



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 21, 2024 – 08:29 AM EDT

PDB ID : 2M7A  
BMRB ID : 19178  
Title : Enteropathogenic Escherichia coli 0111:H- str. 11128 ORF EC0111\_1119 similar to bacteriophage lambda ea8.5  
Authors : Donaldson, L.W.F.  
Deposited on : 2013-04-18

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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

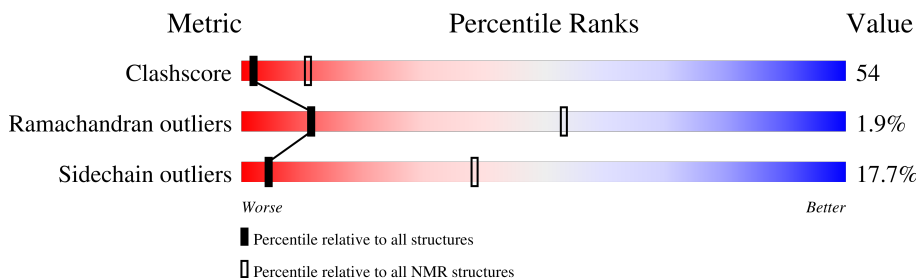
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

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	101	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:16-A:59, A:70-A:89 (64)	0.77	1

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 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1308 atoms, of which 634 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1307	411	634	112	143	7	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP C8UME7
A	0	SER	-	expression tag	UNP C8UME7

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

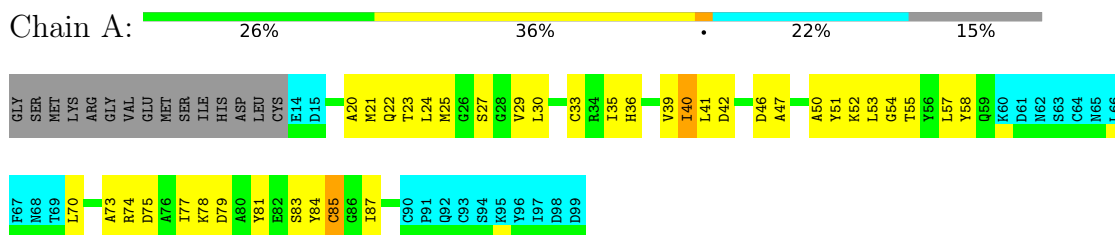
Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Uncharacterized protein

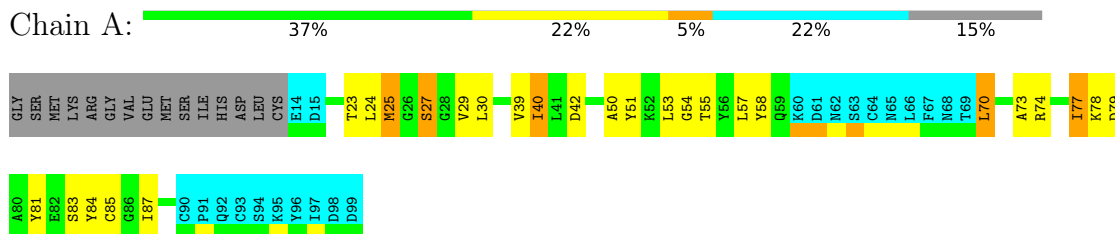


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

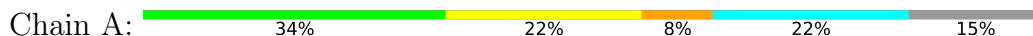
#### 4.2.1 Score per residue for model 1 (medoid)

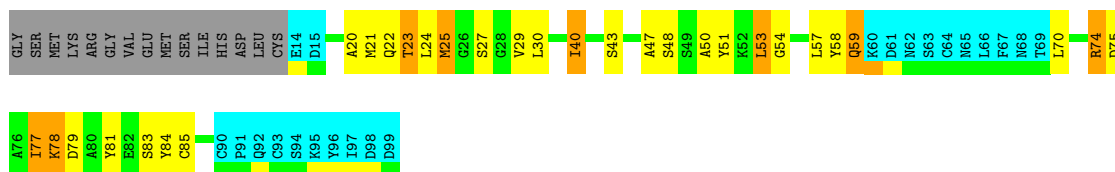
- Molecule 1: Uncharacterized protein



#### 4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein

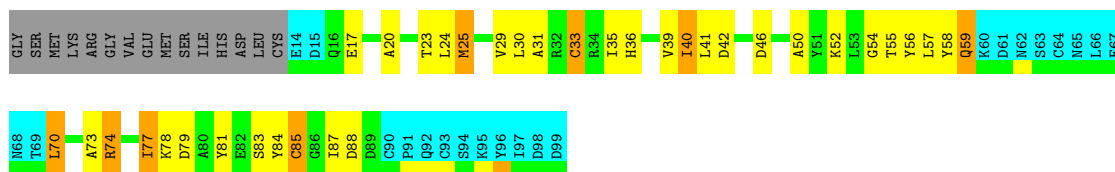




### 4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein

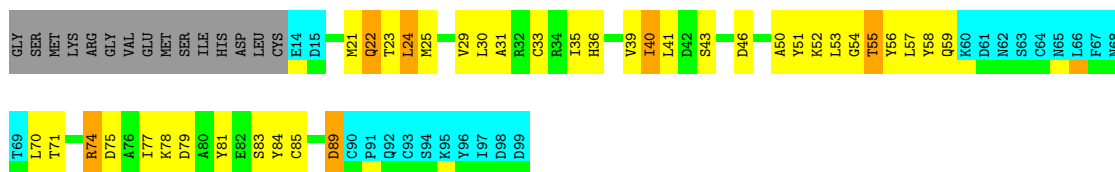
Chain A: 28% 28% 8% 22% 15%



### 4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein

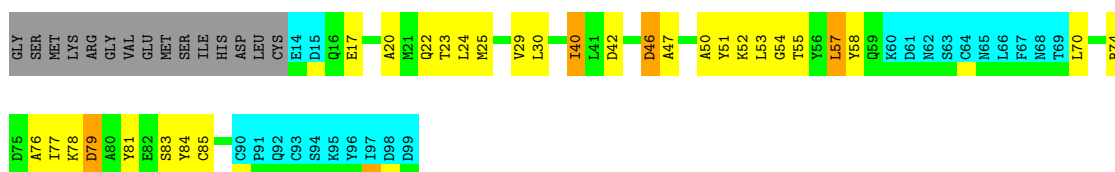
Chain A: 26% 32% 6% 22% 15%



### 4.2.5 Score per residue for model 5

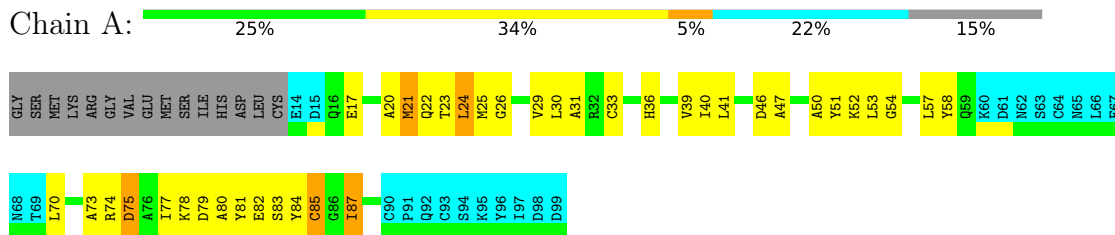
- Molecule 1: Uncharacterized protein

Chain A: 34% 26% 0% 22% 15%

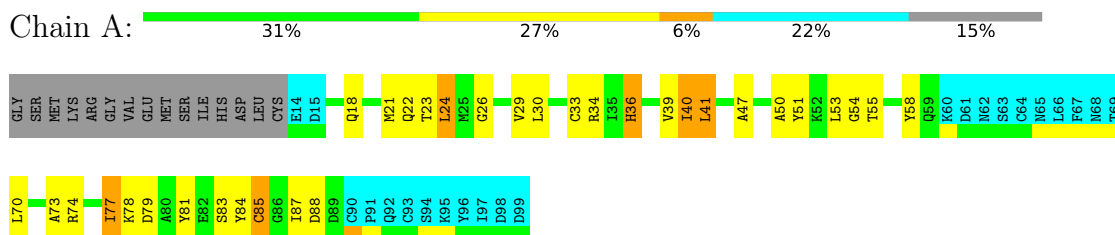


### 4.2.6 Score per residue for model 6

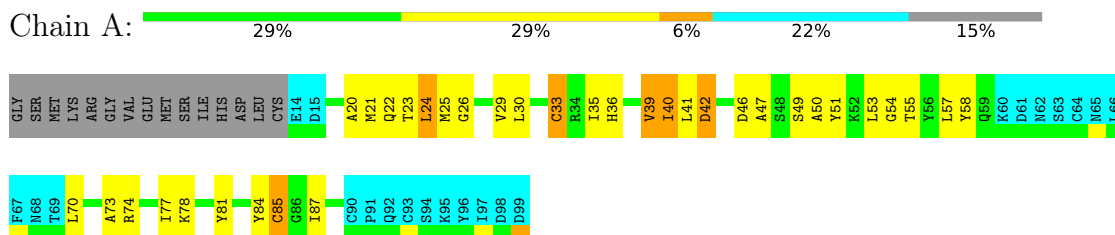
- Molecule 1: Uncharacterized protein



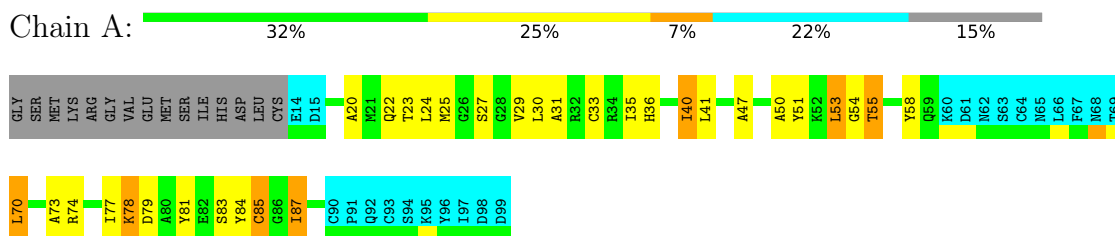
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein

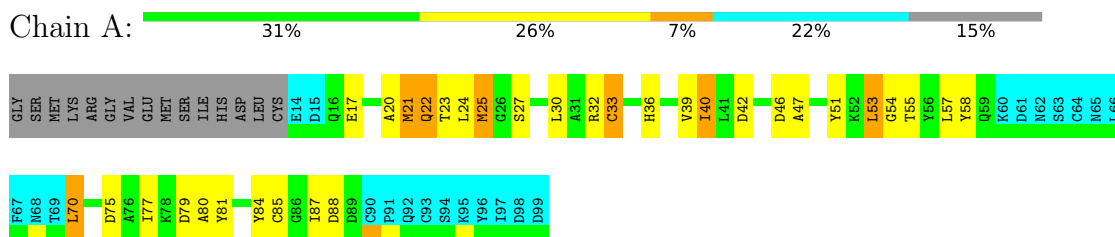


- Molecule 1: Uncharacterized protein



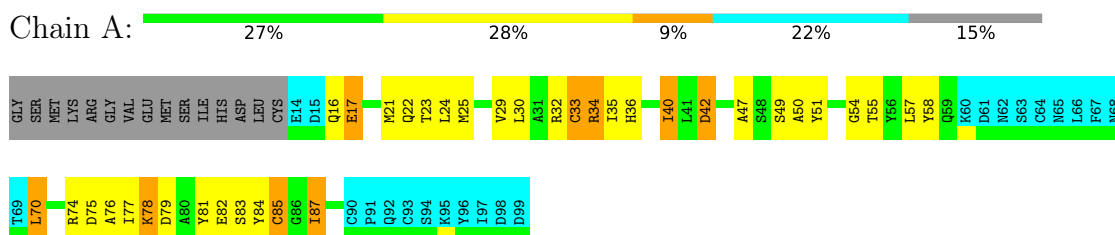
## 4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



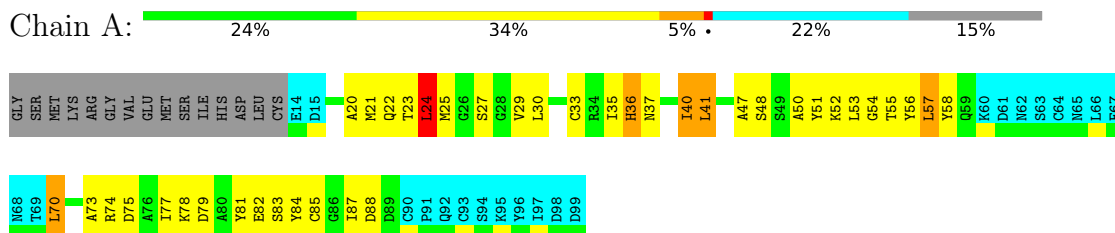
## 4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein



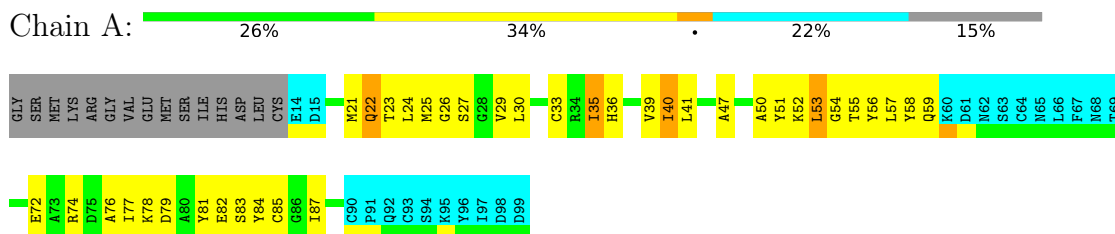
## 4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein



## 4.2.13 Score per residue for model 13

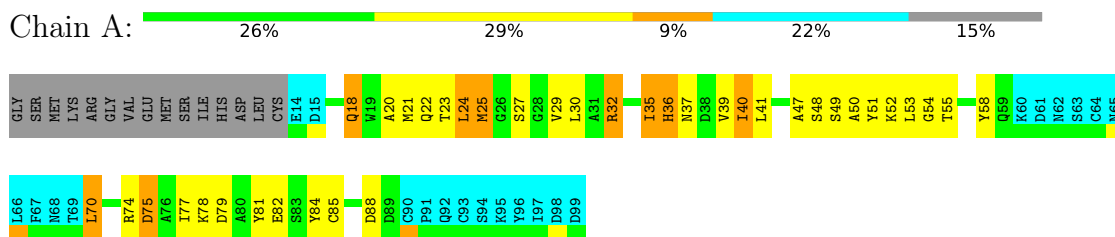
- Molecule 1: Uncharacterized protein





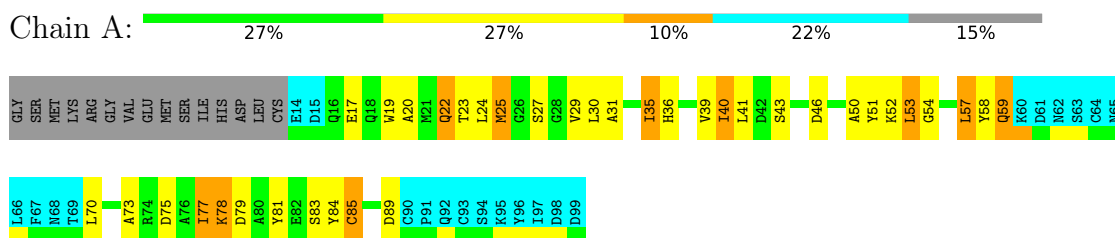
## 4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein



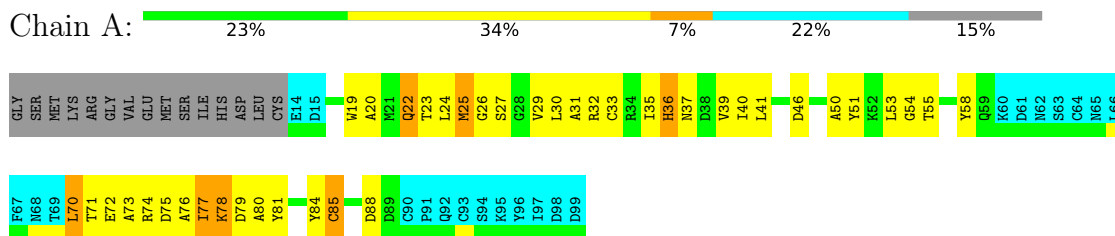
## 4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein



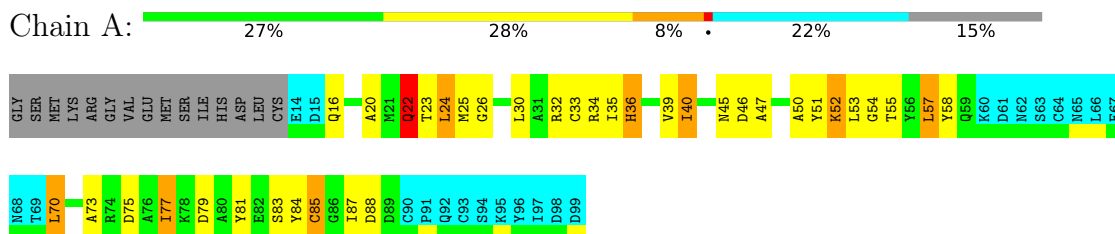
## 4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein



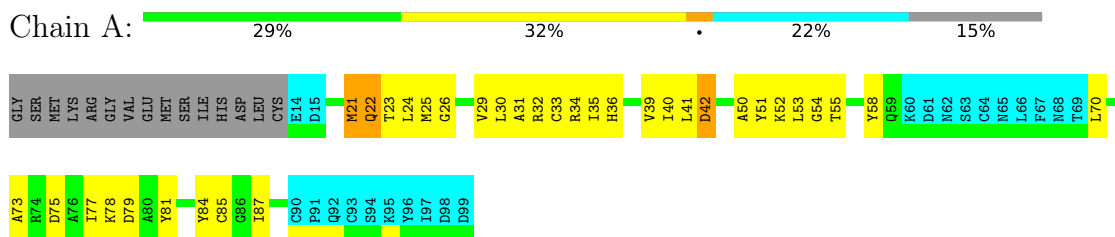
## 4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein



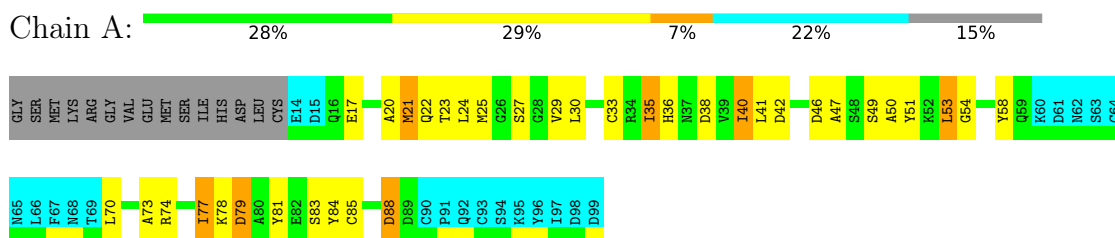
## 4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein



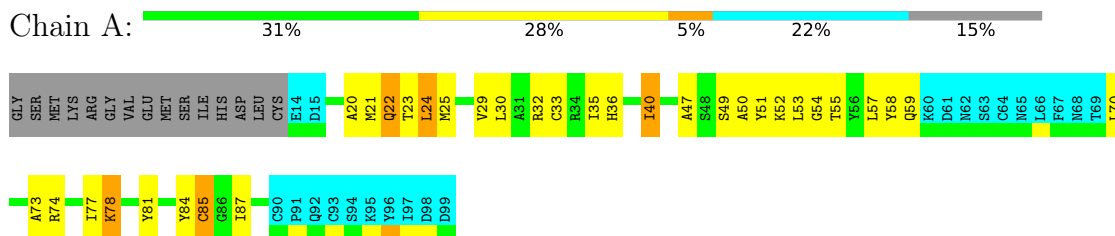
## 4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein



## 4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein



## 5 Refinement protocol and experimental data overview

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

Of the 500 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	structure solution	3
CYANA	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	870
Number of shifts mapped to atoms	825
Number of unparsed shifts	0
Number of shifts with mapping errors	45
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts 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	498	478	468	52±6
All	All	9980	9560	9360	1044

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 54.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG21	1:A:50:ALA:HB2	1.11	1.18	9	13
1:A:30:LEU:HD11	1:A:81:TYR:CE1	1.00	1.92	1	18
1:A:51:TYR:CD1	1:A:77:ILE:HD11	1.00	1.92	4	4
1:A:24:LEU:HD21	1:A:77:ILE:HG23	0.95	1.33	14	2
1:A:30:LEU:HD21	1:A:81:TYR:CZ	0.94	1.98	6	6
1:A:40:ILE:HD12	1:A:84:TYR:CE2	0.93	1.98	16	1
1:A:20:ALA:HB1	1:A:57:LEU:HD11	0.92	1.41	17	1
1:A:23:THR:HG22	1:A:53:LEU:HD11	0.91	1.42	19	4
1:A:51:TYR:O	1:A:55:THR:HG23	0.90	1.66	12	7
1:A:58:TYR:CD2	1:A:73:ALA:HB1	0.89	2.03	15	11
1:A:35:ILE:HG23	1:A:36:HIS:CE1	0.89	2.03	19	6
1:A:29:VAL:HG11	1:A:50:ALA:HB2	0.89	1.44	13	7

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:HD21	1:A:77:ILE:CG2	0.88	1.97	14	5
1:A:40:ILE:HG23	1:A:84:TYR:CD2	0.87	2.04	17	10
1:A:55:THR:HG23	1:A:70:LEU:HD21	0.87	1.46	11	1
1:A:55:THR:CG2	1:A:70:LEU:HD13	0.86	1.99	9	1
1:A:29:VAL:HG21	1:A:50:ALA:CB	0.86	1.99	4	11
1:A:55:THR:OG1	1:A:70:LEU:HD13	0.86	1.69	3	2
1:A:20:ALA:HB1	1:A:57:LEU:HD22	0.85	1.48	6	1
1:A:24:LEU:HD12	1:A:54:GLY:HA3	0.84	1.50	8	14
1:A:29:VAL:HG11	1:A:50:ALA:CB	0.84	2.02	20	6
1:A:57:LEU:O	1:A:57:LEU:HD22	0.83	1.72	17	4
1:A:70:LEU:HD12	1:A:70:LEU:O	0.83	1.74	3	9
1:A:24:LEU:CD2	1:A:77:ILE:HG23	0.83	2.03	14	1
1:A:23:THR:CG2	1:A:57:LEU:HD22	0.82	2.02	3	2
1:A:27:SER:HB2	1:A:53:LEU:HD13	0.82	1.51	9	4
1:A:27:SER:CB	1:A:53:LEU:HD13	0.82	2.04	12	4
1:A:24:LEU:HD23	1:A:25:MET:N	0.81	1.90	8	10
1:A:29:VAL:CG2	1:A:50:ALA:HB2	0.81	2.06	5	12
1:A:47:ALA:HB1	1:A:51:TYR:CZ	0.81	2.09	10	11
1:A:35:ILE:HG23	1:A:36:HIS:CD2	0.80	2.11	3	1
1:A:24:LEU:O	1:A:53:LEU:HD21	0.79	1.77	13	1
1:A:40:ILE:HG23	1:A:84:TYR:CD1	0.78	2.13	1	7
1:A:51:TYR:CE1	1:A:77:ILE:HD11	0.78	2.12	4	2
1:A:29:VAL:CG1	1:A:50:ALA:HB2	0.78	2.09	20	6
1:A:24:LEU:HA	1:A:53:LEU:HD12	0.78	1.56	20	6
1:A:50:ALA:O	1:A:53:LEU:HD23	0.77	1.78	13	1
1:A:77:ILE:HD13	1:A:77:ILE:N	0.76	1.94	17	2
1:A:30:LEU:HD13	1:A:40:ILE:HG21	0.76	1.56	16	1
1:A:24:LEU:HD12	1:A:54:GLY:CA	0.76	2.10	17	17
1:A:55:THR:OG1	1:A:70:LEU:HD21	0.76	1.80	1	2
1:A:51:TYR:CD1	1:A:77:ILE:HD12	0.75	2.16	6	2
1:A:57:LEU:HD23	1:A:57:LEU:O	0.74	1.82	8	2
1:A:33:CYS:SG	1:A:35:ILE:HG22	0.74	2.22	4	5
1:A:30:LEU:HD22	1:A:40:ILE:HG22	0.74	1.58	16	1
1:A:53:LEU:C	1:A:53:LEU:HD12	0.73	2.03	10	1
1:A:40:ILE:HG23	1:A:84:TYR:CE2	0.73	2.18	6	9
1:A:50:ALA:HA	1:A:53:LEU:HD12	0.73	1.60	12	2
1:A:30:LEU:HD22	1:A:40:ILE:CG2	0.73	2.13	16	1
1:A:24:LEU:HD11	1:A:77:ILE:HG21	0.73	1.58	15	10
1:A:27:SER:OG	1:A:29:VAL:HG23	0.72	1.83	12	4
1:A:55:THR:CG2	1:A:70:LEU:HD21	0.72	2.13	11	1
1:A:55:THR:HB	1:A:70:LEU:HD11	0.72	1.62	17	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ILE:CG2	1:A:84:TYR:CE2	0.71	2.73	19	13
1:A:17:GLU:OE1	1:A:76:ALA:HB1	0.71	1.85	11	1
1:A:20:ALA:CB	1:A:58:TYR:CE1	0.71	2.74	3	9
1:A:29:VAL:HG21	1:A:50:ALA:N	0.70	2.00	20	9
1:A:40:ILE:C	1:A:40:ILE:HD13	0.70	2.06	9	5
1:A:20:ALA:CB	1:A:57:LEU:HD11	0.70	2.16	17	1
1:A:35:ILE:HG23	1:A:36:HIS:ND1	0.70	2.00	14	3
1:A:57:LEU:C	1:A:57:LEU:HD13	0.70	2.07	5	3
1:A:57:LEU:HD13	1:A:58:TYR:N	0.70	2.00	12	2
1:A:40:ILE:CG2	1:A:84:TYR:CE1	0.70	2.75	10	2
1:A:57:LEU:HD22	1:A:57:LEU:C	0.70	2.06	12	1
1:A:40:ILE:CG2	1:A:84:TYR:CD1	0.70	2.75	3	3
1:A:23:THR:HG22	1:A:57:LEU:HD22	0.70	1.63	3	1
1:A:77:ILE:HG22	1:A:81:TYR:CE1	0.69	2.22	18	6
1:A:33:CYS:CB	1:A:36:HIS:CE1	0.69	2.74	10	5
1:A:30:LEU:HD21	1:A:81:TYR:CE2	0.69	2.23	10	4
1:A:77:ILE:CG2	1:A:81:TYR:CE1	0.69	2.76	5	7
1:A:31:ALA:HB3	1:A:41:LEU:HB2	0.69	1.64	16	5
1:A:58:TYR:CE2	1:A:77:ILE:HD11	0.68	2.23	14	2
1:A:30:LEU:HD11	1:A:81:TYR:HE1	0.68	1.48	3	7
1:A:55:THR:HG22	1:A:70:LEU:HD11	0.68	1.65	18	2
1:A:24:LEU:N	1:A:53:LEU:HD12	0.68	2.01	6	3
1:A:30:LEU:HD13	1:A:40:ILE:CG1	0.68	2.19	9	5
1:A:24:LEU:HD21	1:A:77:ILE:HG21	0.68	1.66	7	3
1:A:23:THR:HG21	1:A:57:LEU:HD22	0.67	1.64	10	2
1:A:58:TYR:CE2	1:A:73:ALA:HB1	0.67	2.24	15	1
1:A:31:ALA:HB2	1:A:43:SER:OG	0.67	1.89	4	1
1:A:30:LEU:CD1	1:A:81:TYR:CE1	0.67	2.78	4	11
1:A:20:ALA:HB1	1:A:57:LEU:CD1	0.66	2.19	17	1
1:A:24:LEU:HD11	1:A:77:ILE:CG2	0.66	2.21	2	6
1:A:40:ILE:CG2	1:A:84:TYR:CD2	0.66	2.78	17	8
1:A:24:LEU:CD1	1:A:77:ILE:HG21	0.66	2.21	6	3
1:A:24:LEU:C	1:A:24:LEU:HD23	0.65	2.11	9	4
1:A:24:LEU:HD11	1:A:77:ILE:HG12	0.65	1.69	18	5
1:A:58:TYR:CD2	1:A:73:ALA:CB	0.65	2.80	15	8
1:A:77:ILE:O	1:A:81:TYR:CD1	0.65	2.50	2	13
1:A:30:LEU:HD22	1:A:40:ILE:HG23	0.64	1.69	18	1
1:A:70:LEU:HD13	1:A:70:LEU:O	0.64	1.92	14	4
1:A:29:VAL:CB	1:A:50:ALA:HB2	0.64	2.22	13	11
1:A:40:ILE:HG23	1:A:84:TYR:CG	0.64	2.27	5	11
1:A:24:LEU:CA	1:A:53:LEU:HD12	0.64	2.21	17	5

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:CG2	1:A:36:HIS:CE1	0.64	2.80	14	5
1:A:33:CYS:CB	1:A:36:HIS:CD2	0.64	2.81	20	5
1:A:29:VAL:HG21	1:A:50:ALA:CA	0.63	2.23	20	4
1:A:27:SER:OG	1:A:53:LEU:HD13	0.63	1.92	14	2
1:A:30:LEU:HD21	1:A:81:TYR:CE1	0.63	2.29	6	4
1:A:29:VAL:HG21	1:A:50:ALA:H	0.63	1.53	8	3
1:A:51:TYR:CD1	1:A:77:ILE:CD1	0.63	2.81	6	4
1:A:54:GLY:O	1:A:58:TYR:CD2	0.63	2.52	14	17
1:A:24:LEU:HD23	1:A:24:LEU:C	0.63	2.14	8	4
1:A:40:ILE:HD13	1:A:84:TYR:CD2	0.62	2.29	14	2
1:A:30:LEU:CD1	1:A:81:TYR:CZ	0.62	2.83	14	4
1:A:40:ILE:HD13	1:A:80:ALA:HB1	0.62	1.71	6	1
1:A:40:ILE:O	1:A:84:TYR:CD1	0.62	2.52	19	2
1:A:53:LEU:HD13	1:A:53:LEU:O	0.62	1.93	20	3
1:A:30:LEU:HD13	1:A:40:ILE:HG13	0.61	1.71	19	5
1:A:47:ALA:HB1	1:A:51:TYR:CE2	0.61	2.31	13	1
1:A:29:VAL:HG22	1:A:46:ASP:O	0.61	1.96	3	3
1:A:24:LEU:CD2	1:A:50:ALA:HB1	0.61	2.26	8	2
1:A:84:TYR:O	1:A:87:ILE:HD12	0.61	1.96	3	2
1:A:30:LEU:CD2	1:A:81:TYR:CZ	0.61	2.83	17	5
1:A:35:ILE:HD13	1:A:35:ILE:O	0.60	1.96	13	3
1:A:24:LEU:CD2	1:A:77:ILE:CG2	0.60	2.80	7	1
1:A:25:MET:HB2	1:A:30:LEU:HD12	0.60	1.72	17	5
1:A:23:THR:HB	1:A:57:LEU:HD13	0.59	1.72	1	2
1:A:17:GLU:O	1:A:20:ALA:HB3	0.59	1.97	19	2
1:A:47:ALA:O	1:A:51:TYR:CD1	0.59	2.55	9	5
1:A:52:LYS:O	1:A:56:TYR:CD1	0.59	2.55	13	1
1:A:40:ILE:O	1:A:41:LEU:HD12	0.59	1.98	18	2
1:A:55:THR:HB	1:A:70:LEU:HD21	0.58	1.73	10	1
1:A:36:HIS:ND1	1:A:39:VAL:HG21	0.58	2.13	10	1
1:A:47:ALA:O	1:A:51:TYR:CD2	0.58	2.56	13	3
1:A:80:ALA:O	1:A:84:TYR:CD2	0.58	2.57	16	1
1:A:30:LEU:HD22	1:A:41:LEU:O	0.58	1.98	14	3
1:A:57:LEU:C	1:A:57:LEU:HD23	0.58	2.18	11	2
1:A:40:ILE:HG21	1:A:84:TYR:CE2	0.58	2.34	12	6
1:A:20:ALA:CB	1:A:57:LEU:HD22	0.57	2.25	6	1
1:A:47:ALA:CB	1:A:51:TYR:CZ	0.57	2.87	14	7
1:A:58:TYR:HE2	1:A:77:ILE:HD11	0.57	1.57	14	2
1:A:24:LEU:CD1	1:A:54:GLY:CA	0.57	2.83	12	4
1:A:40:ILE:HD13	1:A:40:ILE:O	0.57	2.00	9	2
1:A:31:ALA:HB3	1:A:41:LEU:CB	0.57	2.30	18	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:VAL:CG1	1:A:41:LEU:CD1	0.56	2.83	18	2
1:A:72:GLU:O	1:A:76:ALA:HB2	0.56	2.00	13	2
1:A:40:ILE:HG23	1:A:84:TYR:CE1	0.56	2.35	1	3
1:A:73:ALA:O	1:A:77:ILE:HD13	0.56	1.99	1	2
1:A:20:ALA:CB	1:A:58:TYR:CZ	0.56	2.88	3	1
1:A:17:GLU:OE2	1:A:76:ALA:HB1	0.56	1.99	5	1
1:A:32:ARG:NE	1:A:32:ARG:H	0.56	1.98	14	1
1:A:41:LEU:HD23	1:A:88:ASP:O	0.56	2.01	3	1
1:A:24:LEU:CD2	1:A:25:MET:N	0.56	2.69	18	3
1:A:23:THR:HB	1:A:57:LEU:HD12	0.55	1.78	8	1
1:A:29:VAL:HG11	1:A:81:TYR:OH	0.55	2.00	18	3
1:A:47:ALA:O	1:A:51:TYR:CG	0.55	2.59	6	5
1:A:30:LEU:HD11	1:A:81:TYR:CD1	0.55	2.37	5	2
1:A:77:ILE:N	1:A:77:ILE:CD1	0.55	2.64	17	2
1:A:47:ALA:HB1	1:A:51:TYR:OH	0.55	2.01	7	3
1:A:23:THR:OG1	1:A:53:LEU:HD11	0.55	2.01	17	1
1:A:55:THR:OG1	1:A:70:LEU:HD11	0.55	2.02	11	1
1:A:33:CYS:HB2	1:A:36:HIS:CD2	0.54	2.37	20	2
1:A:74:ARG:O	1:A:78:LYS:CB	0.54	2.56	1	12
1:A:47:ALA:HB1	1:A:51:TYR:CE1	0.54	2.37	9	9
1:A:24:LEU:HA	1:A:53:LEU:HD11	0.54	1.79	10	1
1:A:21:MET:HE1	1:A:25:MET:SD	0.54	2.42	14	2
1:A:35:ILE:HG23	1:A:36:HIS:NE2	0.53	2.18	3	1
1:A:39:VAL:HG12	1:A:41:LEU:HD13	0.53	1.80	18	1
1:A:50:ALA:HB1	1:A:81:TYR:OH	0.53	2.04	13	1
1:A:77:ILE:HG23	1:A:81:TYR:CE1	0.53	2.39	13	5
1:A:30:LEU:HD13	1:A:40:ILE:CD1	0.53	2.34	3	2
1:A:21:MET:CE	1:A:40:ILE:HD11	0.53	2.34	18	1
1:A:40:ILE:C	1:A:41:LEU:HD12	0.53	2.24	18	1
1:A:73:ALA:O	1:A:77:ILE:CD1	0.53	2.57	7	2
1:A:81:TYR:O	1:A:85:CYS:CB	0.52	2.58	17	7
1:A:24:LEU:HD21	1:A:50:ALA:HB1	0.52	1.81	8	2
1:A:40:ILE:HG21	1:A:84:TYR:CD2	0.52	2.40	4	2
1:A:70:LEU:HD12	1:A:74:ARG:NH2	0.52	2.20	12	1
1:A:27:SER:HB3	1:A:53:LEU:HD22	0.52	1.81	14	1
1:A:24:LEU:HD11	1:A:77:ILE:CG1	0.52	2.35	18	3
1:A:33:CYS:HB2	1:A:36:HIS:CE1	0.52	2.38	10	1
1:A:51:TYR:CE1	1:A:77:ILE:HG13	0.51	2.39	1	4
1:A:33:CYS:HB3	1:A:36:HIS:CD2	0.51	2.41	9	6
1:A:27:SER:OG	1:A:53:LEU:CD1	0.51	2.58	14	2
1:A:70:LEU:HD11	1:A:74:ARG:NH2	0.51	2.20	2	1

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ILE:CG2	1:A:84:TYR:CZ	0.51	2.93	10	4
1:A:50:ALA:CB	1:A:81:TYR:OH	0.51	2.59	12	4
1:A:23:THR:O	1:A:24:LEU:C	0.51	2.49	18	18
1:A:30:LEU:HD11	1:A:81:TYR:CZ	0.51	2.39	1	4
1:A:41:LEU:HD23	1:A:87:ILE:HG22	0.51	1.83	13	1
1:A:77:ILE:O	1:A:81:TYR:CG	0.51	2.64	4	3
1:A:29:VAL:CG1	1:A:81:TYR:OH	0.51	2.59	9	7
1:A:77:ILE:HG22	1:A:81:TYR:CZ	0.51	2.41	18	2
1:A:40:ILE:HG12	1:A:84:TYR:CD2	0.51	2.41	8	1
1:A:20:ALA:HB1	1:A:58:TYR:CE1	0.51	2.41	16	4
1:A:55:THR:HG22	1:A:70:LEU:HD13	0.51	1.77	9	1
1:A:24:LEU:CA	1:A:53:LEU:HD11	0.51	2.36	10	1
1:A:55:THR:O	1:A:59:GLN:CG	0.50	2.60	20	1
1:A:55:THR:CB	1:A:70:LEU:HD11	0.50	2.35	17	1
1:A:75:ASP:O	1:A:79:ASP:CB	0.50	2.59	17	9
1:A:79:ASP:O	1:A:83:SER:CB	0.50	2.60	2	9
1:A:23:THR:HG21	1:A:57:LEU:HD13	0.50	1.83	3	1
1:A:24:LEU:HD11	1:A:77:ILE:CD1	0.50	2.36	10	5
1:A:40:ILE:C	1:A:40:ILE:CD1	0.50	2.80	19	2
1:A:51:TYR:CE1	1:A:77:ILE:CD1	0.50	2.92	4	2
1:A:30:LEU:HD13	1:A:40:ILE:CG2	0.50	2.37	18	1
1:A:51:TYR:O	1:A:55:THR:CG2	0.49	2.59	13	2
1:A:34:ARG:HD2	1:A:35:ILE:HD12	0.49	1.83	11	1
1:A:33:CYS:HB3	1:A:36:HIS:CE1	0.49	2.41	3	3
1:A:21:MET:HG3	1:A:24:LEU:HD22	0.49	1.82	18	2
1:A:51:TYR:CD1	1:A:51:TYR:N	0.49	2.78	14	6
1:A:20:ALA:HB1	1:A:58:TYR:CZ	0.49	2.42	3	1
1:A:42:ASP:O	1:A:88:ASP:CB	0.49	2.60	3	2
1:A:87:ILE:CG1	1:A:87:ILE:O	0.49	2.61	18	1
1:A:51:TYR:CE1	1:A:74:ARG:HB2	0.49	2.43	4	1
1:A:71:THR:O	1:A:75:ASP:CB	0.49	2.61	4	1
1:A:72:GLU:O	1:A:76:ALA:CB	0.49	2.60	13	1
1:A:74:ARG:O	1:A:78:LYS:CG	0.49	2.61	13	1
1:A:19:TRP:CD1	1:A:22:GLN:NE2	0.49	2.80	16	1
1:A:51:TYR:CD1	1:A:77:ILE:HG13	0.49	2.43	2	1
1:A:84:TYR:O	1:A:87:ILE:CD1	0.49	2.60	11	3
1:A:81:TYR:O	1:A:85:CYS:N	0.49	2.46	2	20
1:A:25:MET:HE2	1:A:30:LEU:HB2	0.49	1.83	11	1
1:A:36:HIS:ND1	1:A:39:VAL:CG2	0.49	2.75	10	1
1:A:53:LEU:CD2	1:A:53:LEU:O	0.49	2.61	15	2
1:A:78:LYS:O	1:A:82:GLU:CG	0.48	2.61	11	3

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:LEU:C	1:A:57:LEU:CD2	0.48	2.79	12	1
1:A:52:LYS:O	1:A:56:TYR:CG	0.48	2.66	13	1
1:A:29:VAL:HG12	1:A:81:TYR:OH	0.48	2.08	9	4
1:A:58:TYR:CD2	1:A:73:ALA:HB2	0.48	2.43	8	1
1:A:34:ARG:CG	1:A:35:ILE:HD12	0.48	2.38	18	1
1:A:30:LEU:HD13	1:A:40:ILE:HG23	0.48	1.84	18	1
1:A:47:ALA:CB	1:A:51:TYR:OH	0.48	2.62	7	3
1:A:24:LEU:N	1:A:53:LEU:HD11	0.48	2.24	10	1
1:A:20:ALA:HB2	1:A:58:TYR:CE1	0.48	2.44	2	1
1:A:84:TYR:O	1:A:87:ILE:CG1	0.48	2.61	20	2
1:A:53:LEU:HD12	1:A:53:LEU:O	0.48	2.09	10	1
1:A:23:THR:CG2	1:A:53:LEU:HD11	0.48	2.38	16	4
1:A:40:ILE:HG23	1:A:84:TYR:CZ	0.48	2.44	7	5
1:A:77:ILE:CG2	1:A:81:TYR:CZ	0.48	2.96	5	1
1:A:40:ILE:CD1	1:A:80:ALA:HB1	0.48	2.39	6	1
1:A:41:LEU:HD13	1:A:89:ASP:HA	0.48	1.86	4	1
1:A:40:ILE:HD13	1:A:41:LEU:N	0.47	2.24	19	1
1:A:52:LYS:CG	1:A:53:LEU:N	0.47	2.78	5	3
1:A:21:MET:O	1:A:25:MET:CG	0.47	2.62	13	1
1:A:20:ALA:O	1:A:57:LEU:HD13	0.47	2.10	8	1
1:A:55:THR:OG1	1:A:70:LEU:CD2	0.47	2.62	14	1
1:A:78:LYS:O	1:A:78:LYS:CD	0.47	2.63	16	1
1:A:54:GLY:C	1:A:58:TYR:CD2	0.47	2.88	17	1
1:A:52:LYS:O	1:A:55:THR:HG22	0.47	2.09	17	2
1:A:23:THR:HG23	1:A:24:LEU:N	0.46	2.25	10	3
1:A:21:MET:O	1:A:22:GLN:C	0.46	2.53	4	4
1:A:51:TYR:CE1	1:A:77:ILE:HD12	0.46	2.45	6	1
1:A:55:THR:HB	1:A:70:LEU:HD13	0.46	1.87	8	1
1:A:42:ASP:N	1:A:87:ILE:O	0.46	2.49	8	2
1:A:29:VAL:HB	1:A:50:ALA:HB2	0.46	1.86	18	1
1:A:40:ILE:HB	1:A:84:TYR:CD2	0.46	2.45	18	1
1:A:19:TRP:CE2	1:A:22:GLN:OE1	0.46	2.69	15	1
1:A:23:THR:O	1:A:27:SER:N	0.46	2.49	14	1
1:A:79:ASP:O	1:A:83:SER:N	0.46	2.49	3	12
1:A:22:GLN:CG	1:A:23:THR:N	0.46	2.77	6	1
1:A:23:THR:O	1:A:26:GLY:N	0.46	2.49	17	6
1:A:30:LEU:HG	1:A:81:TYR:CZ	0.46	2.46	8	1
1:A:39:VAL:HG12	1:A:41:LEU:CD1	0.46	2.40	13	1
1:A:25:MET:CE	1:A:40:ILE:CG1	0.46	2.94	15	2
1:A:50:ALA:O	1:A:54:GLY:N	0.46	2.48	8	3
1:A:30:LEU:HG	1:A:81:TYR:CE2	0.46	2.46	8	1

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HD12	1:A:70:LEU:C	0.46	2.31	9	1
1:A:40:ILE:HG21	1:A:84:TYR:CE1	0.45	2.44	10	1
1:A:24:LEU:HD11	1:A:77:ILE:HG13	0.45	1.87	17	1
1:A:53:LEU:C	1:A:53:LEU:CD1	0.45	2.78	10	1
1:A:35:ILE:CD1	1:A:36:HIS:CE1	0.45	2.99	15	1
1:A:78:LYS:O	1:A:82:GLU:CB	0.45	2.65	14	2
1:A:32:ARG:NH2	1:A:39:VAL:O	0.45	2.50	16	1
1:A:48:SER:HA	1:A:51:TYR:CD2	0.45	2.47	14	3
1:A:41:LEU:CD2	1:A:87:ILE:HG22	0.45	2.41	13	1
1:A:20:ALA:HA	1:A:57:LEU:HD22	0.45	1.88	2	1
1:A:74:ARG:CD	1:A:74:ARG:C	0.45	2.85	4	1
1:A:42:ASP:OD1	1:A:87:ILE:N	0.45	2.49	18	1
1:A:31:ALA:O	1:A:41:LEU:N	0.45	2.50	15	2
1:A:34:ARG:CG	1:A:35:ILE:CD1	0.45	2.95	18	1
1:A:24:LEU:C	1:A:24:LEU:CD2	0.45	2.84	9	3
1:A:24:LEU:CD1	1:A:54:GLY:N	0.45	2.80	7	1
1:A:33:CYS:SG	1:A:41:LEU:HD11	0.45	2.52	16	2
1:A:21:MET:CE	1:A:40:ILE:HD12	0.44	2.41	6	2
1:A:21:MET:CE	1:A:25:MET:SD	0.44	3.05	12	1
1:A:22:GLN:O	1:A:26:GLY:N	0.44	2.50	18	4
1:A:35:ILE:HG23	1:A:36:HIS:CG	0.44	2.47	14	1
1:A:24:LEU:HA	1:A:53:LEU:HD13	0.44	1.88	19	1
1:A:55:THR:OG1	1:A:70:LEU:CD1	0.44	2.66	4	1
1:A:40:ILE:CD1	1:A:84:TYR:CE2	0.44	2.89	16	1
1:A:23:THR:HB	1:A:53:LEU:HD11	0.44	1.89	6	2
1:A:23:THR:HG23	1:A:53:LEU:HD11	0.44	1.89	20	1
1:A:21:MET:HE1	1:A:80:ALA:HB1	0.44	1.89	10	1
1:A:74:ARG:CG	1:A:75:ASP:N	0.44	2.80	16	1
1:A:24:LEU:HD11	1:A:77:ILE:HD13	0.44	1.88	20	1
1:A:29:VAL:O	1:A:43:SER:CB	0.44	2.66	2	2
1:A:87:ILE:O	1:A:87:ILE:CG1	0.44	2.66	9	3
1:A:51:TYR:N	1:A:51:TYR:CD1	0.44	2.84	12	1
1:A:59:GLN:N	1:A:59:GLN:OE1	0.44	2.50	15	1
1:A:24:LEU:CD1	1:A:58:TYR:CE2	0.44	3.01	5	3
1:A:57:LEU:O	1:A:57:LEU:CD2	0.43	2.62	8	1
1:A:35:ILE:HG22	1:A:36:HIS:ND1	0.43	2.28	16	1
1:A:53:LEU:O	1:A:53:LEU:HD22	0.43	2.12	19	2
1:A:40:ILE:O	1:A:87:ILE:HD11	0.43	2.14	18	1
1:A:75:ASP:O	1:A:79:ASP:N	0.43	2.52	16	5
1:A:51:TYR:CE1	1:A:74:ARG:HG2	0.43	2.49	20	1
1:A:56:TYR:CD1	1:A:57:LEU:N	0.43	2.87	12	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:LEU:HD13	1:A:53:LEU:C	0.43	2.34	20	1
1:A:24:LEU:HD11	1:A:50:ALA:O	0.43	2.14	7	1
1:A:39:VAL:CG1	1:A:41:LEU:HD12	0.43	2.44	8	1
1:A:35:ILE:C	1:A:36:HIS:ND1	0.43	2.72	17	1
1:A:47:ALA:CB	1:A:51:TYR:CE2	0.43	3.02	5	1
1:A:24:LEU:CD1	1:A:54:GLY:HA3	0.43	2.43	12	5
1:A:55:THR:O	1:A:59:GLN:NE2	0.43	2.52	4	1
1:A:34:ARG:CD	1:A:35:ILE:HD12	0.43	2.44	11	1
1:A:59:GLN:NE2	1:A:59:GLN:C	0.42	2.73	3	1
1:A:50:ALA:HA	1:A:53:LEU:HD21	0.42	1.90	14	1
1:A:30:LEU:CD2	1:A:40:ILE:HG23	0.42	2.43	18	1
1:A:30:LEU:HD12	1:A:81:TYR:CZ	0.42	2.50	12	1
1:A:34:ARG:HG2	1:A:35:ILE:HD12	0.42	1.89	18	1
1:A:33:CYS:O	1:A:36:HIS:O	0.42	2.37	9	4
1:A:81:TYR:O	1:A:85:CYS:CA	0.42	2.68	15	2
1:A:45:ASN:O	1:A:47:ALA:N	0.42	2.52	17	1
1:A:35:ILE:HD12	1:A:36:HIS:CE1	0.42	2.48	19	1
1:A:21:MET:HG3	1:A:25:MET:CB	0.42	2.44	4	1
1:A:30:LEU:HD12	1:A:81:TYR:CE1	0.41	2.50	14	1
1:A:35:ILE:HG12	1:A:36:HIS:CE1	0.41	2.50	15	1
1:A:78:LYS:CD	1:A:78:LYS:C	0.41	2.89	15	1
1:A:25:MET:HE1	1:A:40:ILE:HB	0.41	1.90	20	1
1:A:54:GLY:O	1:A:58:TYR:CG	0.41	2.73	17	1
1:A:25:MET:HE2	1:A:30:LEU:CB	0.41	2.45	8	1
1:A:27:SER:HB3	1:A:53:LEU:CD2	0.41	2.46	10	2
1:A:88:ASP:OD2	1:A:88:ASP:N	0.41	2.53	19	1
1:A:25:MET:CE	1:A:40:ILE:HG12	0.41	2.45	15	1
1:A:24:LEU:HD12	1:A:54:GLY:HA2	0.41	1.92	2	1
1:A:16:GLN:CD	1:A:16:GLN:N	0.41	2.74	11	1
1:A:25:MET:CE	1:A:30:LEU:HB2	0.41	2.45	18	1
1:A:41:LEU:CD2	1:A:88:ASP:O	0.41	2.68	3	1
1:A:52:LYS:O	1:A:55:THR:CG2	0.41	2.69	17	1
1:A:20:ALA:HA	1:A:57:LEU:CD2	0.41	2.45	20	1
1:A:21:MET:CG	1:A:25:MET:CB	0.41	2.98	4	1
1:A:50:ALA:HA	1:A:53:LEU:CD2	0.41	2.46	13	1
1:A:54:GLY:O	1:A:58:TYR:N	0.41	2.52	15	1
1:A:84:TYR:O	1:A:85:CYS:C	0.41	2.59	3	1
1:A:24:LEU:HD23	1:A:25:MET:CA	0.41	2.46	8	1
1:A:40:ILE:O	1:A:41:LEU:HD23	0.41	2.16	12	1
1:A:40:ILE:HB	1:A:84:TYR:CG	0.41	2.50	18	1
1:A:41:LEU:CG	1:A:88:ASP:O	0.40	2.68	3	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:HD13	1:A:36:HIS:CE1	0.40	2.52	15	1
1:A:23:THR:CG2	1:A:24:LEU:N	0.40	2.84	3	1
1:A:58:TYR:O	1:A:59:GLN:C	0.40	2.60	2	1
1:A:25:MET:HE1	1:A:30:LEU:CB	0.40	2.46	13	1
1:A:56:TYR:O	1:A:59:GLN:O	0.40	2.40	3	1
1:A:53:LEU:HD22	1:A:53:LEU:O	0.40	2.16	5	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	64/101 (63%)	61±1 (95±1%)	2±1 (3±2%)	1±1 (2±1%)	11	53
All	All	1280/2020 (63%)	1213 (95%)	43 (3%)	24 (2%)	11	53

All 4 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	22	GLN	15
1	A	46	ASP	5
1	A	24	LEU	3
1	A	59	GLN	1

### 6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	52/87 (60%)	43±3 (82±5%)	9±3 (18±5%)	4	38
All	All	1040/1740 (60%)	856 (82%)	184 (18%)	4	38

All 38 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	40	ILE	17
1	A	70	LEU	12
1	A	85	CYS	10
1	A	39	VAL	9
1	A	25	MET	8
1	A	77	ILE	8
1	A	78	LYS	7
1	A	52	LYS	7
1	A	88	ASP	7
1	A	42	ASP	6
1	A	21	MET	6
1	A	53	LEU	6
1	A	24	LEU	6
1	A	32	ARG	6
1	A	87	ILE	5
1	A	36	HIS	5
1	A	49	SER	5
1	A	74	ARG	4
1	A	17	GLU	4
1	A	33	CYS	4
1	A	57	LEU	4
1	A	35	ILE	4
1	A	27	SER	3
1	A	22	GLN	3
1	A	46	ASP	3
1	A	55	THR	3
1	A	37	ASN	3
1	A	23	THR	2
1	A	59	GLN	2
1	A	89	ASP	2
1	A	79	ASP	2
1	A	75	ASP	2
1	A	18	GLN	2
1	A	34	ARG	2
1	A	41	LEU	2
1	A	71	THR	1
1	A	16	GLN	1
1	A	38	ASP	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 75% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 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	870
Number of shifts mapped to atoms	825
Number of unparsed shifts	0
Number of shifts with mapping errors	45
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 45 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	GLY	N	110.601	.	1
1	A	4	GLY	H	8.514	.	1
1	A	5	VAL	N	119.058	.	1
1	A	5	VAL	H	8.028	.	1
1	A	8	SER	H	8.475	.	1
1	A	8	SER	N	117.557	.	1
1	A	6	GLU	N	124.028	.	1
1	A	6	GLU	H	8.576	.	1
1	A	10	HIS	H	8.57	0.011	1
1	A	10	HIS	N	125.53	.	1
1	A	9	ILE	H	8.169	.	1
1	A	9	ILE	N	121.943	.	1
1	A	7	MET	N	121.533	.	1
1	A	7	MET	H	8.354	.	1

*Continued on next page...*



Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	10	HIS	C	174.068	0.012	1
1	A	10	HIS	CA	56.332	.	1
1	A	10	HIS	CB	29.901	0.033	1
1	A	1	MET	CE	16.839	.	1
1	A	1	MET	HE1	2.058	.	1
1	A	1	MET	HE2	2.058	.	1
1	A	1	MET	HE3	2.058	.	1
1	A	5	VAL	CG2	20.331	.	2
1	A	5	VAL	HG21	0.915	.	2
1	A	5	VAL	HG22	0.915	.	2
1	A	5	VAL	HG23	0.915	.	2
1	A	5	VAL	CG1	21.114	.	2
1	A	5	VAL	HG11	0.926	.	2
1	A	5	VAL	HG12	0.926	.	2
1	A	5	VAL	HG13	0.926	.	2
1	A	10	HIS	HA	3.821	.	1
1	A	10	HIS	HD2	6.968	0.002	1
1	A	10	HIS	CD2	119.994	.	1
1	A	10	HIS	CE1	138.311	.	1
1	A	10	HIS	HE1	7.689	.	1
1	A	9	ILE	CA	61.957	0.103	1
1	A	9	ILE	CB	38.522	0.052	1
1	A	9	ILE	CG1	27.221	0.071	1
1	A	9	ILE	CG2	17.375	0.063	1
1	A	9	ILE	HG21	0.815	0.003	1
1	A	9	ILE	HG22	0.815	0.003	1
1	A	9	ILE	HG23	0.815	0.003	1
1	A	9	ILE	CD1	13.129	0.101	1
1	A	9	ILE	HD11	0.808	0.005	1
1	A	9	ILE	HD12	0.808	0.005	1
1	A	9	ILE	HD13	0.808	0.005	1

### 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
$^{13}\text{C}_\alpha$	74	$-0.63 \pm 0.16$	Should be checked
$^{13}\text{C}_\beta$	63	$0.15 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	73	$-0.44 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	80	$-0.72 \pm 0.36$	Should be applied

### 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 81%, i.e. 675 atoms were assigned a chemical shift out of a possible 830. 0 out of 8 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	310/325 (95%)	130/133 (98%)	118/128 (92%)	62/64 (97%)
Sidechain	313/441 (71%)	217/286 (76%)	93/138 (67%)	3/17 (18%)
Aromatic	52/64 (81%)	28/30 (93%)	23/32 (72%)	1/2 (50%)
Overall	675/830 (81%)	375/449 (84%)	234/298 (79%)	66/83 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 825 atoms were assigned a chemical shift out of a possible 1099. 0 out of 9 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	368/433 (85%)	151/176 (86%)	144/172 (84%)	73/85 (86%)
Sidechain	389/583 (67%)	268/374 (72%)	116/186 (62%)	5/23 (22%)
Aromatic	68/83 (82%)	36/39 (92%)	31/42 (74%)	1/2 (50%)
Overall	825/1099 (75%)	455/589 (77%)	291/400 (73%)	79/110 (72%)

### 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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	92	GLN	HB2	0.62	0.80 – 3.29	-5.7
1	A	54	GLY	N	127.82	91.59 – 127.52	5.1

### 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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

