



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 09:12 am BST

PDB ID : 5YQ3
Title : Solution NMR Structure and Backbone Dynamics of the Partially Disordered Arabidopsis thaliana Phloem Protein 16-1, A Putative mRNA Transporter
Authors : Bhuyan, A.K.; Sashi, P.
Deposited on : 2017-11-04

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 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

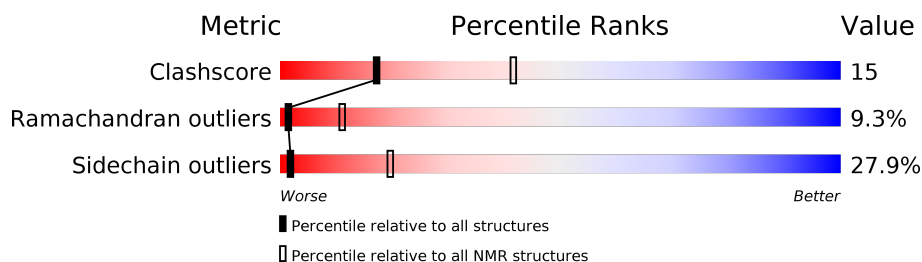
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	162	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 9 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:1-A:17, A:27-A:78, A:86-A:138 (122)	1.06	9

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2522 atoms, of which 1244 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called At3g55470.

Mol	Chain	Residues	Atoms						Trace
1	A	162	Total	C	H	N	O	S	0
			2522	807	1244	223	244	4	

There are 7 discrepancies between the modelled and reference sequences:

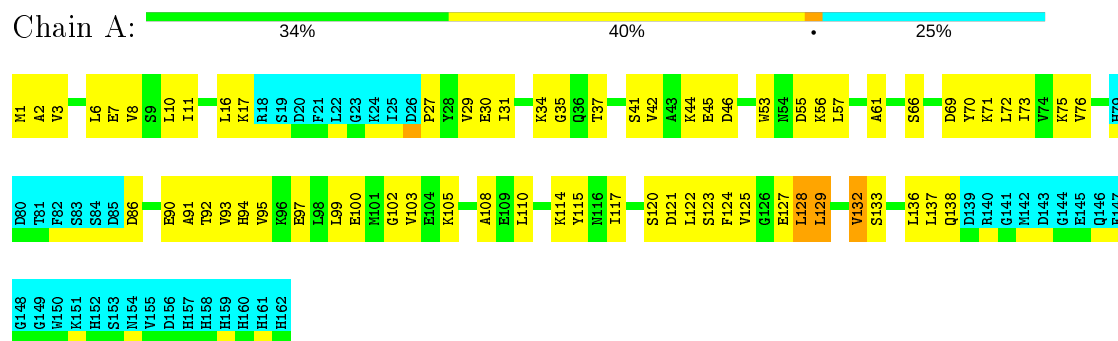
Chain	Residue	Modelled	Actual	Comment	Reference
A	154	ASN	GLN	engineered mutation	UNP Q9M2T2
A	157	HIS	-	expression tag	UNP Q9M2T2
A	158	HIS	-	expression tag	UNP Q9M2T2
A	159	HIS	-	expression tag	UNP Q9M2T2
A	160	HIS	-	expression tag	UNP Q9M2T2
A	161	HIS	-	expression tag	UNP Q9M2T2
A	162	HIS	-	expression tag	UNP Q9M2T2

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: At3g55470

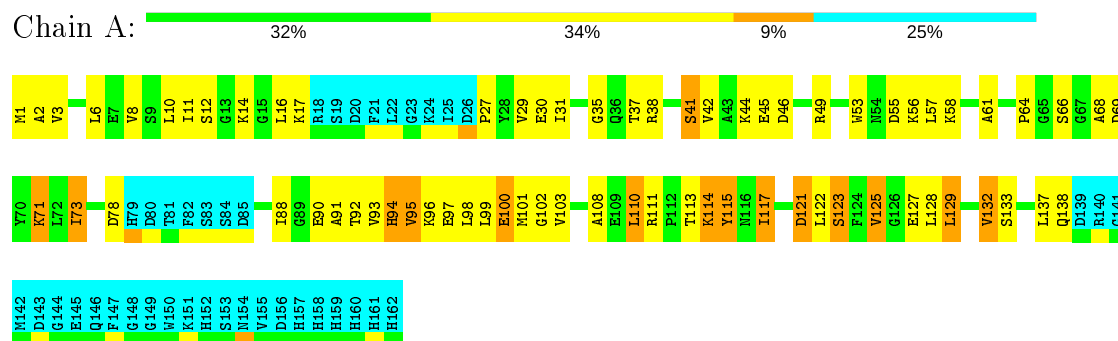


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

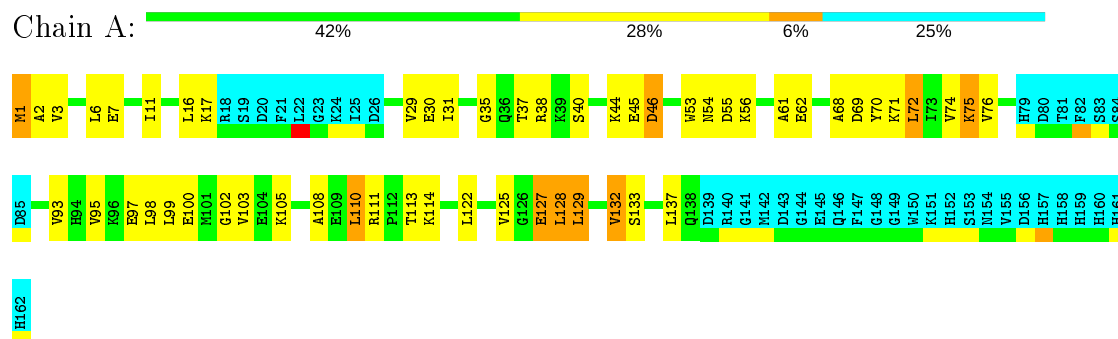
4.2.1 Score per residue for model 1

- Molecule 1: At3g55470



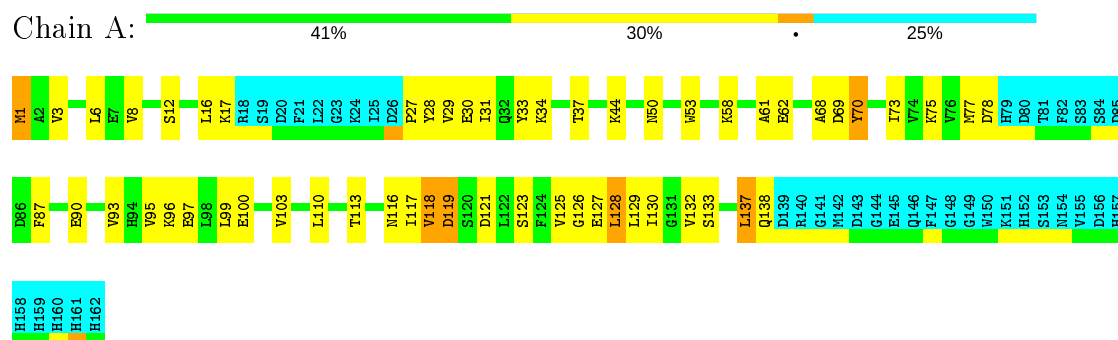
4.2.2 Score per residue for model 2

- Molecule 1: At3g55470



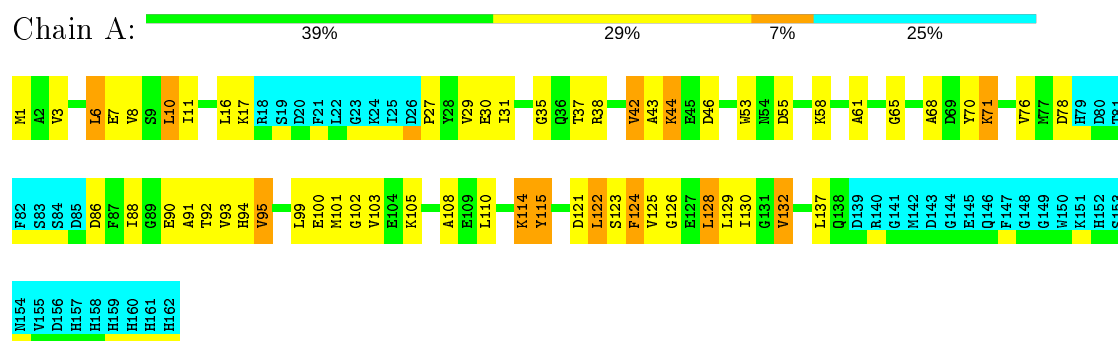
4.2.3 Score per residue for model 3

- Molecule 1: At3g55470



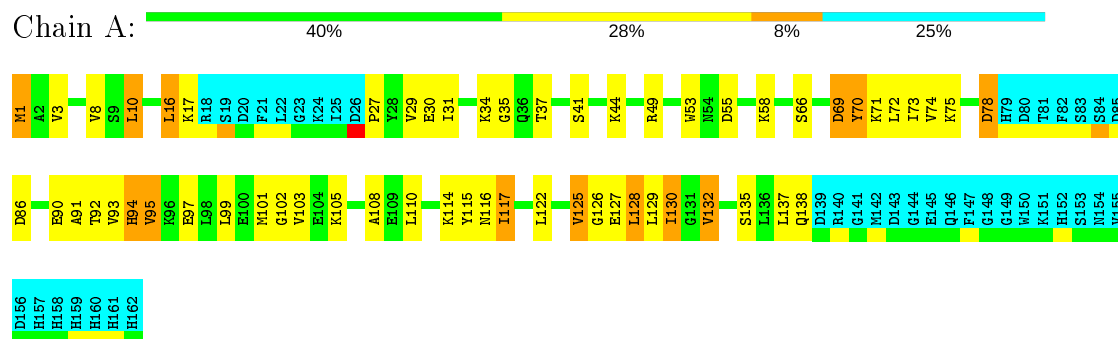
4.2.4 Score per residue for model 4

- Molecule 1: At3g55470



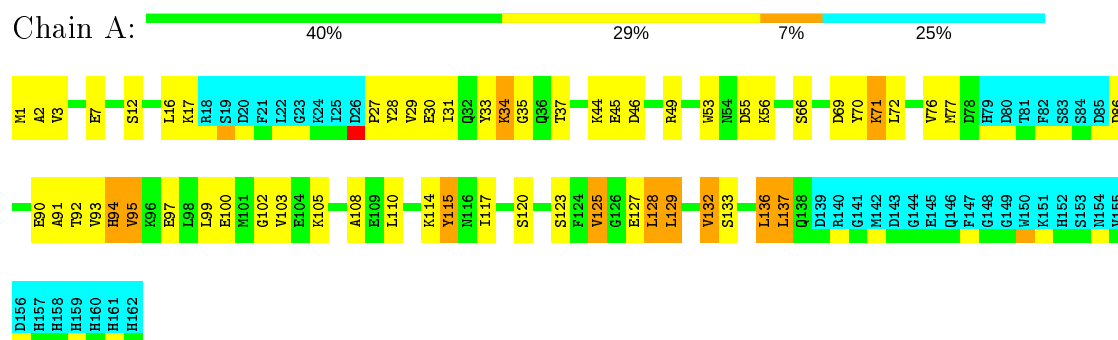
4.2.5 Score per residue for model 5

- Molecule 1: At3g55470



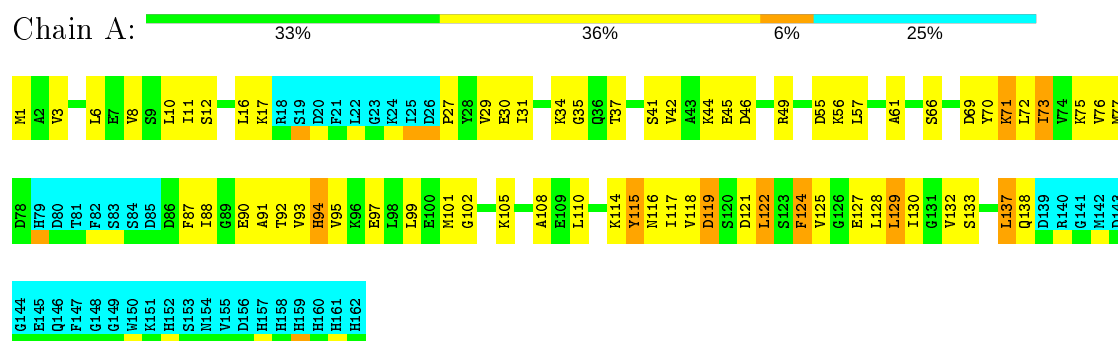
4.2.6 Score per residue for model 6

- Molecule 1: At3g55470



4.2.7 Score per residue for model 7

- Molecule 1: At3g55470



- Molecule 1: At3g55470

Chain A:

Category	Block Range	Count
G	G148-G162	10
H	H148-H162	10
I	I148-I162	10
J	J148-J162	10
K	K148-K162	10
L	L148-L162	10
M	M148-M162	10
N	N148-N162	10
O	O148-O162	10
P	P148-P162	10
Q	Q148-Q162	10
R	R148-R162	10

- Molecule 1: At3g55470

Chain A:

Category	Percentage	Amino Acid Codes
40%	40%	M1, A2, L6, F7, V8, I11, S12, K17, R18, S19, T20, D21, F21, L22, G23, G24, D25, D26, F27, V28, V29, E30, I31, K34, G35, G36, T37, R38, V42, A43, K44, E45, D46, D55, K56, L57, K58, S66, D69, W73, Y74, K75, V76, H79, L80, L81, F82, S83, S84, L85, R86
29%	29%	
7%	7%	
25%	25%	

- Molecule 1: At3g55470

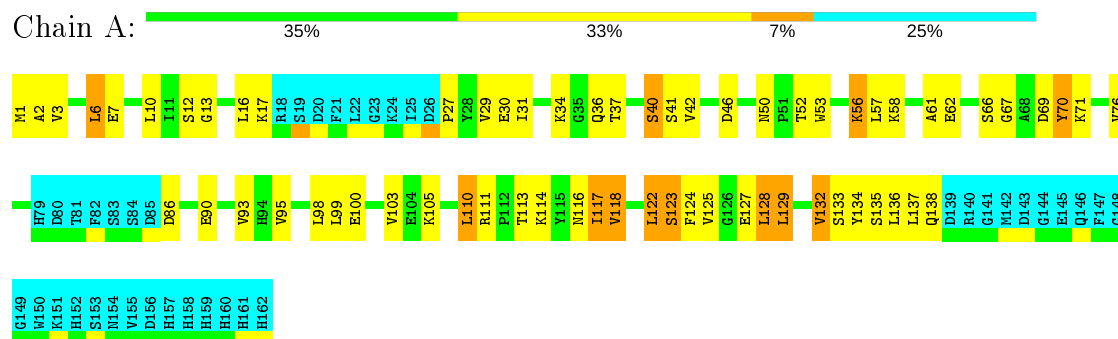
Chain A:

40% 32% 25%

M1 A2 V3 G4 I5 L6 E7 W8 S9 L10 T11 S12 G13 K14 K17 S18 S19 T20 F21 L22 G23 K24 T25 D26 P27 V28 V29 E30 I31 K34 G35 G36 T37 R38 S41 V42 A43 K44 M50 D55 S56 L57 R60 A61 S66 G67 D68 V70 K71 L72 V75 V76 H79 D80 T81 F82 S83 S84 D85 E90 L98 L99 E100 V103 E104 K105 L110 T113 K114 L117 V118 D119 L122 S123 F124 V125 G126 E127 L128 L129 I130 G131 V132 S133 V134 S135 L136 L137 Q138 D139 A140 G141 M142 D143 G144 E145 F146 G148 G149 W150 K151 F152

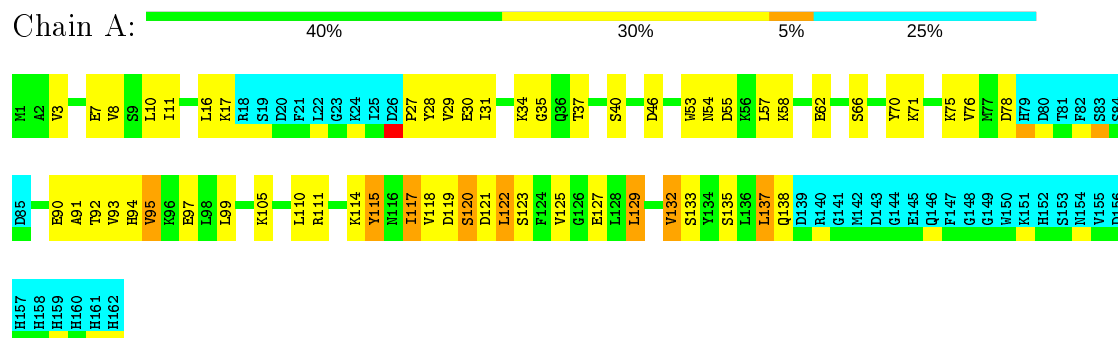
4.2.11 Score per residue for model 11

- Molecule 1: At3g55470



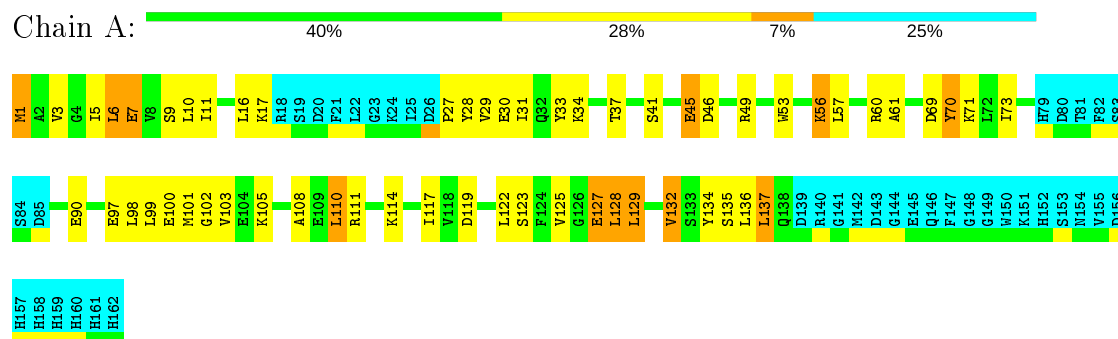
4.2.12 Score per residue for model 12

- Molecule 1: At3g55470



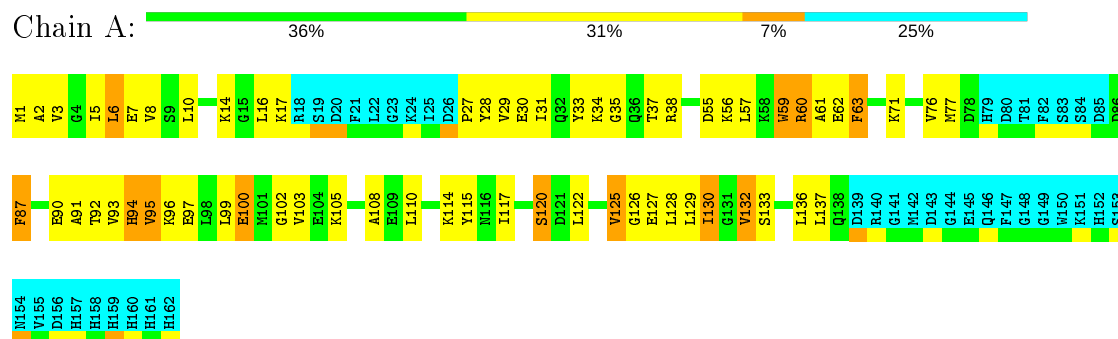
4.2.13 Score per residue for model 13

- Molecule 1: At3g55470



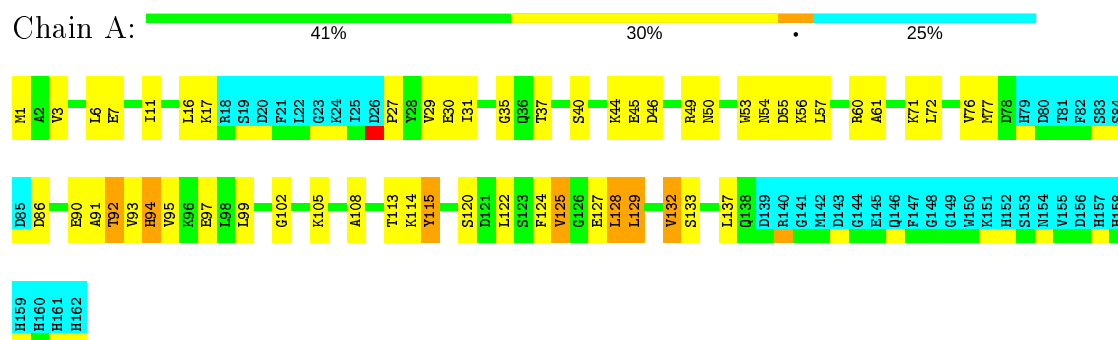
4.2.14 Score per residue for model 14

- Molecule 1: At3g55470



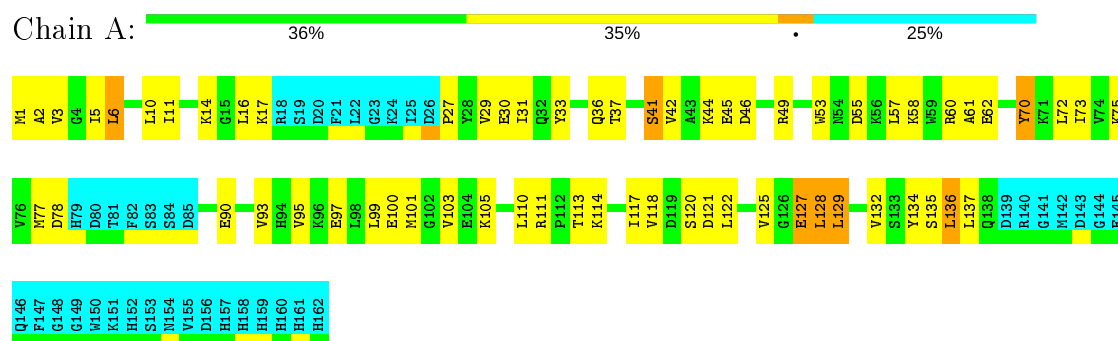
4.2.15 Score per residue for model 15

- Molecule 1: At3g55470



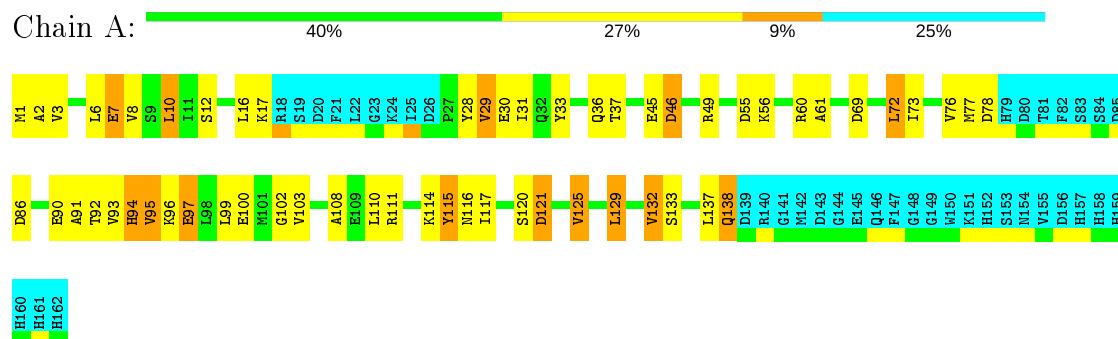
4.2.16 Score per residue for model 16

- Molecule 1: At3g55470



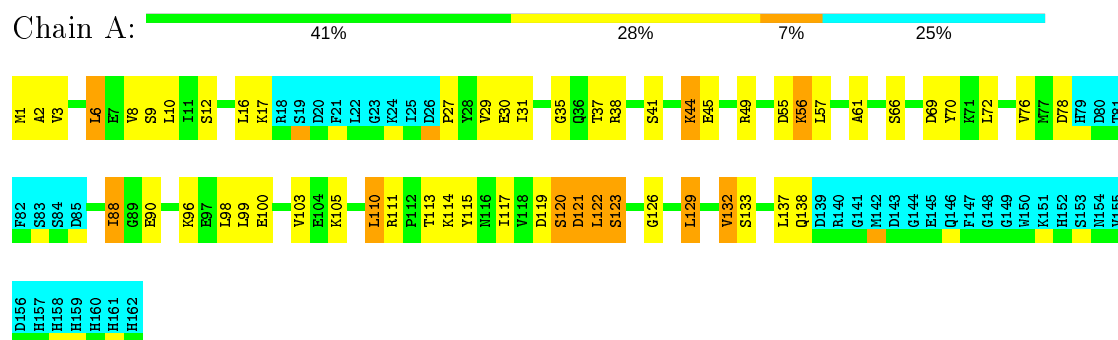
4.2.17 Score per residue for model 17

- Molecule 1: At3g55470



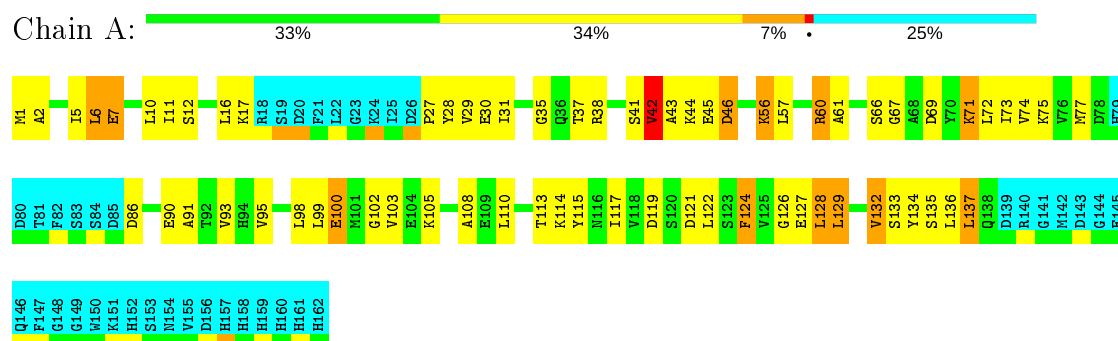
4.2.18 Score per residue for model 18

- Molecule 1: At3g55470



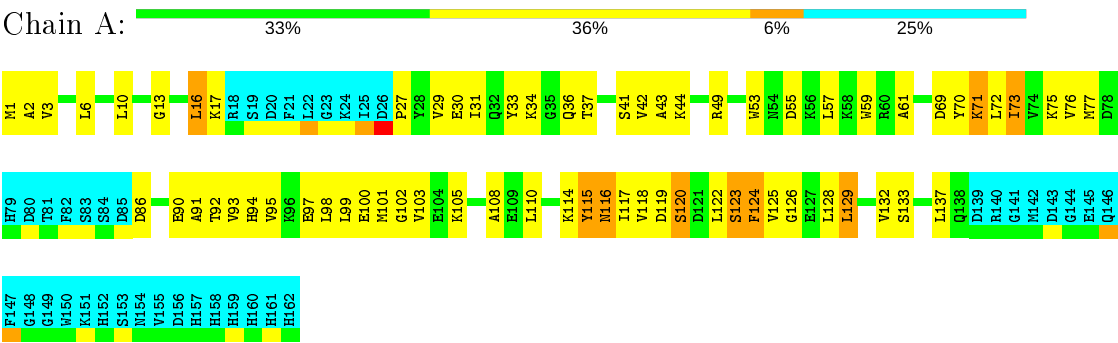
4.2.19 Score per residue for model 19

- Molecule 1: At3g55470



4.2.20 Score per residue for model 20

● Molecule 1: At3g55470



5 Refinement protocol and experimental data overview

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

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
CYANA	refinement	
CYANA	structure calculation	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1658
Number of shifts mapped to atoms	1658
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

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

6 Model quality

6.1 Standard geometry

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	947	969	971	29±5
All	All	18940	19380	19420	587

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LEU:HD22	1:A:110:LEU:HD13	0.96	1.37	18	5
1:A:117:ILE:HG23	1:A:118:VAL:HG23	0.86	1.46	20	2
1:A:10:LEU:HD21	1:A:57:LEU:HD21	0.82	1.51	7	6
1:A:91:ALA:HB3	1:A:125:VAL:HG12	0.81	1.52	4	9
1:A:6:LEU:HD11	1:A:61:ALA:HB2	0.77	1.55	18	10
1:A:76:VAL:HG11	1:A:122:LEU:HD21	0.77	1.55	7	1
1:A:29:VAL:HG13	1:A:31:ILE:HD13	0.76	1.57	11	19
1:A:31:ILE:HD11	1:A:52:THR:HG21	0.76	1.57	11	1
1:A:129:LEU:C	1:A:129:LEU:HD22	0.72	2.04	18	1
1:A:73:ILE:HG22	1:A:76:VAL:HG12	0.70	1.61	20	1
1:A:11:ILE:HD12	1:A:129:LEU:HB2	0.70	1.63	15	11
1:A:29:VAL:CG1	1:A:31:ILE:HD13	0.69	2.17	11	19
1:A:129:LEU:H	1:A:129:LEU:HD13	0.68	1.49	8	9
1:A:6:LEU:HD13	1:A:59:TRP:CE2	0.68	2.24	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:LEU:HD13	1:A:130:ILE:N	0.67	2.04	4	4
1:A:6:LEU:HD12	1:A:59:TRP:O	0.67	1.90	20	1
1:A:129:LEU:HD13	1:A:129:LEU:H	0.66	1.48	15	6
1:A:30:GLU:O	1:A:31:ILE:HD12	0.65	1.92	18	19
1:A:6:LEU:HD21	1:A:61:ALA:CB	0.64	2.22	4	4
1:A:6:LEU:CD1	1:A:61:ALA:HB2	0.64	2.23	10	7
1:A:88:ILE:HD12	1:A:115:TYR:O	0.63	1.94	18	1
1:A:7:GLU:O	1:A:132:VAL:HG13	0.63	1.94	17	5
1:A:96:LYS:HE2	1:A:99:LEU:HD21	0.63	1.67	8	1
1:A:93:VAL:O	1:A:95:VAL:HG13	0.63	1.94	16	5
1:A:8:VAL:HA	1:A:132:VAL:HG12	0.62	1.71	1	8
1:A:73:ILE:HD13	1:A:94:HIS:O	0.62	1.94	1	1
1:A:6:LEU:HD11	1:A:61:ALA:CB	0.62	2.24	14	3
1:A:127:GLU:O	1:A:128:LEU:HD22	0.62	1.95	13	2
1:A:71:LYS:O	1:A:72:LEU:HD22	0.62	1.95	19	2
1:A:93:VAL:O	1:A:95:VAL:HG22	0.62	1.95	12	12
1:A:99:LEU:HD12	1:A:100:GLU:N	0.62	2.10	9	13
1:A:3:VAL:HG13	1:A:62:GLU:HG3	0.61	1.71	16	4
1:A:11:ILE:HD12	1:A:129:LEU:CB	0.61	2.26	16	6
1:A:56:LYS:O	1:A:57:LEU:HD23	0.61	1.96	13	4
1:A:129:LEU:N	1:A:129:LEU:HD13	0.61	2.11	19	8
1:A:10:LEU:HD13	1:A:55:ASP:O	0.61	1.96	18	4
1:A:2:ALA:HA	1:A:136:LEU:HD11	0.61	1.71	9	2
1:A:8:VAL:HG13	1:A:132:VAL:CG2	0.60	2.25	4	3
1:A:91:ALA:O	1:A:92:THR:C	0.60	2.39	15	1
1:A:96:LYS:CE	1:A:99:LEU:HD21	0.60	2.26	8	1
1:A:3:VAL:HG22	1:A:62:GLU:CG	0.60	2.26	16	2
1:A:31:ILE:CD1	1:A:52:THR:HG21	0.60	2.26	11	1
1:A:10:LEU:HD21	1:A:57:LEU:HD11	0.60	1.71	11	4
1:A:40:SER:HB3	1:A:57:LEU:HD21	0.59	1.74	15	1
1:A:129:LEU:O	1:A:129:LEU:HD22	0.58	1.98	18	4
1:A:121:ASP:O	1:A:122:LEU:HD22	0.58	1.98	1	1
1:A:6:LEU:HD22	1:A:134:TYR:CD2	0.58	2.34	13	3
1:A:88:ILE:HD11	1:A:114:LYS:NZ	0.58	2.14	1	1
1:A:129:LEU:HD13	1:A:129:LEU:N	0.58	2.14	6	7
1:A:93:VAL:HB	1:A:122:LEU:HD22	0.58	1.76	15	1
1:A:7:GLU:O	1:A:132:VAL:HG23	0.58	1.99	6	5
1:A:6:LEU:HD22	1:A:134:TYR:CD1	0.57	2.34	11	1
1:A:70:TYR:CE2	1:A:122:LEU:HD11	0.57	2.34	10	1
1:A:63:PHE:O	1:A:99:LEU:HD11	0.57	1.99	14	1
1:A:10:LEU:HD21	1:A:57:LEU:CD2	0.57	2.29	12	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:LEU:O	1:A:110:LEU:HD12	0.57	2.00	14	5
1:A:8:VAL:HG13	1:A:132:VAL:CG1	0.57	2.29	1	5
1:A:5:ILE:HD13	1:A:60:ARG:HA	0.56	1.76	13	5
1:A:30:GLU:C	1:A:31:ILE:HD12	0.56	2.21	17	19
1:A:100:GLU:O	1:A:103:VAL:HG12	0.56	2.01	10	6
1:A:96:LYS:HD3	1:A:99:LEU:HD21	0.56	1.78	17	2
1:A:110:LEU:HD12	1:A:110:LEU:O	0.55	2.02	16	5
1:A:102:GLY:CA	1:A:108:ALA:HB2	0.55	2.32	20	12
1:A:6:LEU:HD13	1:A:59:TRP:CD2	0.55	2.36	20	1
1:A:90:GLU:N	1:A:117:ILE:HD12	0.54	2.17	19	10
1:A:76:VAL:HG11	1:A:122:LEU:CD2	0.54	2.28	7	1
1:A:29:VAL:CG2	1:A:31:ILE:HD13	0.54	2.32	17	1
1:A:74:VAL:HG23	1:A:75:LYS:HD2	0.54	1.77	2	1
1:A:87:PHE:HB2	1:A:130:ILE:HD13	0.54	1.79	8	1
1:A:88:ILE:O	1:A:130:ILE:HD11	0.54	2.01	7	1
1:A:71:LYS:C	1:A:72:LEU:HD12	0.54	2.23	6	2
1:A:1:MET:O	1:A:103:VAL:HG11	0.54	2.03	3	13
1:A:127:GLU:O	1:A:128:LEU:HD12	0.54	2.03	11	7
1:A:73:ILE:HG23	1:A:116:ASN:OD1	0.53	2.02	20	1
1:A:136:LEU:O	1:A:137:LEU:HD12	0.53	2.03	19	2
1:A:6:LEU:HD21	1:A:61:ALA:HB3	0.53	1.80	4	1
1:A:8:VAL:HG13	1:A:132:VAL:HG21	0.53	1.79	14	3
1:A:10:LEU:CD2	1:A:57:LEU:HD11	0.52	2.34	11	1
1:A:116:ASN:ND2	1:A:122:LEU:HD22	0.52	2.20	11	1
1:A:90:GLU:O	1:A:128:LEU:HD22	0.51	2.06	6	5
1:A:116:ASN:OD1	1:A:122:LEU:HD13	0.51	2.06	5	1
1:A:3:VAL:HG13	1:A:62:GLU:CG	0.51	2.36	14	3
1:A:72:LEU:HD23	1:A:74:VAL:CG2	0.51	2.36	2	1
1:A:98:LEU:HD22	1:A:110:LEU:HB3	0.51	1.82	19	2
1:A:102:GLY:HA2	1:A:108:ALA:HB2	0.50	1.83	13	13
1:A:73:ILE:O	1:A:76:VAL:HG12	0.50	2.06	20	1
1:A:72:LEU:HD12	1:A:74:VAL:HG22	0.50	1.82	5	1
1:A:10:LEU:HD11	1:A:57:LEU:HD21	0.50	1.83	11	1
1:A:76:VAL:HG11	1:A:122:LEU:HD11	0.49	1.84	7	1
1:A:12:SER:H	1:A:129:LEU:HD12	0.49	1.68	6	7
1:A:68:ALA:HB1	1:A:96:LYS:HE3	0.49	1.84	3	1
1:A:76:VAL:CG1	1:A:122:LEU:HD11	0.49	2.36	7	1
1:A:129:LEU:HD22	1:A:129:LEU:O	0.49	2.08	13	12
1:A:2:ALA:HB3	1:A:99:LEU:O	0.48	2.08	2	7
1:A:16:LEU:HD22	1:A:126:GLY:HA3	0.48	1.85	20	2
1:A:10:LEU:HD21	1:A:57:LEU:CD1	0.48	2.38	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:VAL:O	1:A:3:VAL:HG13	0.48	2.09	11	6
1:A:11:ILE:HD12	1:A:129:LEU:HG	0.48	1.86	4	1
1:A:93:VAL:HG23	1:A:122:LEU:HD13	0.48	1.85	15	1
1:A:73:ILE:O	1:A:76:VAL:HG13	0.48	2.08	17	1
1:A:2:ALA:HB2	1:A:103:VAL:CG1	0.48	2.39	16	2
1:A:73:ILE:O	1:A:76:VAL:HG23	0.48	2.09	7	2
1:A:13:GLY:C	1:A:42:VAL:HG23	0.48	2.29	11	1
1:A:129:LEU:CD2	1:A:129:LEU:C	0.48	2.77	18	1
1:A:1:MET:H3	1:A:100:GLU:HA	0.48	1.69	2	3
1:A:6:LEU:HD23	1:A:134:TYR:CD2	0.48	2.44	9	1
1:A:56:LYS:C	1:A:57:LEU:HD23	0.47	2.30	11	2
1:A:78:ASP:CG	1:A:118:VAL:HG21	0.47	2.29	12	1
1:A:116:ASN:O	1:A:125:VAL:HG11	0.47	2.09	17	1
1:A:91:ALA:HA	1:A:128:LEU:HD22	0.47	1.86	19	1
1:A:3:VAL:HG22	1:A:62:GLU:HG2	0.47	1.86	16	1
1:A:73:ILE:HG21	1:A:94:HIS:O	0.47	2.10	1	1
1:A:30:GLU:CG	1:A:30:GLU:O	0.47	2.62	8	1
1:A:135:SER:O	1:A:137:LEU:HD23	0.47	2.10	13	2
1:A:6:LEU:HD22	1:A:134:TYR:CE2	0.46	2.45	16	1
1:A:3:VAL:HG23	1:A:62:GLU:HG3	0.46	1.87	2	2
1:A:88:ILE:HD12	1:A:114:LYS:HB2	0.46	1.88	4	1
1:A:16:LEU:HD11	1:A:126:GLY:HA2	0.46	1.84	8	1
1:A:93:VAL:HG23	1:A:123:SER:OG	0.46	2.10	6	1
1:A:3:VAL:HG23	1:A:62:GLU:CG	0.46	2.41	11	1
1:A:98:LEU:HD22	1:A:110:LEU:HD21	0.46	1.87	20	1
1:A:3:VAL:HG13	1:A:3:VAL:O	0.46	2.11	5	8
1:A:10:LEU:HD21	1:A:57:LEU:CG	0.46	2.40	20	4
1:A:90:GLU:C	1:A:117:ILE:HD12	0.46	2.31	6	7
1:A:93:VAL:HG12	1:A:94:HIS:N	0.46	2.26	12	5
1:A:59:TRP:N	1:A:59:TRP:CD1	0.46	2.83	20	1
1:A:10:LEU:HD11	1:A:40:SER:CB	0.45	2.41	11	1
1:A:129:LEU:HD13	1:A:129:LEU:C	0.45	2.32	3	1
1:A:71:LYS:O	1:A:72:LEU:HD12	0.45	2.12	6	1
1:A:73:ILE:HD11	1:A:97:GLU:OE2	0.45	2.11	17	1
1:A:93:VAL:CG1	1:A:122:LEU:HD12	0.45	2.41	1	1
1:A:6:LEU:HD22	1:A:134:TYR:HD2	0.45	1.72	19	2
1:A:3:VAL:HG22	1:A:62:GLU:CB	0.44	2.42	14	1
1:A:72:LEU:O	1:A:74:VAL:HG23	0.44	2.12	19	1
1:A:93:VAL:HG22	1:A:94:HIS:N	0.44	2.27	8	7
1:A:2:ALA:HB2	1:A:103:VAL:HG12	0.44	1.89	14	1
1:A:8:VAL:HG13	1:A:132:VAL:HG11	0.44	1.90	7	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:VAL:O	1:A:94:HIS:C	0.44	2.56	20	4
1:A:13:GLY:O	1:A:43:ALA:HB1	0.44	2.12	20	2
1:A:10:LEU:HD11	1:A:40:SER:OG	0.44	2.13	11	1
1:A:129:LEU:CD1	1:A:129:LEU:N	0.44	2.81	19	2
1:A:93:VAL:CG2	1:A:94:HIS:N	0.44	2.81	15	1
1:A:6:LEU:HD11	1:A:61:ALA:HB3	0.43	1.90	14	1
1:A:31:ILE:HG22	1:A:31:ILE:O	0.43	2.13	3	2
1:A:73:ILE:HD12	1:A:116:ASN:OD1	0.43	2.13	20	1
1:A:87:PHE:CD1	1:A:130:ILE:HD13	0.43	2.49	7	1
1:A:98:LEU:HD22	1:A:110:LEU:CD2	0.43	2.44	20	1
1:A:93:VAL:CG1	1:A:94:HIS:N	0.43	2.82	12	5
1:A:78:ASP:HB2	1:A:88:ILE:HD13	0.43	1.89	18	1
1:A:93:VAL:HG22	1:A:123:SER:OG	0.43	2.14	1	1
1:A:64:PRO:HG3	1:A:99:LEU:HD11	0.42	1.89	1	1
1:A:129:LEU:O	1:A:129:LEU:CD2	0.42	2.67	2	6
1:A:6:LEU:CD1	1:A:61:ALA:HB3	0.42	2.44	2	1
1:A:2:ALA:HB2	1:A:103:VAL:HB	0.42	1.90	11	1
1:A:72:LEU:HD12	1:A:74:VAL:CG2	0.42	2.43	5	1
1:A:129:LEU:CD2	1:A:129:LEU:O	0.42	2.67	15	9
1:A:91:ALA:HB2	1:A:117:ILE:HG13	0.42	1.90	7	3
1:A:11:ILE:HD12	1:A:129:LEU:CG	0.42	2.43	4	1
1:A:10:LEU:CG	1:A:57:LEU:HD21	0.42	2.44	11	1
1:A:129:LEU:CD2	1:A:132:VAL:HG13	0.42	2.44	10	1
1:A:31:ILE:O	1:A:31:ILE:HG22	0.42	2.15	18	4
1:A:29:VAL:HG22	1:A:30:GLU:N	0.42	2.30	14	1
1:A:5:ILE:HD13	1:A:60:ARG:CA	0.42	2.44	14	1
1:A:117:ILE:HG23	1:A:117:ILE:O	0.41	2.15	12	1
1:A:102:GLY:N	1:A:108:ALA:HB2	0.41	2.30	20	1
1:A:91:ALA:O	1:A:93:VAL:N	0.41	2.54	20	3
1:A:8:VAL:HA	1:A:132:VAL:HG22	0.41	1.91	17	1
1:A:87:PHE:CD1	1:A:130:ILE:HG21	0.41	2.50	14	1
1:A:59:TRP:CD1	1:A:59:TRP:N	0.41	2.87	14	1
1:A:42:VAL:HG13	1:A:43:ALA:N	0.41	2.29	19	1
1:A:118:VAL:HG12	1:A:119:ASP:OD2	0.41	2.16	3	1
1:A:6:LEU:HD22	1:A:134:TYR:HD1	0.41	1.73	11	1
1:A:118:VAL:HG12	1:A:118:VAL:O	0.41	2.14	20	1
1:A:129:LEU:N	1:A:129:LEU:CD1	0.41	2.82	11	2
1:A:3:VAL:O	1:A:136:LEU:HD13	0.41	2.16	14	1
1:A:121:ASP:H	1:A:122:LEU:HD22	0.41	1.76	12	1
1:A:16:LEU:HD23	1:A:16:LEU:H	0.41	1.76	17	1
1:A:42:VAL:HG13	1:A:43:ALA:O	0.40	2.17	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ILE:O	1:A:73:ILE:HG22	0.40	2.17	20	2
1:A:92:THR:HG21	1:A:124:PHE:CE1	0.40	2.51	15	1
1:A:132:VAL:O	1:A:132:VAL:HG23	0.40	2.16	8	1
1:A:61:ALA:HB3	1:A:134:TYR:HE2	0.40	1.76	16	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	121/162 (75%)	87±3 (72±3%)	22±3 (19±2%)	11±3 (9±2%)	1	11
All	All	2420/3240 (75%)	1747 (72%)	448 (19%)	225 (9%)	1	11

All 37 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	132	VAL	16
1	A	125	VAL	14
1	A	46	ASP	13
1	A	35	GLY	13
1	A	92	THR	12
1	A	115	TYR	12
1	A	73	ILE	10
1	A	76	VAL	9
1	A	95	VAL	9
1	A	94	HIS	9
1	A	71	LYS	7
1	A	120	SER	7
1	A	138	GLN	7
1	A	70	TYR	7
1	A	126	GLY	6
1	A	45	GLU	6
1	A	42	VAL	6
1	A	34	LYS	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	124	PHE	5
1	A	121	ASP	5
1	A	41	SER	5
1	A	72	LEU	4
1	A	118	VAL	4
1	A	123	SER	4
1	A	119	ASP	4
1	A	69	ASP	3
1	A	117	ILE	3
1	A	68	ALA	3
1	A	67	GLY	3
1	A	78	ASP	2
1	A	137	LEU	2
1	A	65	GLY	2
1	A	122	LEU	2
1	A	44	LYS	2
1	A	77	MET	2
1	A	66	SER	1
1	A	86	ASP	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	103/138 (75%)	74±3 (72±3%)	29±3 (28±3%)	2	19
All	All	2060/2760 (75%)	1486 (72%)	574 (28%)	2	19

All 72 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	37	THR	20
1	A	17	LYS	20
1	A	114	LYS	19
1	A	137	LEU	18
1	A	105	LYS	17
1	A	128	LEU	17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	129	LEU	16
1	A	133	SER	16
1	A	16	LEU	16
1	A	97	GLU	15
1	A	44	LYS	15
1	A	69	ASP	14
1	A	56	LYS	13
1	A	55	ASP	12
1	A	122	LEU	12
1	A	53	TRP	12
1	A	70	TYR	11
1	A	75	LYS	11
1	A	127	GLU	11
1	A	71	LYS	10
1	A	66	SER	10
1	A	49	ARG	10
1	A	115	TYR	10
1	A	86	ASP	10
1	A	113	THR	9
1	A	38	ARG	9
1	A	111	ARG	9
1	A	58	LYS	9
1	A	123	SER	9
1	A	1	MET	9
1	A	34	LYS	8
1	A	33	TYR	8
1	A	41	SER	8
1	A	120	SER	8
1	A	77	MET	8
1	A	121	ASP	8
1	A	28	TYR	8
1	A	101	MET	8
1	A	6	LEU	7
1	A	99	LEU	7
1	A	110	LEU	7
1	A	136	LEU	6
1	A	124	PHE	6
1	A	78	ASP	5
1	A	45	GLU	5
1	A	135	SER	5
1	A	119	ASP	5
1	A	10	LEU	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	50	ASN	4
1	A	72	LEU	4
1	A	100	GLU	4
1	A	46	ASP	4
1	A	138	GLN	4
1	A	36	GLN	4
1	A	60	ARG	4
1	A	14	LYS	4
1	A	130	ILE	3
1	A	96	LYS	3
1	A	54	ASN	3
1	A	40	SER	3
1	A	7	GLU	3
1	A	116	ASN	3
1	A	87	PHE	2
1	A	9	SER	2
1	A	12	SER	2
1	A	42	VAL	2
1	A	63	PHE	1
1	A	29	VAL	1
1	A	90	GLU	1
1	A	117	ILE	1
1	A	88	ILE	1
1	A	59	TRP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *final.str*

7.1.1 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	1658
Number of shifts mapped to atoms	1658
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	152	0.18 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	137	0.56 ± 0.14	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	155	-0.21 ± 0.22	None needed (< 0.5 ppm)

7.1.3 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 77%, i.e. 1141 atoms were assigned a chemical shift out of a possible 1481. 25 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	468/602 (78%)	236/240 (98%)	116/244 (48%)	116/118 (98%)
Sidechain	655/781 (84%)	404/455 (89%)	251/296 (85%)	0/30 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	18/98 (18%)	15/51 (29%)	3/44 (7%)	0/3 (0%)
Overall	1141/1481 (77%)	655/746 (88%)	370/584 (63%)	116/151 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1465 atoms were assigned a chemical shift out of a possible 1974. 27 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	620/802 (77%)	313/320 (98%)	152/324 (47%)	155/158 (98%)
Sidechain	804/979 (82%)	503/573 (88%)	301/366 (82%)	0/40 (0%)
Aromatic	41/193 (21%)	36/104 (35%)	5/77 (6%)	0/12 (0%)
Overall	1465/1974 (74%)	852/997 (85%)	458/767 (60%)	155/210 (74%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:

