:9:CYS:CB	1:A:11:GLN:HG2	0.42	2.44	4	1
1:A:17:TYR:CE1	1:A:101:GLU:HG2	0.42	2.49	17	2
1:A:6:CYS:SG	1:A:8:GLY:N	0.42	2.88	18	2
1:A:16:ARG:HD2	1:A:102:ASN:O	0.42	2.14	20	1
1:A:13:ILE:HG23	1:A:27:HIS:CD2	0.42	2.50	1	1
1:A:33:CYS:CB	1:A:37:GLY:H	0.42	2.27	13	1
1:A:51:LEU:HG	1:A:52:GLY:H	0.42	1.75	16	1
1:A:19:LEU:HG	1:A:99:ARG:HD2	0.42	1.92	19	1
1:A:48:TYR:CD1	1:A:48:TYR:C	0.42	2.93	18	1
1:A:97:ILE:H	1:A:97:ILE:HG13	0.42	1.33	1	1
1:A:22:ILE:HG13	1:A:26:TRP:NE1	0.41	2.29	20	1
1:A:31:LEU:HD13	1:A:97:ILE:CG2	0.41	2.45	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ILE:HD13	1:A:54:LYS:HB3	0.41	1.92	16	1
1:A:99:ARG:HG3	1:A:99:ARG:NH1	0.41	2.30	3	1
1:A:6:CYS:O	1:A:10:GLN:HA	0.41	2.15	1	2
1:A:18:PHE:HE2	1:A:25:TYR:HB3	0.41	1.76	20	1
1:A:55:LEU:HG	1:A:56:CYS:O	0.41	2.15	12	1
1:A:99:ARG:HD2	1:A:99:ARG:HA	0.41	1.64	20	1
1:A:57:ARG:O	1:A:60:TYR:HD1	0.41	1.98	18	1
1:A:19:LEU:HD22	1:A:97:ILE:HG22	0.41	1.93	7	1
1:A:11:GLN:O	1:A:12:ASN:HB2	0.40	2.16	16	2
1:A:57:ARG:HG3	1:A:57:ARG:O	0.40	2.16	15	1
1:A:13:ILE:HG23	1:A:27:HIS:NE2	0.40	2.31	11	1
1:A:17:TYR:HD1	1:A:102:ASN:H	0.40	1.58	20	1
1:A:56:CYS:SG	1:A:59:ASP:CB	0.40	3.09	20	1
1:A:99:ARG:HG3	1:A:99:ARG:HH11	0.40	1.77	3	1
1:A:16:ARG:HA	1:A:18:PHE:CE1	0.40	2.52	20	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	56/114 (49%)	46±2 (83±4%)	7±2 (12±4%)	3±1 (6±2%)	4	23
All	All	1120/2280 (49%)	925 (83%)	132 (12%)	63 (6%)	4	23

All 9 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	23	ASP	20
1	A	21	ALA	20
1	A	12	ASN	12
1	A	51	LEU	4
1	A	3	LEU	2
1	A	102	ASN	2
1	A	97	ILE	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	31	LEU	1
1	A	96	LEU	1

6.3.2 Protein sidechains ⓘ

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	50/91 (55%)	27±3 (54±5%)	23±3 (46±5%)	0	2
All	All	1000/1820 (55%)	542 (54%)	458 (46%)	0	2

All 44 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	CYS	20
1	A	20	LYS	20
1	A	5	THR	20
1	A	17	TYR	20
1	A	60	TYR	20
1	A	97	ILE	18
1	A	4	LEU	18
1	A	101	GLU	17
1	A	24	GLN	17
1	A	100	LEU	16
1	A	98	THR	15
1	A	54	LYS	15
1	A	16	ARG	15
1	A	32	SER	14
1	A	55	LEU	14
1	A	10	GLN	12
1	A	96	LEU	12
1	A	58	ARG	11
1	A	51	LEU	11
1	A	48	TYR	11
1	A	53	ARG	10
1	A	11	GLN	10
1	A	31	LEU	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	50	LYS	10
1	A	56	CYS	8
1	A	103	THR	8
1	A	99	ARG	8
1	A	33	CYS	8
1	A	57	ARG	8
1	A	29	ASP	7
1	A	36	CYS	7
1	A	3	LEU	6
1	A	49	TYR	6
1	A	59	ASP	6
1	A	28	GLU	5
1	A	34	ASP	4
1	A	12	ASN	4
1	A	15	ASP	4
1	A	30	CYS	3
1	A	18	PHE	3
1	A	13	ILE	2
1	A	23	ASP	2
1	A	35	LEU	2
1	A	22	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 82% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5100

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	1033
Number of shifts mapped to atoms	1033
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	105	-0.34 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	86	0.01 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	98	0.05 ± 0.17	None needed (< 0.5 ppm)
^{15}N	104	1.07 ± 0.27	Should be applied

7.1.3 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 74%, i.e. 534 atoms were assigned a chemical shift out of a possible 723. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	274/280 (98%)	109/112 (97%)	110/112 (98%)	55/56 (98%)
Sidechain	255/374 (68%)	169/220 (77%)	81/131 (62%)	5/23 (22%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	5/69 (7%)	3/35 (9%)	0/31 (0%)	2/3 (67%)
Overall	534/723 (74%)	281/367 (77%)	191/274 (70%)	62/82 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 937 atoms were assigned a chemical shift out of a possible 1350. 2 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	514/568 (90%)	207/227 (91%)	203/228 (89%)	104/113 (92%)
Sidechain	416/687 (61%)	272/402 (68%)	137/245 (56%)	7/40 (18%)
Aromatic	7/95 (7%)	3/49 (6%)	0/41 (0%)	4/5 (80%)
Overall	937/1350 (69%)	482/678 (71%)	340/514 (66%)	115/158 (73%)

7.1.4 Statistically unusual chemical shifts [i](#)

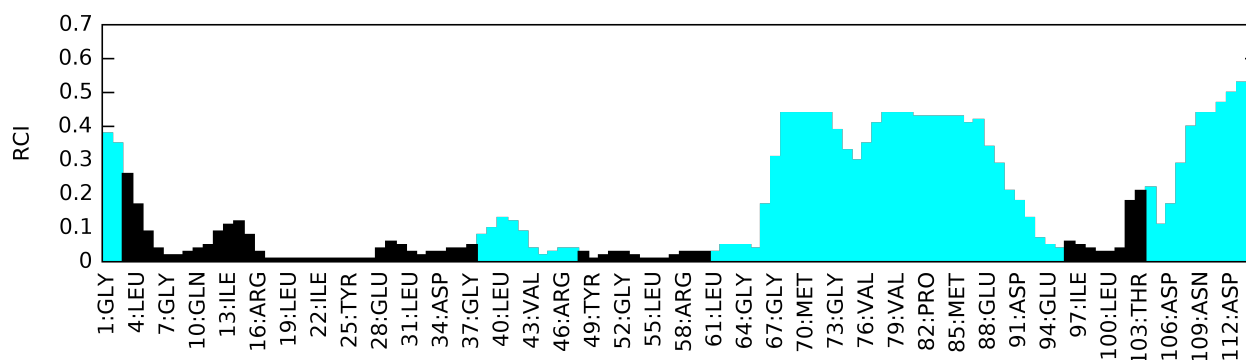
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	31	LEU	HD22	-0.96	2.14 – -0.66	-6.1
1	A	31	LEU	HD23	-0.96	2.14 – -0.66	-6.1
1	A	31	LEU	HD21	-0.96	2.14 – -0.66	-6.1
1	A	20	LYS	HE3	3.96	3.86 – 1.96	5.5
1	A	20	LYS	HE2	3.96	3.87 – 1.97	5.5

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5100

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	742
Number of shifts mapped to atoms	742
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.2.2 Chemical shift referencing [i](#)

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

7.2.3 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 47%, i.e. 341 atoms were assigned a chemical shift out of a possible 722. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	112/280 (40%)	112/112 (100%)	0/112 (0%)	0/56 (0%)
Sidechain	196/374 (52%)	196/220 (89%)	0/131 (0%)	0/23 (0%)
Aromatic	33/68 (49%)	33/35 (94%)	0/31 (0%)	0/2 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Overall	341/722 (47%)	341/367 (93%)	0/274 (0%)	0/81 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 619 atoms were assigned a chemical shift out of a possible 1348. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	226/568 (40%)	226/227 (100%)	0/228 (0%)	0/113 (0%)
Sidechain	351/687 (51%)	351/402 (87%)	0/245 (0%)	0/40 (0%)
Aromatic	42/93 (45%)	42/49 (86%)	0/41 (0%)	0/3 (0%)
Overall	619/1348 (46%)	619/678 (91%)	0/514 (0%)	0/156 (0%)

7.2.4 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	31	LEU	HD22	-0.99	2.14 – -0.66	-6.2
1	A	31	LEU	HD23	-0.99	2.14 – -0.66	-6.2
1	A	31	LEU	HD21	-0.99	2.14 – -0.66	-6.2
1	A	20	LYS	HE3	3.99	3.86 – 1.96	5.7
1	A	20	LYS	HE2	3.99	3.87 – 1.97	5.6

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

