



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 9, 2017 – 11:08 am GMT

PDB ID : 2N8L  
Title : Zipcode-binding-protein-1 KH3KH4(DD) domains in complex with the KH3 RNA target  
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Deposited on : 2015-10-21

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.

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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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : recalc28906  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28906

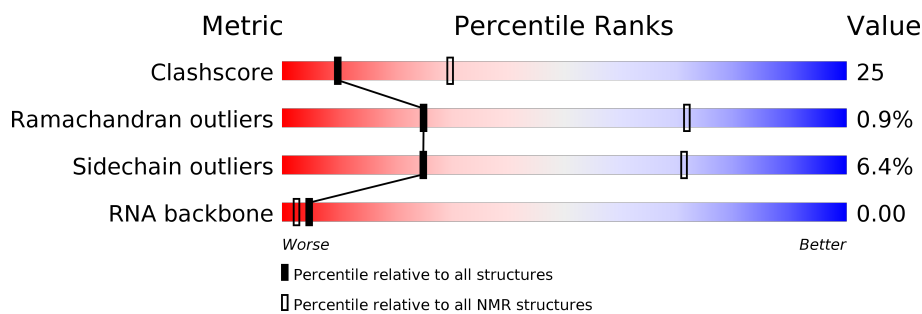
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 53%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367
RNA backbone	3398	623

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	191	
2	B	8	

## 2 Ensemble composition and analysis

This entry contains 12 models. Model 3 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:22-A:61, A:67-A:96, A:102-A:121, A:125-A:179 (145)	0.54	3

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 7, 10, 11, 12
2	5, 6, 8, 9

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3197 atoms, of which 1576 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin-like growth factor 2 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	191	Total	C	H	N	O	S	0
			2941	916	1487	262	272	4	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP O42254
A	2	ALA	-	EXPRESSION TAG	UNP O42254
A	3	MET	-	EXPRESSION TAG	UNP O42254
A	4	GLY	-	EXPRESSION TAG	UNP O42254
A	14	PHE	TYR	ENGINEERED MUTATION	UNP O42254
A	122	ASP	LYS	ENGINEERED MUTATION	UNP O42254
A	123	ASP	GLY	ENGINEERED MUTATION	UNP O42254

- Molecule 2 is a RNA chain called RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3').

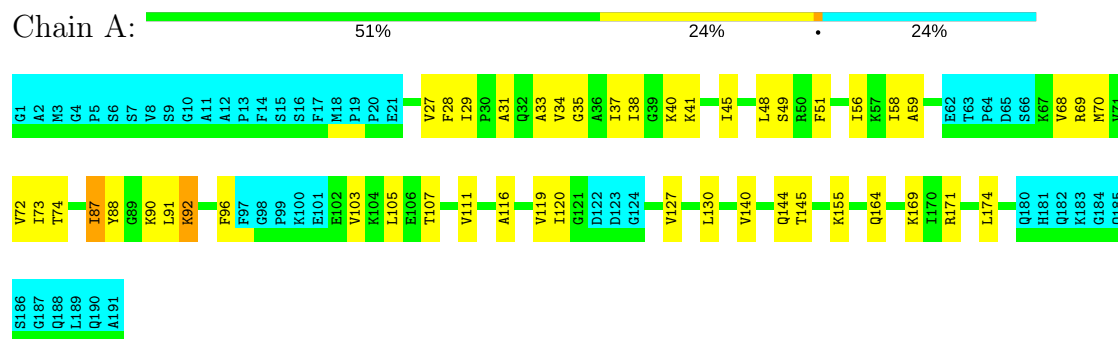
Mol	Chain	Residues	Atoms						Trace
2	B	8	Total	C	H	N	O	P	0
			256	75	89	30	54	8	

## 4 Residue-property plots [i](#)

### 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: Insulin-like growth factor 2 mRNA-binding protein 1



- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

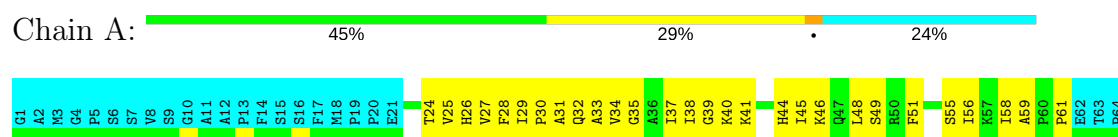


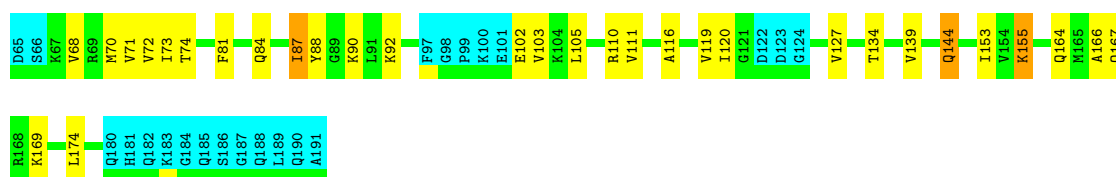
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

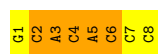
- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1





- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

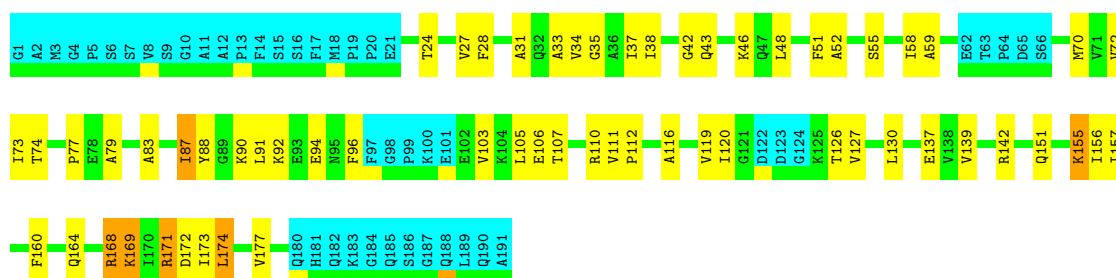
Chain B:



#### 4.2.2 Score per residue for model 2

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A:



- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

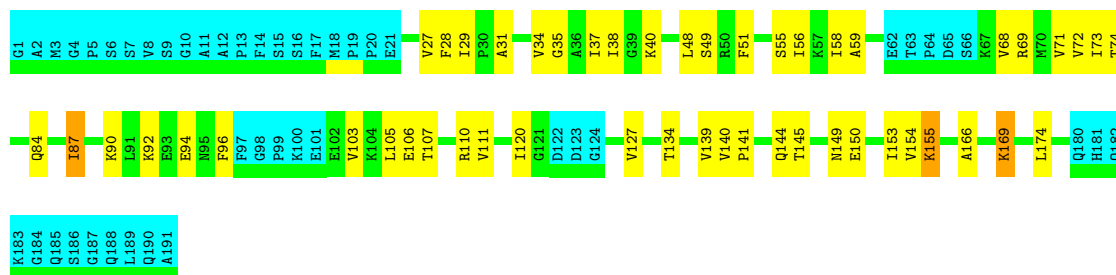
Chain B:



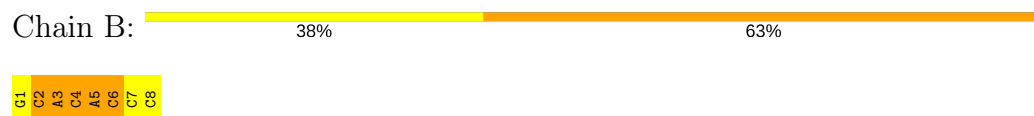
#### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A:

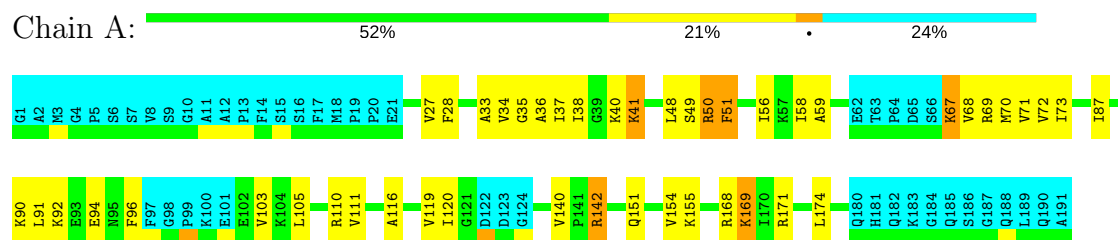


- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

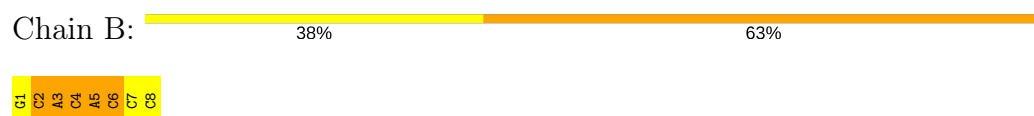


#### 4.2.4 Score per residue for model 4

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

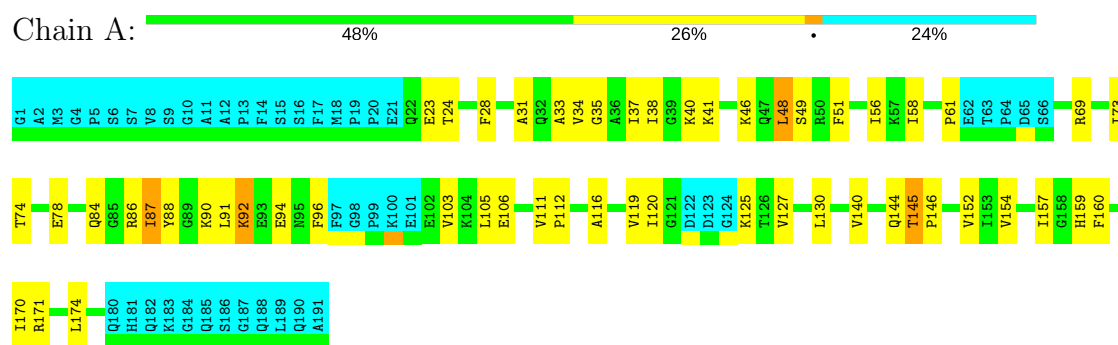


- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

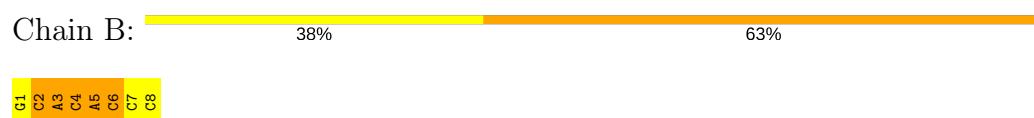


#### 4.2.5 Score per residue for model 5

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

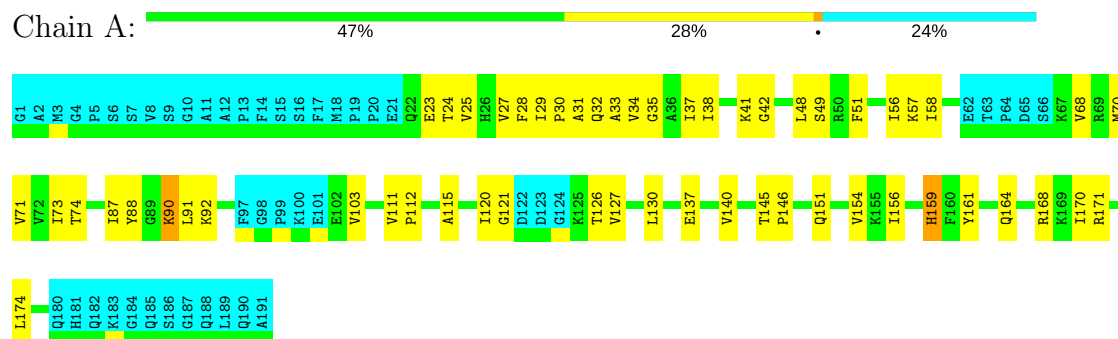


- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

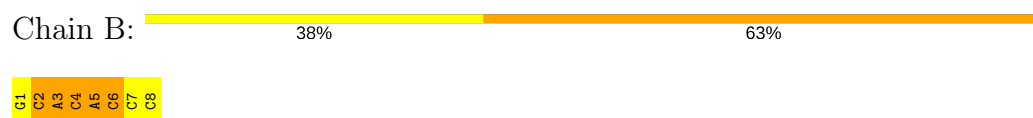


### 4.2.6 Score per residue for model 6

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

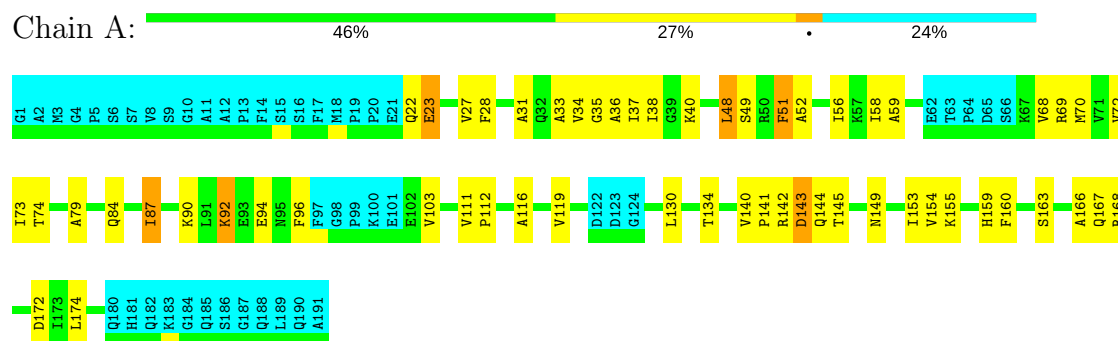


- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')



### 4.2.7 Score per residue for model 7

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1



- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

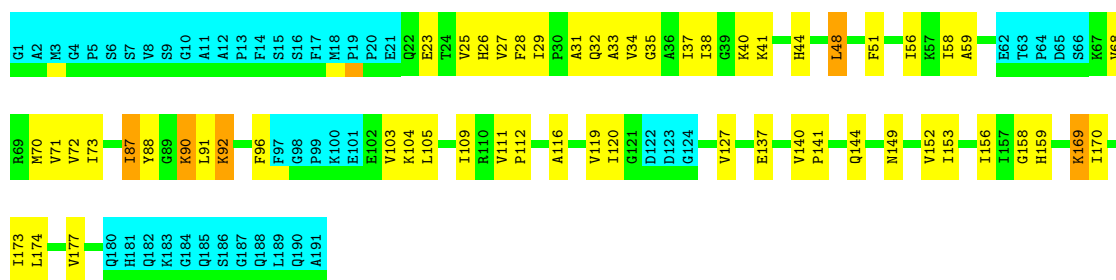


### 4.2.8 Score per residue for model 8

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1







- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

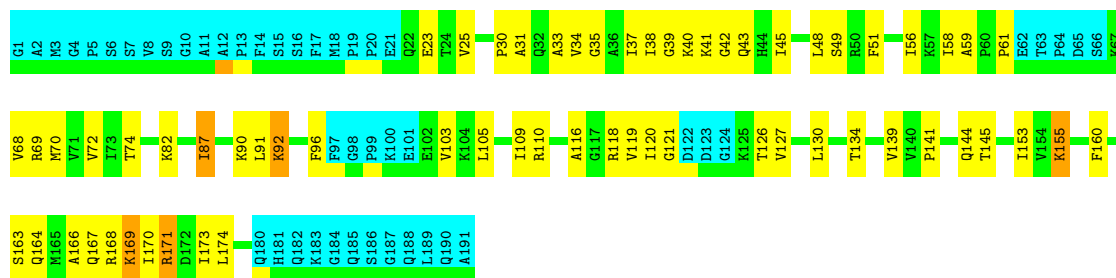
Chain B:



#### 4.2.9 Score per residue for model 9

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A:



- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

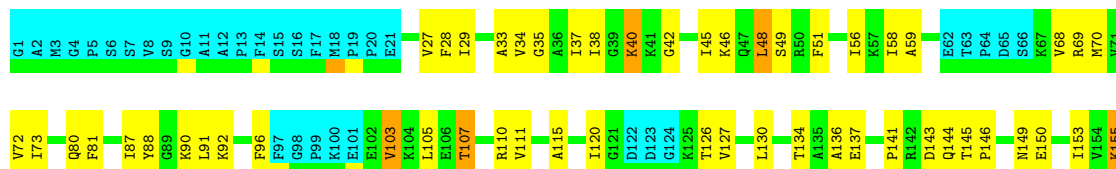
Chain B:

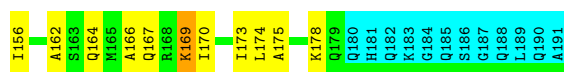


#### 4.2.10 Score per residue for model 10

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A:





- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

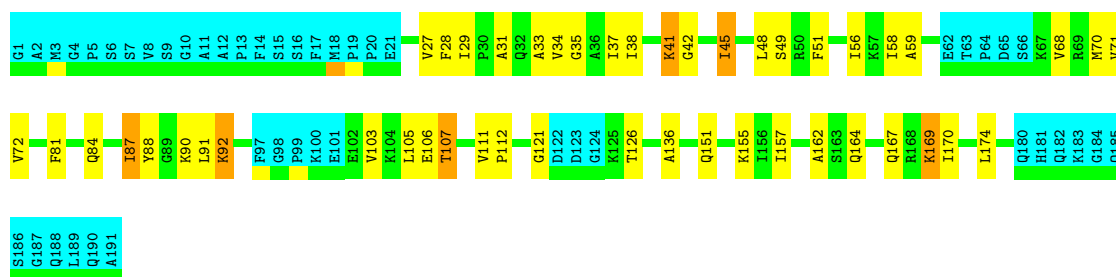
Chain B: 38% 50% 13%



#### 4.2.11 Score per residue for model 11

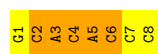
- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A: 51% 21% 24%



- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

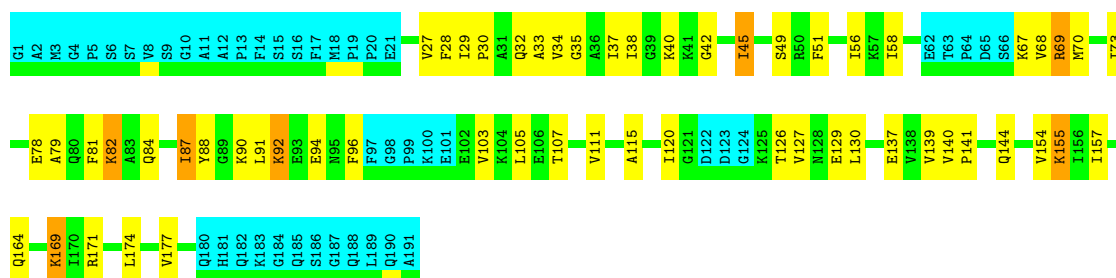
Chain B: 38% 63%



#### 4.2.12 Score per residue for model 12

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A: 46% 26% 24%



- Molecule 2: RNA (5'-R(P\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*C)-3')

Chain B:  13% 25% 63%

G1	C2	A3	C4	A5	C6	C7	C8
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## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 12 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
ARIA	structure solution	
ARIA	refinement	

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)	2n8l_cs.str
Number of chemical shift lists	1
Total number of shifts	1344
Number of shifts mapped to atoms	1344
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	53%

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

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.31±0.01	0±0/1146 (0.0±0.0%)	0.44±0.01	0±0/1548 (0.0±0.0%)
2	B	0.37±0.02	0±0/185 (0.0±0.0%)	1.06±0.03	0±0/285 (0.0±0.1%)
All	All	0.32	0/15972 (0.0%)	0.58	1/21996 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	2	C	P-O3'-C3'	5.12	125.85	119.70	10	1

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1127	1191	1187	47±5
2	B	167	89	89	24±2
All	All	15528	15360	15312	759

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:LYS:HE3	1:A:103:VAL:HB	1.00	1.33	1	11
1:A:120:ILE:HA	1:A:127:VAL:HB	0.98	1.34	1	8
1:A:35:GLY:HA2	2:B:4:C:H41	0.94	1.21	9	12
2:B:1:G:HO2'	2:B:2:C:H6	0.89	0.99	4	11
2:B:1:G:O2'	2:B:2:C:H6	0.88	1.52	11	11
1:A:35:GLY:HA2	2:B:4:C:N4	0.86	1.85	6	12
1:A:141:PRO:HG2	1:A:144:GLN:HB2	0.86	1.48	12	1
2:B:4:C:H4'	2:B:5:A:O4'	0.82	1.74	7	12
1:A:169:LYS:HA	1:A:169:LYS:HE2	0.82	1.50	1	1
1:A:169:LYS:HE3	1:A:169:LYS:HA	0.81	1.50	11	5
1:A:111:VAL:HG23	1:A:174:LEU:HD11	0.80	1.54	3	2
1:A:87:ILE:HA	1:A:90:LYS:HD3	0.78	1.53	3	2
1:A:37:ILE:HD12	1:A:90:LYS:HB3	0.77	1.56	5	9
1:A:30:PRO:HB2	1:A:32:GLN:HG2	0.77	1.56	6	3
1:A:121:GLY:HA3	1:A:126:THR:HB	0.77	1.56	11	2
1:A:38:ILE:HD12	2:B:4:C:C5	0.76	2.15	12	12
1:A:59:ALA:HB2	1:A:72:VAL:HG23	0.75	1.56	10	9
1:A:145:THR:HB	1:A:146:PRO:HD2	0.75	1.54	5	3
2:B:4:C:H4'	2:B:5:A:O5'	0.74	1.81	12	12
1:A:48:LEU:HD23	1:A:56:ILE:HG12	0.74	1.59	9	1
1:A:92:LYS:HE3	1:A:103:VAL:HG22	0.74	1.60	10	1
1:A:110:ARG:HG3	1:A:151:GLN:HG2	0.73	1.59	4	2
2:B:3:A:H1'	2:B:4:C:C5	0.73	2.19	4	12
1:A:144:GLN:HG2	1:A:153:ILE:H	0.73	1.44	1	2
1:A:144:GLN:HE21	1:A:153:ILE:HB	0.72	1.42	3	1
2:B:2:C:O2'	2:B:3:A:H5'	0.72	1.84	10	1
1:A:56:ILE:HG13	1:A:73:ILE:HG22	0.69	1.62	6	5
1:A:140:VAL:HG22	1:A:154:VAL:HG13	0.69	1.63	3	1
1:A:112:PRO:HD2	1:A:174:LEU:HG	0.69	1.64	8	2
1:A:92:LYS:HE3	1:A:103:VAL:CB	0.69	2.18	7	4
1:A:48:LEU:HA	1:A:51:PHE:CE2	0.69	2.23	11	4
1:A:38:ILE:HG22	1:A:42:GLY:HA2	0.68	1.64	10	3
1:A:106:GLU:HG2	1:A:157:ILE:HG13	0.68	1.66	2	1
1:A:48:LEU:HA	1:A:51:PHE:CD1	0.67	2.25	4	3
1:A:28:PHE:CZ	1:A:68:VAL:HG11	0.67	2.25	6	3
1:A:169:LYS:CE	1:A:169:LYS:HA	0.67	2.20	1	3
2:B:1:G:O2'	2:B:2:C:C6	0.67	2.47	12	8
1:A:106:GLU:HG3	1:A:157:ILE:HG13	0.67	1.66	5	2
1:A:38:ILE:HD12	2:B:4:C:C4	0.66	2.25	6	8
1:A:28:PHE:CE1	1:A:68:VAL:HG11	0.66	2.25	4	2
1:A:92:LYS:CE	1:A:103:VAL:HB	0.66	2.19	9	7
1:A:88:TYR:HA	1:A:91:LEU:HD22	0.66	1.66	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ALA:HB2	1:A:96:PHE:HE2	0.66	1.48	9	5
1:A:41:LYS:HA	2:B:4:C:OP2	0.66	1.91	4	3
1:A:103:VAL:HG13	1:A:159:HIS:HA	0.65	1.68	7	3
1:A:49:SER:HB2	1:A:56:ILE:HB	0.65	1.68	5	1
2:B:3:A:C1'	2:B:4:C:C5	0.65	2.80	3	12
1:A:112:PRO:HA	1:A:151:GLN:HG2	0.64	1.68	6	1
1:A:168:ARG:O	1:A:172:ASP:HB2	0.64	1.93	7	1
1:A:28:PHE:CE2	1:A:68:VAL:HG11	0.64	2.27	3	3
1:A:48:LEU:HG	1:A:51:PHE:HE1	0.64	1.53	6	3
1:A:48:LEU:HA	1:A:51:PHE:CZ	0.64	2.28	1	4
2:B:4:C:C4'	2:B:5:A:O4'	0.64	2.46	9	12
1:A:61:PRO:HD3	1:A:69:ARG:HG3	0.64	1.67	5	2
1:A:121:GLY:HA3	1:A:126:THR:CB	0.64	2.23	11	1
1:A:59:ALA:HB3	1:A:70:MET:HG3	0.64	1.70	11	1
1:A:48:LEU:HD12	1:A:56:ILE:HG12	0.63	1.68	10	1
1:A:94:GLU:HB2	1:A:96:PHE:CE2	0.63	2.27	7	3
1:A:169:LYS:HE2	1:A:169:LYS:HA	0.63	1.69	9	3
1:A:91:LEU:HD21	1:A:105:LEU:HG	0.63	1.68	8	1
1:A:45:ILE:HD12	1:A:58:ILE:HG12	0.63	1.68	10	1
1:A:144:GLN:HB2	1:A:152:VAL:HB	0.63	1.71	5	1
1:A:48:LEU:HA	1:A:51:PHE:CD2	0.62	2.28	10	2
1:A:168:ARG:HA	1:A:171:ARG:HB2	0.62	1.70	4	2
1:A:50:ARG:HA	1:A:50:ARG:HE	0.62	1.54	4	1
2:B:1:G:O5'	2:B:1:G:H8	0.62	1.77	5	3
2:B:4:C:O4'	2:B:5:A:C8	0.61	2.53	2	12
1:A:141:PRO:HD2	1:A:155:LYS:HE3	0.61	1.70	3	1
1:A:33:ALA:HB2	1:A:96:PHE:CE2	0.61	2.31	9	4
1:A:58:ILE:HB	2:B:5:A:N6	0.61	2.10	8	1
1:A:112:PRO:CD	1:A:174:LEU:HG	0.61	2.26	5	2
1:A:81:PHE:HA	1:A:164:GLN:HE22	0.61	1.55	12	1
1:A:34:VAL:HG21	1:A:69:ARG:HB3	0.60	1.73	4	6
1:A:48:LEU:HD22	1:A:56:ILE:HG12	0.60	1.72	1	3
1:A:140:VAL:HB	1:A:154:VAL:HG22	0.60	1.70	5	3
1:A:27:VAL:HB	1:A:71:VAL:CG1	0.60	2.27	11	2
1:A:46:LYS:HE2	2:B:6:C:H4'	0.60	1.73	5	2
1:A:58:ILE:HB	2:B:5:A:N1	0.60	2.11	3	9
1:A:111:VAL:HG12	1:A:174:LEU:HD21	0.60	1.73	5	3
1:A:116:ALA:HB1	1:A:140:VAL:HG21	0.60	1.72	8	2
1:A:111:VAL:HG23	1:A:174:LEU:CD2	0.60	2.26	12	2
1:A:25:VAL:HG22	1:A:73:ILE:HD11	0.59	1.73	6	1
1:A:48:LEU:HA	1:A:51:PHE:HD1	0.59	1.52	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ALA:HA	1:A:34:VAL:HG12	0.59	1.74	8	9
1:A:55:SER:HB3	1:A:74:THR:HB	0.58	1.74	1	1
1:A:35:GLY:CA	2:B:4:C:H41	0.58	2.10	2	12
1:A:139:VAL:HG13	1:A:155:LYS:HD3	0.58	1.75	9	3
2:B:6:C:H6	2:B:6:C:O5'	0.58	1.82	1	3
1:A:58:ILE:HB	2:B:5:A:C6	0.58	2.34	10	9
1:A:40:LYS:HA	2:B:3:A:OP2	0.57	1.98	10	1
1:A:90:LYS:HD2	1:A:90:LYS:C	0.57	2.19	6	2
1:A:88:TYR:CE2	1:A:105:LEU:HB3	0.57	2.35	5	6
1:A:48:LEU:HG	1:A:51:PHE:CE1	0.57	2.35	1	3
1:A:23:GLU:OE1	1:A:171:ARG:HG3	0.57	2.00	9	1
1:A:25:VAL:HG13	1:A:109:ILE:HG22	0.56	1.77	9	1
1:A:36:ALA:HB2	2:B:2:C:O2'	0.56	2.00	4	1
1:A:167:GLN:O	1:A:171:ARG:HG2	0.56	2.01	9	1
1:A:24:THR:HA	1:A:73:ILE:O	0.56	2.01	2	4
1:A:91:LEU:HG	1:A:105:LEU:HG	0.56	1.77	9	3
1:A:110:ARG:HD3	1:A:153:ILE:HG12	0.55	1.77	9	3
1:A:141:PRO:HG3	1:A:155:LYS:HE3	0.55	1.76	12	3
1:A:116:ALA:O	1:A:119:VAL:HG12	0.55	2.00	1	5
1:A:171:ARG:HA	1:A:174:LEU:HD23	0.55	1.77	2	1
1:A:48:LEU:HA	1:A:51:PHE:CE1	0.55	2.37	8	2
2:B:2:C:O2'	2:B:3:A:C5'	0.55	2.55	10	1
1:A:35:GLY:HA3	2:B:3:A:C8	0.55	2.37	6	7
1:A:109:ILE:HG21	1:A:171:ARG:NH2	0.55	2.17	9	1
1:A:23:GLU:O	1:A:74:THR:HA	0.55	2.02	9	4
1:A:27:VAL:HB	1:A:71:VAL:HG22	0.55	1.79	3	1
1:A:25:VAL:HG21	1:A:171:ARG:NH1	0.55	2.15	9	1
1:A:90:LYS:HG3	1:A:91:LEU:HD22	0.54	1.78	6	1
1:A:163:SER:O	1:A:167:GLN:HG3	0.54	2.02	9	2
2:B:1:G:C2	2:B:2:C:N4	0.54	2.75	10	1
1:A:37:ILE:HD12	1:A:90:LYS:CG	0.54	2.32	9	3
1:A:170:ILE:O	1:A:174:LEU:HD13	0.54	2.03	8	2
1:A:111:VAL:HG12	1:A:174:LEU:HD22	0.54	1.78	2	1
1:A:120:ILE:HA	1:A:127:VAL:HG23	0.53	1.80	12	1
1:A:81:PHE:HD1	1:A:164:GLN:HG3	0.53	1.61	11	1
1:A:137:GLU:O	1:A:156:ILE:HA	0.53	2.03	10	4
2:B:5:A:H2'	2:B:6:C:O5'	0.53	2.03	3	8
1:A:111:VAL:HG23	1:A:174:LEU:CD1	0.53	2.31	3	2
1:A:111:VAL:HG23	1:A:174:LEU:HD21	0.53	1.79	12	1
1:A:141:PRO:HG3	1:A:155:LYS:HE2	0.53	1.79	7	1
1:A:88:TYR:O	1:A:91:LEU:HB2	0.53	2.04	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:VAL:O	1:A:70:MET:HA	0.53	2.04	2	9
2:B:5:A:H8	2:B:5:A:O5'	0.53	1.86	1	3
1:A:115:ALA:HB1	1:A:174:LEU:HD22	0.52	1.79	10	1
1:A:88:TYR:HA	1:A:91:LEU:HD23	0.52	1.81	2	3
1:A:112:PRO:CD	1:A:174:LEU:HD13	0.52	2.34	2	1
1:A:119:VAL:HG22	1:A:130:LEU:HD11	0.52	1.81	7	1
1:A:46:LYS:HE2	2:B:6:C:C4'	0.52	2.35	5	1
1:A:33:ALA:O	1:A:37:ILE:HG12	0.52	2.04	8	11
2:B:3:A:O4'	2:B:4:C:C5	0.52	2.63	2	9
2:B:2:C:H4'	2:B:3:A:OP1	0.52	2.04	10	2
1:A:111:VAL:HG23	1:A:174:LEU:HD22	0.52	1.82	6	1
1:A:130:LEU:HD21	1:A:170:ILE:HD11	0.52	1.80	6	3
1:A:119:VAL:HG22	1:A:173:ILE:HD11	0.52	1.81	2	1
1:A:37:ILE:HD12	1:A:90:LYS:HG2	0.52	1.80	9	1
1:A:126:THR:O	1:A:130:LEU:HG	0.51	2.05	2	3
1:A:41:LYS:HE2	1:A:43:GLN:HB3	0.51	1.81	9	1
1:A:81:PHE:HA	1:A:164:GLN:NE2	0.51	2.21	10	3
1:A:55:SER:HB2	1:A:74:THR:HB	0.51	1.82	2	2
1:A:91:LEU:HD23	1:A:103:VAL:CG2	0.51	2.36	8	1
1:A:48:LEU:HD22	1:A:51:PHE:HZ	0.51	1.65	5	1
1:A:139:VAL:CG1	1:A:155:LYS:HD3	0.51	2.35	9	1
1:A:94:GLU:HG2	1:A:96:PHE:CE2	0.51	2.40	4	1
1:A:121:GLY:HA3	1:A:126:THR:HG22	0.51	1.82	6	1
1:A:94:GLU:HA	1:A:94:GLU:OE1	0.51	2.05	2	1
2:B:4:C:O5'	2:B:4:C:H6	0.51	1.88	4	1
1:A:112:PRO:HD2	1:A:174:LEU:HD22	0.51	1.82	11	2
1:A:49:SER:HA	1:A:56:ILE:HD13	0.50	1.83	1	10
1:A:29:ILE:C	1:A:68:VAL:HB	0.50	2.27	12	2
1:A:84:GLN:HA	1:A:87:ILE:HG22	0.50	1.84	12	1
1:A:144:GLN:OE1	1:A:153:ILE:HB	0.50	2.07	7	2
1:A:110:ARG:CD	1:A:153:ILE:HG12	0.50	2.37	9	2
1:A:41:LYS:HA	2:B:4:C:C5'	0.50	2.36	8	1
1:A:136:ALA:HB2	1:A:162:ALA:HB1	0.50	1.83	11	2
1:A:142:ARG:H	1:A:142:ARG:HD2	0.50	1.67	4	1
1:A:120:ILE:HA	1:A:127:VAL:CG2	0.49	2.37	12	1
1:A:170:ILE:O	1:A:174:LEU:HG	0.49	2.06	10	3
1:A:48:LEU:HD22	1:A:51:PHE:CZ	0.49	2.41	5	1
1:A:164:GLN:O	1:A:168:ARG:HG2	0.49	2.07	6	1
1:A:48:LEU:HA	1:A:51:PHE:HE1	0.49	1.67	8	1
1:A:88:TYR:CZ	1:A:105:LEU:HB3	0.49	2.41	8	1
1:A:39:GLY:HA2	2:B:3:A:OP1	0.49	2.07	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:6:C:O5'	2:B:6:C:H6	0.49	1.89	12	3
2:B:1:G:O5'	2:B:1:G:C8	0.49	2.62	5	1
2:B:5:A:O2'	2:B:6:C:P	0.49	2.70	5	1
1:A:82:LYS:H	1:A:82:LYS:HD2	0.49	1.68	12	1
1:A:87:ILE:O	1:A:90:LYS:HG3	0.49	2.06	8	1
1:A:37:ILE:HD12	1:A:90:LYS:CB	0.48	2.38	11	2
1:A:144:GLN:HB2	1:A:152:VAL:CB	0.48	2.36	5	1
1:A:175:ALA:HA	1:A:178:LYS:HD3	0.48	1.84	10	1
1:A:73:ILE:HD12	1:A:73:ILE:O	0.48	2.08	3	2
1:A:77:PRO:HA	1:A:168:ARG:NH2	0.48	2.24	2	1
2:B:4:C:C5'	2:B:5:A:O4'	0.48	2.61	9	3
2:B:6:C:C5	2:B:7:C:C4	0.48	3.02	9	1
1:A:34:VAL:HA	1:A:37:ILE:HG12	0.48	1.86	10	2
1:A:37:ILE:CD1	1:A:90:LYS:HB3	0.48	2.39	10	1
1:A:137:GLU:HB3	1:A:157:ILE:HB	0.48	1.86	12	1
1:A:40:LYS:O	1:A:41:LYS:HG2	0.48	2.08	5	1
2:B:3:A:H1'	2:B:4:C:C6	0.48	2.44	10	12
2:B:5:A:C5	2:B:6:C:C5	0.48	3.02	3	8
2:B:4:C:H4'	2:B:5:A:C5'	0.48	2.39	6	3
1:A:111:VAL:HG22	1:A:115:ALA:HB3	0.47	1.86	10	3
2:B:5:A:C2'	2:B:6:C:O5'	0.47	2.62	3	7
2:B:4:C:H5'	2:B:5:A:O4'	0.47	2.09	12	2
1:A:144:GLN:HG2	1:A:152:VAL:HB	0.47	1.85	8	1
1:A:142:ARG:HA	1:A:142:ARG:NE	0.47	2.24	2	1
1:A:134:THR:HB	1:A:166:ALA:HB2	0.47	1.84	9	2
1:A:121:GLY:CA	1:A:126:THR:HB	0.47	2.35	11	1
2:B:1:G:H2'	2:B:2:C:C6	0.47	2.43	10	1
1:A:45:ILE:CD1	1:A:58:ILE:HG12	0.47	2.39	9	2
1:A:79:ALA:HA	1:A:82:LYS:HD3	0.47	1.86	12	1
1:A:73:ILE:O	1:A:73:ILE:HD12	0.47	2.10	4	3
1:A:84:GLN:O	1:A:87:ILE:HG22	0.47	2.09	11	5
1:A:144:GLN:NE2	1:A:153:ILE:HB	0.47	2.19	3	1
1:A:42:GLY:O	1:A:45:ILE:HG22	0.47	2.10	11	2
1:A:59:ALA:HB3	1:A:70:MET:HB2	0.46	1.87	9	1
1:A:49:SER:CB	1:A:56:ILE:HB	0.46	2.39	5	1
1:A:145:THR:HB	1:A:146:PRO:CD	0.46	2.35	5	1
1:A:48:LEU:HD22	1:A:51:PHE:HE1	0.46	1.69	7	2
1:A:25:VAL:HG21	1:A:167:GLN:NE2	0.46	2.26	1	1
1:A:169:LYS:CA	1:A:169:LYS:HE3	0.46	2.38	8	1
1:A:52:ALA:O	1:A:79:ALA:HB1	0.46	2.10	7	2
1:A:39:GLY:HA3	1:A:44:HIS:NE2	0.46	2.26	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:TYR:O	1:A:164:GLN:HG3	0.46	2.11	6	1
1:A:94:GLU:HG2	1:A:96:PHE:CZ	0.46	2.45	4	1
1:A:116:ALA:HB1	1:A:140:VAL:HG11	0.46	1.87	7	1
1:A:86:ARG:NE	1:A:86:ARG:HA	0.46	2.26	5	1
1:A:143:ASP:CG	1:A:144:GLN:H	0.45	2.15	10	1
1:A:141:PRO:CG	1:A:155:LYS:HE2	0.45	2.41	7	1
1:A:78:GLU:HG3	1:A:79:ALA:N	0.45	2.26	12	1
1:A:25:VAL:HB	1:A:109:ILE:HG22	0.45	1.87	8	1
1:A:29:ILE:O	1:A:68:VAL:HB	0.45	2.12	10	2
1:A:141:PRO:CD	1:A:155:LYS:HE3	0.45	2.41	3	1
1:A:29:ILE:C	1:A:68:VAL:HG23	0.45	2.31	1	4
1:A:155:LYS:N	1:A:155:LYS:HD2	0.45	2.26	3	2
1:A:30:PRO:HA	1:A:68:VAL:HA	0.45	1.89	6	3
1:A:111:VAL:HG12	1:A:174:LEU:HD11	0.45	1.88	7	2
1:A:140:VAL:HG12	1:A:154:VAL:HG22	0.45	1.89	6	1
2:B:4:C:H6	2:B:4:C:O5'	0.45	1.95	3	1
2:B:1:G:O2'	2:B:2:C:C5'	0.45	2.65	5	1
2:B:1:G:C8	2:B:1:G:O5'	0.45	2.69	4	1
1:A:134:THR:HG21	1:A:166:ALA:HA	0.45	1.87	3	3
1:A:49:SER:OG	1:A:56:ILE:HB	0.45	2.11	7	1
1:A:103:VAL:O	1:A:159:HIS:HA	0.45	2.12	8	1
1:A:57:LYS:HD2	2:B:6:C:O2	0.44	2.13	6	1
1:A:28:PHE:CG	1:A:68:VAL:HG21	0.44	2.47	3	1
2:B:1:G:O2'	2:B:2:C:H5'	0.44	2.12	5	2
1:A:141:PRO:CG	1:A:155:LYS:HE3	0.44	2.43	12	1
1:A:170:ILE:O	1:A:173:ILE:HG13	0.44	2.12	9	2
2:B:4:C:C4'	2:B:5:A:O5'	0.44	2.61	8	5
1:A:139:VAL:HG13	1:A:155:LYS:HB2	0.44	1.89	12	1
1:A:87:ILE:O	1:A:90:LYS:HB2	0.44	2.13	2	2
1:A:35:GLY:O	2:B:3:A:H5'	0.44	2.12	4	1
1:A:144:GLN:HG3	1:A:153:ILE:H	0.44	1.72	3	1
1:A:141:PRO:HD2	1:A:153:ILE:O	0.44	2.13	8	1
1:A:48:LEU:HD22	1:A:51:PHE:CE1	0.44	2.48	7	1
1:A:115:ALA:HB2	1:A:177:VAL:HG11	0.43	1.89	12	1
1:A:139:VAL:HG22	1:A:141:PRO:HD3	0.43	1.89	3	1
1:A:38:ILE:CG2	1:A:42:GLY:HA2	0.43	2.41	10	1
1:A:27:VAL:HB	1:A:71:VAL:HG12	0.43	1.88	11	1
1:A:107:THR:HG21	1:A:167:GLN:NE2	0.43	2.28	11	2
1:A:38:ILE:HG23	1:A:45:ILE:HG21	0.43	1.89	1	1
1:A:110:ARG:HD2	1:A:153:ILE:HG12	0.43	1.90	1	1
2:B:1:G:H8	2:B:1:G:O5'	0.43	1.96	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ILE:HD11	1:A:90:LYS:CG	0.43	2.44	8	1
1:A:52:ALA:HB1	1:A:83:ALA:HB2	0.43	1.89	2	1
1:A:88:TYR:CG	1:A:160:PHE:HB3	0.43	2.48	2	2
1:A:171:ARG:HA	1:A:174:LEU:HG	0.43	1.91	6	2
1:A:58:ILE:HG12	1:A:71:VAL:HG22	0.43	1.91	6	1
1:A:73:ILE:HG23	1:A:73:ILE:O	0.43	2.14	2	1
1:A:25:VAL:HG21	1:A:167:GLN:HE21	0.42	1.74	1	1
1:A:104:LYS:HD2	1:A:158:GLY:HA2	0.42	1.89	8	1
2:B:1:G:C4'	2:B:2:C:OP1	0.42	2.67	2	4
1:A:32:GLN:HB2	1:A:96:PHE:HZ	0.42	1.73	8	1
1:A:160:PHE:O	1:A:164:GLN:HG2	0.42	2.13	9	1
1:A:94:GLU:O	1:A:94:GLU:HG3	0.42	2.14	4	1
1:A:142:ARG:HD2	1:A:142:ARG:N	0.42	2.29	4	1
1:A:149:ASN:O	1:A:150:GLU:HG2	0.42	2.15	3	2
1:A:26:HIS:HB3	1:A:70:MET:HB3	0.42	1.92	1	1
1:A:171:ARG:HA	1:A:174:LEU:HD22	0.42	1.89	5	1
2:B:5:A:C5	2:B:6:C:C4	0.42	3.07	12	1
1:A:59:ALA:HB2	1:A:72:VAL:CG2	0.42	2.42	1	1
1:A:140:VAL:CG1	1:A:154:VAL:HG22	0.42	2.44	3	1
1:A:155:LYS:HD2	1:A:155:LYS:H	0.42	1.73	1	1
1:A:29:ILE:HD13	1:A:87:ILE:HD11	0.41	1.92	8	1
1:A:110:ARG:HH11	1:A:153:ILE:HG13	0.41	1.75	1	1
1:A:171:ARG:HG3	1:A:171:ARG:HH11	0.41	1.75	9	1
1:A:116:ALA:O	1:A:119:VAL:HB	0.41	2.15	2	1
1:A:140:VAL:CG2	1:A:154:VAL:HG22	0.41	2.45	3	1
1:A:67:LYS:HD2	1:A:67:LYS:O	0.41	2.14	4	1
1:A:140:VAL:HG22	1:A:154:VAL:HB	0.41	1.91	7	1
1:A:94:GLU:HB3	1:A:96:PHE:CE2	0.41	2.50	5	1
1:A:69:ARG:NH1	2:B:4:C:N3	0.41	2.67	5	1
1:A:41:LYS:HA	2:B:4:C:H5''	0.41	1.91	8	1
1:A:169:LYS:HA	1:A:169:LYS:CE	0.41	2.45	4	1
1:A:38:ILE:HG23	1:A:45:ILE:HB	0.41	1.93	12	1
1:A:140:VAL:HG22	1:A:154:VAL:CG1	0.41	2.39	3	1
1:A:173:ILE:O	1:A:177:VAL:HG23	0.41	2.14	8	1
1:A:26:HIS:HA	1:A:71:VAL:O	0.41	2.16	8	1
1:A:36:ALA:HA	2:B:3:A:H5'	0.41	1.91	7	1
1:A:111:VAL:O	1:A:151:GLN:HG3	0.41	2.16	11	1
1:A:37:ILE:HD11	1:A:90:LYS:HG2	0.41	1.93	8	1
1:A:112:PRO:HD2	1:A:174:LEU:HD13	0.41	1.93	2	1
1:A:91:LEU:HD22	1:A:91:LEU:N	0.41	2.31	6	1
1:A:38:ILE:HD12	2:B:4:C:C6	0.41	2.50	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:GLN:HB3	1:A:160:PHE:HE1	0.41	1.76	7	1
2:B:5:A:O2'	2:B:6:C:O5'	0.41	2.39	5	1
1:A:31:ALA:HA	1:A:34:VAL:CG1	0.41	2.46	2	1
2:B:5:A:C4	2:B:6:C:C6	0.40	3.09	10	2
1:A:141:PRO:HD3	1:A:155:LYS:HE3	0.40	1.93	12	1
2:B:5:A:C4	2:B:6:C:C5	0.40	3.08	9	1
1:A:27:VAL:HB	1:A:71:VAL:HB	0.40	1.93	1	1
1:A:116:ALA:HB2	1:A:152:VAL:CG2	0.40	2.46	5	1
1:A:28:PHE:HB3	1:A:106:GLU:O	0.40	2.16	3	1
1:A:91:LEU:HD23	1:A:105:LEU:HD11	0.40	1.91	5	1
1:A:50:ARG:HA	1:A:50:ARG:NE	0.40	2.28	4	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	145/191 (76%)	139±2 (96±1%)	5±1 (3±1%)	1±1 (1±1%)	25	72
All	All	1740/2292 (76%)	1669 (96%)	55 (3%)	16 (1%)	25	72

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	40	LYS	8
1	A	145	THR	1
1	A	125	LYS	1
1	A	61	PRO	1
1	A	42	GLY	1
1	A	43	GLN	1
1	A	39	GLY	1
1	A	143	ASP	1
1	A	144	GLN	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	120/155 (77%)	112±3 (94±2%)	8±3 (6±2%)	25	71
All	All	1440/1860 (77%)	1348 (94%)	92 (6%)	25	71

All 36 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	87	ILE	12
1	A	169	LYS	8
1	A	155	LYS	8
1	A	92	LYS	6
1	A	107	THR	5
1	A	28	PHE	4
1	A	48	LEU	4
1	A	145	THR	3
1	A	51	PHE	3
1	A	41	LYS	3
1	A	168	ARG	2
1	A	23	GLU	2
1	A	46	LYS	2
1	A	149	ASN	2
1	A	90	LYS	2
1	A	142	ARG	2
1	A	171	ARG	2
1	A	82	LYS	2
1	A	45	ILE	2
1	A	67	LYS	2
1	A	159	HIS	1
1	A	80	GLN	1
1	A	22	GLN	1
1	A	174	LEU	1
1	A	129	GLU	1
1	A	44	HIS	1
1	A	102	GLU	1
1	A	50	ARG	1
1	A	73	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	105	LEU	1
1	A	69	ARG	1
1	A	164	GLN	1
1	A	103	VAL	1
1	A	172	ASP	1
1	A	78	GLU	1
1	A	143	ASP	1

### 6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	7/8 (88%)	7±0 (98±5%)	0±0 (0±0%)	0.00±0.01
All	All	84/96 (88%)	82 (98%)	0 (0%)	0.00

The overall RNA backbone suiteness is 0.00.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	6	C	12
2	B	2	C	12
2	B	8	C	12
2	B	4	C	12
2	B	5	A	12
2	B	7	C	11
2	B	3	A	11

There are no RNA pucker outliers to report.

## 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](#)

There are no ligands in this entry.

## 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 53% for the well-defined parts and 46% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2n8l\_cs.str

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	1344
Number of shifts mapped to atoms	1344
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	128	$-0.06 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	122	$0.19 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	0	—	None (insufficient data)

#### 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 53%, i.e. 1055 atoms were assigned a chemical shift out of a possible 1985. 17 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	316/709 (45%)	197/282 (70%)	119/290 (41%)	0/137 (0%)
Sidechain	715/1030 (69%)	461/603 (76%)	254/373 (68%)	0/54 (0%)

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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	24/93 (26%)	24/49 (49%)	0/36 (0%)	0/8 (0%)
Overall	1055/1985 (53%)	682/1023 (67%)	373/754 (49%)	0/208 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 1133 atoms were assigned a chemical shift out of a possible 2477. 17 out of 24 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	339/927 (37%)	211/368 (57%)	128/382 (34%)	0/177 (0%)
Sidechain	766/1269 (60%)	496/749 (66%)	270/459 (59%)	0/61 (0%)
Aromatic	28/128 (22%)	28/68 (41%)	0/50 (0%)	0/10 (0%)
Overall	1133/2477 (46%)	735/1274 (58%)	398/946 (42%)	0/257 (0%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	164	GLN	HB3	14.78	3.37 – 0.67	47.3
1	A	164	GLN	HB2	10.46	3.30 – 0.80	33.6
1	A	164	GLN	CB	6.59	38.36 – 19.96	-12.3
1	A	119	VAL	CG2	8.16	29.20 – 13.40	-8.3

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

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

Random coil index (RCI) for chain A:

