



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:35 PM BST

PDB ID : 2JTN  
Title : NMR Solution Structure of a ldb1-LID:Lhx3-LIM complex  
Authors : Lee, C.; Nancarrow, A.L.; Mackay, J.P.; Matthews, J.M.  
Deposited on : 2007-08-03

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : unknown  
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

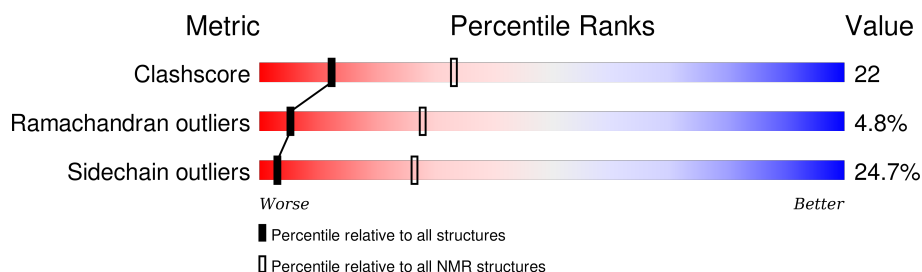
# 1 Overall quality at a glance

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
Sidechain outliers	111093	9958

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  $\geq 3$ , 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	182	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:38, A:57-A:182 (158)	1.00	6

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 5 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2750 atoms, of which 1337 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LIM domain-binding protein 1, LIM/homeobox protein Lhx3.

Mol	Chain	Residues	Atoms						Trace
1	A	182	Total	C	H	N	O	S	0
			2746	873	1337	249	269	18	

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLY	-	SEE REMARK 999	UNP P50481
A	47	GLY	-	SEE REMARK 999	UNP P50481
A	48	SER	-	SEE REMARK 999	UNP P50481
A	49	GLY	-	SEE REMARK 999	UNP P50481
A	50	GLY	-	SEE REMARK 999	UNP P50481
A	51	HIS	-	SEE REMARK 999	UNP P50481
A	52	MET	-	SEE REMARK 999	UNP P50481
A	53	GLY	-	SEE REMARK 999	UNP P50481
A	54	SER	-	SEE REMARK 999	UNP P50481
A	55	GLY	-	SEE REMARK 999	UNP P50481
A	56	GLY	-	SEE REMARK 999	UNP P50481

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

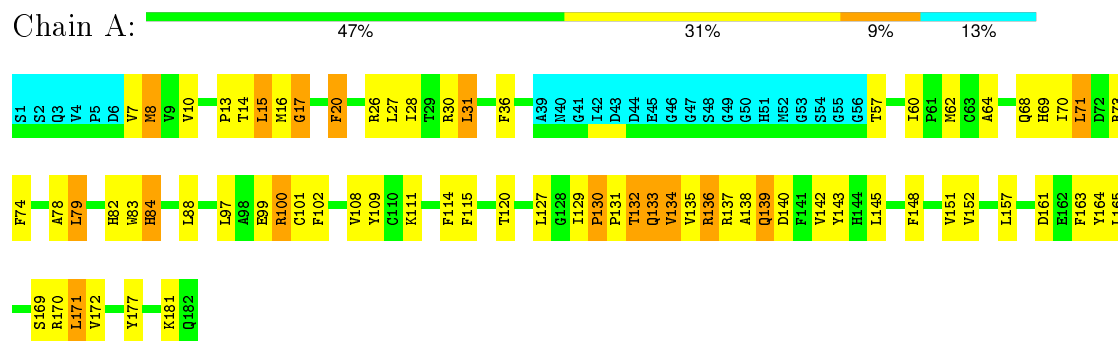
Mol	Chain	Residues	Atoms	
2	A	4	Total	Zn
			4	4

## 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: LIM domain-binding protein 1, LIM/homeobox protein Lhx3

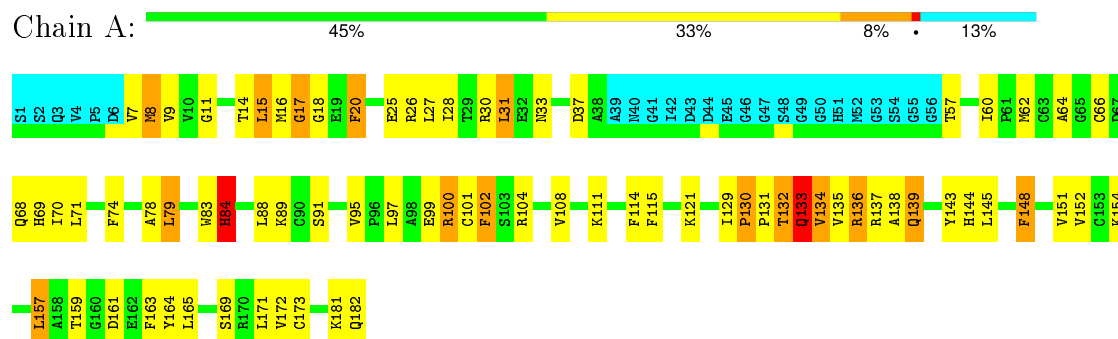


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

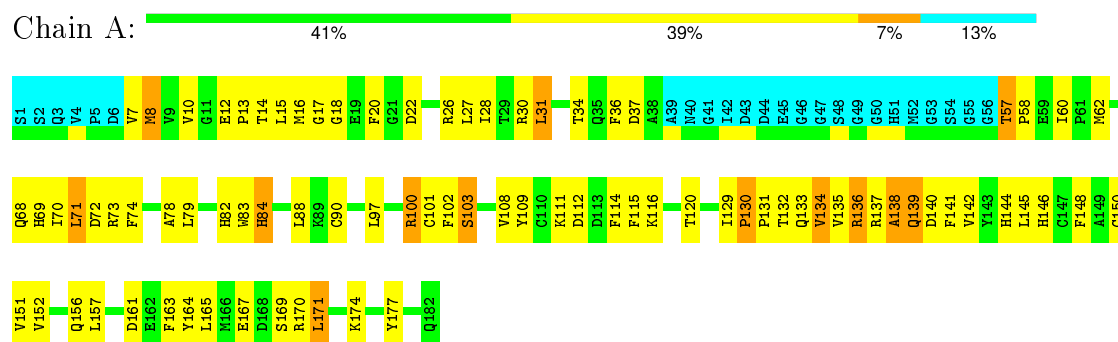
#### 4.2.1 Score per residue for model 1

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



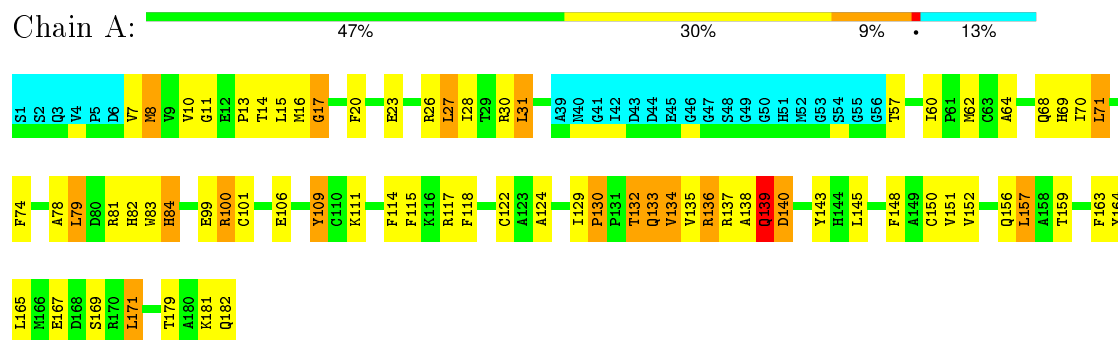
### 4.2.2 Score per residue for model 2

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



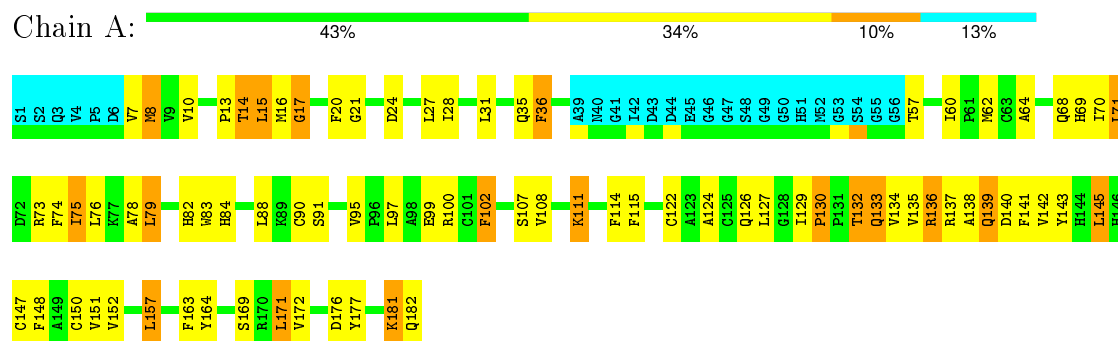
### 4.2.3 Score per residue for model 3

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



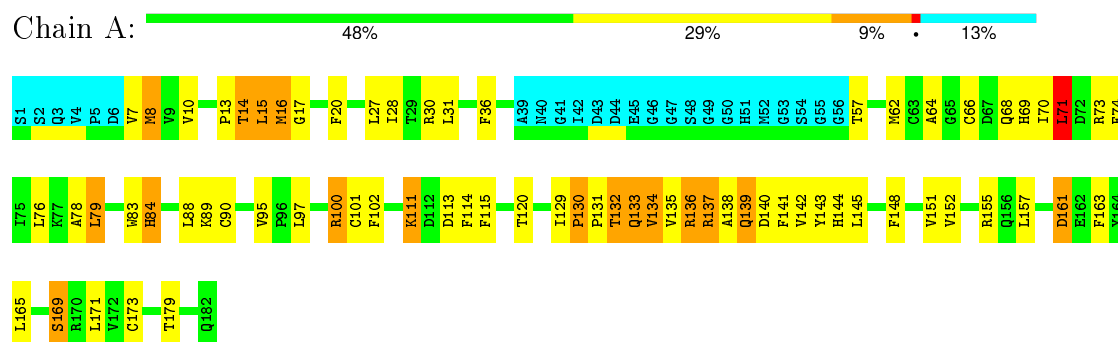
### 4.2.4 Score per residue for model 4

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



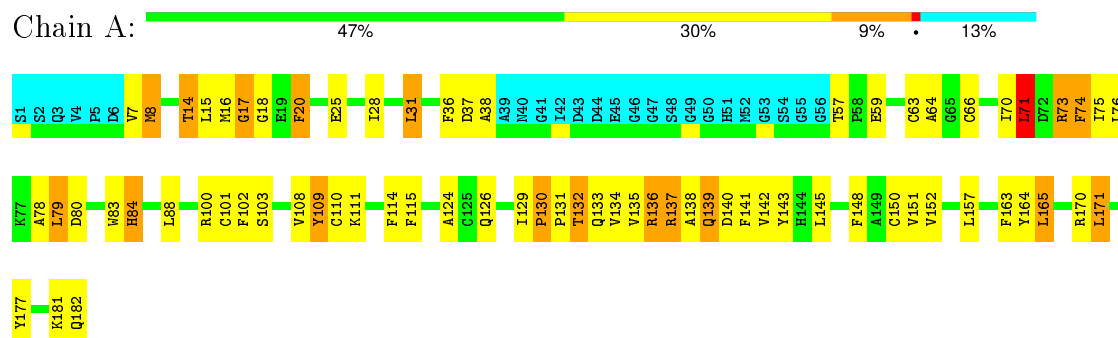
### 4.2.5 Score per residue for model 5

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



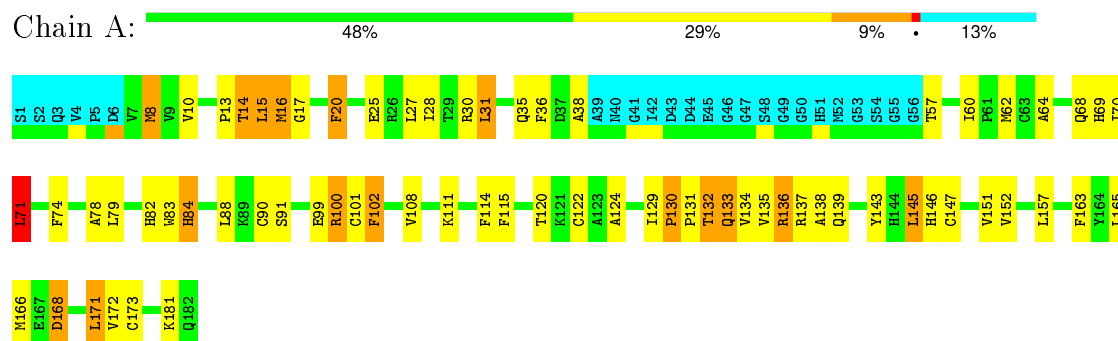
### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



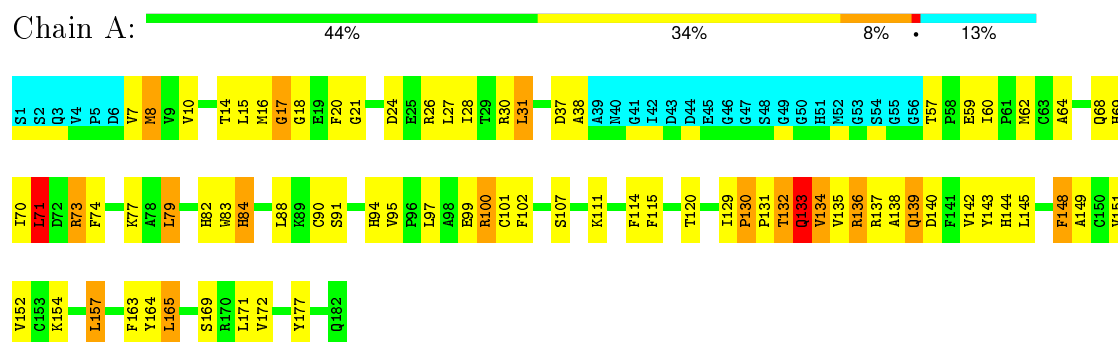
### 4.2.7 Score per residue for model 7

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



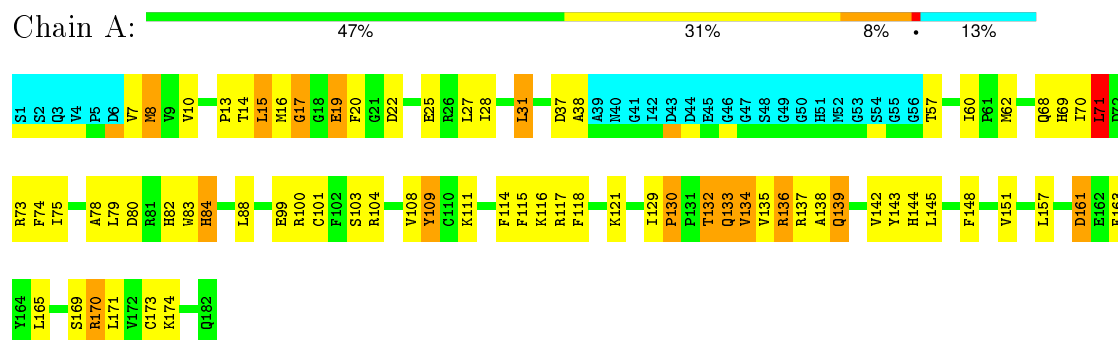
#### 4.2.8 Score per residue for model 8

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



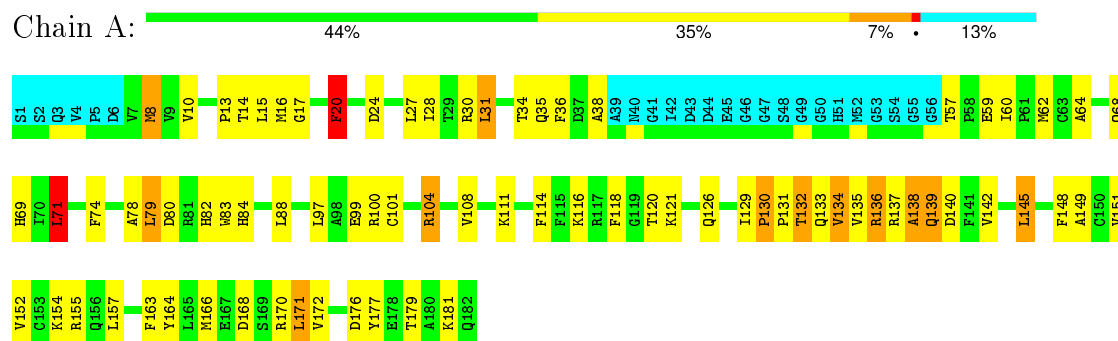
#### 4.2.9 Score per residue for model 9

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



#### 4.2.10 Score per residue for model 10

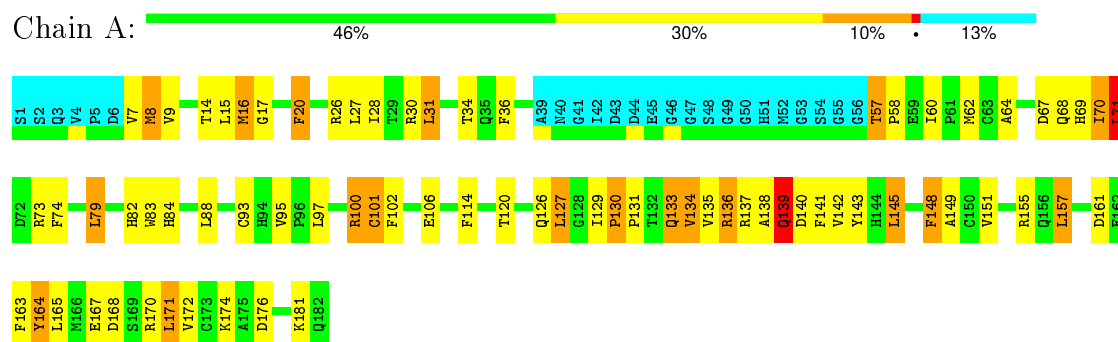
- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3





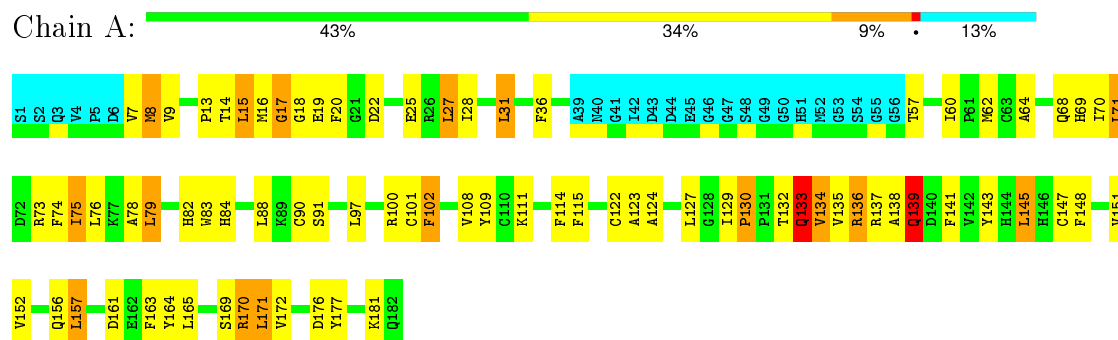
### 4.2.11 Score per residue for model 11

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



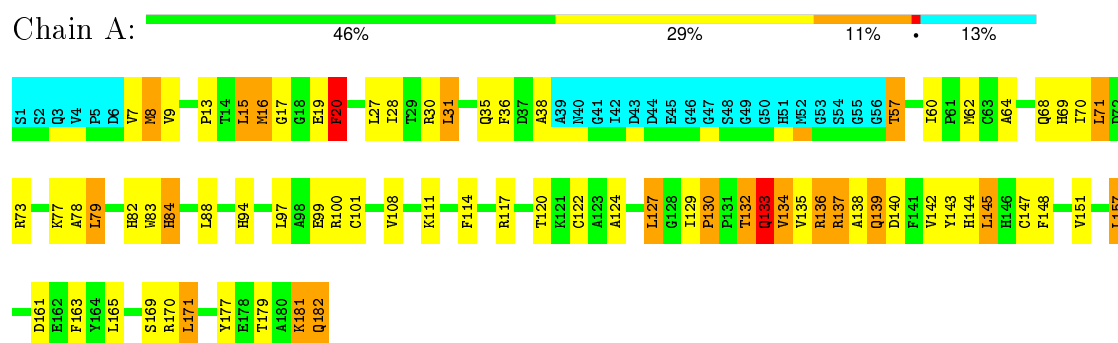
### 4.2.12 Score per residue for model 12

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



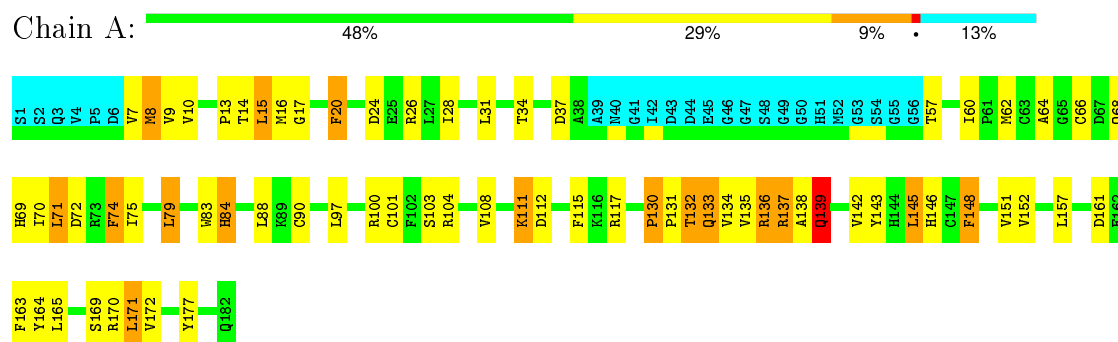
### 4.2.13 Score per residue for model 13

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



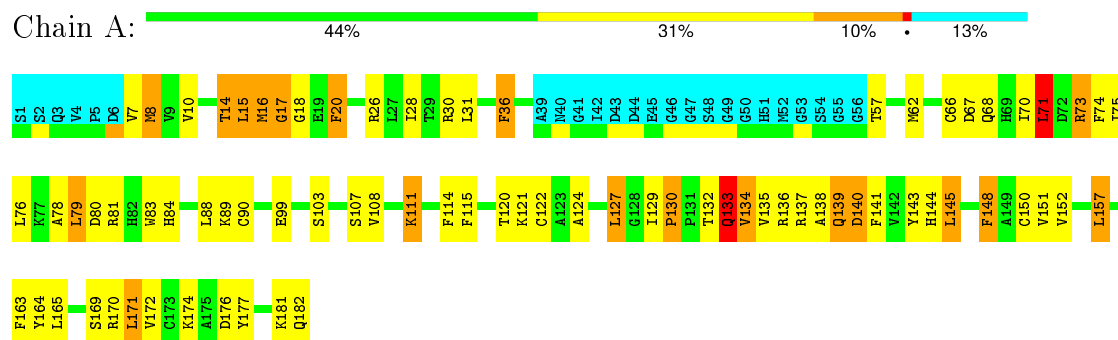
#### 4.2.14 Score per residue for model 14

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



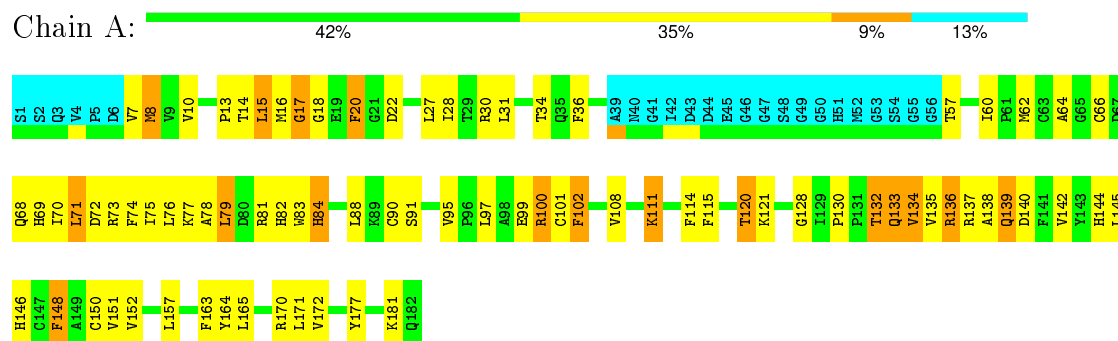
#### 4.2.15 Score per residue for model 15

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



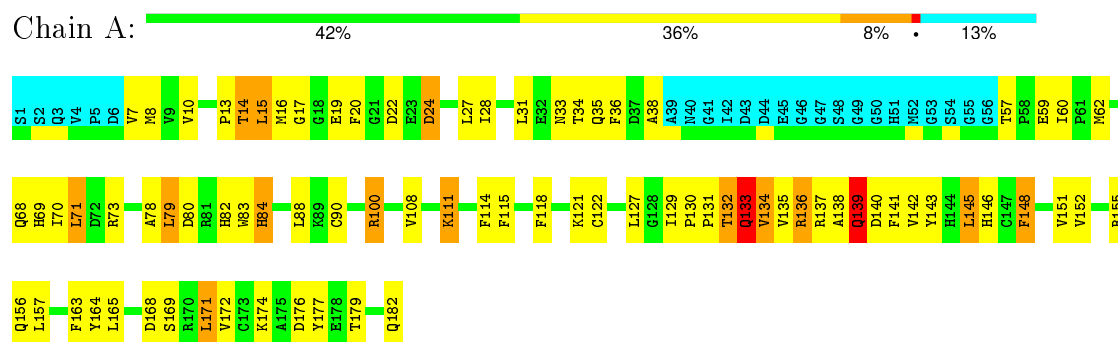
#### 4.2.16 Score per residue for model 16

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



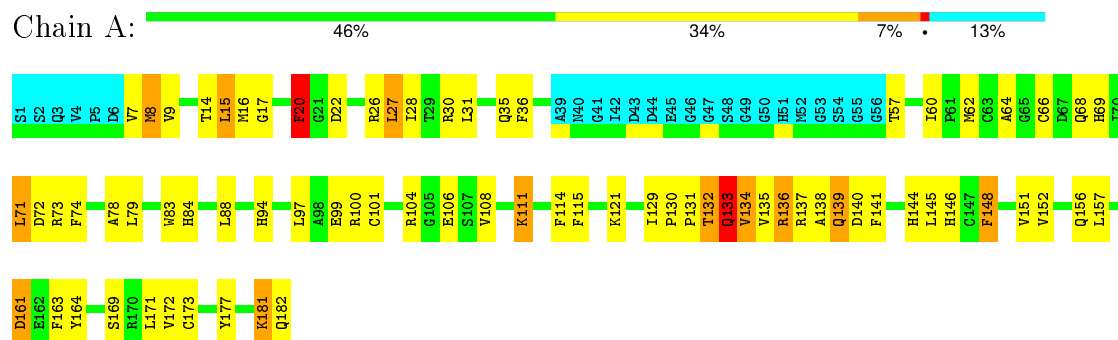
### 4.2.17 Score per residue for model 17

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



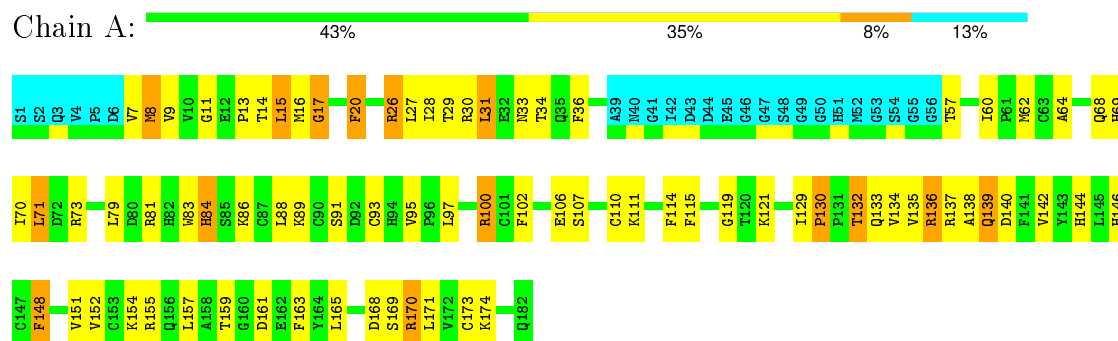
### 4.2.18 Score per residue for model 18

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



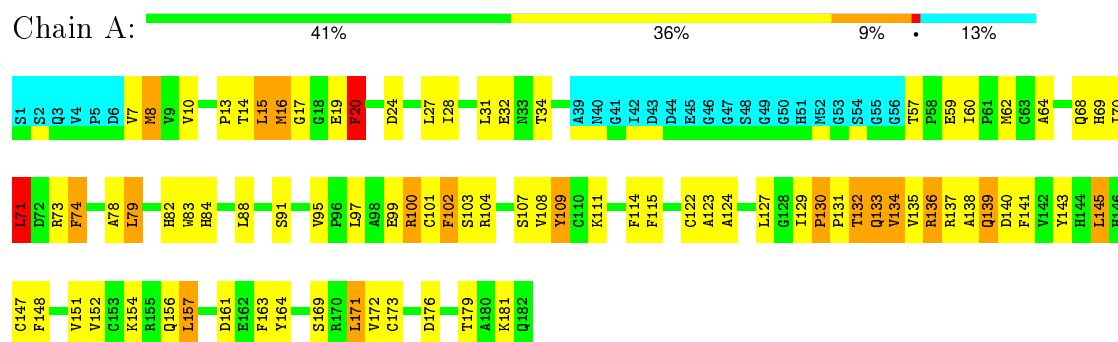
### 4.2.19 Score per residue for model 19

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



### 4.2.20 Score per residue for model 20

- Molecule 1: LIM domain-binding protein 1, LIM/homeobox protein Lhx3



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics, cartesian 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
CNS	refinement	1.1
ARIA	refinement	1.2

No chemical shift data was provided. 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.

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	1258	1210	1209	55±6
All	All	25240	24200	24180	1098

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HD12	1:A:88:LEU:HD21	0.85	1.47	19	1
1:A:28:ILE:HG21	1:A:88:LEU:HD21	0.83	1.50	17	14
1:A:134:VAL:O	1:A:145:LEU:HD21	0.81	1.76	12	13
1:A:17:GLY:CA	1:A:132:THR:HG23	0.80	2.07	13	19
1:A:17:GLY:HA3	1:A:132:THR:HG23	0.80	1.53	14	18
1:A:163:PHE:CD2	1:A:171:LEU:HD23	0.79	2.13	18	19
1:A:139:GLN:CG	1:A:165:LEU:HD13	0.78	2.08	17	2
1:A:148:PHE:CZ	1:A:171:LEU:HD21	0.77	2.14	20	18
1:A:124:ALA:HB2	1:A:143:TYR:CE2	0.77	2.15	15	7
1:A:79:LEU:HD12	1:A:83:TRP:CZ2	0.77	2.14	6	4
1:A:15:LEU:HD12	1:A:133:GLN:HG3	0.76	1.57	17	8
1:A:70:ILE:HD11	1:A:82:HIS:NE2	0.76	1.95	11	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:PHE:CE1	1:A:171:LEU:HD11	0.74	2.16	14	9
1:A:137:ARG:CB	1:A:142:VAL:HG22	0.74	2.12	5	1
1:A:79:LEU:HD21	1:A:101:CYS:SG	0.72	2.24	10	8
1:A:151:VAL:HG13	1:A:171:LEU:O	0.72	1.83	15	3
1:A:79:LEU:HD12	1:A:83:TRP:NE1	0.72	1.99	12	17
1:A:148:PHE:CE1	1:A:171:LEU:HD21	0.72	2.19	4	14
1:A:13:PRO:HB2	1:A:134:VAL:HG12	0.71	1.62	4	12
1:A:126:GLN:O	1:A:127:LEU:HD12	0.71	1.86	11	2
1:A:28:ILE:HD11	1:A:99:GLU:C	0.71	2.07	4	11
1:A:79:LEU:HD12	1:A:83:TRP:CE2	0.70	2.21	11	12
1:A:83:TRP:CB	1:A:88:LEU:HD13	0.69	2.17	9	10
1:A:133:GLN:OE1	1:A:145:LEU:HD11	0.69	1.88	20	2
1:A:28:ILE:HD11	1:A:99:GLU:N	0.68	2.03	8	2
1:A:138:ALA:HB1	1:A:165:LEU:HD11	0.68	1.65	3	10
1:A:28:ILE:HG23	1:A:101:CYS:HB2	0.68	1.64	14	14
1:A:27:LEU:HD21	1:A:100:ARG:HG2	0.68	1.66	4	4
1:A:28:ILE:CD1	1:A:88:LEU:HD21	0.68	2.19	19	1
1:A:129:ILE:CD1	1:A:142:VAL:HG13	0.68	2.19	6	4
1:A:15:LEU:HD11	1:A:129:ILE:HG22	0.68	1.65	1	8
1:A:88:LEU:HD23	1:A:97:LEU:O	0.67	1.90	10	7
1:A:34:THR:HG23	1:A:38:ALA:HB2	0.67	1.66	17	1
1:A:60:ILE:HG21	1:A:69:HIS:CD2	0.67	2.25	11	15
1:A:157:LEU:N	1:A:157:LEU:HD22	0.66	2.05	3	11
1:A:172:VAL:HG23	1:A:176:ASP:OD2	0.66	1.90	17	4
1:A:70:ILE:HD11	1:A:82:HIS:CD2	0.66	2.26	11	1
1:A:120:THR:HG22	1:A:142:VAL:HG11	0.66	1.66	2	1
1:A:157:LEU:HD22	1:A:157:LEU:N	0.65	2.06	17	9
1:A:148:PHE:CD1	1:A:171:LEU:HD11	0.64	2.28	15	3
1:A:151:VAL:HG11	1:A:170:ARG:NH1	0.64	2.07	10	1
1:A:88:LEU:HD11	1:A:101:CYS:SG	0.64	2.33	5	3
1:A:16:MET:SD	1:A:120:THR:HG21	0.64	2.33	11	4
1:A:22:ASP:CB	1:A:27:LEU:HD13	0.63	2.24	2	1
1:A:28:ILE:HA	1:A:78:ALA:HB2	0.62	1.72	7	13
1:A:122:CYS:HB2	1:A:129:ILE:HD11	0.62	1.71	13	3
1:A:138:ALA:HB3	1:A:143:TYR:CE1	0.61	2.30	14	6
1:A:15:LEU:HG	1:A:135:VAL:HG12	0.61	1.72	14	12
1:A:28:ILE:HG23	1:A:101:CYS:CB	0.61	2.26	7	10
1:A:139:GLN:OE1	1:A:165:LEU:HD22	0.61	1.95	3	3
1:A:28:ILE:HG22	1:A:78:ALA:HB2	0.60	1.72	4	5
1:A:156:GLN:C	1:A:157:LEU:HD22	0.60	2.17	2	4
1:A:28:ILE:CG2	1:A:88:LEU:HD21	0.59	2.27	16	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LEU:HD23	1:A:100:ARG:O	0.59	1.97	11	1
1:A:124:ALA:HB2	1:A:143:TYR:CZ	0.59	2.33	7	1
1:A:27:LEU:HD11	1:A:100:ARG:CB	0.59	2.27	11	4
1:A:27:LEU:HD12	1:A:100:ARG:CB	0.59	2.27	8	2
1:A:120:THR:CG2	1:A:142:VAL:HG11	0.59	2.28	2	3
1:A:22:ASP:HB3	1:A:27:LEU:HD22	0.59	1.74	17	3
1:A:139:GLN:HG2	1:A:165:LEU:HD13	0.59	1.74	17	1
1:A:137:ARG:HB3	1:A:142:VAL:HG22	0.59	1.75	5	1
1:A:70:ILE:C	1:A:71:LEU:HD23	0.59	2.17	6	6
1:A:64:ALA:HB3	1:A:83:TRP:CD2	0.58	2.33	11	8
1:A:8:MET:HE1	1:A:163:PHE:CE2	0.58	2.33	7	11
1:A:38:ALA:O	1:A:71:LEU:HD22	0.58	1.98	10	1
1:A:17:GLY:HA2	1:A:132:THR:HG23	0.57	1.74	6	2
1:A:11:GLY:HA2	1:A:159:THR:HG23	0.57	1.75	19	2
1:A:79:LEU:HD22	1:A:103:SER:HB2	0.57	1.74	14	1
1:A:135:VAL:HG21	1:A:143:TYR:O	0.57	1.99	12	8
1:A:151:VAL:HG23	1:A:152:VAL:HG23	0.57	1.77	15	15
1:A:22:ASP:HB2	1:A:27:LEU:HD13	0.57	1.76	2	1
1:A:28:ILE:HD12	1:A:88:LEU:CD2	0.57	2.27	19	1
1:A:135:VAL:HG23	1:A:145:LEU:HG	0.57	1.77	17	11
1:A:10:VAL:HG21	1:A:157:LEU:HB3	0.56	1.76	5	2
1:A:28:ILE:HG21	1:A:88:LEU:CD2	0.56	2.30	6	10
1:A:27:LEU:HD12	1:A:100:ARG:HB3	0.56	1.78	10	3
1:A:26:ARG:HD2	1:A:79:LEU:HD23	0.55	1.78	19	1
1:A:7:VAL:HG23	1:A:164:TYR:CE1	0.55	2.36	3	3
1:A:97:LEU:HD21	1:A:110:CYS:HB3	0.55	1.77	19	1
1:A:172:VAL:HG23	1:A:176:ASP:HB3	0.55	1.78	15	2
1:A:122:CYS:N	1:A:129:ILE:HD11	0.55	2.16	7	6
1:A:164:TYR:HB2	1:A:172:VAL:HG13	0.55	1.77	17	8
1:A:138:ALA:O	1:A:140:ASP:N	0.55	2.40	17	14
1:A:15:LEU:HD11	1:A:129:ILE:CG2	0.55	2.32	12	9
1:A:60:ILE:HD13	1:A:69:HIS:CD2	0.55	2.36	18	2
1:A:31:LEU:O	1:A:31:LEU:HD12	0.54	2.02	3	8
1:A:143:TYR:OH	1:A:165:LEU:HD11	0.54	2.02	11	1
1:A:124:ALA:HB2	1:A:143:TYR:CD2	0.54	2.36	3	4
1:A:28:ILE:HG22	1:A:78:ALA:CB	0.54	2.32	4	2
1:A:139:GLN:HG3	1:A:165:LEU:HD22	0.54	1.80	11	2
1:A:79:LEU:N	1:A:79:LEU:HD23	0.54	2.18	16	7
1:A:27:LEU:HD21	1:A:100:ARG:CG	0.54	2.32	4	2
1:A:22:ASP:HB2	1:A:27:LEU:HD22	0.54	1.78	2	1
1:A:130:PRO:CB	1:A:133:GLN:HG2	0.54	2.33	2	4

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ARG:HB3	1:A:142:VAL:HG23	0.53	1.80	13	1
1:A:129:ILE:HD12	1:A:142:VAL:HG13	0.53	1.80	6	2
1:A:151:VAL:HG11	1:A:170:ARG:CG	0.53	2.32	11	3
1:A:79:LEU:HD22	1:A:103:SER:OG	0.53	2.03	20	4
1:A:27:LEU:HD11	1:A:100:ARG:HB3	0.53	1.79	19	6
1:A:151:VAL:HG22	1:A:171:LEU:O	0.53	2.04	13	1
1:A:164:TYR:CG	1:A:177:TYR:CE1	0.52	2.96	17	6
1:A:20:PHE:CZ	1:A:115:PHE:CE1	0.52	2.98	8	3
1:A:137:ARG:HB2	1:A:142:VAL:HG22	0.52	1.79	5	1
1:A:20:PHE:CE2	1:A:114:PHE:CD2	0.52	2.98	17	1
1:A:157:LEU:HD12	1:A:161:ASP:OD2	0.52	2.04	1	1
1:A:135:VAL:HB	1:A:145:LEU:HD11	0.52	1.80	1	1
1:A:120:THR:HG22	1:A:142:VAL:CG1	0.52	2.35	16	2
1:A:152:VAL:HG21	1:A:176:ASP:HB2	0.52	1.81	10	2
1:A:20:PHE:CE2	1:A:114:PHE:CD1	0.52	2.98	8	5
1:A:133:GLN:OE1	1:A:135:VAL:HG12	0.52	2.05	18	3
1:A:70:ILE:HD11	1:A:84:HIS:CD2	0.51	2.40	3	7
1:A:74:PHE:C	1:A:75:ILE:HD12	0.51	2.25	14	1
1:A:70:ILE:O	1:A:71:LEU:HD23	0.51	2.05	5	2
1:A:123:ALA:HB3	1:A:141:PHE:HB3	0.51	1.81	20	2
1:A:31:LEU:HD12	1:A:31:LEU:O	0.51	2.05	2	4
1:A:164:TYR:CD2	1:A:177:TYR:CD1	0.51	2.99	10	9
1:A:156:GLN:O	1:A:157:LEU:HD13	0.51	2.05	3	2
1:A:22:ASP:CB	1:A:27:LEU:HD22	0.51	2.35	2	1
1:A:20:PHE:CZ	1:A:114:PHE:CE1	0.51	2.99	16	11
1:A:136:ARG:HD3	1:A:145:LEU:HD12	0.51	1.83	9	1
1:A:129:ILE:HG23	1:A:133:GLN:HE21	0.51	1.66	9	5
1:A:83:TRP:HB3	1:A:88:LEU:HD13	0.51	1.83	2	7
1:A:114:PHE:CZ	1:A:118:PHE:CD2	0.51	2.99	3	2
1:A:130:PRO:HB2	1:A:133:GLN:HB3	0.50	1.83	19	13
1:A:20:PHE:CE2	1:A:114:PHE:CE2	0.50	2.99	17	1
1:A:102:PHE:CE1	1:A:114:PHE:CE2	0.50	3.00	1	4
1:A:20:PHE:CE2	1:A:115:PHE:CE1	0.50	2.99	12	2
1:A:20:PHE:CE1	1:A:115:PHE:CD1	0.50	2.99	2	1
1:A:135:VAL:HG22	1:A:136:ARG:N	0.50	2.22	6	19
1:A:102:PHE:CZ	1:A:114:PHE:CD2	0.50	3.00	12	1
1:A:102:PHE:CE2	1:A:114:PHE:CD2	0.50	3.00	12	2
1:A:135:VAL:HB	1:A:145:LEU:HD23	0.50	1.82	13	1
1:A:34:THR:HG23	1:A:34:THR:O	0.50	2.07	11	2
1:A:22:ASP:O	1:A:27:LEU:HD13	0.50	2.07	12	1
1:A:79:LEU:HD22	1:A:103:SER:CB	0.50	2.37	14	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:PHE:CE1	1:A:114:PHE:CE1	0.50	3.00	19	1
1:A:114:PHE:CE2	1:A:118:PHE:CE2	0.50	3.00	3	2
1:A:15:LEU:HD22	1:A:16:MET:HE3	0.50	1.84	20	1
1:A:151:VAL:HG11	1:A:170:ARG:CZ	0.50	2.36	10	1
1:A:15:LEU:HD12	1:A:133:GLN:CG	0.49	2.37	12	5
1:A:13:PRO:O	1:A:134:VAL:HG12	0.49	2.06	3	2
1:A:34:THR:O	1:A:34:THR:HG22	0.49	2.07	16	1
1:A:10:VAL:HG23	1:A:161:ASP:O	0.49	2.07	20	4
1:A:139:GLN:CD	1:A:165:LEU:HD13	0.49	2.27	17	1
1:A:114:PHE:CE2	1:A:118:PHE:CD2	0.49	3.00	3	1
1:A:137:ARG:HB3	1:A:142:VAL:HG13	0.49	1.83	5	1
1:A:20:PHE:CE2	1:A:114:PHE:CE1	0.49	3.01	11	3
1:A:74:PHE:O	1:A:75:ILE:HD13	0.49	2.08	15	4
1:A:22:ASP:HB3	1:A:27:LEU:HD13	0.48	1.85	18	1
1:A:164:TYR:CD2	1:A:177:TYR:CE1	0.48	3.01	2	1
1:A:60:ILE:HD13	1:A:69:HIS:CG	0.48	2.44	18	1
1:A:108:VAL:O	1:A:108:VAL:HG13	0.48	2.08	10	6
1:A:157:LEU:N	1:A:157:LEU:CD2	0.48	2.76	18	9
1:A:15:LEU:HD21	1:A:135:VAL:CG1	0.48	2.39	2	2
1:A:7:VAL:HG11	1:A:174:LYS:CE	0.48	2.37	11	1
1:A:102:PHE:CZ	1:A:114:PHE:CE2	0.48	3.02	19	1
1:A:97:LEU:HD23	1:A:101:CYS:SG	0.48	2.47	2	1
1:A:151:VAL:HG11	1:A:170:ARG:HG2	0.48	1.85	9	3
1:A:133:GLN:NE2	1:A:135:VAL:HG11	0.48	2.23	10	1
1:A:102:PHE:O	1:A:108:VAL:HG23	0.48	2.08	2	3
1:A:64:ALA:CB	1:A:83:TRP:CD2	0.48	2.97	6	11
1:A:149:ALA:HB1	1:A:155:ARG:O	0.48	2.08	10	1
1:A:11:GLY:C	1:A:159:THR:HG23	0.48	2.30	3	1
1:A:108:VAL:HG13	1:A:108:VAL:O	0.47	2.09	18	8
1:A:9:VAL:HG23	1:A:161:ASP:C	0.47	2.30	13	7
1:A:149:ALA:HB1	1:A:155:ARG:C	0.47	2.29	11	2
1:A:136:ARG:NE	1:A:148:PHE:CZ	0.47	2.82	2	1
1:A:64:ALA:HB1	1:A:83:TRP:CH2	0.47	2.43	10	1
1:A:129:ILE:HD12	1:A:142:VAL:CG1	0.47	2.39	2	3
1:A:20:PHE:CE1	1:A:114:PHE:CD1	0.47	3.03	2	1
1:A:7:VAL:HG11	1:A:174:LYS:HE2	0.47	1.84	11	1
1:A:157:LEU:CD2	1:A:157:LEU:N	0.47	2.78	6	10
1:A:114:PHE:CE1	1:A:118:PHE:CD2	0.47	3.02	9	1
1:A:109:TYR:CD1	1:A:109:TYR:N	0.47	2.82	3	4
1:A:95:VAL:O	1:A:97:LEU:HD13	0.47	2.10	8	6
1:A:16:MET:HE3	1:A:120:THR:HB	0.47	1.86	5	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HD11	1:A:99:GLU:O	0.47	2.10	3	3
1:A:38:ALA:HB3	1:A:71:LEU:HD22	0.47	1.87	7	1
1:A:22:ASP:OD1	1:A:27:LEU:HD11	0.47	2.10	9	1
1:A:27:LEU:HD12	1:A:100:ARG:CG	0.46	2.40	8	1
1:A:79:LEU:HD23	1:A:79:LEU:N	0.46	2.24	20	4
1:A:120:THR:HG22	1:A:142:VAL:HG12	0.46	1.85	16	1
1:A:8:MET:CE	1:A:163:PHE:CE2	0.46	2.99	7	7
1:A:129:ILE:HG23	1:A:130:PRO:HD2	0.46	1.87	11	3
1:A:109:TYR:N	1:A:109:TYR:CD1	0.46	2.83	6	1
1:A:70:ILE:CD1	1:A:84:HIS:CE1	0.46	2.98	17	3
1:A:34:THR:HG22	1:A:34:THR:O	0.46	2.10	20	1
1:A:60:ILE:CG2	1:A:69:HIS:CD2	0.46	2.98	17	5
1:A:28:ILE:HD11	1:A:99:GLU:CA	0.46	2.40	9	3
1:A:70:ILE:CD1	1:A:84:HIS:CD2	0.46	2.99	8	6
1:A:164:TYR:CG	1:A:177:TYR:CD1	0.46	3.04	18	2
1:A:148:PHE:CZ	1:A:171:LEU:CD2	0.46	2.98	17	7
1:A:124:ALA:CB	1:A:143:TYR:CE2	0.45	2.99	7	3
1:A:143:TYR:CE2	1:A:171:LEU:CD1	0.45	3.00	7	1
1:A:127:LEU:CB	1:A:144:HIS:CE1	0.45	3.00	15	2
1:A:148:PHE:CE1	1:A:171:LEU:CD2	0.45	3.00	11	5
1:A:137:ARG:CG	1:A:142:VAL:HG23	0.45	2.40	6	1
1:A:130:PRO:CB	1:A:133:GLN:CG	0.45	2.94	2	4
1:A:70:ILE:CD1	1:A:82:HIS:CD2	0.45	3.00	11	1
1:A:122:CYS:CA	1:A:129:ILE:HD11	0.45	2.41	7	3
1:A:10:VAL:HG23	1:A:163:PHE:CD1	0.45	2.47	16	5
1:A:177:TYR:CE2	1:A:182:GLN:CB	0.45	3.00	18	2
1:A:32:GLU:CG	1:A:74:PHE:CE1	0.45	3.00	20	1
1:A:36:PHE:CE1	1:A:73:ARG:CZ	0.45	3.00	15	1
1:A:36:PHE:CE2	1:A:73:ARG:NH1	0.45	2.85	6	1
1:A:163:PHE:CD2	1:A:171:LEU:CD2	0.45	3.00	1	6
1:A:25:GLU:CG	1:A:102:PHE:CE2	0.45	3.00	7	1
1:A:64:ALA:HB1	1:A:83:TRP:CE3	0.45	2.47	6	1
1:A:104:ARG:CD	1:A:118:PHE:CE2	0.45	3.00	10	1
1:A:14:THR:N	1:A:135:VAL:O	0.45	2.49	6	6
1:A:111:LYS:O	1:A:115:PHE:CD2	0.45	2.70	5	3
1:A:138:ALA:HB1	1:A:165:LEU:CD1	0.45	2.41	3	2
1:A:68:GLN:CG	1:A:69:HIS:CE1	0.45	2.99	18	1
1:A:109:TYR:CD2	1:A:117:ARG:NH1	0.45	2.85	9	1
1:A:141:PHE:N	1:A:141:PHE:CD1	0.44	2.85	18	1
1:A:33:ASN:O	1:A:34:THR:HG22	0.44	2.13	19	1
1:A:172:VAL:HG13	1:A:172:VAL:O	0.44	2.11	7	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ALA:CB	1:A:83:TRP:CE3	0.44	3.00	6	2
1:A:69:HIS:CE1	1:A:71:LEU:HD23	0.44	2.48	9	2
1:A:8:MET:HE2	1:A:163:PHE:O	0.44	2.11	18	1
1:A:75:ILE:HD13	1:A:76:LEU:H	0.44	1.72	4	2
1:A:20:PHE:CZ	1:A:114:PHE:CD1	0.44	3.06	8	1
1:A:57:THR:HG22	1:A:58:PRO:HD2	0.44	1.90	11	2
1:A:10:VAL:HG22	1:A:163:PHE:CE1	0.44	2.48	4	3
1:A:7:VAL:HG22	1:A:8:MET:N	0.44	2.28	15	17
1:A:117:ARG:CD	1:A:118:PHE:CE2	0.44	3.01	3	1
1:A:20:PHE:CD1	1:A:21:GLY:N	0.44	2.86	8	2
1:A:38:ALA:CB	1:A:71:LEU:HD22	0.43	2.43	7	1
1:A:122:CYS:CB	1:A:129:ILE:HD11	0.43	2.41	7	1
1:A:114:PHE:CE1	1:A:118:PHE:CG	0.43	3.06	17	1
1:A:69:HIS:ND1	1:A:71:LEU:HD23	0.43	2.28	9	1
1:A:7:VAL:HG23	1:A:164:TYR:CZ	0.43	2.49	1	2
1:A:151:VAL:HG11	1:A:170:ARG:HG3	0.43	1.91	11	1
1:A:15:LEU:CD1	1:A:133:GLN:HG3	0.43	2.43	3	4
1:A:70:ILE:HD11	1:A:84:HIS:CE1	0.43	2.48	5	2
1:A:11:GLY:CA	1:A:159:THR:HG23	0.43	2.42	19	2
1:A:129:ILE:CG2	1:A:130:PRO:HD2	0.43	2.44	11	2
1:A:138:ALA:HB3	1:A:143:TYR:HE1	0.43	1.74	6	1
1:A:148:PHE:CE1	1:A:171:LEU:CD1	0.43	3.00	20	4
1:A:129:ILE:CD1	1:A:142:VAL:CG1	0.43	2.97	19	1
1:A:135:VAL:HG23	1:A:145:LEU:CD2	0.42	2.44	10	1
1:A:165:LEU:HD21	1:A:168:ASP:O	0.42	2.13	7	1
1:A:148:PHE:CE2	1:A:171:LEU:HD21	0.42	2.48	1	1
1:A:28:ILE:HG22	1:A:29:THR:N	0.42	2.29	19	1
1:A:142:VAL:O	1:A:142:VAL:HG13	0.42	2.14	17	1
1:A:102:PHE:CD1	1:A:114:PHE:CD2	0.42	3.07	20	1
1:A:140:ASP:OD1	1:A:141:PHE:CD2	0.42	2.72	4	1
1:A:148:PHE:CE2	1:A:171:LEU:HD11	0.42	2.49	10	1
1:A:142:VAL:HG13	1:A:142:VAL:O	0.42	2.14	13	1
1:A:148:PHE:CD1	1:A:171:LEU:CD1	0.42	3.00	15	1
1:A:7:VAL:CB	1:A:164:TYR:CE1	0.42	3.03	20	3
1:A:75:ILE:C	1:A:76:LEU:HD12	0.42	2.35	16	2
1:A:130:PRO:HB2	1:A:133:GLN:HG2	0.42	1.91	2	1
1:A:111:LYS:O	1:A:115:PHE:CE2	0.42	2.73	16	10
1:A:72:ASP:HB2	1:A:75:ILE:HD11	0.42	1.91	14	1
1:A:149:ALA:HB1	1:A:154:LYS:C	0.42	2.36	8	1
1:A:102:PHE:CD2	1:A:114:PHE:CD2	0.42	3.07	2	1
1:A:70:ILE:CG2	1:A:71:LEU:N	0.41	2.83	5	6

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:ASP:OD2	1:A:141:PHE:CE2	0.41	2.73	4	2
1:A:140:ASP:OD2	1:A:141:PHE:CZ	0.41	2.73	20	2
1:A:111:LYS:O	1:A:115:PHE:CE1	0.41	2.73	3	2
1:A:140:ASP:O	1:A:141:PHE:CD1	0.41	2.73	17	1
1:A:138:ALA:HB1	1:A:139:GLN:OE1	0.41	2.15	7	1
1:A:100:ARG:N	1:A:100:ARG:CD	0.41	2.84	2	1
1:A:27:LEU:HD11	1:A:100:ARG:HB2	0.41	1.93	2	2
1:A:27:LEU:HD12	1:A:101:CYS:O	0.41	2.14	13	1
1:A:82:HIS:O	1:A:82:HIS:CD2	0.41	2.73	8	8
1:A:120:THR:CG2	1:A:142:VAL:CG1	0.41	2.99	8	1
1:A:138:ALA:N	1:A:141:PHE:O	0.41	2.54	5	3
1:A:122:CYS:N	1:A:129:ILE:CD1	0.41	2.83	17	1
1:A:25:GLU:CB	1:A:102:PHE:CE2	0.41	3.04	1	1
1:A:172:VAL:HG23	1:A:176:ASP:CB	0.41	2.46	4	1
1:A:82:HIS:CD2	1:A:82:HIS:O	0.41	2.74	3	5
1:A:33:ASN:ND2	1:A:70:ILE:HG21	0.41	2.29	17	1
1:A:93:CYS:SG	1:A:95:VAL:HG23	0.41	2.56	11	1
1:A:93:CYS:HB2	1:A:95:VAL:HG22	0.41	1.92	19	1
1:A:143:TYR:CE2	1:A:171:LEU:HD12	0.41	2.51	7	1
1:A:15:LEU:HB2	1:A:133:GLN:O	0.41	2.16	3	3
1:A:64:ALA:HB1	1:A:83:TRP:CE2	0.41	2.51	14	1
1:A:138:ALA:C	1:A:139:GLN:HG2	0.41	2.36	17	1
1:A:78:ALA:O	1:A:83:TRP:CD1	0.41	2.74	6	1
1:A:137:ARG:HG2	1:A:142:VAL:HG22	0.41	1.91	14	1
1:A:69:HIS:CE1	1:A:71:LEU:CD2	0.41	3.04	9	1
1:A:10:VAL:CG2	1:A:163:PHE:CD1	0.41	3.04	17	1
1:A:70:ILE:HD11	1:A:82:HIS:CE1	0.41	2.51	11	1
1:A:136:ARG:CD	1:A:148:PHE:CZ	0.41	3.04	2	1
1:A:140:ASP:OD2	1:A:141:PHE:CE1	0.41	2.73	20	1
1:A:20:PHE:CD1	1:A:25:GLU:OE2	0.41	2.74	12	1
1:A:15:LEU:HA	1:A:15:LEU:HD23	0.41	1.81	13	1
1:A:138:ALA:CB	1:A:139:GLN:OE1	0.40	2.69	7	1
1:A:69:HIS:ND1	1:A:71:LEU:CD2	0.40	2.85	5	4
1:A:129:ILE:HD13	1:A:142:VAL:CG1	0.40	2.46	4	1
1:A:15:LEU:HD13	1:A:16:MET:HE2	0.40	1.91	15	1
1:A:76:LEU:N	1:A:76:LEU:CD1	0.40	2.84	6	2
1:A:64:ALA:O	1:A:83:TRP:CZ3	0.40	2.74	20	2
1:A:111:LYS:O	1:A:115:PHE:CZ	0.40	2.74	18	2
1:A:140:ASP:OD1	1:A:141:PHE:CE2	0.40	2.74	20	1
1:A:28:ILE:CG2	1:A:88:LEU:CD2	0.40	3.00	9	1
1:A:15:LEU:HD12	1:A:133:GLN:HB2	0.40	1.93	6	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:GLN:NE2	1:A:165:LEU:CB	0.40	2.85	11	1
1:A:64:ALA:O	1:A:83:TRP:CE3	0.40	2.74	19	1
1:A:94:HIS:O	1:A:94:HIS:CG	0.40	2.75	8	1
1:A:25:GLU:OE1	1:A:102:PHE:CZ	0.40	2.74	12	1
1:A:36:PHE:CD2	1:A:71:LEU:O	0.40	2.75	17	1
1:A:151:VAL:CG1	1:A:170:ARG:CG	0.40	3.00	11	2
1:A:68:GLN:HG2	1:A:69:HIS:CE1	0.40	2.52	18	1
1:A:94:HIS:O	1:A:94:HIS:CD2	0.40	2.74	18	1
1:A:145:LEU:HD12	1:A:145:LEU:N	0.40	2.31	5	1
1:A:143:TYR:N	1:A:143:TYR:CD1	0.40	2.90	5	1
1:A:94:HIS:CD2	1:A:94:HIS:O	0.40	2.75	13	1
1:A:164:TYR:N	1:A:172:VAL:O	0.40	2.55	11	1
1:A:76:LEU:N	1:A:76:LEU:HD12	0.40	2.31	5	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	157/182 (86%)	127±3 (81±2%)	22±3 (14±2%)	8±1 (5±1%)	5	28
All	All	3140/3640 (86%)	2542 (81%)	446 (14%)	152 (5%)	5	28

All 28 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	130	PRO	20
1	A	139	GLN	19
1	A	71	LEU	14
1	A	131	PRO	12
1	A	17	GLY	11
1	A	133	GLN	9
1	A	18	GLY	7
1	A	173	CYS	7
1	A	36	PHE	6

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	20	PHE	6
1	A	19	GLU	5
1	A	169	SER	4
1	A	38	ALA	4
1	A	181	LYS	3
1	A	24	ASP	3
1	A	84	HIS	3
1	A	106	GLU	3
1	A	166	MET	2
1	A	148	PHE	2
1	A	168	ASP	2
1	A	37	ASP	2
1	A	138	ALA	2
1	A	110	CYS	1
1	A	73	ARG	1
1	A	128	GLY	1
1	A	34	THR	1
1	A	119	GLY	1
1	A	35	GLN	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	138/153 (90%)	104±3 (75±2%)	34±3 (25±2%)	3	26
All	All	2760/3060 (90%)	2078 (75%)	682 (25%)	3	26

All 88 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	84	HIS	20
1	A	136	ARG	20
1	A	57	THR	20
1	A	8	MET	20
1	A	31	LEU	20
1	A	71	LEU	20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	16	MET	20
1	A	137	ARG	20
1	A	62	MET	19
1	A	139	GLN	19
1	A	14	THR	19
1	A	68	GLN	18
1	A	134	VAL	16
1	A	132	THR	16
1	A	73	ARG	15
1	A	15	LEU	15
1	A	79	LEU	15
1	A	100	ARG	15
1	A	133	GLN	14
1	A	74	PHE	14
1	A	181	LYS	13
1	A	30	ARG	13
1	A	171	LEU	13
1	A	169	SER	12
1	A	20	PHE	12
1	A	145	LEU	12
1	A	111	LYS	10
1	A	90	CYS	10
1	A	102	PHE	9
1	A	157	LEU	9
1	A	26	ARG	9
1	A	144	HIS	8
1	A	170	ARG	8
1	A	91	SER	8
1	A	121	LYS	8
1	A	148	PHE	7
1	A	66	CYS	7
1	A	146	HIS	7
1	A	182	GLN	7
1	A	104	ARG	6
1	A	150	CYS	6
1	A	36	PHE	6
1	A	179	THR	6
1	A	127	LEU	6
1	A	109	TYR	5
1	A	59	GLU	5
1	A	174	LYS	5
1	A	35	GLN	5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	80	ASP	5
1	A	147	CYS	5
1	A	107	SER	5
1	A	24	ASP	4
1	A	81	ARG	4
1	A	89	LYS	4
1	A	165	LEU	4
1	A	154	LYS	4
1	A	168	ASP	3
1	A	77	LYS	3
1	A	72	ASP	3
1	A	161	ASP	3
1	A	167	GLU	3
1	A	140	ASP	3
1	A	27	LEU	3
1	A	116	LYS	3
1	A	155	ARG	3
1	A	37	ASP	3
1	A	25	GLU	2
1	A	67	ASP	2
1	A	141	PHE	2
1	A	103	SER	2
1	A	117	ARG	2
1	A	75	ILE	2
1	A	112	ASP	2
1	A	126	GLN	2
1	A	63	CYS	1
1	A	164	TYR	1
1	A	23	GLU	1
1	A	86	LYS	1
1	A	19	GLU	1
1	A	12	GLU	1
1	A	113	ASP	1
1	A	33	ASN	1
1	A	156	GLN	1
1	A	120	THR	1
1	A	106	GLU	1
1	A	34	THR	1
1	A	101	CYS	1
1	A	70	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 4 ligands modelled in this entry, 4 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

No chemical shift data were provided