



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:05 pm BST

PDB ID : 2LGL  
Title : NMR structure of the UHRF1 PHD domain  
Authors : Wang, C.; Shen, J.; Yang, Z.; Chen, P.; Zhao, B.; Hu, W.; Lan, W.; Tong, X.;  
Wu, H.; Li, G.; Cao, C.  
Deposited on : 2011-07-28

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 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

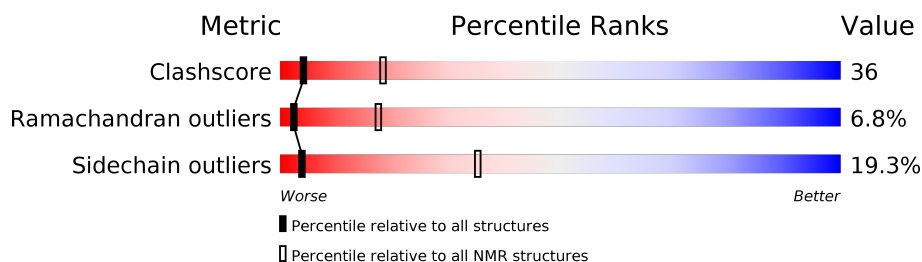
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 80%.

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	69	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:317-A:379 (63)	0.90	15

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 4 clusters and 3 single-model clusters were found.

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

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

There are 2 unique types of molecules in this entry. The entry contains 1023 atoms, of which 482 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms						Trace
1	A	69	Total	C	H	N	O	S	0
			1020	323	482	95	107	13	

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

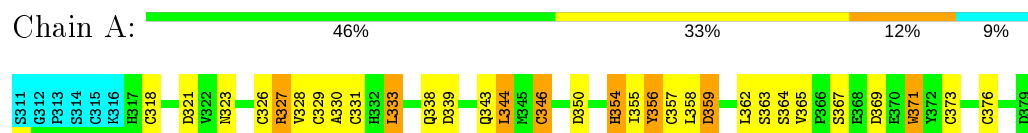
Mol	Chain	Residues	Atoms	
2	A	3	Total	Zn
			3	3

## 4 Residue-property plots

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

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

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

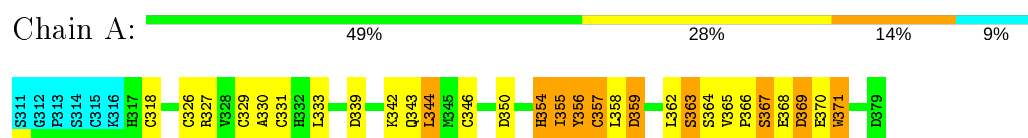


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

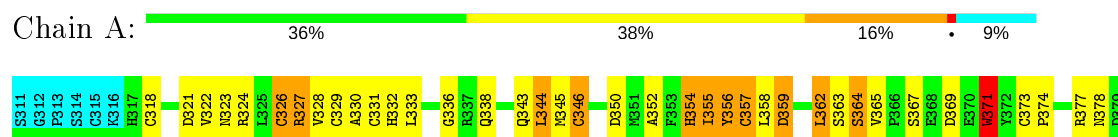
#### 4.2.1 Score per residue for model 1

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



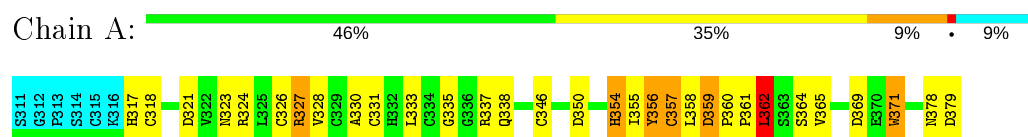
#### 4.2.2 Score per residue for model 2

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



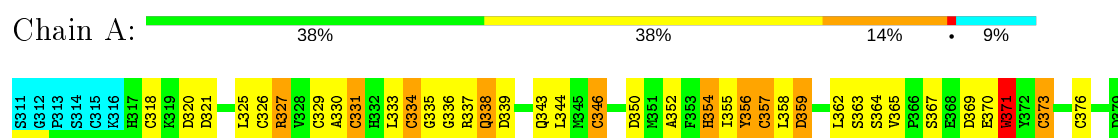
### 4.2.3 Score per residue for model 3

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



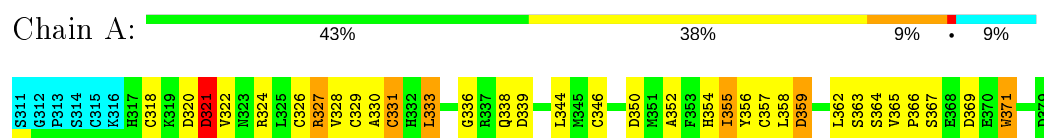
### 4.2.4 Score per residue for model 4

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



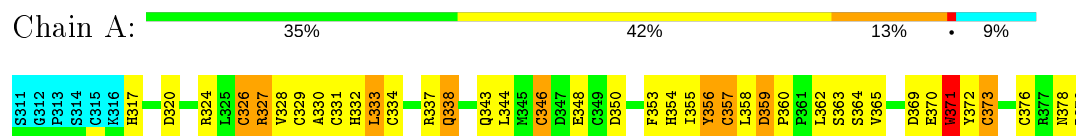
### 4.2.5 Score per residue for model 5

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



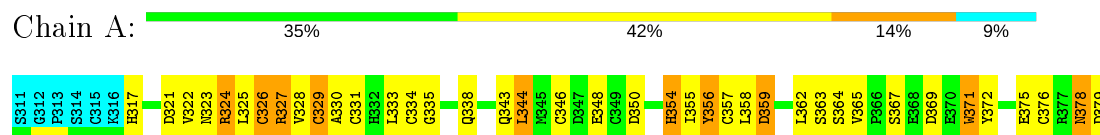
### 4.2.6 Score per residue for model 6

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



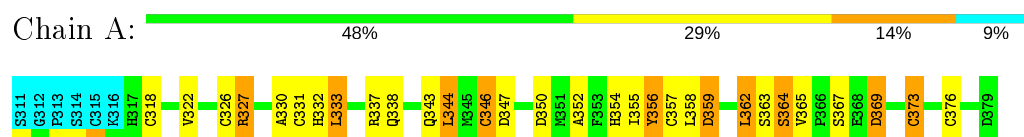
### 4.2.7 Score per residue for model 7

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



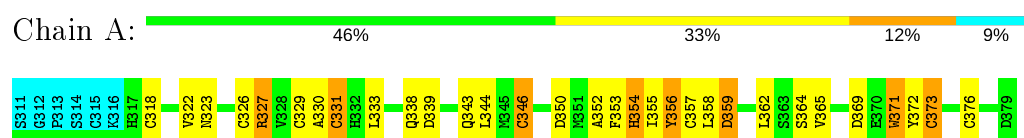
### 4.2.8 Score per residue for model 8

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



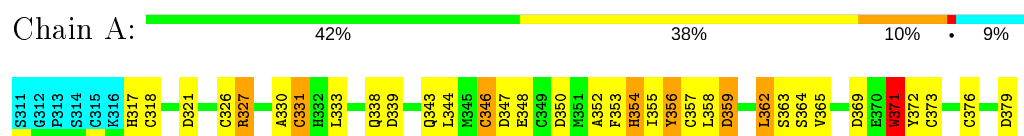
### 4.2.9 Score per residue for model 9

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



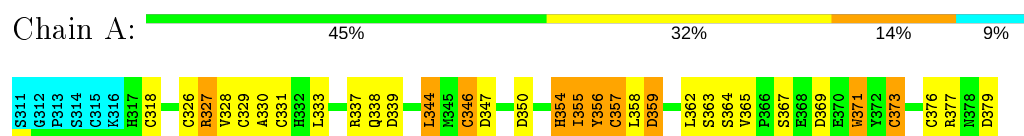
### 4.2.10 Score per residue for model 10

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



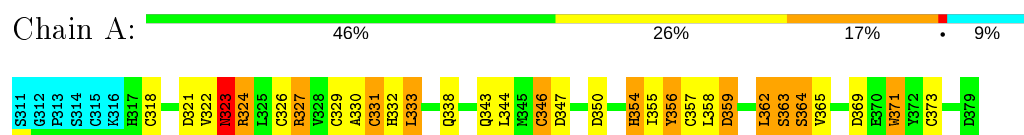
### 4.2.11 Score per residue for model 11

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



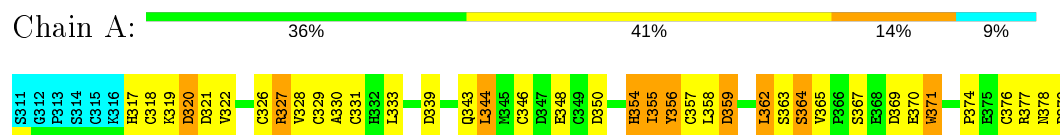
### 4.2.12 Score per residue for model 12

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



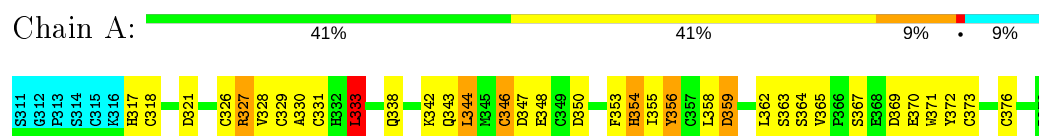
### 4.2.13 Score per residue for model 13

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



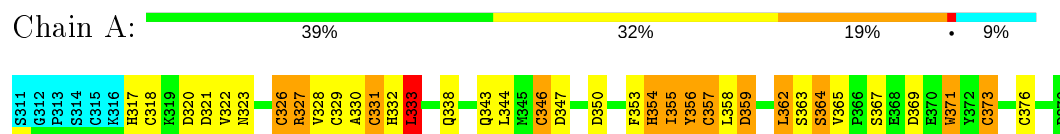
### 4.2.14 Score per residue for model 14

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



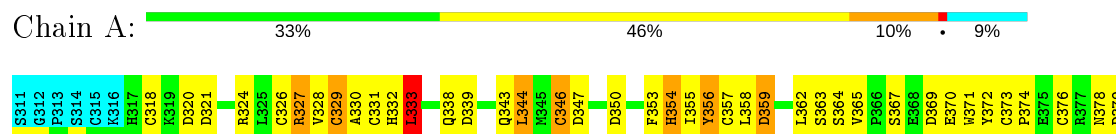
### 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



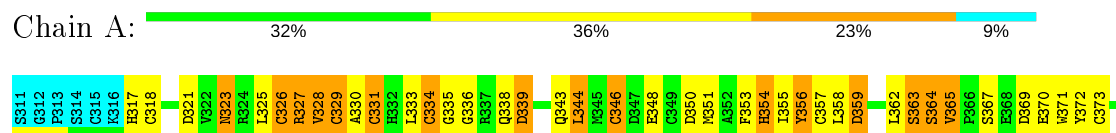
### 4.2.16 Score per residue for model 16

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



### 4.2.17 Score per residue for model 17

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

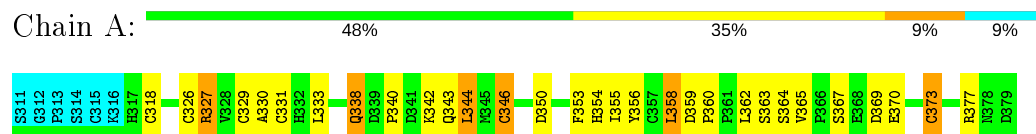






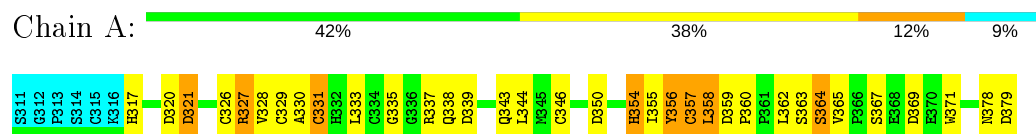
#### 4.2.18 Score per residue for model 18

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



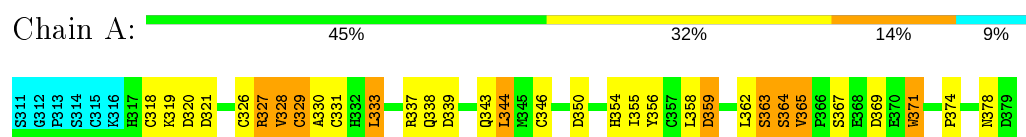
#### 4.2.19 Score per residue for model 19

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



#### 4.2.20 Score per residue for model 20

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



## 5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	688
Number of shifts mapped to atoms	688
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	500	443	441	34±5
All	All	10060	8860	8820	685

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:330:ALA:HB1	1:A:338:GLN:NE2	0.90	1.81	15	1
1:A:333:LEU:HD23	1:A:354:HIS:CE1	0.89	2.02	10	6
1:A:317:HIS:ND1	1:A:328:VAL:HG21	0.86	1.85	19	1
1:A:326:CYS:O	1:A:330:ALA:HB3	0.83	1.74	6	8
1:A:344:LEU:HD23	1:A:344:LEU:N	0.78	1.94	17	6
1:A:344:LEU:N	1:A:344:LEU:HD12	0.77	1.95	9	5
1:A:344:LEU:HD12	1:A:344:LEU:N	0.77	1.95	6	2
1:A:344:LEU:N	1:A:344:LEU:HD23	0.77	1.94	13	4
1:A:333:LEU:HD13	1:A:354:HIS:CE1	0.76	2.15	14	5
1:A:362:LEU:HD23	1:A:364:SER:H	0.75	1.41	19	2
1:A:333:LEU:HD23	1:A:354:HIS:ND1	0.72	1.98	17	4
1:A:331:CYS:N	1:A:352:ALA:HB3	0.72	2.00	10	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:365:VAL:HG12	1:A:367:SER:O	0.68	1.88	14	14
1:A:326:CYS:O	1:A:328:VAL:N	0.68	2.27	7	6
1:A:331:CYS:SG	1:A:343:GLN:NE2	0.67	2.69	10	4
1:A:346:CYS:O	1:A:350:ASP:N	0.65	2.30	20	20
1:A:343:GLN:C	1:A:344:LEU:HD23	0.65	2.12	1	10
1:A:333:LEU:HD22	1:A:354:HIS:CE1	0.65	2.27	2	3
1:A:330:ALA:HB1	1:A:338:GLN:HE22	0.65	1.51	15	1
1:A:322:VAL:HG12	1:A:337:ARG:NH2	0.65	2.07	8	1
1:A:327:ARG:HE	1:A:332:HIS:CE1	0.64	2.09	12	1
1:A:327:ARG:H	1:A:327:ARG:CD	0.64	2.06	6	1
1:A:362:LEU:O	1:A:364:SER:N	0.63	2.31	18	16
1:A:362:LEU:HD23	1:A:364:SER:N	0.62	2.10	19	2
1:A:344:LEU:N	1:A:344:LEU:CD2	0.62	2.60	14	6
1:A:356:TYR:CG	1:A:356:TYR:O	0.62	2.53	15	4
1:A:331:CYS:H	1:A:338:GLN:HE22	0.62	1.36	16	3
1:A:344:LEU:HD21	1:A:355:ILE:HD11	0.61	1.70	17	2
1:A:344:LEU:CD2	1:A:344:LEU:N	0.61	2.61	18	4
1:A:334:CYS:SG	1:A:336:GLY:N	0.61	2.74	4	2
1:A:326:CYS:O	1:A:330:ALA:N	0.60	2.34	1	12
1:A:323:ASN:O	1:A:325:LEU:N	0.60	2.34	7	1
1:A:356:TYR:O	1:A:356:TYR:CG	0.60	2.53	2	12
1:A:354:HIS:O	1:A:356:TYR:N	0.60	2.35	5	6
1:A:327:ARG:NE	1:A:332:HIS:CE1	0.60	2.69	12	1
1:A:371:TRP:CG	1:A:372:TYR:N	0.60	2.68	10	7
1:A:331:CYS:H	1:A:338:GLN:HE21	0.60	1.38	18	1
1:A:371:TRP:CE2	1:A:372:TYR:O	0.59	2.55	9	7
1:A:328:VAL:HG23	1:A:329:CYS:N	0.59	2.12	6	1
1:A:356:TYR:O	1:A:356:TYR:CD1	0.59	2.56	15	8
1:A:353:PHE:CD1	1:A:355:ILE:HG23	0.59	2.32	16	6
1:A:331:CYS:SG	1:A:331:CYS:O	0.59	2.61	18	5
1:A:319:LYS:O	1:A:321:ASP:N	0.59	2.36	13	2
1:A:344:LEU:CD1	1:A:344:LEU:N	0.59	2.65	6	4
1:A:331:CYS:H	1:A:338:GLN:NE2	0.59	1.96	15	3
1:A:327:ARG:O	1:A:330:ALA:O	0.59	2.20	7	14
1:A:327:ARG:NE	1:A:332:HIS:ND1	0.59	2.50	12	1
1:A:333:LEU:HD12	1:A:333:LEU:N	0.59	2.13	13	3
1:A:326:CYS:O	1:A:326:CYS:SG	0.59	2.60	4	1
1:A:320:ASP:O	1:A:321:ASP:CB	0.58	2.51	5	3
1:A:332:HIS:O	1:A:332:HIS:ND1	0.58	2.36	6	1
1:A:375:GLU:O	1:A:378:ASN:ND2	0.58	2.36	7	1
1:A:333:LEU:N	1:A:333:LEU:HD12	0.57	2.14	2	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:322:VAL:O	1:A:323:ASN:CB	0.57	2.51	15	3
1:A:332:HIS:NE2	1:A:352:ALA:O	0.57	2.37	8	1
1:A:331:CYS:SG	1:A:343:GLN:OE1	0.57	2.62	12	1
1:A:326:CYS:O	1:A:329:CYS:N	0.57	2.38	7	1
1:A:348:GLU:OE1	1:A:376:CYS:SG	0.57	2.62	7	3
1:A:331:CYS:SG	1:A:338:GLN:NE2	0.57	2.77	15	1
1:A:331:CYS:O	1:A:335:GLY:N	0.57	2.37	17	4
1:A:344:LEU:HD21	1:A:355:ILE:CD1	0.57	2.30	17	4
1:A:338:GLN:OE1	1:A:357:CYS:SG	0.56	2.63	5	1
1:A:365:VAL:O	1:A:365:VAL:HG12	0.56	2.01	16	3
1:A:373:CYS:N	1:A:376:CYS:SG	0.56	2.78	9	5
1:A:371:TRP:CD1	1:A:371:TRP:C	0.56	2.79	11	8
1:A:373:CYS:O	1:A:376:CYS:SG	0.56	2.64	9	4
1:A:344:LEU:N	1:A:344:LEU:CD1	0.56	2.68	12	3
1:A:373:CYS:O	1:A:377:ARG:N	0.56	2.38	18	1
1:A:371:TRP:NE1	1:A:372:TYR:O	0.56	2.39	6	2
1:A:331:CYS:O	1:A:331:CYS:SG	0.56	2.64	20	1
1:A:331:CYS:SG	1:A:338:GLN:OE1	0.56	2.64	14	2
1:A:328:VAL:HG22	1:A:329:CYS:N	0.56	2.16	20	2
1:A:342:LYS:NZ	1:A:356:TYR:CE2	0.56	2.70	1	1
1:A:371:TRP:C	1:A:371:TRP:CD1	0.56	2.80	6	6
1:A:331:CYS:N	1:A:338:GLN:HE22	0.56	1.98	15	2
1:A:364:SER:O	1:A:365:VAL:C	0.55	2.43	3	13
1:A:334:CYS:SG	1:A:338:GLN:OE1	0.55	2.64	7	1
1:A:327:ARG:NH2	1:A:332:HIS:CE1	0.55	2.74	2	1
1:A:362:LEU:O	1:A:363:SER:CB	0.55	2.55	1	1
1:A:356:TYR:CD1	1:A:356:TYR:O	0.55	2.58	5	3
1:A:365:VAL:HG12	1:A:365:VAL:O	0.55	2.01	3	3
1:A:342:LYS:CE	1:A:356:TYR:CE2	0.55	2.89	18	1
1:A:362:LEU:CD2	1:A:365:VAL:H	0.55	2.14	3	1
1:A:356:TYR:C	1:A:356:TYR:CD1	0.55	2.80	20	10
1:A:331:CYS:O	1:A:333:LEU:N	0.55	2.39	15	2
1:A:356:TYR:CD1	1:A:356:TYR:C	0.54	2.80	12	5
1:A:359:ASP:N	1:A:359:ASP:OD1	0.54	2.40	5	3
1:A:328:VAL:CG2	1:A:329:CYS:N	0.54	2.71	6	1
1:A:378:ASN:C	1:A:378:ASN:ND2	0.53	2.59	7	1
1:A:354:HIS:O	1:A:355:ILE:C	0.53	2.46	5	18
1:A:338:GLN:HE22	1:A:343:GLN:HE22	0.53	1.47	18	1
1:A:356:TYR:CD1	1:A:357:CYS:N	0.53	2.77	6	2
1:A:328:VAL:CG1	1:A:329:CYS:N	0.53	2.71	16	1
1:A:339:ASP:N	1:A:356:TYR:OH	0.53	2.39	17	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:362:LEU:C	1:A:364:SER:N	0.52	2.62	11	13
1:A:359:ASP:OD1	1:A:359:ASP:N	0.52	2.40	4	1
1:A:343:GLN:C	1:A:344:LEU:HD12	0.52	2.25	19	7
1:A:322:VAL:HG13	1:A:324:ARG:HH11	0.52	1.64	5	1
1:A:326:CYS:O	1:A:330:ALA:CB	0.52	2.56	18	3
1:A:331:CYS:SG	1:A:338:GLN:CD	0.52	2.88	15	1
1:A:367:SER:CB	1:A:370:GLU:O	0.52	2.57	17	1
1:A:322:VAL:HG13	1:A:324:ARG:NH1	0.52	2.19	5	1
1:A:333:LEU:CB	1:A:354:HIS:NE2	0.52	2.72	6	5
1:A:333:LEU:CD1	1:A:354:HIS:CE1	0.52	2.93	3	5
1:A:323:ASN:O	1:A:324:ARG:C	0.51	2.49	12	2
1:A:319:LYS:C	1:A:321:ASP:N	0.51	2.63	13	2
1:A:326:CYS:O	1:A:327:ARG:C	0.51	2.49	7	4
1:A:370:GLU:O	1:A:371:TRP:CB	0.51	2.56	4	2
1:A:362:LEU:C	1:A:364:SER:H	0.51	2.09	5	18
1:A:359:ASP:CB	1:A:360:PRO:CD	0.50	2.89	19	2
1:A:320:ASP:CB	1:A:324:ARG:NH1	0.50	2.74	6	1
1:A:356:TYR:CE1	1:A:357:CYS:SG	0.50	3.04	17	3
1:A:358:LEU:HD12	1:A:360:PRO:O	0.50	2.06	19	2
1:A:326:CYS:N	1:A:335:GLY:O	0.50	2.45	7	1
1:A:336:GLY:CA	1:A:343:GLN:NE2	0.50	2.74	17	1
1:A:317:HIS:CE1	1:A:328:VAL:HG21	0.50	2.42	19	1
1:A:333:LEU:HD22	1:A:354:HIS:ND1	0.50	2.22	2	3
1:A:354:HIS:CD2	1:A:357:CYS:CB	0.50	2.95	3	5
1:A:323:ASN:O	1:A:324:ARG:O	0.50	2.29	12	1
1:A:317:HIS:O	1:A:321:ASP:OD2	0.50	2.30	17	4
1:A:331:CYS:CA	1:A:352:ALA:HB3	0.50	2.35	10	3
1:A:325:LEU:O	1:A:327:ARG:N	0.50	2.44	17	1
1:A:364:SER:O	1:A:365:VAL:O	0.49	2.30	20	4
1:A:330:ALA:CB	1:A:338:GLN:NE2	0.49	2.67	15	1
1:A:327:ARG:CZ	1:A:332:HIS:CE1	0.49	2.95	2	1
1:A:354:HIS:O	1:A:358:LEU:CD2	0.49	2.60	3	1
1:A:367:SER:OG	1:A:370:GLU:O	0.49	2.31	18	4
1:A:365:VAL:CG1	1:A:367:SER:O	0.49	2.61	16	4
1:A:318:CYS:O	1:A:321:ASP:O	0.49	2.30	12	1
1:A:338:GLN:OE1	1:A:343:GLN:OE1	0.49	2.31	18	1
1:A:320:ASP:O	1:A:321:ASP:OD1	0.49	2.31	4	2
1:A:354:HIS:CG	1:A:357:CYS:HB2	0.49	2.43	10	7
1:A:328:VAL:HG13	1:A:329:CYS:N	0.49	2.22	16	1
1:A:323:ASN:O	1:A:323:ASN:OD1	0.49	2.31	17	1
1:A:362:LEU:HD22	1:A:365:VAL:H	0.48	1.68	3	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:333:LEU:CD2	1:A:354:HIS:CE1	0.48	2.95	2	1
1:A:379:ASP:OD1	1:A:379:ASP:O	0.48	2.31	7	1
1:A:317:HIS:CD2	1:A:327:ARG:NH1	0.48	2.81	6	1
1:A:331:CYS:SG	1:A:336:GLY:N	0.48	2.87	17	2
1:A:371:TRP:CD2	1:A:372:TYR:O	0.48	2.66	10	1
1:A:328:VAL:CG1	1:A:329:CYS:SG	0.48	3.02	16	1
1:A:368:GLU:C	1:A:370:GLU:H	0.48	2.11	1	1
1:A:337:ARG:O	1:A:338:GLN:C	0.48	2.52	4	7
1:A:338:GLN:OE1	1:A:340:PRO:N	0.48	2.47	18	1
1:A:348:GLU:OE2	1:A:376:CYS:O	0.48	2.31	17	2
1:A:374:PRO:O	1:A:378:ASN:OD1	0.48	2.31	20	2
1:A:369:ASP:O	1:A:369:ASP:OD1	0.47	2.31	1	1
1:A:342:LYS:NZ	1:A:356:TYR:CZ	0.47	2.79	1	1
1:A:321:ASP:OD2	1:A:323:ASN:ND2	0.47	2.47	7	1
1:A:328:VAL:HG13	1:A:329:CYS:H	0.47	1.68	17	2
1:A:343:GLN:NE2	1:A:357:CYS:SG	0.47	2.88	9	1
1:A:336:GLY:C	1:A:338:GLN:N	0.47	2.67	5	1
1:A:371:TRP:CD1	1:A:371:TRP:O	0.47	2.68	2	1
1:A:321:ASP:OD1	1:A:321:ASP:O	0.47	2.32	5	1
1:A:378:ASN:HD22	1:A:378:ASN:C	0.47	2.12	7	1
1:A:371:TRP:CD1	1:A:372:TYR:N	0.47	2.83	9	3
1:A:319:LYS:C	1:A:321:ASP:H	0.47	2.12	20	2
1:A:333:LEU:HD13	1:A:354:HIS:ND1	0.47	2.25	3	1
1:A:333:LEU:HB3	1:A:354:HIS:NE2	0.47	2.25	6	3
1:A:368:GLU:O	1:A:370:GLU:N	0.47	2.48	1	1
1:A:321:ASP:CG	1:A:323:ASN:ND2	0.47	2.69	7	1
1:A:358:LEU:O	1:A:359:ASP:C	0.47	2.53	3	18
1:A:332:HIS:ND1	1:A:332:HIS:O	0.47	2.48	8	1
1:A:321:ASP:CG	1:A:322:VAL:H	0.46	2.14	2	1
1:A:322:VAL:HG23	1:A:324:ARG:H	0.46	1.70	2	1
1:A:323:ASN:C	1:A:325:LEU:N	0.46	2.67	7	1
1:A:355:ILE:HD12	1:A:356:TYR:N	0.46	2.25	18	1
1:A:326:CYS:CB	1:A:330:ALA:HB2	0.46	2.40	7	1
1:A:336:GLY:CA	1:A:343:GLN:HE22	0.46	2.24	17	1
1:A:362:LEU:HD22	1:A:364:SER:OG	0.46	2.09	6	2
1:A:320:ASP:O	1:A:321:ASP:CG	0.46	2.54	19	1
1:A:317:HIS:CE1	1:A:321:ASP:OD2	0.46	2.68	15	1
1:A:331:CYS:O	1:A:335:GLY:CA	0.46	2.64	4	1
1:A:321:ASP:OD2	1:A:324:ARG:NH1	0.46	2.49	16	1
1:A:343:GLN:HB3	1:A:352:ALA:HB1	0.46	1.88	4	1
1:A:336:GLY:C	1:A:338:GLN:H	0.46	2.14	5	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:324:ARG:CD	1:A:327:ARG:HH21	0.45	2.24	3	1
1:A:365:VAL:O	1:A:367:SER:N	0.45	2.50	5	2
1:A:338:GLN:HE22	1:A:343:GLN:NE2	0.45	2.09	18	1
1:A:353:PHE:CD2	1:A:354:HIS:N	0.45	2.84	18	1
1:A:331:CYS:SG	1:A:343:GLN:CD	0.45	2.95	10	1
1:A:374:PRO:O	1:A:378:ASN:ND2	0.45	2.50	16	2
1:A:368:GLU:C	1:A:370:GLU:N	0.45	2.69	1	1
1:A:328:VAL:HG13	1:A:329:CYS:SG	0.45	2.51	16	1
1:A:362:LEU:HD22	1:A:364:SER:CB	0.45	2.42	10	1
1:A:376:CYS:O	1:A:379:ASP:CG	0.45	2.55	6	1
1:A:379:ASP:C	1:A:379:ASP:OD1	0.45	2.55	13	4
1:A:374:PRO:O	1:A:378:ASN:CG	0.45	2.55	2	2
1:A:330:ALA:O	1:A:331:CYS:C	0.45	2.54	6	9
1:A:333:LEU:CD1	1:A:354:HIS:ND1	0.45	2.80	3	1
1:A:320:ASP:OD1	1:A:320:ASP:C	0.45	2.55	15	1
1:A:337:ARG:O	1:A:338:GLN:O	0.45	2.36	6	1
1:A:338:GLN:O	1:A:339:ASP:OD1	0.44	2.35	4	1
1:A:344:LEU:HD13	1:A:355:ILE:HG12	0.44	1.88	9	1
1:A:327:ARG:C	1:A:327:ARG:CD	0.44	2.85	12	1
1:A:344:LEU:CD2	1:A:371:TRP:CD1	0.44	3.00	11	1
1:A:378:ASN:O	1:A:379:ASP:C	0.44	2.56	6	2
1:A:325:LEU:C	1:A:327:ARG:H	0.44	2.16	4	1
1:A:322:VAL:CG1	1:A:324:ARG:HH11	0.44	2.24	5	1
1:A:347:ASP:O	1:A:350:ASP:OD1	0.44	2.36	12	5
1:A:321:ASP:O	1:A:321:ASP:CG	0.44	2.56	5	1
1:A:336:GLY:O	1:A:338:GLN:N	0.44	2.51	5	1
1:A:353:PHE:CD1	1:A:354:HIS:N	0.44	2.86	15	1
1:A:348:GLU:OE1	1:A:379:ASP:OD2	0.44	2.35	6	1
1:A:317:HIS:O	1:A:321:ASP:CG	0.44	2.55	17	2
1:A:359:ASP:OD1	1:A:359:ASP:C	0.44	2.56	6	1
1:A:324:ARG:CD	1:A:327:ARG:NH2	0.44	2.80	3	1
1:A:359:ASP:C	1:A:359:ASP:OD1	0.44	2.56	3	1
1:A:317:HIS:NE2	1:A:321:ASP:OD2	0.44	2.51	15	1
1:A:357:CYS:O	1:A:358:LEU:C	0.44	2.56	5	1
1:A:354:HIS:CG	1:A:357:CYS:CB	0.44	3.00	11	1
1:A:366:PRO:C	1:A:368:GLU:H	0.43	2.15	1	1
1:A:375:GLU:O	1:A:378:ASN:CG	0.43	2.56	7	1
1:A:317:HIS:CD2	1:A:328:VAL:HG21	0.43	2.48	13	1
1:A:376:CYS:O	1:A:379:ASP:OD1	0.43	2.36	6	1
1:A:322:VAL:O	1:A:323:ASN:C	0.43	2.54	7	1
1:A:362:LEU:HD23	1:A:362:LEU:O	0.43	2.13	7	3

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:342:LYS:O	1:A:355:ILE:HD11	0.43	2.14	18	1
1:A:333:LEU:CD1	1:A:333:LEU:N	0.43	2.79	13	4
1:A:345:MET:SD	1:A:352:ALA:HB2	0.43	2.53	2	1
1:A:354:HIS:C	1:A:356:TYR:N	0.43	2.70	15	2
1:A:362:LEU:CD2	1:A:362:LEU:C	0.43	2.87	3	1
1:A:317:HIS:O	1:A:322:VAL:CG2	0.43	2.66	13	1
1:A:333:LEU:CB	1:A:354:HIS:CE1	0.43	3.02	11	1
1:A:378:ASN:O	1:A:379:ASP:OD1	0.43	2.36	19	1
1:A:378:ASN:O	1:A:379:ASP:OXT	0.42	2.37	16	1
1:A:359:ASP:N	1:A:360:PRO:HD2	0.42	2.29	3	1
1:A:361:PRO:O	1:A:362:LEU:O	0.42	2.37	3	1
1:A:355:ILE:O	1:A:362:LEU:N	0.42	2.52	5	1
1:A:322:VAL:CG1	1:A:323:ASN:N	0.42	2.82	9	2
1:A:333:LEU:HD22	1:A:354:HIS:CG	0.42	2.49	19	1
1:A:344:LEU:HD11	1:A:365:VAL:HG13	0.42	1.92	5	2
1:A:344:LEU:HD23	1:A:371:TRP:CD1	0.42	2.49	11	2
1:A:326:CYS:HB2	1:A:330:ALA:HB2	0.42	1.92	7	1
1:A:327:ARG:CZ	1:A:332:HIS:ND1	0.41	2.83	2	1
1:A:362:LEU:HD21	1:A:364:SER:OG	0.41	2.15	13	1
1:A:347:ASP:O	1:A:347:ASP:OD1	0.41	2.38	8	2
1:A:354:HIS:CD2	1:A:357:CYS:HB3	0.41	2.50	8	1
1:A:343:GLN:OE1	1:A:356:TYR:CE1	0.41	2.73	6	1
1:A:354:HIS:CD2	1:A:357:CYS:HB2	0.41	2.49	15	2
1:A:344:LEU:HD13	1:A:355:ILE:CD1	0.41	2.45	19	1
1:A:333:LEU:HB2	1:A:354:HIS:NE2	0.41	2.31	14	3
1:A:370:GLU:OE2	1:A:372:TYR:OH	0.41	2.31	14	1
1:A:330:ALA:HB1	1:A:336:GLY:CA	0.41	2.46	2	1
1:A:366:PRO:O	1:A:367:SER:CB	0.41	2.68	1	1
1:A:337:ARG:NH1	1:A:337:ARG:CB	0.41	2.85	11	1
1:A:366:PRO:O	1:A:368:GLU:N	0.40	2.55	1	1
1:A:354:HIS:O	1:A:357:CYS:N	0.40	2.52	11	1
1:A:354:HIS:CE1	1:A:357:CYS:HB3	0.40	2.51	16	1
1:A:347:ASP:OD1	1:A:347:ASP:O	0.40	2.39	16	1
1:A:373:CYS:O	1:A:376:CYS:N	0.40	2.54	10	1
1:A:331:CYS:H	1:A:338:GLN:CD	0.40	2.20	15	1
1:A:359:ASP:N	1:A:360:PRO:CD	0.40	2.85	3	2
1:A:338:GLN:CD	1:A:343:GLN:OE1	0.40	2.60	18	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	62/69 (90%)	52±2 (84±3%)	6±2 (9±3%)	4±1 (7±2%)	2	17
All	All	1240/1380 (90%)	1045 (84%)	111 (9%)	84 (7%)	2	17

All 16 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	369	ASP	20
1	A	363	SER	16
1	A	333	LEU	9
1	A	338	GLN	7
1	A	327	ARG	6
1	A	355	ILE	6
1	A	371	TRP	4
1	A	323	ASN	3
1	A	365	VAL	2
1	A	324	ARG	2
1	A	332	HIS	2
1	A	321	ASP	2
1	A	320	ASP	2
1	A	366	PRO	1
1	A	326	CYS	1
1	A	362	LEU	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	59/64 (92%)	48±2 (81±4%)	11±2 (19±4%)	4	35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1180/1280 (92%)	952 (81%)	228 (19%)	<b>4</b> 35

All 32 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	359	ASP	18
1	A	356	TYR	17
1	A	329	CYS	16
1	A	318	CYS	16
1	A	371	TRP	15
1	A	354	HIS	15
1	A	327	ARG	14
1	A	346	CYS	13
1	A	331	CYS	12
1	A	373	CYS	12
1	A	344	LEU	11
1	A	339	ASP	10
1	A	357	CYS	10
1	A	364	SER	8
1	A	362	LEU	7
1	A	363	SER	5
1	A	326	CYS	4
1	A	328	VAL	4
1	A	334	CYS	3
1	A	377	ARG	3
1	A	333	LEU	3
1	A	358	LEU	2
1	A	367	SER	1
1	A	342	LYS	1
1	A	376	CYS	1
1	A	378	ASN	1
1	A	323	ASN	1
1	A	338	GLN	1
1	A	317	HIS	1
1	A	369	ASP	1
1	A	321	ASP	1
1	A	351	MET	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

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

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 79% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

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	688
Number of shifts mapped to atoms	688
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	66	$-0.95 \pm 0.25$	Should be applied
$^{13}\text{C}_\beta$	64	$0.20 \pm 0.31$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	59	$-0.40 \pm 0.36$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	63	$-0.59 \pm 0.59$	None needed (imprecise)

#### 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 80%, i.e. 608 atoms were assigned a chemical shift out of a possible 758. 5 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	295/305 (97%)	120/121 (99%)	117/126 (93%)	58/58 (100%)
Sidechain	285/393 (73%)	183/235 (78%)	102/140 (73%)	0/18 (0%)

*Continued on next page...*

Continued from previous page...

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	28/60 (47%)	13/31 (42%)	14/23 (61%)	1/6 (17%)
Overall	608/758 (80%)	316/387 (82%)	233/289 (81%)	59/82 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 642 atoms were assigned a chemical shift out of a possible 817. 5 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	316/333 (95%)	128/132 (97%)	125/138 (91%)	63/63 (100%)
Sidechain	298/424 (70%)	191/255 (75%)	107/150 (71%)	0/19 (0%)
Aromatic	28/60 (47%)	13/31 (42%)	14/23 (61%)	1/6 (17%)
Overall	642/817 (79%)	332/418 (79%)	246/311 (79%)	64/88 (73%)

#### 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:

