



Full wwPDB NMR Structure Validation Report ⓘ

Nov 2, 2021 – 01:26 AM EDT

PDB ID : 1M3V
Title : FLIN4: Fusion of the LIM binding domain of Ldb1 and the N-terminal LIM domain of LMO4
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Deposited on : 2002-06-30

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:

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

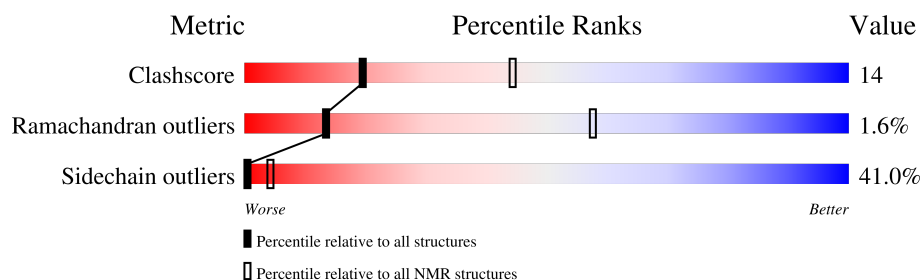
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	122	<div> <div>20%</div> <div>35%</div> <div>.</div> <div>43%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:7-A:67, A:102-A:109 (69)	0.67	2

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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1749 atoms, of which 842 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4.

Mol	Chain	Residues	Atoms						Trace
1	A	122	Total	C	H	N	O	S	0
			1747	551	842	160	183	11	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	SER	CYS	engineered mutation	UNP P70662
A	49	SER	CYS	engineered mutation	UNP P70662

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

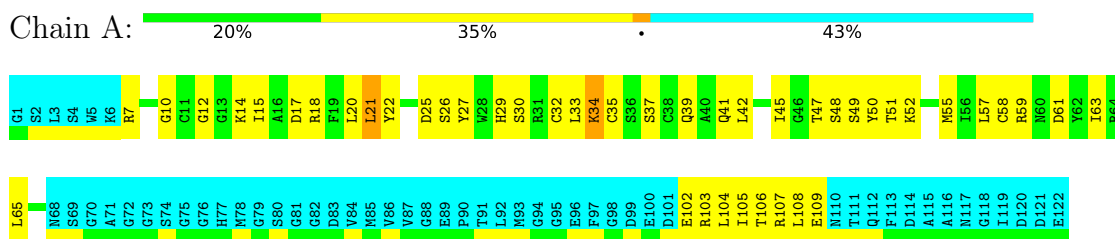
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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 the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4

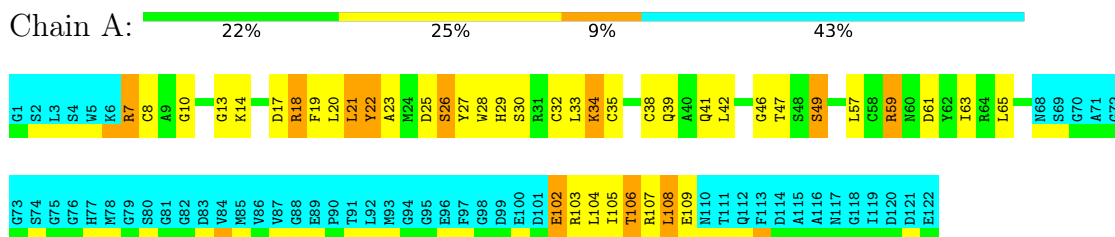


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

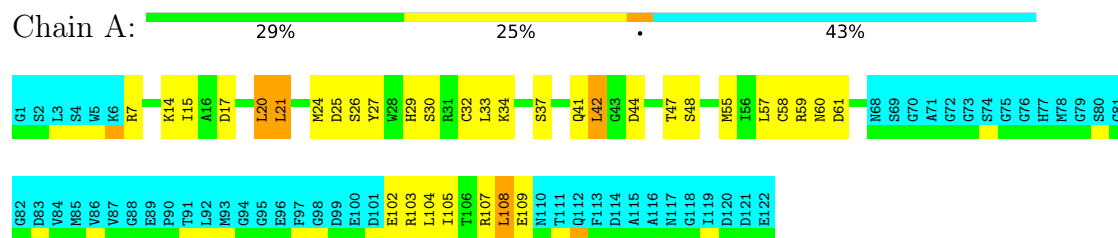
4.2.1 Score per residue for model 1

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



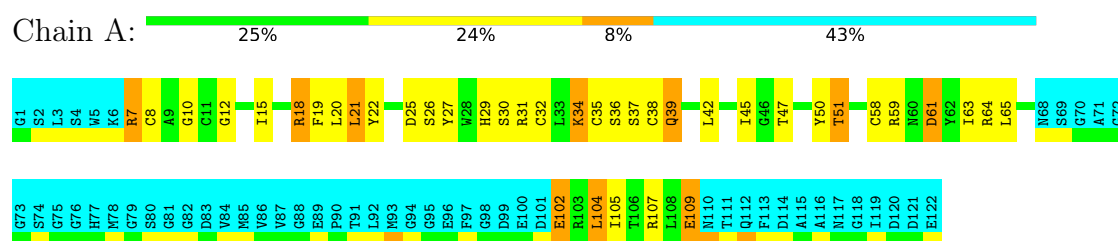
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



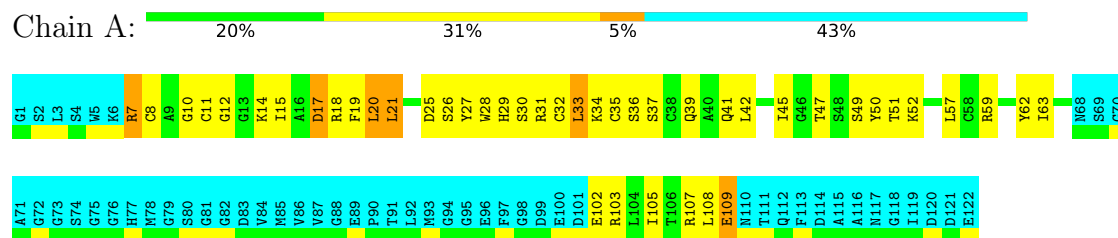
4.2.3 Score per residue for model 3

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



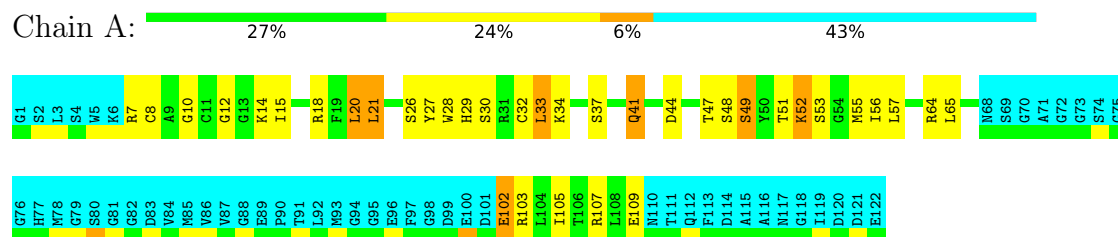
4.2.4 Score per residue for model 4

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



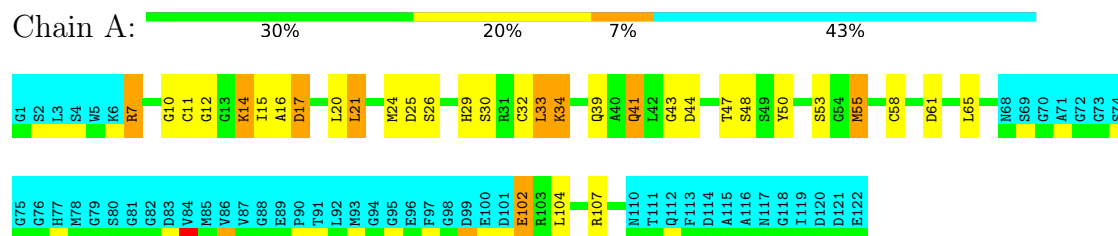
4.2.5 Score per residue for model 5

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



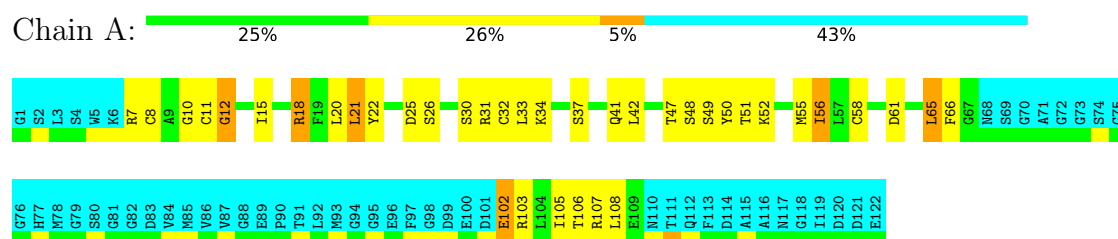
4.2.6 Score per residue for model 6

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



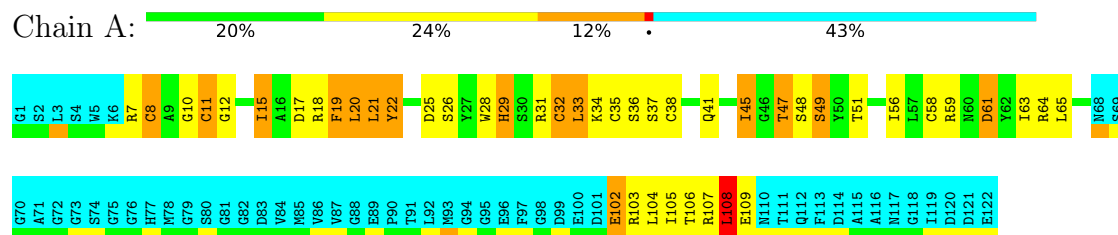
4.2.7 Score per residue for model 7

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



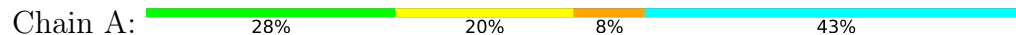
4.2.8 Score per residue for model 8

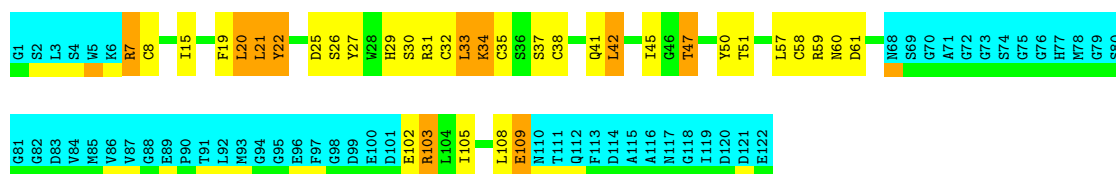
- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



4.2.9 Score per residue for model 9

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4

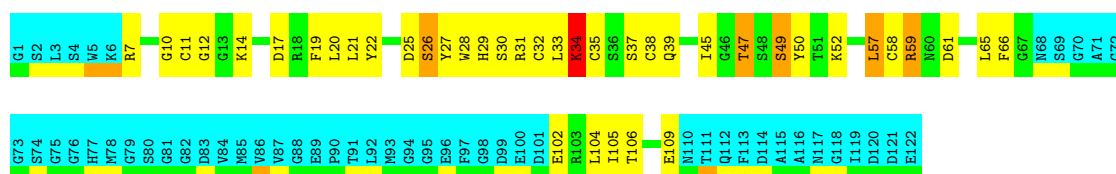




4.2.10 Score per residue for model 10

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4

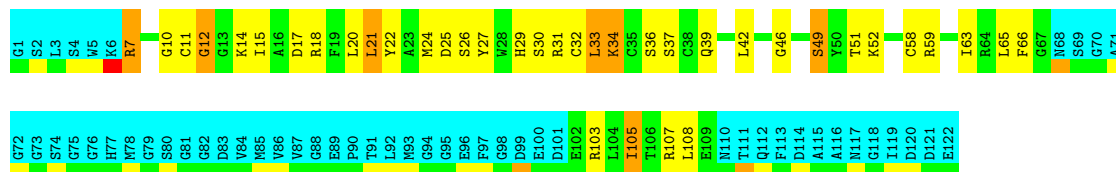
Chain A: 24% 28% 43%



4.2.11 Score per residue for model 11

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4

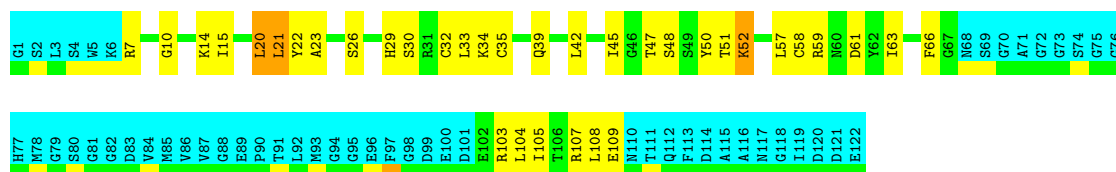
Chain A: 25% 25% 6% 43%



4.2.12 Score per residue for model 12

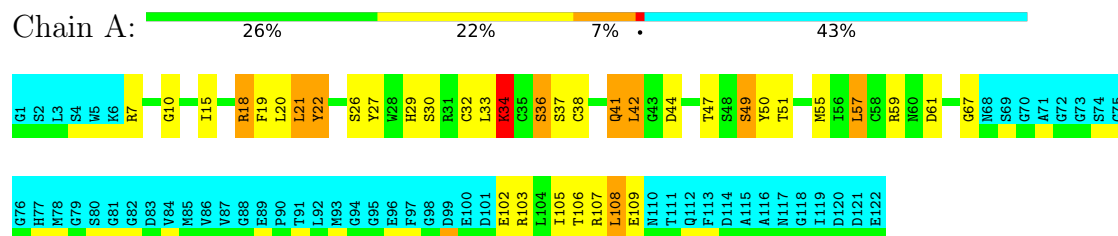
- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4

Chain A: 28% 26% 43%



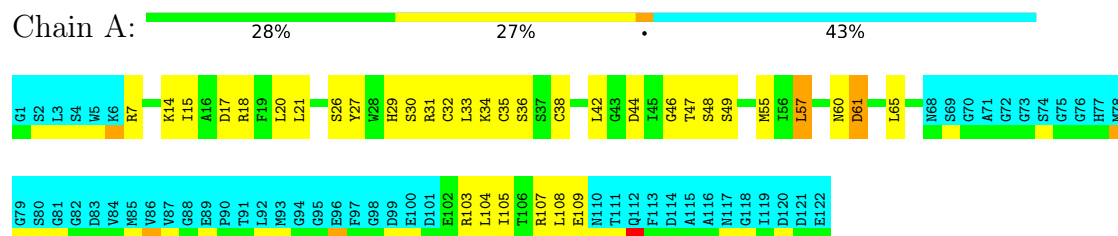
4.2.13 Score per residue for model 13

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



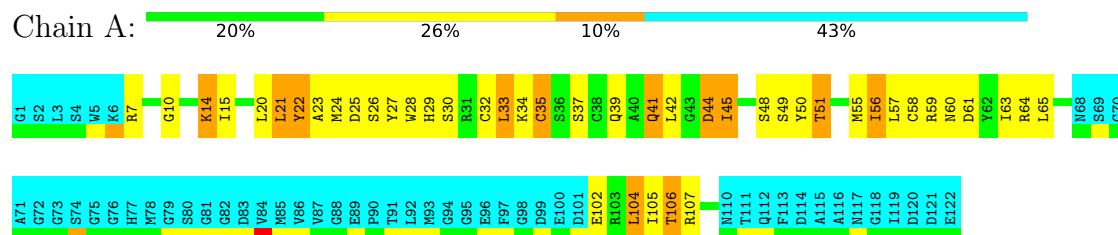
4.2.14 Score per residue for model 14

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



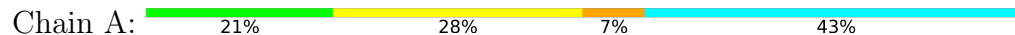
4.2.15 Score per residue for model 15

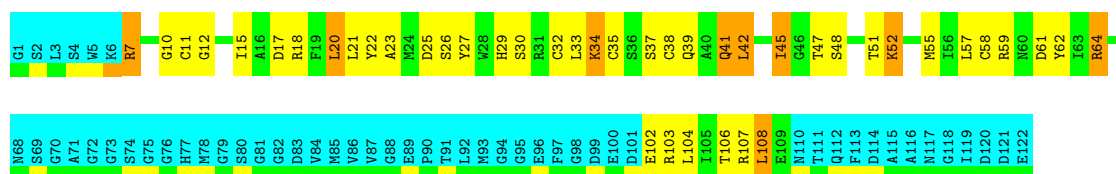
- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



4.2.16 Score per residue for model 16

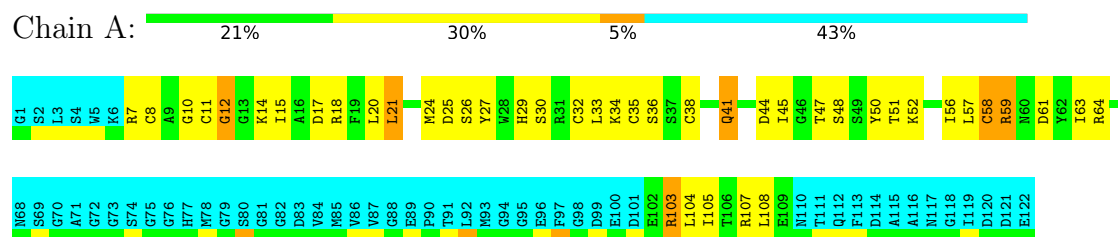
- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4





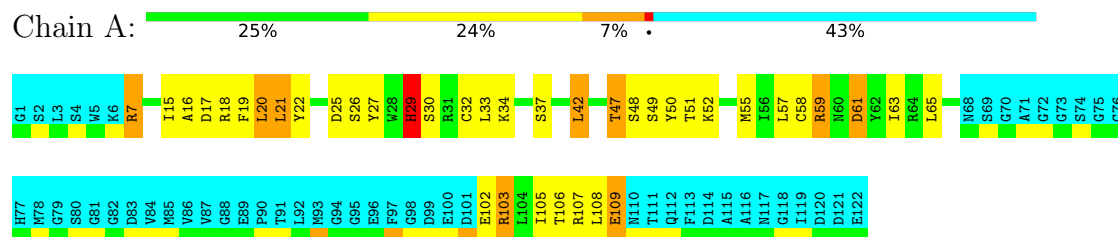
4.2.17 Score per residue for model 17

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



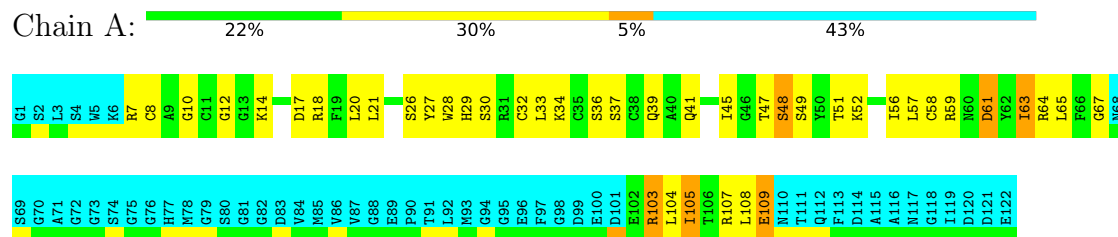
4.2.18 Score per residue for model 18

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



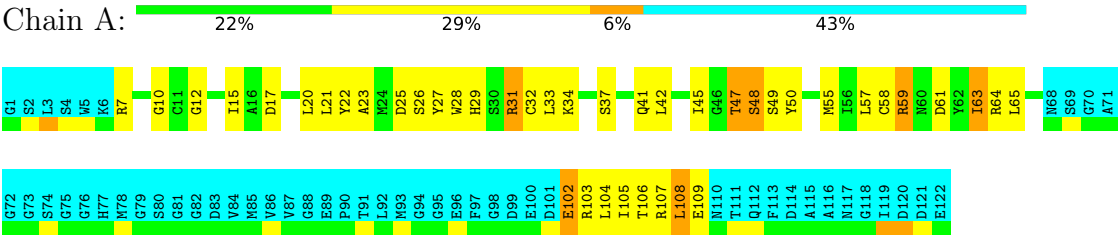
4.2.19 Score per residue for model 19

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



4.2.20 Score per residue for model 20

- Molecule 1: fusion of the LIM interacting domain of ldb1 and the N-terminal LIM domain of LMO4



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing molecular dynamics torsion angle dynamics*.

Of the 200 calculated structures, 20 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
DYANA	refinement	1.5
ARIA	structure solution	1.1.2
TALOS	structure solution	98.040.21.02

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1202
Number of shifts mapped to atoms	1202
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%

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.

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	541	528	533	15±5
All	All	10860	10560	10660	302

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:CYS:SG	1:A:61:ASP:HB2	0.97	2.00	17	14
1:A:21:LEU:HD21	1:A:105:ILE:HG23	0.89	1.45	15	12
1:A:10:GLY:HA3	1:A:32:CYS:HB3	0.85	1.46	17	16
1:A:41:GLN:HG2	1:A:44:ASP:HB2	0.77	1.52	15	1
1:A:21:LEU:HD22	1:A:33:LEU:HG	0.74	1.59	5	5
1:A:52:LYS:HE2	1:A:57:LEU:HD12	0.72	1.60	16	3
1:A:42:LEU:HD21	1:A:58:CYS:HA	0.72	1.62	11	1
1:A:20:LEU:HD23	1:A:109:GLU:HG3	0.72	1.60	4	1
1:A:29:HIS:HB2	1:A:32:CYS:SG	0.71	2.26	8	17
1:A:7:ARG:HG3	1:A:14:LYS:HG3	0.69	1.65	17	1
1:A:20:LEU:O	1:A:108:LEU:HA	0.68	1.88	13	2
1:A:19:PHE:HA	1:A:109:GLU:HB3	0.67	1.66	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD22	1:A:33:LEU:HD13	0.67	1.64	9	1
1:A:41:GLN:HB3	1:A:44:ASP:HB2	0.66	1.67	17	4
1:A:57:LEU:HB3	1:A:61:ASP:HB3	0.66	1.66	14	3
1:A:34:LYS:HG3	1:A:39:GLN:HA	0.65	1.68	3	4
1:A:42:LEU:HD11	1:A:58:CYS:HA	0.65	1.68	18	1
1:A:51:THR:HB	1:A:103:ARG:HD3	0.62	1.71	19	1
1:A:108:LEU:H	1:A:108:LEU:HD13	0.62	1.55	8	1
1:A:21:LEU:HD22	1:A:33:LEU:HD22	0.61	1.71	13	3
1:A:21:LEU:HD11	1:A:105:ILE:HG23	0.61	1.72	4	2
1:A:41:GLN:HG3	1:A:45:ILE:HG12	0.61	1.70	16	1
1:A:42:LEU:HG	1:A:105:ILE:HD11	0.61	1.70	4	1
1:A:34:LYS:HB2	1:A:39:GLN:HA	0.61	1.71	16	1
1:A:20:LEU:HD12	1:A:109:GLU:HG2	0.61	1.72	18	1
1:A:50:TYR:CD1	1:A:102:GLU:HB2	0.61	2.31	18	1
1:A:108:LEU:HD22	1:A:108:LEU:H	0.60	1.56	13	1
1:A:104:LEU:HD22	1:A:104:LEU:H	0.60	1.55	15	1
1:A:31:ARG:HA	1:A:41:GLN:NE2	0.58	2.13	20	1
1:A:59:ARG:O	1:A:63:ILE:HG12	0.57	1.99	18	6
1:A:7:ARG:O	1:A:7:ARG:HG3	0.57	1.99	4	2
1:A:23:ALA:HB3	1:A:28:TRP:CD1	0.57	2.35	20	2
1:A:15:ILE:HG23	1:A:29:HIS:CD2	0.57	2.34	8	2
1:A:8:CYS:HA	1:A:27:TYR:O	0.56	1.99	3	6
1:A:8:CYS:HB2	1:A:15:ILE:HG12	0.56	1.77	3	4
1:A:41:GLN:HG3	1:A:44:ASP:HB3	0.56	1.77	6	1
1:A:35:CYS:HB3	1:A:39:GLN:H	0.55	1.60	12	3
1:A:42:LEU:O	1:A:45:ILE:HG12	0.55	2.01	9	2
1:A:22:TYR:O	1:A:106:THR:HB	0.55	2.02	20	1
1:A:21:LEU:HD21	1:A:105:ILE:HG12	0.55	1.77	13	2
1:A:46:GLY:HA2	1:A:105:ILE:HG21	0.55	1.78	14	1
1:A:20:LEU:HG	1:A:27:TYR:HB3	0.54	1.79	9	1
1:A:104:LEU:HG	1:A:104:LEU:O	0.54	2.03	19	1
1:A:47:THR:HG22	1:A:105:ILE:HG21	0.54	1.80	20	4
1:A:35:CYS:HB3	1:A:38:CYS:HB2	0.54	1.79	3	4
1:A:29:HIS:HB2	1:A:32:CYS:HB2	0.53	1.80	20	9
1:A:22:TYR:HD2	1:A:27:TYR:CD1	0.53	2.22	16	4
1:A:29:HIS:H	1:A:32:CYS:HB2	0.53	1.64	1	4
1:A:18:ARG:O	1:A:18:ARG:HG3	0.53	2.04	13	1
1:A:22:TYR:HB2	1:A:26:SER:O	0.52	2.04	10	1
1:A:52:LYS:O	1:A:55:MET:HG2	0.52	2.04	7	1
1:A:7:ARG:HG2	1:A:8:CYS:N	0.52	2.19	3	1
1:A:48:SER:H	1:A:105:ILE:HD12	0.52	1.65	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD23	1:A:33:LEU:HD23	0.52	1.81	16	1
1:A:52:LYS:HG3	1:A:66:PHE:CZ	0.51	2.41	12	1
1:A:8:CYS:SG	1:A:12:GLY:N	0.51	2.83	8	1
1:A:10:GLY:HA3	1:A:32:CYS:CB	0.51	2.32	8	1
1:A:22:TYR:HD1	1:A:27:TYR:CD1	0.51	2.23	18	1
1:A:18:ARG:C	1:A:109:GLU:HB2	0.51	2.26	13	1
1:A:22:TYR:CB	1:A:27:TYR:HA	0.51	2.35	10	1
1:A:33:LEU:O	1:A:42:LEU:HB2	0.51	2.06	14	1
1:A:19:PHE:HB2	1:A:109:GLU:HG2	0.51	1.82	9	1
1:A:50:TYR:HE2	1:A:59:ARG:HA	0.50	1.66	18	2
1:A:28:TRP:CD2	1:A:33:LEU:HD23	0.50	2.42	4	2
1:A:29:HIS:N	1:A:32:CYS:SG	0.50	2.80	8	1
1:A:19:PHE:HA	1:A:108:LEU:HB3	0.49	1.83	13	1
1:A:50:TYR:CE1	1:A:102:GLU:HB3	0.49	2.41	3	1
1:A:42:LEU:HB3	1:A:105:ILE:HD11	0.49	1.83	2	2
1:A:22:TYR:HD2	1:A:106:THR:HG22	0.49	1.67	7	1
1:A:22:TYR:CD2	1:A:27:TYR:HE1	0.49	2.25	1	1
1:A:33:LEU:O	1:A:33:LEU:HG	0.49	2.07	8	1
1:A:19:PHE:HA	1:A:109:GLU:HG2	0.49	1.84	10	1
1:A:49:SER:OG	1:A:105:ILE:HG13	0.48	2.08	20	7
1:A:20:LEU:C	1:A:20:LEU:HD13	0.48	2.28	18	1
1:A:15:ILE:HG22	1:A:17:ASP:H	0.48	1.67	6	1
1:A:8:CYS:O	1:A:12:GLY:HA2	0.48	2.08	8	1
1:A:109:GLU:OE1	1:A:109:GLU:HA	0.48	2.08	18	1
1:A:11:CYS:SG	1:A:12:GLY:N	0.48	2.85	17	7
1:A:50:TYR:HE2	1:A:59:ARG:HD3	0.47	1.69	17	2
1:A:19:PHE:HD1	1:A:108:LEU:HB2	0.47	1.67	13	1
1:A:7:ARG:O	1:A:27:TYR:HB2	0.47	2.09	16	3
1:A:8:CYS:SG	1:A:28:TRP:HA	0.47	2.50	1	2
1:A:15:ILE:HA	1:A:29:HIS:CE1	0.47	2.44	4	1
1:A:23:ALA:HA	1:A:104:LEU:O	0.47	2.08	16	2
1:A:29:HIS:HB2	1:A:32:CYS:CB	0.47	2.40	20	2
1:A:19:PHE:HA	1:A:109:GLU:HB2	0.47	1.86	4	1
1:A:22:TYR:CD2	1:A:27:TYR:CE1	0.46	3.02	9	2
1:A:104:LEU:H	1:A:104:LEU:HD23	0.46	1.70	19	1
1:A:21:LEU:HD21	1:A:105:ILE:HA	0.46	1.88	4	1
1:A:41:GLN:HB3	1:A:44:ASP:CB	0.46	2.40	13	1
1:A:48:SER:HA	1:A:102:GLU:O	0.46	2.10	5	1
1:A:21:LEU:HD13	1:A:43:GLY:HA3	0.46	1.87	6	1
1:A:22:TYR:CD1	1:A:22:TYR:N	0.46	2.83	8	3
1:A:48:SER:N	1:A:105:ILE:HD12	0.46	2.26	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:SER:HB3	1:A:102:GLU:HG2	0.46	1.86	20	1
1:A:28:TRP:HE3	1:A:32:CYS:HB2	0.46	1.70	8	1
1:A:50:TYR:O	1:A:56:ILE:HA	0.45	2.11	17	2
1:A:36:SER:OG	1:A:57:LEU:HD23	0.45	2.10	13	1
1:A:33:LEU:HG	1:A:42:LEU:HD12	0.45	1.88	16	1
1:A:50:TYR:CE2	1:A:59:ARG:HD3	0.45	2.46	9	1
1:A:28:TRP:HB3	1:A:33:LEU:HB2	0.45	1.87	20	1
1:A:52:LYS:HG2	1:A:62:TYR:HE1	0.45	1.71	16	1
1:A:38:CYS:CB	1:A:41:GLN:HB2	0.45	2.42	16	1
1:A:28:TRP:CE3	1:A:33:LEU:HA	0.45	2.47	1	2
1:A:53:SER:HB2	1:A:55:MET:HG3	0.45	1.89	6	1
1:A:21:LEU:HD13	1:A:33:LEU:HD21	0.44	1.89	8	1
1:A:49:SER:O	1:A:102:GLU:HA	0.44	2.12	8	2
1:A:33:LEU:HD21	1:A:105:ILE:HG12	0.44	1.90	17	1
1:A:49:SER:OG	1:A:105:ILE:HG12	0.44	2.12	11	1
1:A:52:LYS:NZ	1:A:55:MET:HB3	0.44	2.26	5	1
1:A:50:TYR:CE1	1:A:59:ARG:HA	0.44	2.47	10	1
1:A:20:LEU:HD22	1:A:21:LEU:N	0.44	2.27	18	1
1:A:8:CYS:SG	1:A:11:CYS:N	0.44	2.90	8	1
1:A:61:ASP:HA	1:A:64:ARG:HB2	0.44	1.90	16	1
1:A:19:PHE:HD1	1:A:109:GLU:CG	0.44	2.25	8	1
1:A:42:LEU:HD23	1:A:45:ILE:HD11	0.44	1.88	12	1
1:A:15:ILE:CD1	1:A:27:TYR:HB3	0.44	2.42	20	1
1:A:14:LYS:HD3	1:A:16:ALA:HB2	0.43	1.88	6	1
1:A:31:ARG:O	1:A:34:LYS:HB3	0.43	2.13	9	1
1:A:20:LEU:HD12	1:A:109:GLU:CG	0.43	2.42	18	1
1:A:19:PHE:CD1	1:A:109:GLU:HB3	0.43	2.48	1	1
1:A:18:ARG:C	1:A:109:GLU:HG3	0.43	2.33	18	1
1:A:49:SER:HB2	1:A:57:LEU:O	0.43	2.13	4	1
1:A:15:ILE:HG21	1:A:20:LEU:HB2	0.43	1.89	12	1
1:A:47:THR:O	1:A:105:ILE:HD12	0.43	2.14	9	1
1:A:22:TYR:HD2	1:A:27:TYR:CE1	0.43	2.32	3	1
1:A:35:CYS:HB2	1:A:39:GLN:N	0.42	2.29	1	1
1:A:35:CYS:HB2	1:A:39:GLN:H	0.42	1.74	4	1
1:A:109:GLU:HA	1:A:109:GLU:OE1	0.42	2.14	4	1
1:A:15:ILE:HA	1:A:29:HIS:NE2	0.42	2.29	4	1
1:A:65:LEU:HB3	1:A:66:PHE:CD1	0.42	2.49	7	1
1:A:15:ILE:HB	1:A:20:LEU:HD23	0.42	1.90	5	1
1:A:20:LEU:HD22	1:A:20:LEU:N	0.42	2.29	9	1
1:A:50:TYR:HB2	1:A:52:LYS:HE3	0.42	1.91	12	1
1:A:18:ARG:O	1:A:109:GLU:HB2	0.42	2.14	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ARG:O	1:A:19:PHE:CD1	0.42	2.72	13	1
1:A:24:MET:HG3	1:A:104:LEU:HD21	0.42	1.90	17	1
1:A:58:CYS:SG	1:A:61:ASP:CB	0.42	3.07	2	1
1:A:19:PHE:CD1	1:A:108:LEU:HB2	0.42	2.48	13	1
1:A:22:TYR:CG	1:A:106:THR:HB	0.42	2.50	1	1
1:A:19:PHE:CE1	1:A:109:GLU:O	0.41	2.73	4	1
1:A:7:ARG:HD3	1:A:7:ARG:H	0.41	1.75	9	1
1:A:63:ILE:O	1:A:67:GLY:HA3	0.41	2.16	19	1
1:A:42:LEU:HB3	1:A:48:SER:O	0.41	2.14	20	1
1:A:35:CYS:HB3	1:A:39:GLN:N	0.41	2.29	12	1
1:A:19:PHE:HD1	1:A:108:LEU:CB	0.41	2.28	13	1
1:A:22:TYR:HB3	1:A:27:TYR:HA	0.41	1.91	10	1
1:A:51:THR:OG1	1:A:104:LEU:HD22	0.41	2.16	3	1
1:A:57:LEU:HD13	1:A:65:LEU:HD12	0.41	1.92	5	1
1:A:32:CYS:O	1:A:34:LYS:HG3	0.41	2.16	16	1
1:A:22:TYR:HD1	1:A:106:THR:HB	0.41	1.75	15	1
1:A:33:LEU:C	1:A:34:LYS:HG3	0.41	2.37	13	1
1:A:50:TYR:CE2	1:A:102:GLU:HG3	0.41	2.51	13	1
1:A:20:LEU:CD1	1:A:27:TYR:HB3	0.40	2.46	4	1
1:A:108:LEU:HD13	1:A:108:LEU:HA	0.40	1.76	2	1
1:A:19:PHE:CG	1:A:109:GLU:HA	0.40	2.51	9	1
1:A:34:LYS:HD3	1:A:34:LYS:H	0.40	1.77	9	1
1:A:57:LEU:HD11	1:A:66:PHE:CE2	0.40	2.52	10	1
1:A:61:ASP:HA	1:A:64:ARG:NH1	0.40	2.31	3	1
1:A:52:LYS:HG3	1:A:62:TYR:CE1	0.40	2.52	4	1
1:A:41:GLN:HG3	1:A:44:ASP:CB	0.40	2.45	6	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	69/122 (57%)	62±3 (90±4%)	6±2 (9±3%)	1±1 (2±1%)	13	57
All	All	1380/2440 (57%)	1239 (90%)	119 (9%)	22 (2%)	13	57

All 10 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	12	GLY	7
1	A	34	LYS	3
1	A	45	ILE	3
1	A	29	HIS	2
1	A	15	ILE	2
1	A	7	ARG	1
1	A	13	GLY	1
1	A	102	GLU	1
1	A	108	LEU	1
1	A	103	ARG	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	58/94 (62%)	34±4 (59±7%)	24±4 (41±7%)	0	4
All	All	1160/1880 (62%)	684 (59%)	476 (41%)	0	4

All 55 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	26	SER	20
1	A	34	LYS	20
1	A	7	ARG	19
1	A	20	LEU	19
1	A	21	LEU	18
1	A	30	SER	18
1	A	47	THR	18
1	A	107	ARG	18
1	A	103	ARG	16
1	A	25	ASP	15
1	A	108	LEU	15
1	A	37	SER	15
1	A	17	ASP	13
1	A	51	THR	13

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Mol	Chain	Res	Type	Models (Total)
1	A	41	GLN	12
1	A	65	LEU	12
1	A	102	GLU	12
1	A	48	SER	12
1	A	18	ARG	11
1	A	59	ARG	11
1	A	33	LEU	11
1	A	57	LEU	10
1	A	49	SER	9
1	A	104	LEU	9
1	A	14	LYS	8
1	A	42	LEU	8
1	A	55	MET	8
1	A	31	ARG	8
1	A	36	SER	8
1	A	52	LYS	8
1	A	106	THR	7
1	A	109	GLU	7
1	A	64	ARG	7
1	A	22	TYR	6
1	A	45	ILE	6
1	A	61	ASP	5
1	A	56	ILE	5
1	A	38	CYS	4
1	A	24	MET	4
1	A	60	ASN	4
1	A	15	ILE	4
1	A	63	ILE	4
1	A	35	CYS	3
1	A	19	PHE	2
1	A	39	GLN	2
1	A	105	ILE	2
1	A	44	ASP	2
1	A	50	TYR	1
1	A	53	SER	1
1	A	8	CYS	1
1	A	11	CYS	1
1	A	32	CYS	1
1	A	66	PHE	1
1	A	58	CYS	1
1	A	29	HIS	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 monosaccharides 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 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	1202
Number of shifts mapped to atoms	1202
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	118	-0.14 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	98	0.43 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}'$	106	0.05 ± 0.15	None needed (< 0.5 ppm)
^{15}N	114	1.08 ± 0.42	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 82%, i.e. 698 atoms were assigned a chemical shift out of a possible 852. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	339/345 (98%)	136/138 (99%)	134/138 (97%)	69/69 (100%)
Sidechain	325/438 (74%)	211/260 (81%)	114/151 (75%)	0/27 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	34/69 (49%)	33/36 (92%)	0/31 (0%)	1/2 (50%)
Overall	698/852 (82%)	380/434 (88%)	248/320 (78%)	70/98 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1082 atoms were assigned a chemical shift out of a possible 1368. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	555/608 (91%)	217/243 (89%)	224/244 (92%)	114/121 (94%)
Sidechain	480/653 (74%)	315/384 (82%)	165/237 (70%)	0/32 (0%)
Aromatic	47/107 (44%)	45/56 (80%)	0/46 (0%)	2/5 (40%)
Overall	1082/1368 (79%)	577/683 (84%)	389/527 (74%)	116/158 (73%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	33	LEU	HD21	-0.82	2.14 – -0.66	-5.6
1	A	33	LEU	HD22	-0.82	2.14 – -0.66	-5.6
1	A	33	LEU	HD23	-0.82	2.14 – -0.66	-5.6

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

