



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:30 am BST

PDB ID : 2MY1  
Title : Solution structure of Bud31p  
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Deposited on : 2015-01-19

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

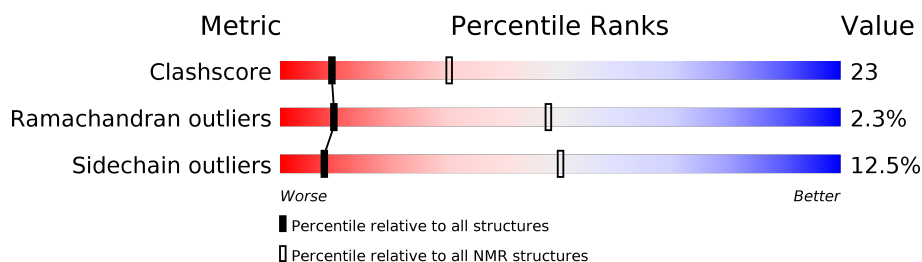
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 76%.

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  $\geq 3$ , 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	159	

## 2 Ensemble composition and analysis ⓘ

This entry contains 35 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:12-A:36, A:45-A:110, A:119-A:155 (128)	0.35	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 6 clusters and 5 single-model clusters were found.

Cluster number	Models
1	2, 4, 6, 7, 9, 10, 11, 14, 15, 16, 20, 22, 26, 27, 30, 35
2	1, 8, 17, 29
3	12, 18, 28, 34
4	5, 23
5	31, 32
6	3, 24
Single-model clusters	13; 19; 21; 25; 33

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2614 atoms, of which 1314 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms						Trace
1	A	159	Total	C	H	N	O	S	0
			2611	810	1314	242	235	10	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P25337
A	0	GLY	-	EXPRESSION TAG	UNP P25337
A	1	SER	-	EXPRESSION TAG	UNP P25337

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

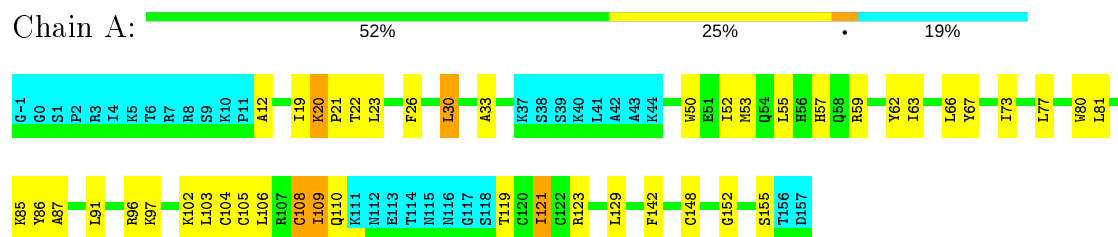
Mol	Chain	Residues	Atoms	
2	A	3	Total	Zn
			3	3

## 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: Pre-mRNA-splicing factor BUD31

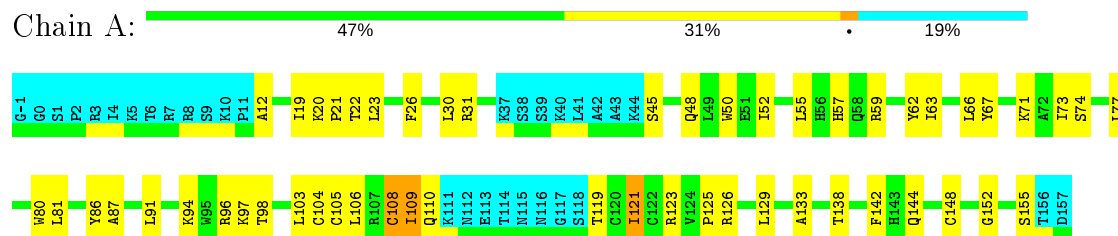


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

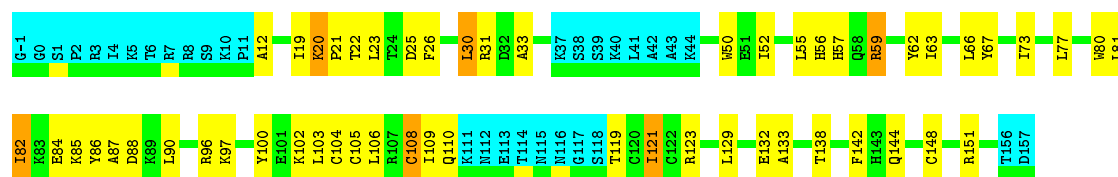
- Molecule 1: Pre-mRNA-splicing factor BUD31



#### 4.2.2 Score per residue for model 2 (medoid)

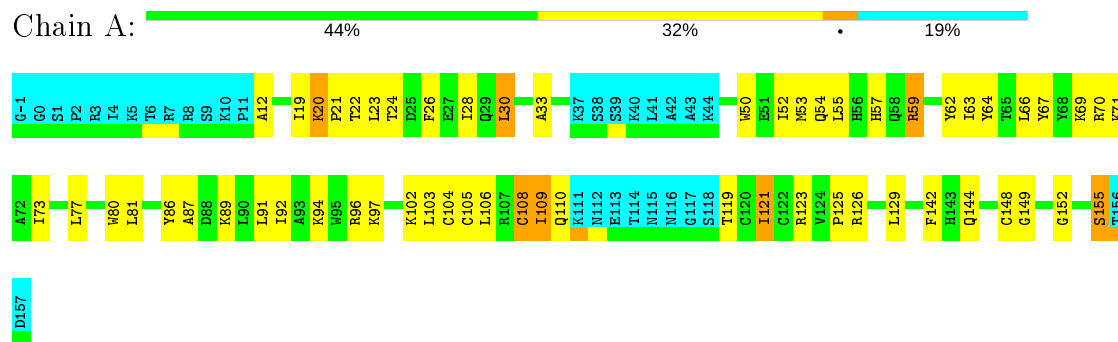
- Molecule 1: Pre-mRNA-splicing factor BUD31





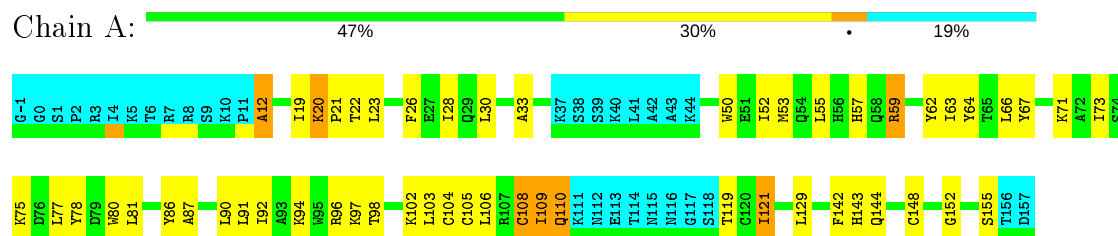
### 4.2.3 Score per residue for model 3

- Molecule 1: Pre-mRNA-splicing factor BUD31



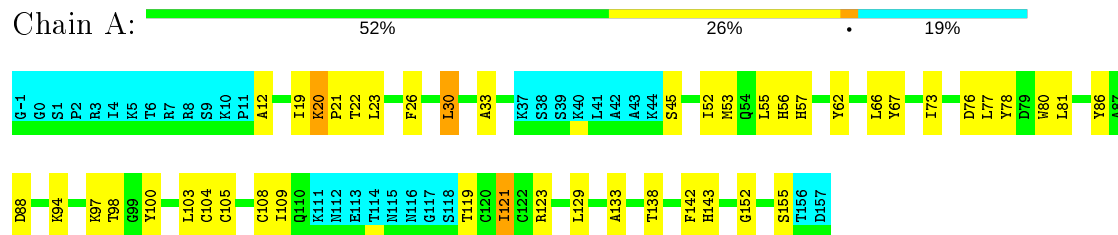
### 4.2.4 Score per residue for model 4

- Molecule 1: Pre-mRNA-splicing factor BUD31



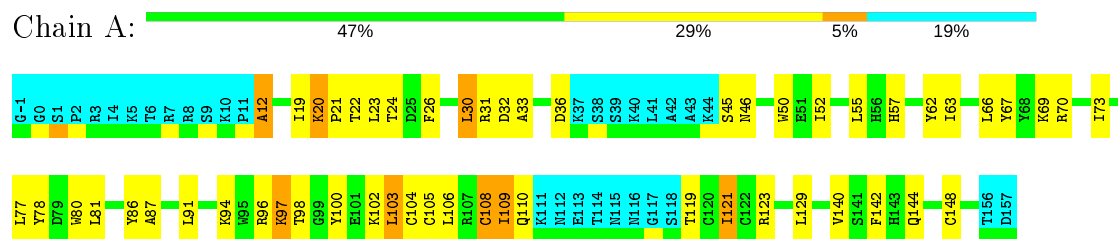
### 4.2.5 Score per residue for model 5

- Molecule 1: Pre-mRNA-splicing factor BUD31



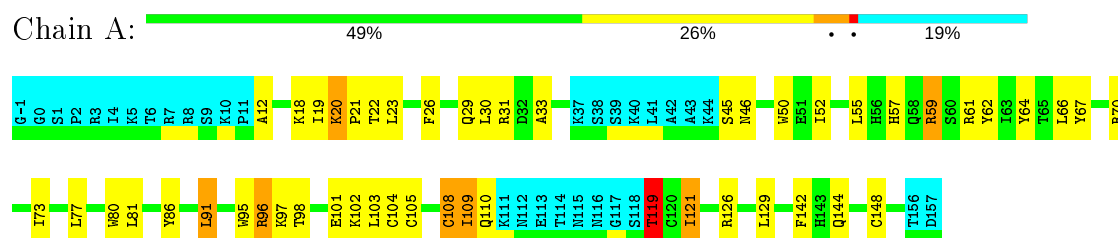
### 4.2.6 Score per residue for model 6

- Molecule 1: Pre-mRNA-splicing factor BUD31



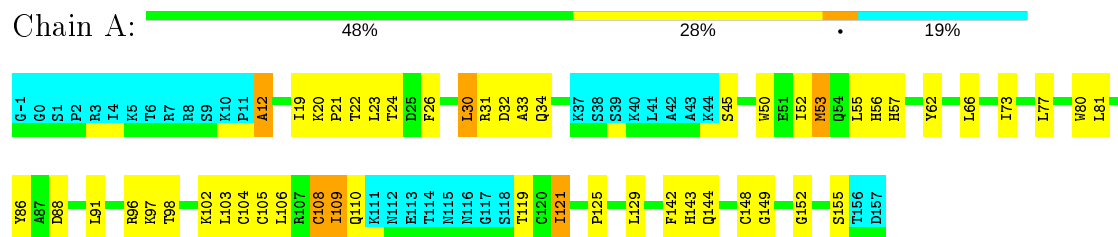
### 4.2.7 Score per residue for model 7

- Molecule 1: Pre-mRNA-splicing factor BUD31



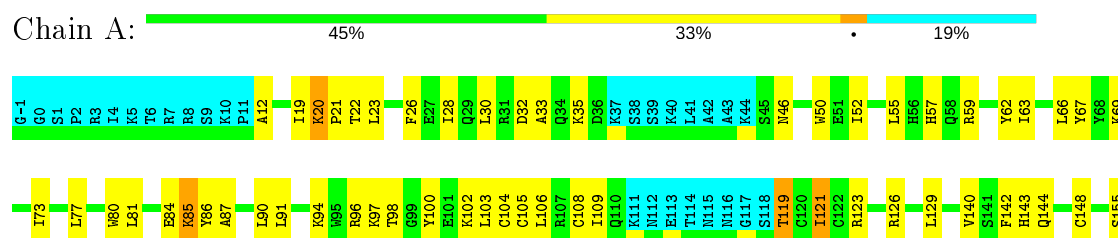
### 4.2.8 Score per residue for model 8

- Molecule 1: Pre-mRNA-splicing factor BUD31



### 4.2.9 Score per residue for model 9

- Molecule 1: Pre-mRNA-splicing factor BUD31

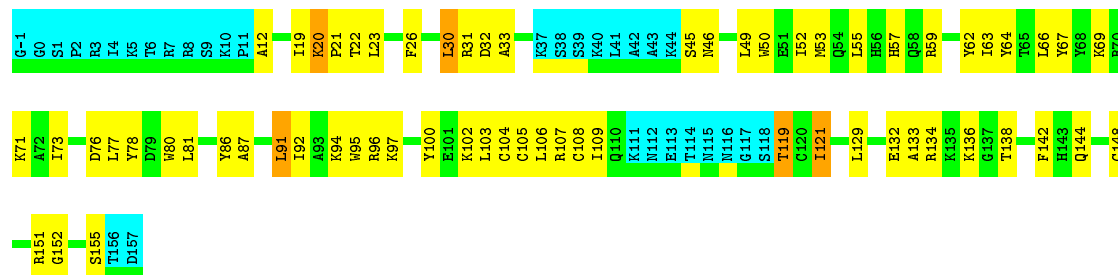


T156  
D157

#### 4.2.10 Score per residue for model 10

- Molecule 1: Pre-mRNA-splicing factor BUD31

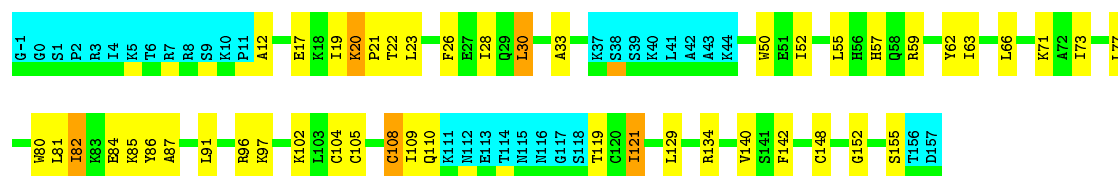
Chain A: 



#### 4.2.11 Score per residue for model 11

- Molecule 1: Pre-mRNA-splicing factor BUD31

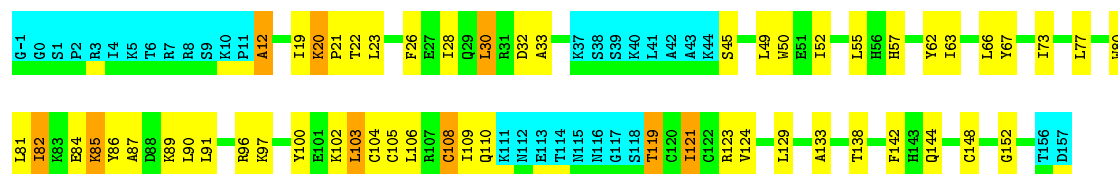
Chain A: 



#### 4.2.12 Score per residue for model 12

- Molecule 1: Pre-mRNA-splicing factor BUD31

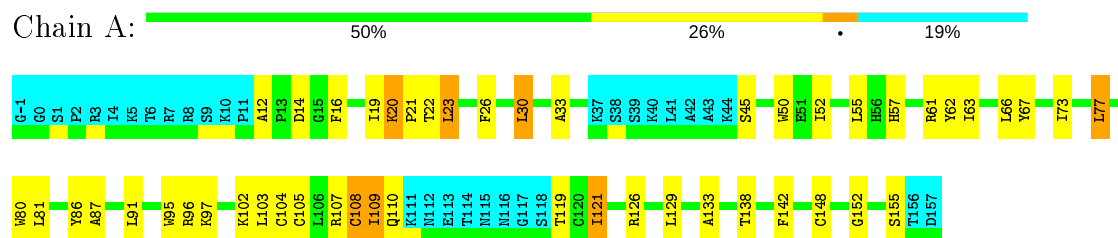
Chain A: 



#### 4.2.13 Score per residue for model 13

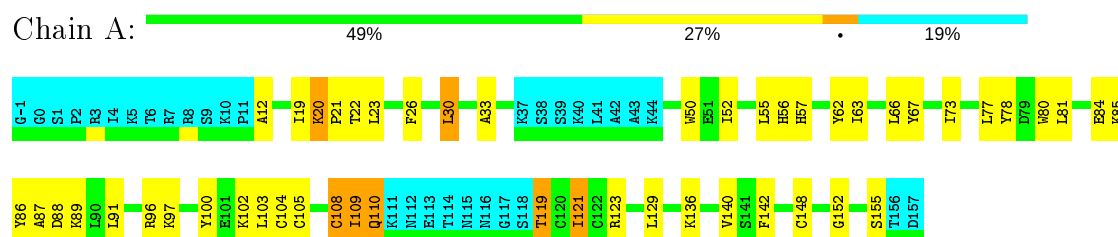
- Molecule 1: Pre-mRNA-splicing factor BUD31





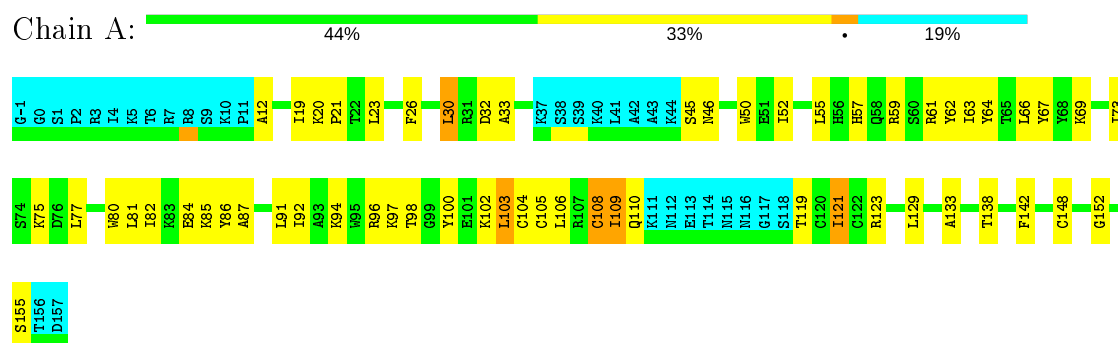
#### 4.2.14 Score per residue for model 14

- Molecule 1: Pre-mRNA-splicing factor BUD31



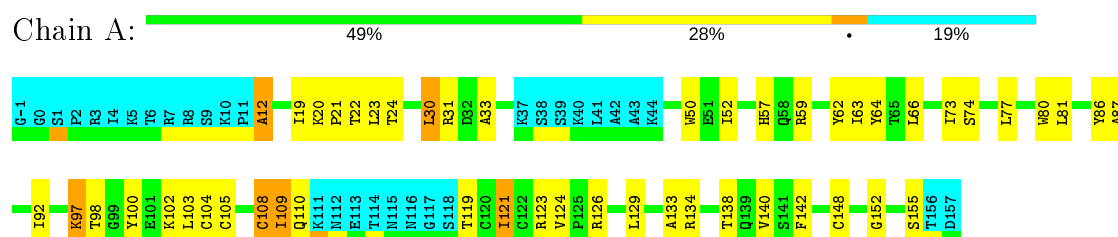
#### 4.2.15 Score per residue for model 15

- Molecule 1: Pre-mRNA-splicing factor BUD31



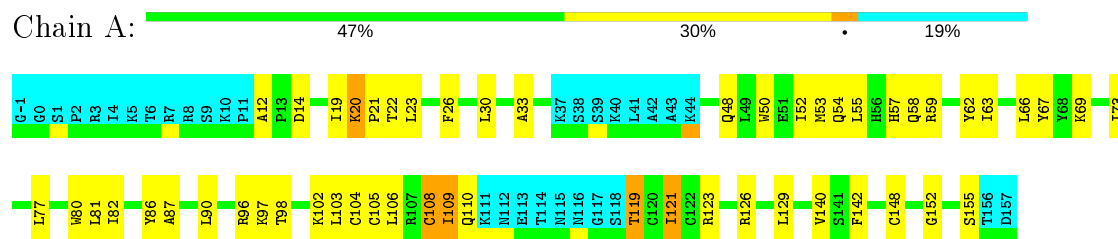
#### 4.2.16 Score per residue for model 16

- Molecule 1: Pre-mRNA-splicing factor BUD31



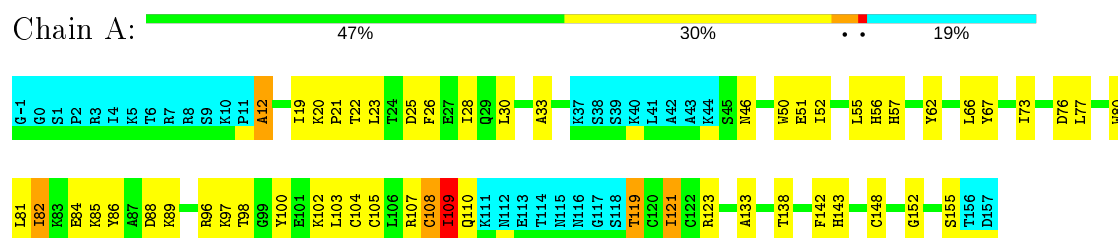
### 4.2.17 Score per residue for model 17

- Molecule 1: Pre-mRNA-splicing factor BUD31



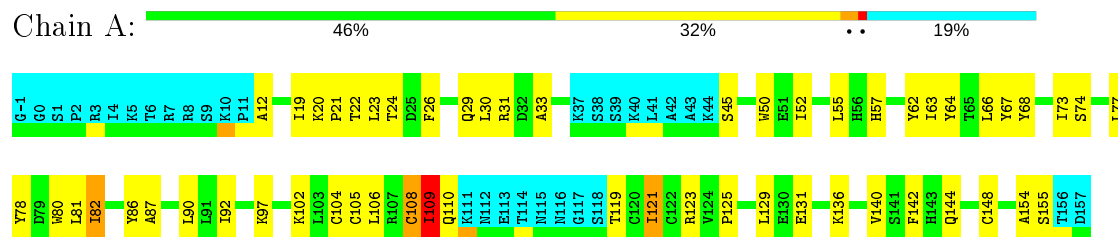
### 4.2.18 Score per residue for model 18

- Molecule 1: Pre-mRNA-splicing factor BUD31



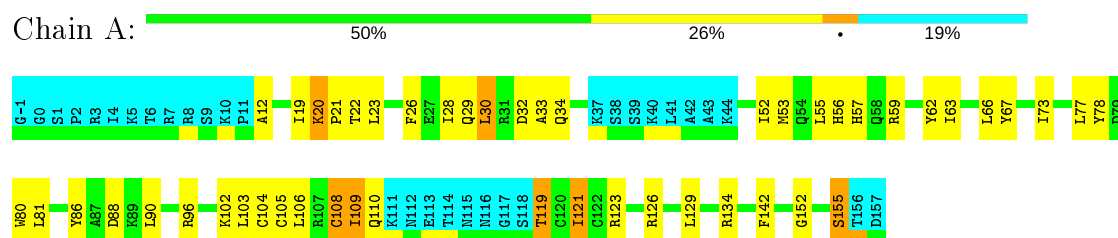
### 4.2.19 Score per residue for model 19

- Molecule 1: Pre-mRNA-splicing factor BUD31



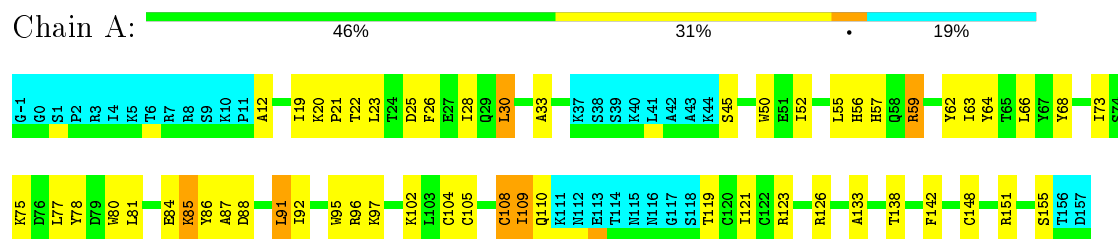
### 4.2.20 Score per residue for model 20

- Molecule 1: Pre-mRNA-splicing factor BUD31



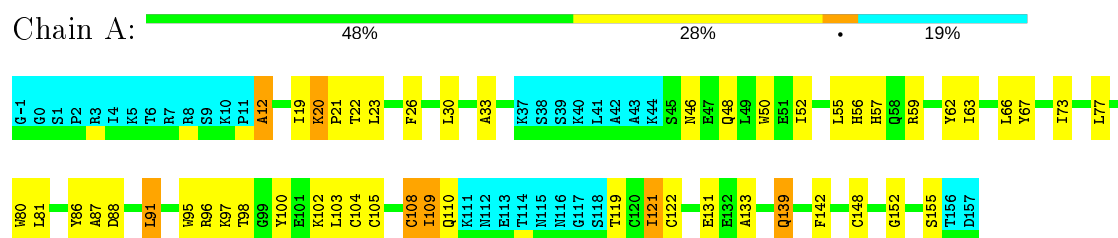
### 4.2.21 Score per residue for model 21

- Molecule 1: Pre-mRNA-splicing factor BUD31



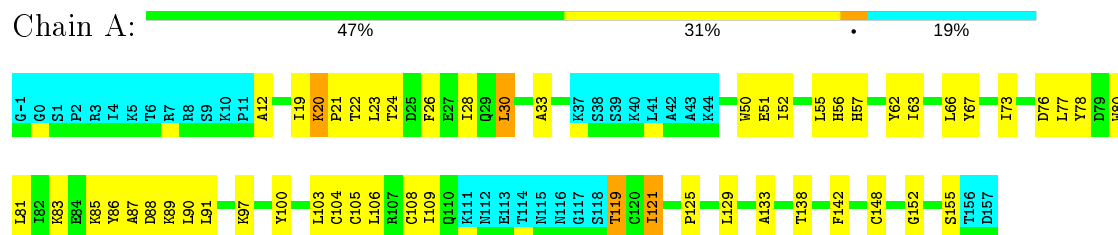
### 4.2.22 Score per residue for model 22

- Molecule 1: Pre-mRNA-splicing factor BUD31



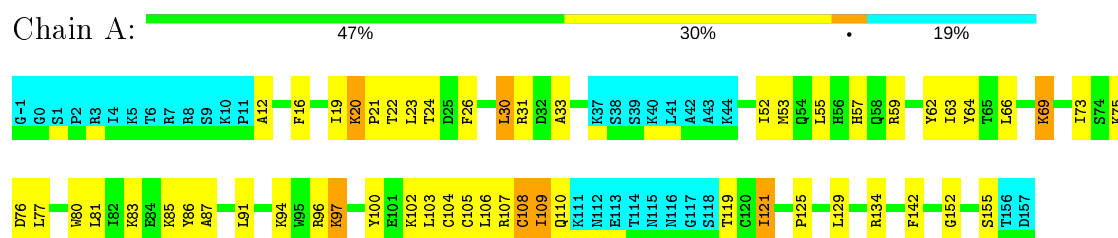
### 4.2.23 Score per residue for model 23

- Molecule 1: Pre-mRNA-splicing factor BUD31



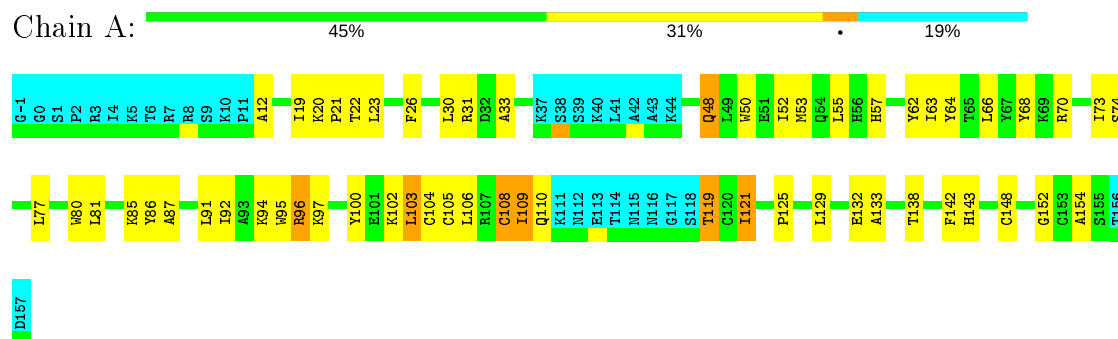
### 4.2.24 Score per residue for model 24

- Molecule 1: Pre-mRNA-splicing factor BUD31



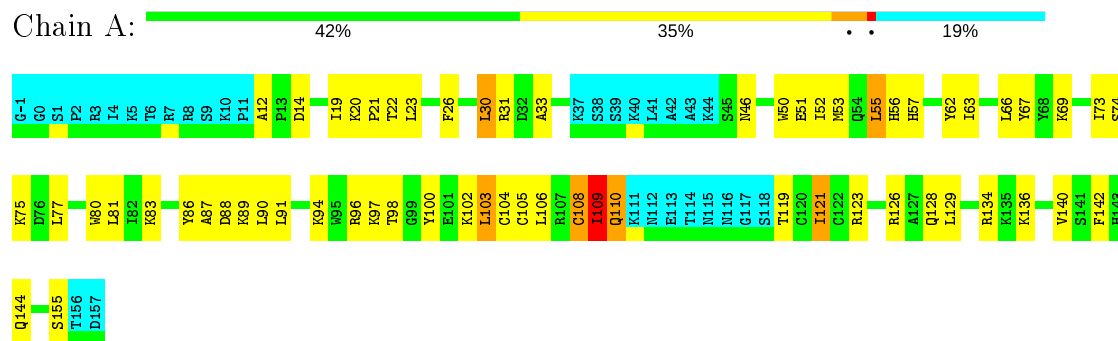
### 4.2.25 Score per residue for model 25

- Molecule 1: Pre-mRNA-splicing factor BUD31



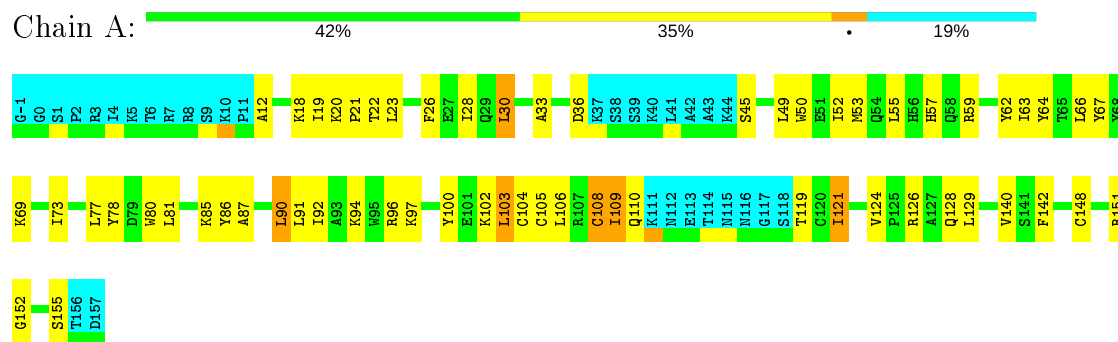
### 4.2.26 Score per residue for model 26

- Molecule 1: Pre-mRNA-splicing factor BUD31



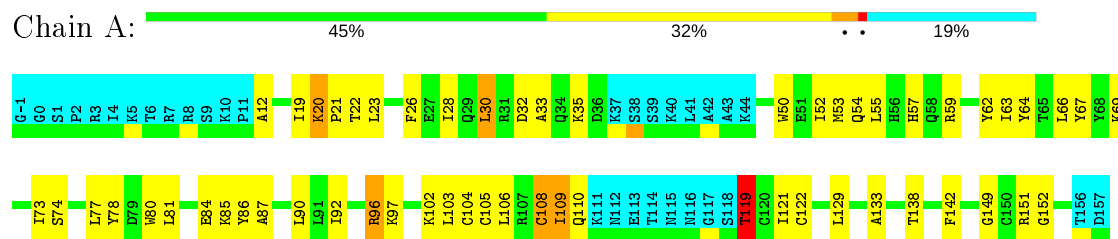
### 4.2.27 Score per residue for model 27

- Molecule 1: Pre-mRNA-splicing factor BUD31



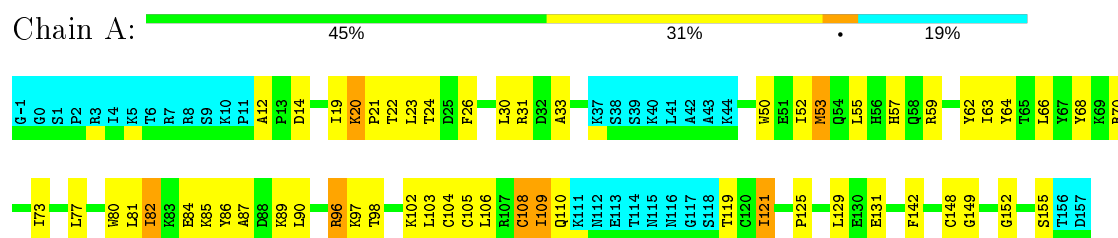
### 4.2.28 Score per residue for model 28

- Molecule 1: Pre-mRNA-splicing factor BUD31



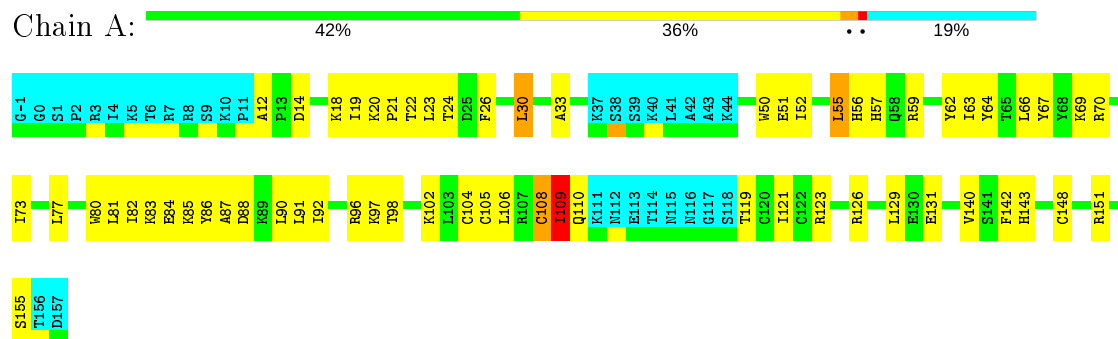
### 4.2.29 Score per residue for model 29

- Molecule 1: Pre-mRNA-splicing factor BUD31



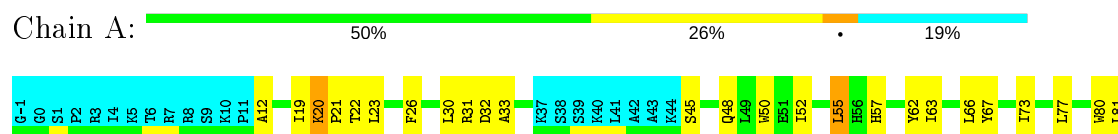
### 4.2.30 Score per residue for model 30

- Molecule 1: Pre-mRNA-splicing factor BUD31



### 4.2.31 Score per residue for model 31

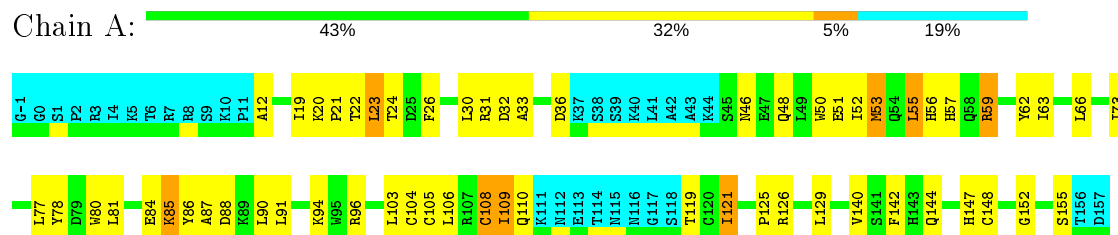
- Molecule 1: Pre-mRNA-splicing factor BUD31





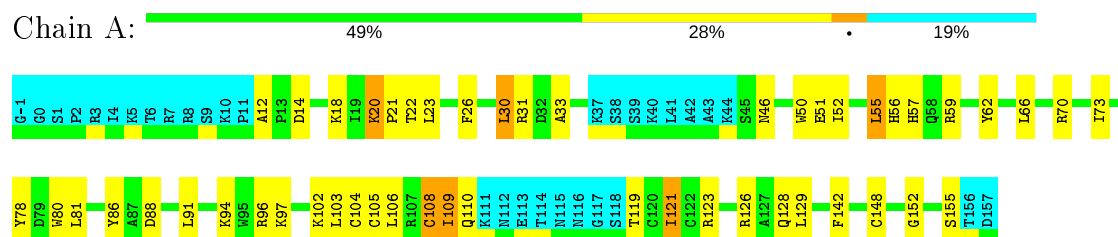
#### 4.2.32 Score per residue for model 32

- Molecule 1: Pre-mRNA-splicing factor BUD31



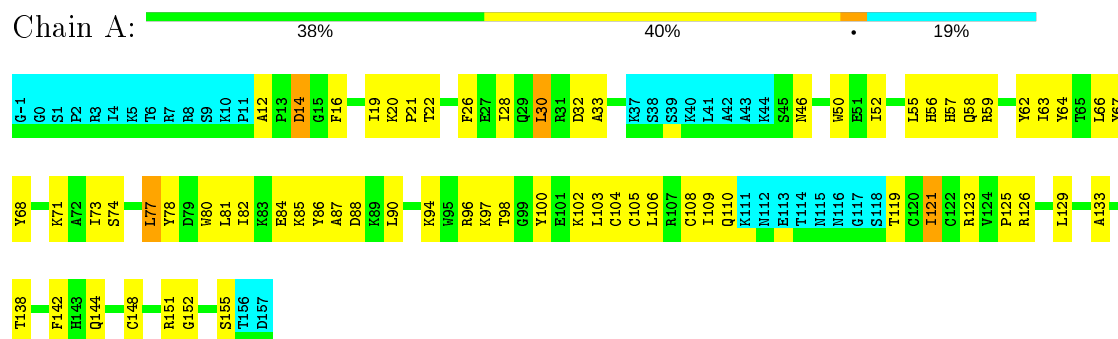
#### 4.2.33 Score per residue for model 33

- Molecule 1: Pre-mRNA-splicing factor BUD31



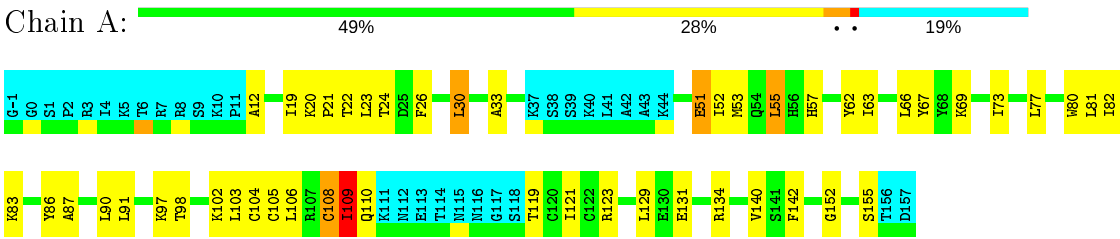
#### 4.2.34 Score per residue for model 34

- Molecule 1: Pre-mRNA-splicing factor BUD31



#### 4.2.35 Score per residue for model 35

- Molecule 1: Pre-mRNA-splicing factor BUD31



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 35 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
X-PLOR NIH	structure solution	2.28
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1698
Number of shifts mapped to atoms	1698
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 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	1065	1066	1066	49±4
All	All	37380	37310	37310	1704

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 23.

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



Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:HD11	1:A:52:ILE:HG23	1.05	1.26	13	15
1:A:22:THR:HG21	1:A:62:TYR:CE2	0.86	2.05	32	34
1:A:121:ILE:HD12	1:A:142:PHE:CD1	0.86	2.06	15	17
1:A:63:ILE:HD12	1:A:87:ALA:HB2	0.84	1.47	26	29
1:A:30:LEU:CD1	1:A:52:ILE:HG23	0.83	2.03	29	15
1:A:103:LEU:HD12	1:A:109:ILE:HD13	0.82	1.48	33	1
1:A:103:LEU:HD13	1:A:109:ILE:HD13	0.81	1.53	28	11
1:A:30:LEU:HD12	1:A:55:LEU:HD23	0.78	1.55	35	3
1:A:19:ILE:O	1:A:23:LEU:HD12	0.77	1.79	20	31
1:A:103:LEU:HD11	1:A:105:CYS:O	0.76	1.81	3	12
1:A:12:ALA:HB2	1:A:80:TRP:CH2	0.75	2.16	34	35
1:A:121:ILE:HD13	1:A:121:ILE:O	0.75	1.81	27	19
1:A:30:LEU:HD21	1:A:52:ILE:HG23	0.75	1.59	30	19
1:A:121:ILE:O	1:A:121:ILE:HD13	0.74	1.81	14	12
1:A:121:ILE:HD11	1:A:129:LEU:HD11	0.74	1.59	2	23
1:A:133:ALA:HB1	1:A:138:THR:O	0.73	1.84	15	14
1:A:103:LEU:HD13	1:A:109:ILE:CD1	0.72	2.15	20	12
1:A:121:ILE:HD12	1:A:142:PHE:CG	0.72	2.19	19	30
1:A:51:GLU:O	1:A:55:LEU:HD22	0.72	1.84	26	4
1:A:81:LEU:HD22	1:A:86:TYR:CD2	0.71	2.20	31	14
1:A:19:ILE:HD12	1:A:23:LEU:HD11	0.71	1.61	17	27
1:A:90:LEU:HD23	1:A:106:LEU:HD13	0.71	1.60	35	10
1:A:90:LEU:HD23	1:A:106:LEU:HD22	0.70	1.61	29	5
1:A:109:ILE:O	1:A:119:THR:HG21	0.69	1.87	23	5
1:A:30:LEU:CD2	1:A:52:ILE:HG23	0.69	2.17	33	19
1:A:110:GLN:C	1:A:119:THR:HG23	0.68	2.08	14	27
1:A:30:LEU:HD11	1:A:52:ILE:CG2	0.68	2.16	1	11
1:A:19:ILE:HG22	1:A:62:TYR:OH	0.68	1.88	15	24
1:A:91:LEU:HA	1:A:106:LEU:HD21	0.67	1.67	1	13
1:A:26:PHE:CD2	1:A:55:LEU:HD12	0.67	2.24	32	4
1:A:26:PHE:CD2	1:A:55:LEU:HD22	0.66	2.26	28	23
1:A:121:ILE:HG23	1:A:142:PHE:CE1	0.66	2.25	27	35
1:A:30:LEU:CG	1:A:52:ILE:HG23	0.65	2.22	27	21
1:A:73:ILE:HG13	1:A:77:LEU:HD23	0.65	1.69	12	31
1:A:103:LEU:HD12	1:A:109:ILE:CD1	0.64	2.21	33	1
1:A:26:PHE:CD1	1:A:55:LEU:HD22	0.64	2.28	23	5
1:A:30:LEU:CD1	1:A:55:LEU:HD23	0.63	2.23	35	3
1:A:90:LEU:CD2	1:A:106:LEU:HD22	0.62	2.25	29	2
1:A:103:LEU:HB2	1:A:109:ILE:HD13	0.62	1.71	10	2
1:A:91:LEU:HD12	1:A:95:TRP:CZ3	0.62	2.29	21	4
1:A:91:LEU:HD21	1:A:95:TRP:CH2	0.61	2.31	25	2
1:A:91:LEU:CA	1:A:106:LEU:HD21	0.60	2.25	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:LEU:O	1:A:140:VAL:HG11	0.60	1.96	30	12
1:A:30:LEU:HD21	1:A:52:ILE:CG2	0.60	2.25	26	18
1:A:78:TYR:HA	1:A:81:LEU:HD12	0.60	1.74	5	11
1:A:19:ILE:HD12	1:A:23:LEU:CD1	0.59	2.26	2	21
1:A:30:LEU:HD12	1:A:55:LEU:HD12	0.59	1.75	6	1
1:A:66:LEU:CD1	1:A:73:ILE:HG21	0.59	2.28	35	33
1:A:103:LEU:HD12	1:A:104:CYS:N	0.58	2.13	35	1
1:A:12:ALA:HB2	1:A:80:TRP:CZ2	0.58	2.32	32	35
1:A:110:GLN:O	1:A:119:THR:HG23	0.58	1.99	35	19
1:A:121:ILE:HD12	1:A:142:PHE:CD2	0.58	2.34	3	19
1:A:30:LEU:HG	1:A:52:ILE:HG23	0.58	1.76	27	15
1:A:12:ALA:HB2	1:A:80:TRP:CZ3	0.57	2.34	13	27
1:A:33:ALA:CB	1:A:52:ILE:HD11	0.57	2.28	24	23
1:A:105:CYS:HB2	1:A:108:CYS:HB2	0.55	1.77	23	35
1:A:66:LEU:HD12	1:A:67:TYR:N	0.54	2.17	6	26
1:A:91:LEU:N	1:A:106:LEU:HD11	0.54	2.18	9	2
1:A:124:VAL:HG13	1:A:128:GLN:CD	0.54	2.23	27	1
1:A:125:PRO:O	1:A:129:LEU:HD12	0.53	2.02	24	8
1:A:66:LEU:HD12	1:A:73:ILE:HG21	0.53	1.81	30	22
1:A:125:PRO:HD3	1:A:154:ALA:HB1	0.53	1.81	19	2
1:A:23:LEU:HD13	1:A:86:TYR:HE2	0.52	1.64	11	16
1:A:30:LEU:HD23	1:A:34:GLN:HG3	0.52	1.81	8	1
1:A:121:ILE:HD11	1:A:129:LEU:CD1	0.51	2.36	17	15
1:A:30:LEU:HD12	1:A:55:LEU:CD1	0.51	2.35	6	1
1:A:66:LEU:HD12	1:A:66:LEU:C	0.51	2.26	27	15
1:A:23:LEU:HD13	1:A:86:TYR:CE2	0.51	2.41	11	12
1:A:121:ILE:HD13	1:A:121:ILE:C	0.50	2.26	34	20
1:A:66:LEU:C	1:A:66:LEU:HD12	0.50	2.27	5	20
1:A:16:PHE:N	1:A:77:LEU:HD21	0.50	2.21	13	2
1:A:28:ILE:N	1:A:28:ILE:HD12	0.50	2.22	3	5
1:A:26:PHE:CE2	1:A:55:LEU:HD12	0.50	2.42	31	5
1:A:121:ILE:C	1:A:121:ILE:HD13	0.50	2.27	9	11
1:A:64:TYR:CD1	1:A:68:TYR:CD2	0.50	3.00	19	4
1:A:28:ILE:HD12	1:A:28:ILE:N	0.49	2.22	23	7
1:A:100:TYR:HB3	1:A:103:LEU:HD23	0.48	1.85	25	16
1:A:23:LEU:HD22	1:A:86:TYR:CD2	0.48	2.43	20	7
1:A:33:ALA:HB3	1:A:52:ILE:CG1	0.48	2.38	31	27
1:A:57:HIS:CD2	1:A:91:LEU:HD21	0.48	2.43	12	5
1:A:81:LEU:CD2	1:A:86:TYR:CD2	0.48	2.97	26	34
1:A:81:LEU:HD23	1:A:86:TYR:CE2	0.48	2.44	12	9
1:A:33:ALA:HB1	1:A:48:GLN:O	0.47	2.09	31	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:HD12	1:A:106:LEU:CD2	0.47	2.39	27	1
1:A:29:GLN:OE1	1:A:55:LEU:HD21	0.47	2.10	20	1
1:A:56:HIS:NE2	1:A:88:ASP:CB	0.47	2.78	22	3
1:A:91:LEU:HD11	1:A:103:LEU:HD11	0.47	1.86	6	1
1:A:82:ILE:HD12	1:A:87:ALA:HB3	0.46	1.87	11	3
1:A:64:TYR:CE1	1:A:92:ILE:HG23	0.46	2.45	4	9
1:A:91:LEU:HD11	1:A:103:LEU:HD21	0.46	1.86	33	1
1:A:82:ILE:CD1	1:A:87:ALA:HB3	0.46	2.40	17	1
1:A:121:ILE:CG2	1:A:142:PHE:CE1	0.46	2.98	27	34
1:A:50:TRP:CD1	1:A:148:CYS:HA	0.46	2.45	25	28
1:A:103:LEU:HD12	1:A:103:LEU:C	0.46	2.31	24	5
1:A:33:ALA:HB3	1:A:52:ILE:HD11	0.46	1.87	27	9
1:A:121:ILE:CD1	1:A:129:LEU:HD11	0.46	2.41	13	3
1:A:81:LEU:HD23	1:A:86:TYR:CD2	0.46	2.46	27	8
1:A:82:ILE:HD11	1:A:89:LYS:N	0.46	2.25	18	3
1:A:64:TYR:OH	1:A:96:ARG:NE	0.46	2.49	29	1
1:A:50:TRP:CE3	1:A:149:GLY:CA	0.46	2.99	29	4
1:A:57:HIS:NE2	1:A:91:LEU:HD21	0.46	2.26	26	3
1:A:91:LEU:CD1	1:A:95:TRP:CZ3	0.46	2.99	22	4
1:A:56:HIS:NE2	1:A:88:ASP:N	0.45	2.64	20	1
1:A:91:LEU:CD1	1:A:103:LEU:HD21	0.45	2.41	33	1
1:A:57:HIS:NE2	1:A:104:CYS:O	0.45	2.48	32	31
1:A:63:ILE:CG2	1:A:78:TYR:CD1	0.45	3.00	20	3
1:A:81:LEU:HD22	1:A:86:TYR:CE2	0.45	2.46	31	3
1:A:64:TYR:CE1	1:A:92:ILE:CG2	0.45	2.99	30	5
1:A:108:CYS:O	1:A:109:ILE:HG23	0.45	2.12	17	19
1:A:49:LEU:HD23	1:A:52:ILE:HD12	0.45	1.89	10	3
1:A:26:PHE:CD2	1:A:59:ARG:CD	0.45	2.99	20	5
1:A:26:PHE:CD1	1:A:59:ARG:CD	0.45	3.00	4	1
1:A:124:VAL:HG12	1:A:129:LEU:HG	0.45	1.89	12	1
1:A:16:PHE:HB2	1:A:77:LEU:HD11	0.45	1.87	24	1
1:A:94:LYS:HB3	1:A:103:LEU:HD22	0.45	1.88	10	2
1:A:62:TYR:CE1	1:A:66:LEU:CD2	0.45	3.00	21	1
1:A:57:HIS:CE1	1:A:104:CYS:O	0.45	2.70	3	34
1:A:67:TYR:CE2	1:A:78:TYR:CD2	0.45	3.05	10	1
1:A:22:THR:HG21	1:A:62:TYR:CD2	0.45	2.46	22	1
1:A:73:ILE:CG1	1:A:77:LEU:HD23	0.45	2.40	10	19
1:A:103:LEU:C	1:A:103:LEU:HD12	0.45	2.33	5	8
1:A:64:TYR:OH	1:A:96:ARG:NH1	0.44	2.50	28	3
1:A:20:LYS:N	1:A:21:PRO:CD	0.44	2.81	22	35
1:A:103:LEU:C	1:A:103:LEU:HD23	0.44	2.32	33	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:GLN:CA	1:A:119:THR:HG23	0.44	2.42	12	1
1:A:94:LYS:CD	1:A:100:TYR:CZ	0.44	3.01	27	3
1:A:33:ALA:CB	1:A:52:ILE:CG1	0.44	2.96	26	32
1:A:64:TYR:CE2	1:A:68:TYR:CD2	0.44	3.05	34	1
1:A:81:LEU:CD2	1:A:86:TYR:CE2	0.43	3.01	22	4
1:A:91:LEU:HD12	1:A:95:TRP:CE3	0.43	2.48	10	1
1:A:33:ALA:HB1	1:A:48:GLN:HG2	0.43	1.89	31	2
1:A:53:MET:HE1	1:A:147:HIS:O	0.43	2.14	32	1
1:A:94:LYS:CD	1:A:106:LEU:CD2	0.43	2.97	10	11
1:A:50:TRP:CD1	1:A:50:TRP:N	0.43	2.86	3	4
1:A:19:ILE:CG2	1:A:62:TYR:OH	0.43	2.64	21	2
1:A:91:LEU:CD2	1:A:95:TRP:CZ3	0.43	3.01	25	1
1:A:50:TRP:O	1:A:53:MET:HE3	0.43	2.14	29	1
1:A:78:TYR:CE1	1:A:82:ILE:CD1	0.43	3.02	34	2
1:A:56:HIS:NE2	1:A:88:ASP:HB2	0.42	2.29	33	12
1:A:63:ILE:CG2	1:A:78:TYR:CE1	0.42	3.02	20	2
1:A:66:LEU:HD12	1:A:73:ILE:CG2	0.42	2.44	10	4
1:A:45:SER:OG	1:A:46:ASN:N	0.42	2.52	10	2
1:A:108:CYS:C	1:A:109:ILE:HG23	0.42	2.35	32	19
1:A:121:ILE:CD1	1:A:142:PHE:CG	0.42	3.01	2	13
1:A:66:LEU:CD1	1:A:73:ILE:CG2	0.42	2.97	24	22
1:A:26:PHE:CE1	1:A:55:LEU:HD22	0.42	2.50	1	2
1:A:84:GLU:O	1:A:85:LYS:CB	0.42	2.68	34	14
1:A:63:ILE:HD11	1:A:86:TYR:HB3	0.42	1.90	30	2
1:A:46:ASN:O	1:A:50:TRP:CD1	0.42	2.73	22	6
1:A:108:CYS:O	1:A:109:ILE:CG2	0.42	2.68	35	9
1:A:26:PHE:CD2	1:A:59:ARG:HD3	0.42	2.50	32	4
1:A:26:PHE:CE2	1:A:55:LEU:HD22	0.42	2.49	18	2
1:A:46:ASN:O	1:A:50:TRP:CG	0.42	2.73	18	2
1:A:63:ILE:HG22	1:A:78:TYR:CE1	0.41	2.50	34	1
1:A:26:PHE:CD2	1:A:59:ARG:HD2	0.41	2.51	28	2
1:A:56:HIS:NE2	1:A:88:ASP:OD2	0.41	2.53	26	1
1:A:64:TYR:CE1	1:A:68:TYR:CD2	0.41	3.08	29	1
1:A:62:TYR:O	1:A:66:LEU:HD23	0.41	2.15	21	1
1:A:26:PHE:CE1	1:A:55:LEU:HD12	0.41	2.50	26	1
1:A:50:TRP:N	1:A:50:TRP:CD1	0.41	2.87	17	1
1:A:26:PHE:CG	1:A:59:ARG:CD	0.41	3.04	7	1
1:A:81:LEU:O	1:A:86:TYR:CD1	0.41	2.73	14	2
1:A:69:LYS:CD	1:A:69:LYS:N	0.41	2.84	24	1
1:A:73:ILE:CD1	1:A:77:LEU:HD23	0.41	2.46	24	1
1:A:30:LEU:HD23	1:A:34:GLN:CG	0.41	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ILE:HD11	1:A:81:LEU:CD2	0.41	2.46	34	1
1:A:94:LYS:HD3	1:A:106:LEU:HD23	0.41	1.93	4	1
1:A:64:TYR:OH	1:A:96:ARG:CD	0.41	2.69	25	1
1:A:50:TRP:CZ3	1:A:144:GLN:OE1	0.41	2.74	34	1
1:A:133:ALA:HB1	1:A:139:GLN:CA	0.40	2.46	22	1
1:A:94:LYS:CE	1:A:100:TYR:CZ	0.40	3.04	5	1
1:A:46:ASN:OD1	1:A:50:TRP:CZ2	0.40	2.75	6	1
1:A:66:LEU:HD11	1:A:73:ILE:CD1	0.40	2.46	13	1
1:A:94:LYS:HD2	1:A:100:TYR:CZ	0.40	2.52	27	1
1:A:129:LEU:CD1	1:A:142:PHE:CB	0.40	3.00	28	1
1:A:63:ILE:HD12	1:A:87:ALA:CB	0.40	2.41	30	1
1:A:53:MET:CE	1:A:148:CYS:HB2	0.40	2.47	8	1
1:A:122:CYS:HA	1:A:142:PHE:CE2	0.40	2.52	22	2

## 5.2 Torsion angles ⓘ

### 5.2.1 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	128/159 (81%)	111±2 (87±2%)	14±2 (11±2%)	3±1 (2±1%)	9	48
All	All	4480/5565 (81%)	3894 (87%)	483 (11%)	103 (2%)	9	48

All 8 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	97	LYS	32
1	A	109	ILE	30
1	A	152	GLY	27
1	A	12	ALA	7
1	A	14	ASP	3
1	A	119	THR	2
1	A	85	LYS	1
1	A	139	GLN	1

### 5.2.2 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	115/141 (82%)	101±3 (87±3%)	14±3 (13±3%)	8	50
All	All	4025/4935 (82%)	3520 (87%)	505 (13%)	8	50

All 59 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	121	ILE	31
1	A	102	LYS	31
1	A	155	SER	29
1	A	96	ARG	28
1	A	30	LEU	23
1	A	123	ARG	21
1	A	20	LYS	21
1	A	59	ARG	20
1	A	98	THR	17
1	A	126	ARG	15
1	A	31	ARG	15
1	A	53	MET	15
1	A	144	GLN	13
1	A	69	LYS	12
1	A	119	THR	12
1	A	32	ASP	11
1	A	24	THR	11
1	A	45	SER	10
1	A	82	ILE	9
1	A	85	LYS	7
1	A	70	ARG	7
1	A	143	HIS	7
1	A	74	SER	7
1	A	103	LEU	7
1	A	134	ARG	7
1	A	151	ARG	7
1	A	71	LYS	6
1	A	55	LEU	6
1	A	83	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	48	GLN	5
1	A	109	ILE	5
1	A	14	ASP	5
1	A	131	GLU	5
1	A	76	ASP	5
1	A	75	LYS	5
1	A	107	ARG	4
1	A	91	LEU	4
1	A	89	LYS	4
1	A	18	LYS	4
1	A	97	LYS	4
1	A	136	LYS	4
1	A	51	GLU	4
1	A	77	LEU	3
1	A	132	GLU	3
1	A	61	ARG	3
1	A	110	GLN	3
1	A	25	ASP	3
1	A	54	GLN	3
1	A	23	LEU	3
1	A	58	GLN	2
1	A	35	LYS	2
1	A	36	ASP	2
1	A	29	GLN	2
1	A	128	GLN	2
1	A	101	GLU	1
1	A	17	GLU	1
1	A	90	LEU	1
1	A	34	GLN	1
1	A	135	LYS	1

### 5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.5 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

## 5.6 Other polymers [i](#)

There are no such molecules in this entry.

## 5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 73% for the entire structure.

### 6.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 6.1.1 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	1698
Number of shifts mapped to atoms	1698
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

#### 6.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	158	$-0.45 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	149	$0.17 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	151	$-0.31 \pm 0.33$	None needed ( $< 0.5$ ppm)

#### 6.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 1291 atoms were assigned a chemical shift out of a possible 1706. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	502/634 (79%)	251/253 (99%)	127/256 (50%)	124/125 (99%)
Sidechain	654/925 (71%)	408/549 (74%)	236/322 (73%)	10/54 (19%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	135/147 (92%)	69/77 (90%)	63/63 (100%)	3/7 (43%)
Overall	1291/1706 (76%)	728/879 (83%)	426/641 (66%)	137/186 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1525 atoms were assigned a chemical shift out of a possible 2088. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	618/785 (79%)	309/313 (99%)	158/318 (50%)	151/154 (98%)
Sidechain	772/1156 (67%)	483/688 (70%)	276/396 (70%)	13/72 (18%)
Aromatic	135/147 (92%)	69/77 (90%)	63/63 (100%)	3/7 (43%)
Overall	1525/2088 (73%)	861/1078 (80%)	497/777 (64%)	167/233 (72%)

#### 6.1.4 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	84	GLU	HG2	0.50	3.33 – 1.23	-8.5
1	A	84	GLU	HG3	1.07	3.31 – 1.21	-5.7
1	A	12	ALA	HB3	0.01	2.61 – 0.11	-5.4
1	A	12	ALA	HB1	0.01	2.61 – 0.11	-5.4
1	A	12	ALA	HB2	0.01	2.61 – 0.11	-5.4
1	A	91	LEU	HG	-0.20	3.16 – -0.14	-5.2

#### 6.1.5 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:

