



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 01:37 am GMT

PDB ID : 2N3W  
Title : Solution structure of the Rpn1 T1 site with K48-linked diubiquitin in the contracted binding mode  
Authors : Chen, X.; Walters, K.J.  
Deposited on : 2015-06-10

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

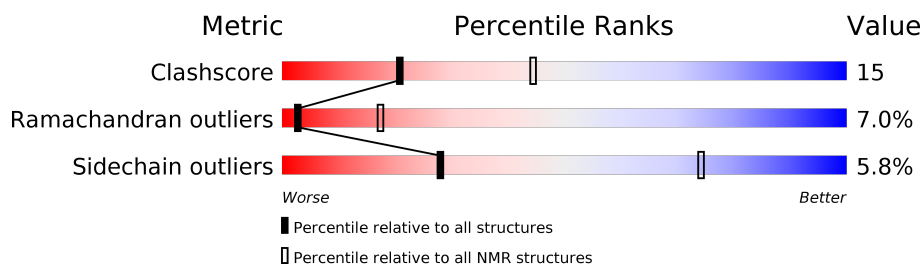
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 24%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	131	
2	B	76	
2	C	76	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 6 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:489-A:553, A:561-A:608, B:1-B:76, C:1-C:76 (265)	0.60	6

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. No single-model clusters were found.

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

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

There are 2 unique types of molecules in this entry. The entry contains 4380 atoms, of which 2223 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			1921	606	967	150	192	6	

- Molecule 2 is a protein called Ubiquitin-60S ribosomal protein L40.

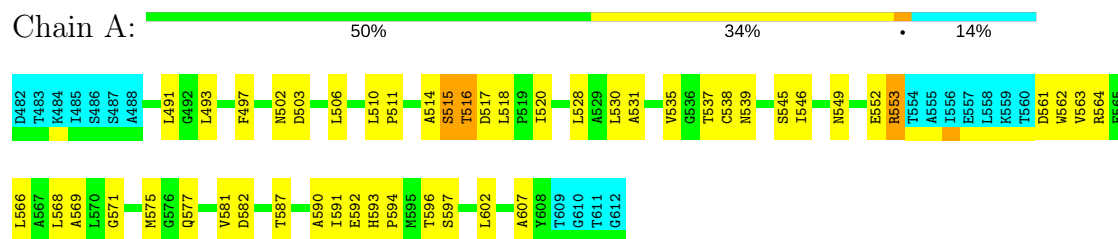
Mol	Chain	Residues	Atoms						Trace
2	B	76	Total	C	H	N	O	S	0
			1229	378	627	105	118	1	
2	C	76	Total	C	H	N	O	S	0
			1230	378	629	105	117	1	

## 4 Residue-property plots

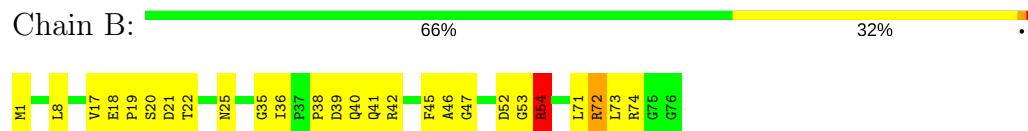
### 4.1 Average score per residue in the NMR ensemble

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.

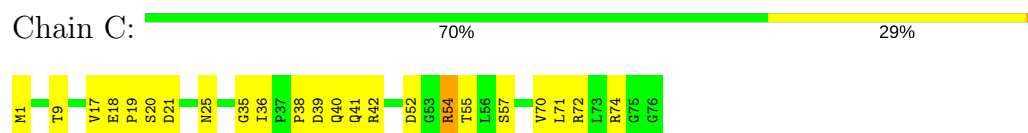
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40



- Molecule 2: Ubiquitin-60S ribosomal protein L40



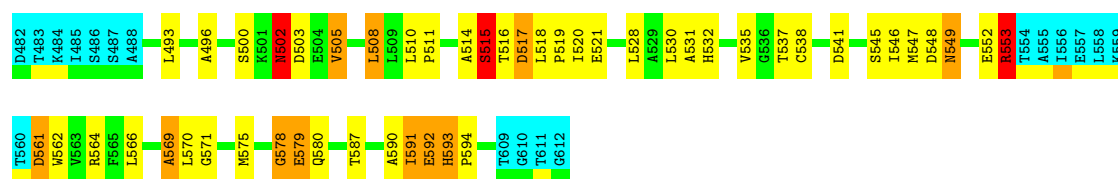
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

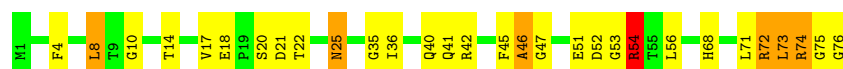
- Molecule 1: 26S proteasome regulatory subunit RPN1





- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain B: 61% 30% 8% •



- Molecule 2: Ubiquitin-60S ribosomal protein L40

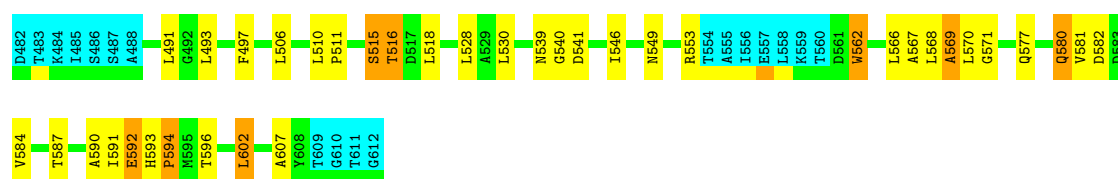
Chain C: 67% 32% •



#### 4.2.2 Score per residue for model 2

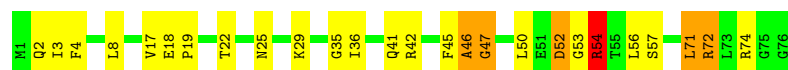
- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 57% 23% 6% 14% •



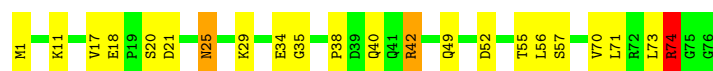
- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain B: 66% 26% 7% •



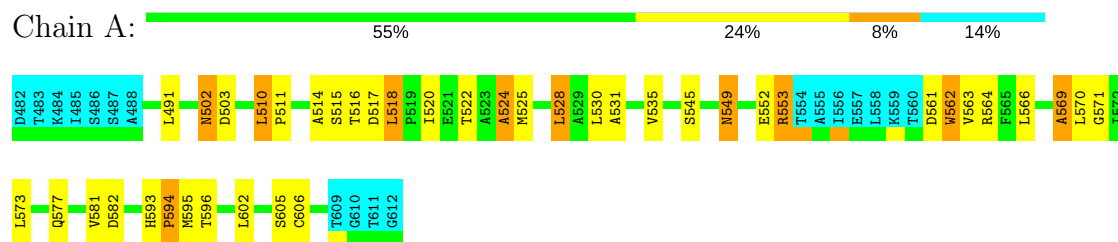
- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain C: 71% 25% •

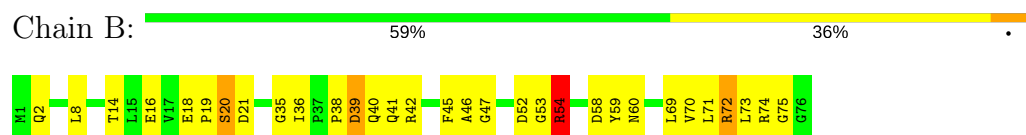


#### 4.2.3 Score per residue for model 3

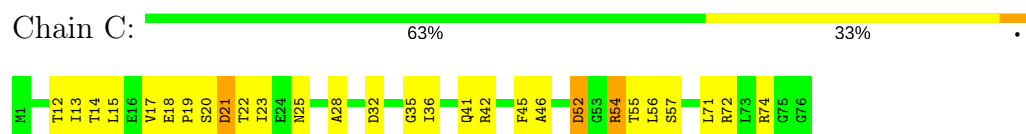
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

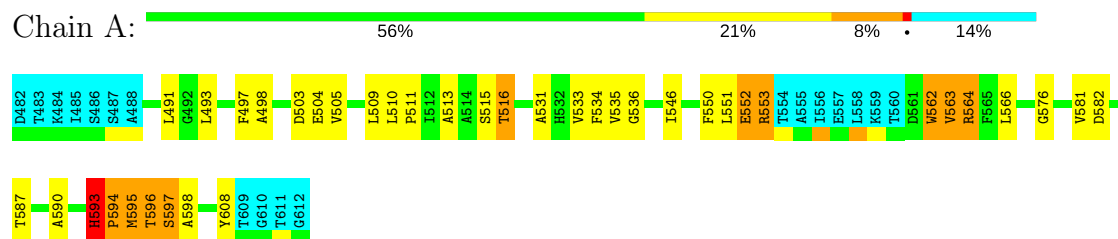


- Molecule 2: Ubiquitin-60S ribosomal protein L40

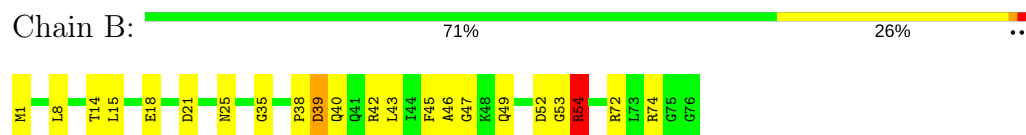


#### 4.2.4 Score per residue for model 4

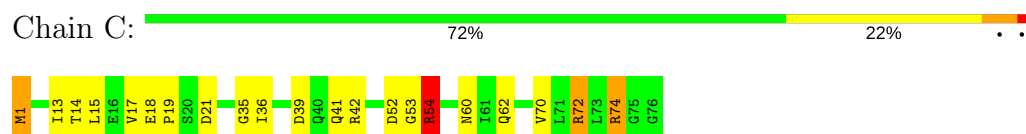
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

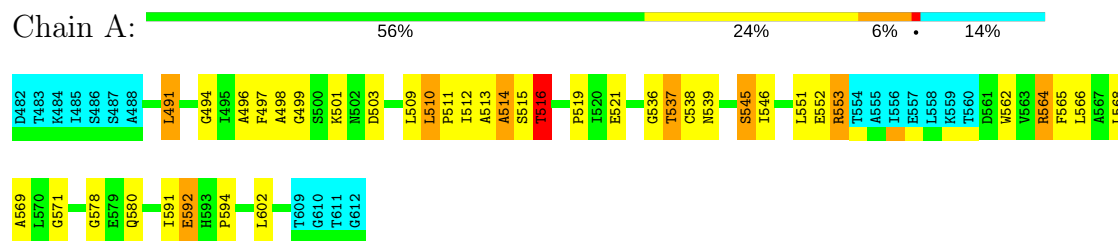


- Molecule 2: Ubiquitin-60S ribosomal protein L40

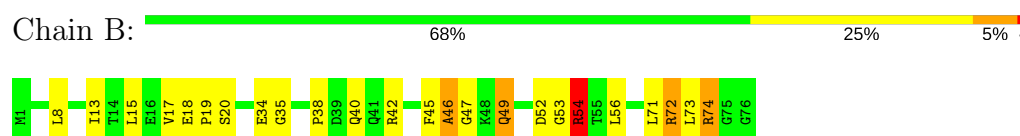


### 4.2.5 Score per residue for model 5

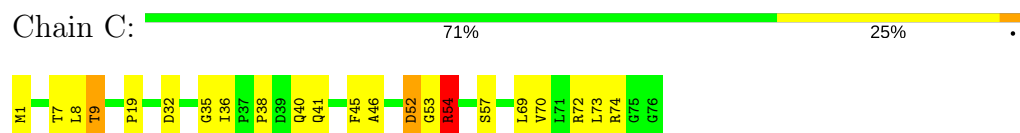
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

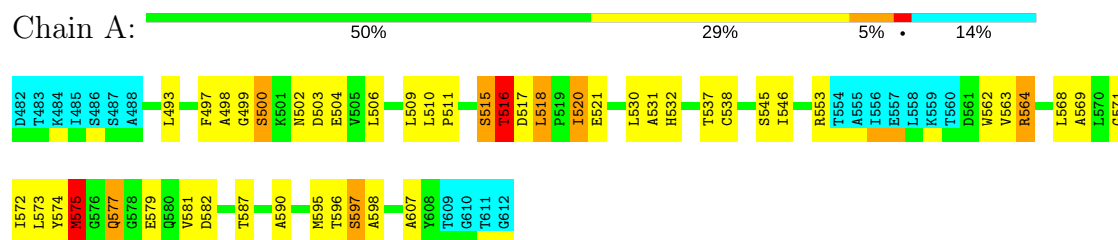


- Molecule 2: Ubiquitin-60S ribosomal protein L40

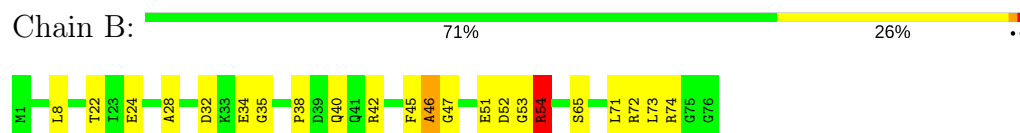


### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: 26S proteasome regulatory subunit RPN1



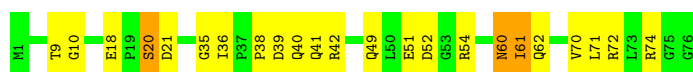
- Molecule 2: Ubiquitin-60S ribosomal protein L40



- Molecule 2: Ubiquitin-60S ribosomal protein L40

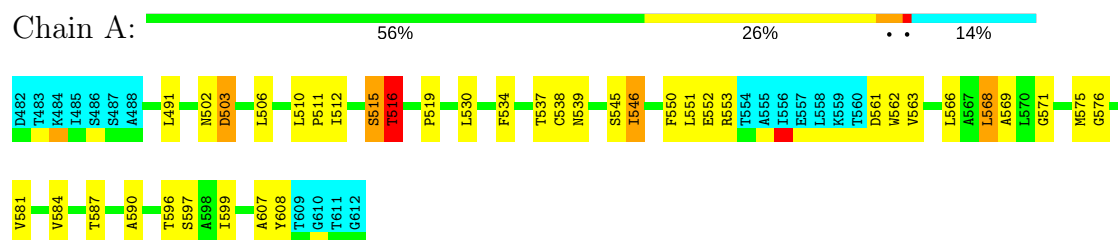




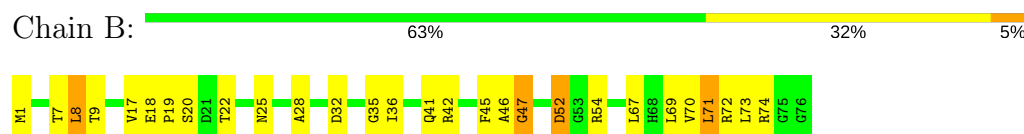


#### 4.2.7 Score per residue for model 7

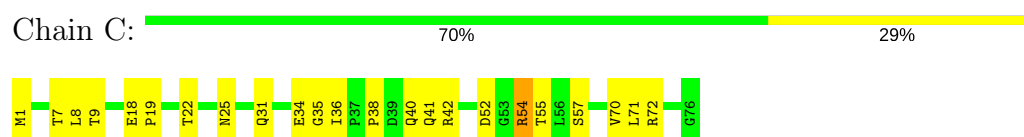
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

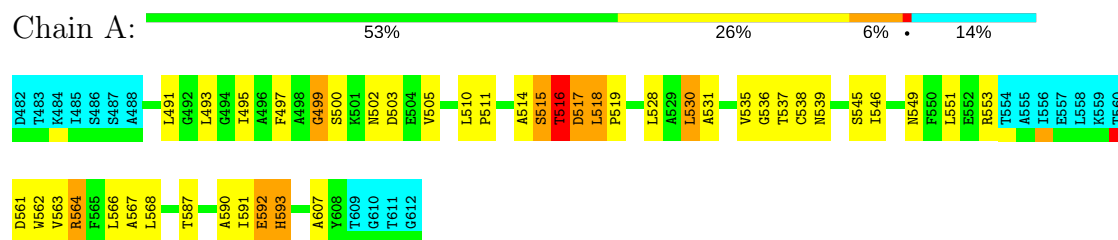


- Molecule 2: Ubiquitin-60S ribosomal protein L40

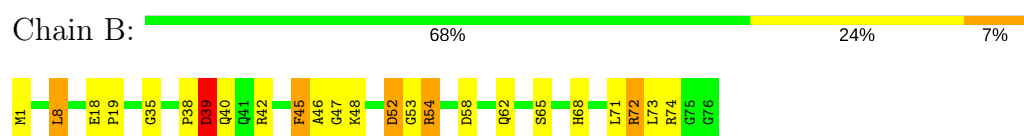


#### 4.2.8 Score per residue for model 8

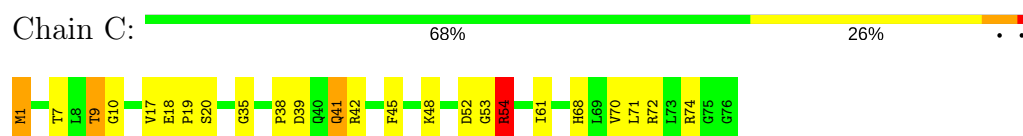
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

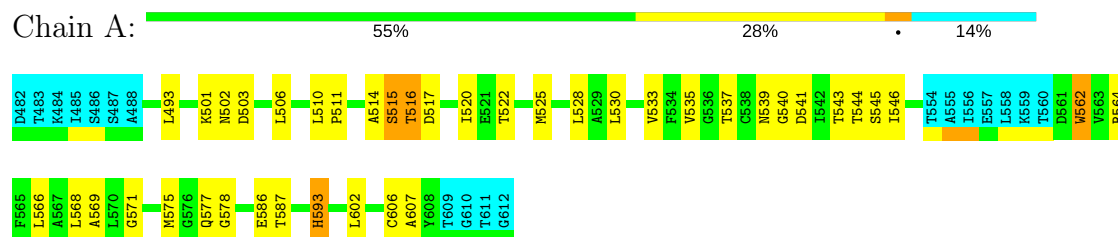


- Molecule 2: Ubiquitin-60S ribosomal protein L40

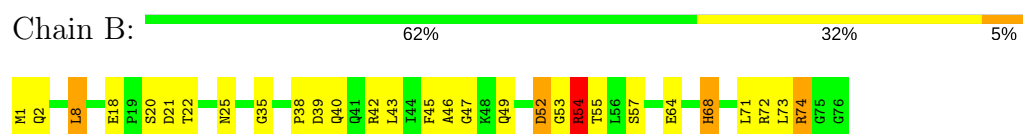


#### 4.2.9 Score per residue for model 9

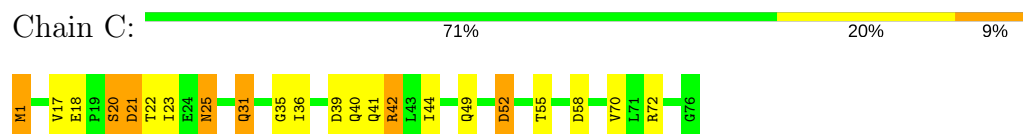
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

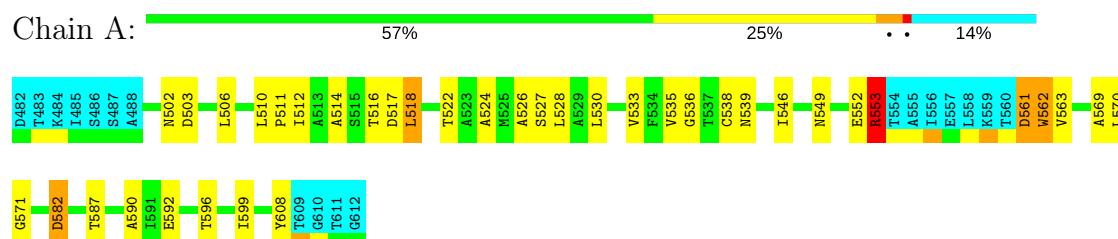


- Molecule 2: Ubiquitin-60S ribosomal protein L40



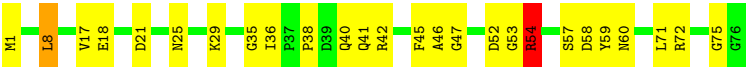
#### 4.2.10 Score per residue for model 10

- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40





● Molecule 2: Ubiquitin-60S ribosomal protein L40



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure solution	

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)	2n3w_cs.str
Number of chemical shift lists	1
Total number of shifts	1034
Number of shifts mapped to atoms	1034
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	24%

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

## 6 Model quality [i](#)

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.5±0.5
2	B	0.0±0.0	3.5±0.5
2	C	0.0±0.0	3.1±0.7
All	All	0	81

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	B	72	ARG	Sidechain	10
2	B	42	ARG	Sidechain	9
1	A	553	ARG	Sidechain	9
2	C	72	ARG	Sidechain	9
2	C	74	ARG	Sidechain	8
2	B	54	ARG	Sidechain	8
2	B	74	ARG	Sidechain	8
2	C	54	ARG	Sidechain	7
2	C	42	ARG	Sidechain	7
1	A	564	ARG	Sidechain	6

### 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	829	835	835	32±5
2	B	602	627	627	18±5
2	C	601	629	629	14±3
All	All	20320	20910	20907	623

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
2:C:15:LEU:HD22	2:C:15:LEU:N	0.77	1.94	1	1
1:A:512:ILE:O	1:A:518:LEU:HD22	0.74	1.81	10	1
1:A:578:GLY:O	1:A:580:GLN:N	0.71	2.24	1	1
2:B:15:LEU:N	2:B:15:LEU:HD22	0.68	2.03	4	1
2:B:69:LEU:HD23	2:B:69:LEU:C	0.68	2.09	7	1
2:C:15:LEU:N	2:C:15:LEU:HD22	0.68	2.04	3	1
2:B:69:LEU:C	2:B:69:LEU:HD23	0.68	2.08	3	1
2:B:71:LEU:HD23	2:B:71:LEU:H	0.68	1.47	3	2
2:B:45:PHE:CG	2:B:46:ALA:N	0.68	2.62	10	8
1:A:591:ILE:HG22	1:A:592:GLU:H	0.66	1.49	5	2
2:B:71:LEU:H	2:B:71:LEU:HD23	0.65	1.50	10	2
1:A:575:MET:N	1:A:575:MET:SD	0.64	2.70	6	1
2:B:71:LEU:CD2	2:B:71:LEU:H	0.64	2.05	3	1
2:C:69:LEU:C	2:C:69:LEU:HD23	0.63	2.13	5	1
2:B:54:ARG:NE	2:B:54:ARG:N	0.63	2.47	3	1
2:B:49:GLN:N	2:B:49:GLN:NE2	0.62	2.47	5	1
2:B:45:PHE:O	2:B:47:GLY:N	0.62	2.32	2	8
2:B:71:LEU:HD23	2:B:71:LEU:N	0.61	2.09	3	2
2:B:71:LEU:H	2:B:71:LEU:CD2	0.61	2.09	10	2
2:C:15:LEU:CD2	2:C:15:LEU:N	0.61	2.63	1	1
2:C:69:LEU:HD23	2:C:70:VAL:N	0.61	2.11	5	1
1:A:511:PRO:O	1:A:515:SER:N	0.61	2.34	5	7
2:B:71:LEU:N	2:B:71:LEU:HD12	0.61	2.11	1	3
2:B:71:LEU:N	2:B:71:LEU:HD23	0.60	2.11	10	1
1:A:562:TRP:CG	1:A:563:VAL:N	0.60	2.69	7	5
2:B:71:LEU:HD12	2:B:71:LEU:N	0.60	2.11	9	1
1:A:591:ILE:HG22	1:A:592:GLU:N	0.60	2.12	5	2
1:A:518:LEU:O	1:A:518:LEU:HD12	0.59	1.97	6	1
1:A:564:ARG:NE	1:A:565:PHE:CZ	0.58	2.72	5	1
1:A:593:HIS:N	1:A:594:PRO:CD	0.58	2.66	4	1
2:B:38:PRO:C	2:B:40:GLN:H	0.57	2.02	8	5
2:C:15:LEU:N	2:C:15:LEU:CD2	0.57	2.67	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:69:LEU:HD23	2:B:70:VAL:N	0.57	2.15	7	2
1:A:593:HIS:ND1	1:A:593:HIS:N	0.57	2.51	8	1
2:B:15:LEU:N	2:B:15:LEU:CD2	0.57	2.67	4	1
1:A:493:LEU:O	1:A:497:PHE:CD2	0.56	2.57	2	2
1:A:515:SER:O	1:A:516:THR:OG1	0.56	2.23	1	8
2:C:41:GLN:O	2:C:42:ARG:NH1	0.56	2.37	10	1
1:A:517:ASP:N	1:A:517:ASP:OD1	0.56	2.39	8	1
2:B:36:ILE:O	2:B:41:GLN:NE2	0.56	2.37	2	5
2:C:60:ASN:OD1	2:C:60:ASN:N	0.56	2.39	6	1
1:A:535:VAL:HG13	1:A:536:GLY:N	0.56	2.16	4	2
2:B:15:LEU:N	2:B:15:LEU:HD12	0.55	2.16	5	1
2:C:38:PRO:O	2:C:40:GLN:N	0.55	2.40	1	1
1:A:538:CYS:SG	1:A:539:ASN:N	0.55	2.79	8	1
1:A:510:LEU:HB3	1:A:511:PRO:CD	0.55	2.31	9	7
1:A:502:ASN:ND2	1:A:503:ASP:H	0.55	1.99	1	2
2:C:71:LEU:CD2	2:C:71:LEU:N	0.55	2.70	3	2
1:A:510:LEU:CB	1:A:511:PRO:CD	0.55	2.85	1	4
1:A:593:HIS:N	1:A:593:HIS:ND1	0.55	2.53	4	2
1:A:528:LEU:HD23	1:A:528:LEU:O	0.55	2.02	3	2
1:A:562:TRP:CD2	1:A:563:VAL:N	0.55	2.75	4	1
1:A:512:ILE:C	1:A:518:LEU:HD22	0.54	2.22	10	1
2:C:71:LEU:HD22	2:C:71:LEU:N	0.54	2.17	3	2
1:A:578:GLY:O	1:A:579:GLU:C	0.54	2.46	1	1
2:B:2:GLN:HE21	2:B:3:ILE:N	0.54	2.00	2	1
1:A:593:HIS:CG	1:A:593:HIS:O	0.54	2.59	1	1
2:C:1:MET:N	2:C:17:VAL:O	0.54	2.37	10	6
1:A:508:LEU:HD23	1:A:508:LEU:O	0.54	2.03	1	1
1:A:608:TYR:CD2	1:A:608:TYR:O	0.54	2.60	4	1
1:A:587:THR:O	1:A:590:ALA:N	0.54	2.41	7	7
2:C:60:ASN:O	2:C:62:GLN:NE2	0.54	2.41	4	2
2:C:36:ILE:O	2:C:41:GLN:NE2	0.53	2.42	10	7
2:B:40:GLN:NE2	2:B:72:ARG:O	0.53	2.40	1	1
2:B:25:ASN:OD1	2:B:29:LYS:NZ	0.53	2.41	2	2
1:A:537:THR:OG1	1:A:538:CYS:N	0.53	2.41	7	5
2:B:8:LEU:HD23	2:B:8:LEU:O	0.53	2.03	8	3
2:B:40:GLN:NE2	2:B:73:LEU:O	0.53	2.42	1	2
1:A:502:ASN:ND2	1:A:503:ASP:N	0.53	2.56	1	2
1:A:566:LEU:HD12	1:A:566:LEU:N	0.53	2.19	2	4
2:B:38:PRO:O	2:B:40:GLN:N	0.53	2.42	4	4
2:B:54:ARG:HE	2:B:54:ARG:N	0.53	2.02	3	1
1:A:596:THR:O	1:A:598:ALA:N	0.53	2.42	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:18:GLU:H	2:B:21:ASP:CG	0.53	2.07	4	3
1:A:551:LEU:N	1:A:551:LEU:CD1	0.53	2.71	7	1
1:A:608:TYR:CG	1:A:608:TYR:O	0.53	2.61	4	1
1:A:493:LEU:O	1:A:497:PHE:CE2	0.53	2.62	2	2
1:A:512:ILE:HG13	2:C:8:LEU:HD12	0.53	1.80	7	1
2:B:42:ARG:NH1	2:B:72:ARG:NH1	0.52	2.57	5	1
1:A:591:ILE:O	1:A:593:HIS:N	0.52	2.41	2	1
2:B:71:LEU:HD12	2:B:71:LEU:O	0.52	2.04	2	1
2:B:71:LEU:N	2:B:71:LEU:CD1	0.52	2.71	1	1
2:C:45:PHE:CG	2:C:46:ALA:N	0.52	2.76	5	1
2:C:42:ARG:NH1	2:C:49:GLN:OE1	0.52	2.42	2	1
2:C:42:ARG:NE	2:C:49:GLN:OE1	0.52	2.43	9	1
1:A:566:LEU:N	1:A:566:LEU:HD12	0.52	2.19	1	2
1:A:538:CYS:O	1:A:539:ASN:ND2	0.52	2.42	7	3
1:A:518:LEU:O	1:A:553:ARG:NH1	0.52	2.43	1	1
1:A:506:LEU:HD12	1:A:506:LEU:N	0.52	2.20	6	1
1:A:539:ASN:OD1	1:A:540:GLY:N	0.52	2.43	9	2
1:A:549:ASN:HD21	1:A:553:ARG:NH1	0.52	2.03	3	1
2:C:52:ASP:N	2:C:52:ASP:OD1	0.52	2.42	10	3
2:C:18:GLU:N	2:C:21:ASP:OD2	0.52	2.42	2	3
2:C:45:PHE:O	2:C:46:ALA:HB3	0.52	2.05	3	1
2:B:71:LEU:CD1	2:B:71:LEU:N	0.52	2.73	9	2
1:A:602:LEU:HD12	1:A:602:LEU:N	0.51	2.21	2	1
1:A:551:LEU:N	1:A:551:LEU:HD12	0.51	2.20	7	1
1:A:569:ALA:O	1:A:571:GLY:N	0.51	2.43	3	5
2:C:45:PHE:CD2	2:C:46:ALA:N	0.51	2.78	5	1
2:B:18:GLU:O	2:B:20:SER:N	0.51	2.43	3	1
1:A:493:LEU:O	1:A:497:PHE:CD1	0.51	2.63	8	1
1:A:591:ILE:C	1:A:593:HIS:N	0.51	2.64	2	1
1:A:591:ILE:O	1:A:592:GLU:O	0.51	2.29	5	3
1:A:510:LEU:HB3	1:A:511:PRO:HD3	0.51	1.83	5	4
1:A:582:ASP:N	1:A:582:ASP:OD1	0.51	2.44	10	1
1:A:502:ASN:C	1:A:504:GLU:H	0.51	2.09	6	1
2:B:69:LEU:C	2:B:69:LEU:CD2	0.51	2.79	3	2
1:A:516:THR:O	1:A:517:ASP:O	0.51	2.29	1	1
2:C:49:GLN:H	2:C:49:GLN:NE2	0.51	2.03	1	1
1:A:550:PHE:CZ	1:A:553:ARG:NH2	0.51	2.79	4	1
2:C:45:PHE:O	2:C:48:LYS:N	0.51	2.42	8	1
2:B:52:ASP:N	2:B:52:ASP:OD1	0.50	2.43	7	3
2:B:73:LEU:N	2:B:73:LEU:CD1	0.50	2.74	5	1
2:B:19:PRO:O	2:B:57:SER:OG	0.50	2.30	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:71:LEU:CD2	2:B:71:LEU:N	0.50	2.72	8	3
1:A:493:LEU:O	1:A:497:PHE:CE1	0.50	2.63	8	1
2:B:38:PRO:C	2:B:40:GLN:N	0.50	2.64	9	3
1:A:562:TRP:CD1	1:A:562:TRP:N	0.50	2.80	6	2
1:A:561:ASP:OD1	1:A:561:ASP:N	0.50	2.44	1	1
2:C:18:GLU:H	2:C:21:ASP:CG	0.50	2.10	9	4
1:A:595:MET:O	1:A:597:SER:N	0.50	2.45	4	1
2:C:12:THR:HG22	2:C:13:ILE:N	0.50	2.22	3	1
1:A:510:LEU:N	1:A:511:PRO:HD2	0.49	2.22	10	8
2:C:38:PRO:C	2:C:40:GLN:N	0.49	2.65	1	2
2:B:73:LEU:N	2:B:73:LEU:HD12	0.49	2.22	5	1
1:A:516:THR:OG1	2:C:42:ARG:NH1	0.49	2.44	6	2
1:A:578:GLY:C	1:A:580:GLN:N	0.49	2.66	1	2
2:B:4:PHE:CE2	2:B:14:THR:OG1	0.49	2.62	1	1
1:A:541:ASP:OD1	2:B:74:ARG:NH2	0.49	2.46	9	1
1:A:586:GLU:OE1	2:B:68:HIS:ND1	0.49	2.44	9	1
1:A:545:SER:OG	2:B:73:LEU:CD1	0.49	2.60	9	1
1:A:595:MET:C	1:A:597:SER:N	0.49	2.65	4	2
2:C:17:VAL:HG21	2:C:56:LEU:CD1	0.49	2.37	2	3
1:A:506:LEU:N	1:A:506:LEU:HD12	0.49	2.21	2	2
2:C:22:THR:O	2:C:25:ASN:N	0.49	2.45	9	2
2:B:45:PHE:CD2	2:B:46:ALA:N	0.49	2.81	3	3
1:A:497:PHE:CD1	1:A:497:PHE:N	0.49	2.74	5	1
1:A:493:LEU:O	1:A:496:ALA:N	0.49	2.45	1	1
1:A:516:THR:O	1:A:517:ASP:CB	0.49	2.60	6	1
1:A:596:THR:O	1:A:599:ILE:N	0.49	2.45	7	2
2:C:69:LEU:CD2	2:C:69:LEU:C	0.49	2.81	5	1
2:B:45:PHE:O	2:B:46:ALA:C	0.48	2.50	10	7
2:B:18:GLU:N	2:B:21:ASP:OD2	0.48	2.46	10	1
1:A:593:HIS:CD2	1:A:593:HIS:N	0.48	2.81	3	1
2:C:62:GLN:H	2:C:62:GLN:CD	0.48	2.12	6	1
1:A:549:ASN:O	1:A:553:ARG:N	0.48	2.46	10	1
1:A:491:LEU:N	1:A:491:LEU:HD12	0.48	2.23	4	1
1:A:562:TRP:CD1	1:A:563:VAL:N	0.48	2.81	3	1
1:A:551:LEU:C	1:A:553:ARG:N	0.48	2.67	5	1
2:C:32:ASP:OD1	2:C:32:ASP:N	0.48	2.46	5	1
2:C:39:ASP:OD1	2:C:40:GLN:N	0.48	2.46	9	1
1:A:596:THR:C	1:A:598:ALA:N	0.48	2.66	6	2
2:C:51:GLU:N	2:C:51:GLU:CD	0.48	2.67	6	1
2:B:53:GLY:O	2:B:54:ARG:O	0.48	2.31	6	9
2:B:2:GLN:NE2	2:B:3:ILE:N	0.48	2.61	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:581:VAL:HG13	1:A:582:ASP:N	0.48	2.23	3	2
2:C:8:LEU:N	2:C:8:LEU:HD22	0.48	2.23	7	1
1:A:566:LEU:CD1	1:A:566:LEU:N	0.48	2.76	2	5
2:B:2:GLN:HE21	2:B:3:ILE:CA	0.48	2.20	2	1
2:C:52:ASP:OD1	2:C:52:ASP:N	0.48	2.45	9	1
1:A:538:CYS:C	1:A:539:ASN:ND2	0.48	2.68	5	1
2:B:45:PHE:CE2	2:B:46:ALA:HB3	0.47	2.43	10	1
1:A:564:ARG:O	1:A:567:ALA:HB3	0.47	2.09	8	1
2:C:55:THR:OG1	2:C:57:SER:OG	0.47	2.32	7	2
1:A:587:THR:OG1	2:B:68:HIS:CE1	0.47	2.67	9	1
2:C:72:ARG:CG	2:C:73:LEU:N	0.47	2.77	1	1
2:B:17:VAL:HG21	2:B:56:LEU:CD1	0.47	2.38	2	3
2:B:18:GLU:CB	2:B:19:PRO:CD	0.47	2.92	7	4
1:A:551:LEU:O	1:A:553:ARG:N	0.47	2.48	5	1
2:C:18:GLU:O	2:C:20:SER:N	0.47	2.47	3	2
1:A:552:GLU:OE1	1:A:552:GLU:N	0.47	2.47	10	1
2:B:2:GLN:O	2:B:2:GLN:CG	0.47	2.62	3	1
2:C:70:VAL:HG12	2:C:71:LEU:H	0.47	1.70	2	3
2:B:58:ASP:O	2:B:59:TYR:CD2	0.47	2.67	3	1
2:B:58:ASP:O	2:B:59:TYR:CG	0.47	2.68	3	1
1:A:515:SER:OG	1:A:516:THR:N	0.47	2.48	5	2
1:A:579:GLU:N	1:A:579:GLU:CD	0.47	2.69	6	1
2:C:53:GLY:O	2:C:54:ARG:O	0.47	2.33	10	4
1:A:569:ALA:C	1:A:571:GLY:N	0.46	2.69	10	8
2:B:2:GLN:NE2	2:B:3:ILE:CA	0.46	2.78	2	1
1:A:562:TRP:O	1:A:564:ARG:N	0.46	2.48	4	2
2:C:18:GLU:CB	2:C:19:PRO:CD	0.46	2.93	10	5
2:C:14:THR:C	2:C:15:LEU:HD12	0.46	2.30	10	2
1:A:551:LEU:HD12	1:A:551:LEU:N	0.46	2.24	8	1
1:A:562:TRP:C	1:A:564:ARG:N	0.46	2.69	4	3
2:B:2:GLN:C	2:B:2:GLN:NE2	0.46	2.68	2	1
1:A:512:ILE:O	1:A:518:LEU:HD13	0.46	2.10	10	1
2:C:15:LEU:HD12	2:C:15:LEU:N	0.46	2.25	4	1
2:B:18:GLU:O	2:B:21:ASP:N	0.46	2.47	3	2
2:C:7:THR:O	2:C:9:THR:N	0.46	2.49	5	2
1:A:591:ILE:C	1:A:593:HIS:H	0.46	2.14	2	1
1:A:602:LEU:CD1	1:A:602:LEU:N	0.46	2.78	2	1
2:C:71:LEU:N	2:C:71:LEU:HD12	0.46	2.25	10	1
1:A:506:LEU:CD2	1:A:530:LEU:HD22	0.46	2.41	10	2
1:A:514:ALA:O	1:A:515:SER:C	0.46	2.53	3	2
1:A:520:ILE:O	1:A:520:ILE:HG22	0.46	2.11	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:593:HIS:O	1:A:593:HIS:CG	0.46	2.67	9	1
2:C:39:ASP:O	2:C:72:ARG:CZ	0.46	2.64	4	1
1:A:493:LEU:N	1:A:493:LEU:HD12	0.46	2.25	9	2
1:A:501:LYS:NZ	1:A:501:LYS:CB	0.46	2.78	9	1
1:A:533:VAL:C	1:A:535:VAL:H	0.46	2.15	4	3
1:A:491:LEU:N	1:A:491:LEU:CD1	0.46	2.79	4	1
1:A:579:GLU:CD	1:A:579:GLU:N	0.46	2.69	1	1
1:A:530:LEU:HD23	1:A:530:LEU:C	0.46	2.32	9	2
2:B:51:GLU:N	2:B:51:GLU:CD	0.45	2.69	1	1
2:B:46:ALA:C	2:B:48:LYS:H	0.45	2.14	8	1
2:C:71:LEU:N	2:C:71:LEU:CD1	0.45	2.80	10	1
1:A:531:ALA:O	1:A:535:VAL:N	0.45	2.49	3	3
2:B:22:THR:O	2:B:25:ASN:N	0.45	2.50	1	3
1:A:500:SER:O	1:A:500:SER:OG	0.45	2.33	6	1
1:A:568:LEU:HD12	1:A:568:LEU:N	0.45	2.25	8	1
1:A:517:ASP:CG	1:A:518:LEU:H	0.45	2.14	8	1
2:C:38:PRO:C	2:C:40:GLN:H	0.45	2.14	6	4
1:A:515:SER:C	1:A:516:THR:OG1	0.45	2.55	6	4
2:B:50:LEU:N	2:B:50:LEU:HD23	0.45	2.26	2	1
1:A:587:THR:OG1	2:B:68:HIS:NE2	0.45	2.49	9	1
1:A:581:VAL:CG1	1:A:582:ASP:N	0.45	2.79	3	3
1:A:572:ILE:O	1:A:574:TYR:N	0.45	2.50	6	1
1:A:497:PHE:CD2	1:A:505:VAL:HG11	0.45	2.46	8	1
1:A:520:ILE:HG22	1:A:520:ILE:O	0.45	2.11	1	1
2:B:15:LEU:N	2:B:15:LEU:CD1	0.45	2.80	5	1
2:B:45:PHE:C	2:B:47:GLY:N	0.45	2.70	5	1
2:B:14:THR:C	2:B:15:LEU:HD22	0.45	2.31	4	1
1:A:509:LEU:CD1	1:A:509:LEU:N	0.45	2.80	6	1
1:A:566:LEU:H	1:A:566:LEU:CD1	0.45	2.25	1	1
1:A:509:LEU:CD2	1:A:509:LEU:N	0.45	2.79	5	1
1:A:491:LEU:C	1:A:491:LEU:HD23	0.45	2.32	8	1
1:A:510:LEU:HD13	1:A:510:LEU:C	0.45	2.32	5	1
1:A:567:ALA:O	1:A:571:GLY:N	0.45	2.50	2	1
2:C:22:THR:O	2:C:23:ILE:C	0.45	2.54	9	2
1:A:551:LEU:C	1:A:553:ARG:H	0.44	2.15	4	2
1:A:502:ASN:C	1:A:504:GLU:N	0.44	2.70	6	1
1:A:545:SER:OG	2:B:73:LEU:CD2	0.44	2.65	7	4
1:A:502:ASN:CG	1:A:503:ASP:H	0.44	2.16	3	3
2:B:42:ARG:NH1	2:B:72:ARG:CZ	0.44	2.80	5	1
1:A:577:GLN:OE1	1:A:579:GLU:OE1	0.44	2.35	6	1
2:C:31:GLN:OE1	2:C:36:ILE:C	0.44	2.55	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:55:THR:C	2:C:57:SER:H	0.44	2.15	2	2
2:B:43:LEU:O	2:B:49:GLN:OE1	0.44	2.35	9	2
1:A:546:ILE:O	1:A:550:PHE:CD1	0.44	2.70	7	1
2:C:8:LEU:N	2:C:8:LEU:CD2	0.44	2.80	7	1
2:C:49:GLN:N	2:C:49:GLN:CD	0.44	2.71	1	1
1:A:528:LEU:HD23	1:A:528:LEU:C	0.44	2.33	1	3
1:A:602:LEU:HD23	1:A:602:LEU:C	0.44	2.32	9	1
2:B:2:GLN:O	2:B:64:GLU:OE1	0.44	2.36	9	1
1:A:535:VAL:CG1	1:A:536:GLY:N	0.44	2.80	4	1
2:C:14:THR:C	2:C:15:LEU:HD22	0.44	2.32	1	2
1:A:545:SER:O	1:A:548:ASP:N	0.44	2.51	1	1
2:C:62:GLN:O	2:C:65:SER:OG	0.44	2.35	1	1
1:A:517:ASP:O	1:A:518:LEU:O	0.44	2.36	3	2
1:A:605:SER:OG	1:A:606:CYS:N	0.44	2.51	3	1
2:B:60:ASN:N	2:B:60:ASN:OD1	0.44	2.50	3	1
2:C:18:GLU:O	2:C:21:ASP:OD1	0.44	2.36	3	1
2:B:52:ASP:OD1	2:B:52:ASP:N	0.44	2.50	8	1
1:A:512:ILE:HG22	1:A:512:ILE:O	0.44	2.12	5	1
2:C:8:LEU:O	2:C:9:THR:CG2	0.44	2.66	5	1
2:B:18:GLU:C	2:B:20:SER:N	0.44	2.71	3	1
1:A:572:ILE:C	1:A:574:TYR:N	0.44	2.70	6	1
1:A:566:LEU:N	1:A:566:LEU:CD1	0.43	2.80	1	1
2:C:18:GLU:O	2:C:21:ASP:N	0.43	2.50	3	2
1:A:497:PHE:C	1:A:499:GLY:N	0.43	2.72	8	1
2:B:2:GLN:NE2	2:B:4:PHE:CE2	0.43	2.86	2	1
1:A:510:LEU:HD13	1:A:510:LEU:O	0.43	2.13	5	1
2:C:25:ASN:HD21	2:C:29:LYS:NZ	0.43	2.12	2	1
1:A:568:LEU:O	1:A:571:GLY:N	0.43	2.51	9	1
2:C:21:ASP:OD1	2:C:21:ASP:N	0.43	2.51	6	1
2:C:38:PRO:O	2:C:39:ASP:C	0.43	2.56	8	1
1:A:516:THR:O	1:A:552:GLU:CD	0.43	2.57	7	1
2:C:8:LEU:O	2:C:9:THR:HG23	0.43	2.13	5	1
1:A:606:CYS:O	1:A:607:ALA:HB2	0.43	2.13	9	1
2:C:55:THR:OG1	2:C:58:ASP:OD1	0.43	2.36	9	1
1:A:564:ARG:O	1:A:567:ALA:N	0.43	2.47	8	1
1:A:595:MET:C	1:A:597:SER:H	0.43	2.15	4	2
1:A:497:PHE:C	1:A:499:GLY:H	0.43	2.17	8	1
1:A:530:LEU:O	1:A:530:LEU:HD13	0.43	2.14	8	1
2:C:1:MET:SD	2:C:18:GLU:C	0.43	2.97	8	1
1:A:590:ALA:O	2:B:46:ALA:O	0.43	2.36	2	1
2:C:38:PRO:O	2:C:41:GLN:N	0.43	2.52	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:502:ASN:HD22	1:A:503:ASP:N	0.43	2.12	1	1
2:C:70:VAL:HG12	2:C:71:LEU:N	0.43	2.28	2	1
1:A:499:GLY:O	1:A:500:SER:OG	0.43	2.34	6	1
1:A:521:GLU:N	1:A:521:GLU:CD	0.43	2.72	6	1
2:C:73:LEU:O	2:C:74:ARG:O	0.43	2.37	2	1
2:B:55:THR:C	2:B:57:SER:H	0.43	2.17	9	1
1:A:526:ALA:C	1:A:528:LEU:N	0.43	2.71	10	1
1:A:530:LEU:O	1:A:532:HIS:N	0.43	2.52	6	1
1:A:519:PRO:C	1:A:521:GLU:N	0.43	2.72	1	1
1:A:562:TRP:N	1:A:562:TRP:CD1	0.43	2.86	2	1
1:A:594:PRO:C	1:A:596:THR:H	0.43	2.16	3	2
2:C:31:GLN:OE1	2:C:31:GLN:O	0.43	2.37	9	1
1:A:581:VAL:O	1:A:584:VAL:N	0.42	2.52	2	2
2:B:72:ARG:O	2:B:73:LEU:O	0.42	2.36	1	1
1:A:506:LEU:N	1:A:506:LEU:CD1	0.42	2.82	2	1
2:B:19:PRO:C	2:B:57:SER:OG	0.42	2.57	2	1
2:C:48:LYS:NZ	2:C:48:LYS:CB	0.42	2.82	8	1
1:A:534:PHE:O	1:A:537:THR:O	0.42	2.37	7	1
2:C:22:THR:OG1	2:C:25:ASN:OD1	0.42	2.37	7	1
1:A:524:ALA:O	1:A:525:MET:C	0.42	2.58	3	1
2:C:42:ARG:NH1	2:C:49:GLN:NE2	0.42	2.66	6	1
1:A:517:ASP:OD1	1:A:552:GLU:O	0.42	2.37	1	1
1:A:591:ILE:CG2	1:A:592:GLU:N	0.42	2.82	5	1
2:B:62:GLN:O	2:B:65:SER:OG	0.42	2.36	8	1
1:A:549:ASN:O	1:A:552:GLU:N	0.42	2.52	1	1
1:A:516:THR:O	1:A:552:GLU:OE2	0.42	2.37	3	1
1:A:550:PHE:CE2	1:A:566:LEU:HD21	0.42	2.50	4	1
2:B:22:THR:OG1	2:B:24:GLU:CG	0.42	2.68	6	1
1:A:596:THR:O	1:A:597:SER:C	0.42	2.58	7	1
1:A:525:MET:O	1:A:528:LEU:CB	0.42	2.67	9	1
2:C:1:MET:O	2:C:17:VAL:O	0.42	2.37	10	1
2:B:40:GLN:OE1	2:B:72:ARG:NE	0.42	2.53	3	1
2:C:62:GLN:N	2:C:62:GLN:CD	0.42	2.72	6	1
2:B:22:THR:OG1	2:B:25:ASN:OD1	0.42	2.37	7	1
2:B:75:GLY:O	2:B:76:GLY:OXT	0.42	2.38	1	1
1:A:516:THR:O	1:A:552:GLU:OE1	0.42	2.37	4	1
2:B:7:THR:C	2:B:9:THR:H	0.42	2.17	7	1
2:B:54:ARG:NE	2:B:54:ARG:CA	0.42	2.82	3	1
1:A:543:THR:O	1:A:544:THR:C	0.42	2.58	9	1
1:A:524:ALA:O	1:A:527:SER:OG	0.42	2.36	10	1
2:B:18:GLU:C	2:B:20:SER:H	0.42	2.18	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:506:LEU:O	1:A:511:PRO:CD	0.42	2.68	7	1
1:A:568:LEU:C	1:A:568:LEU:CD1	0.42	2.88	7	1
1:A:512:ILE:CG2	1:A:512:ILE:O	0.42	2.68	5	1
1:A:504:GLU:O	1:A:505:VAL:C	0.42	2.58	4	1
1:A:530:LEU:HD23	1:A:530:LEU:O	0.41	2.14	1	1
2:C:60:ASN:O	2:C:62:GLN:N	0.41	2.53	6	1
2:B:7:THR:O	2:B:9:THR:N	0.41	2.51	7	1
2:B:8:LEU:O	2:B:8:LEU:HD23	0.41	2.15	1	1
1:A:520:ILE:O	1:A:522:THR:N	0.41	2.53	3	1
1:A:509:LEU:O	1:A:510:LEU:C	0.41	2.58	4	1
1:A:553:ARG:NH1	1:A:562:TRP:CH2	0.41	2.87	4	1
1:A:519:PRO:C	1:A:521:GLU:H	0.41	2.18	5	1
1:A:518:LEU:HD12	1:A:518:LEU:O	0.41	2.15	10	1
1:A:528:LEU:O	1:A:528:LEU:HD23	0.41	2.15	10	1
1:A:530:LEU:C	1:A:532:HIS:N	0.41	2.73	6	1
1:A:561:ASP:OD1	1:A:561:ASP:O	0.41	2.38	7	1
2:C:19:PRO:O	2:C:57:SER:CB	0.41	2.69	5	1
2:B:38:PRO:O	2:B:39:ASP:C	0.41	2.58	4	2
1:A:497:PHE:CE1	1:A:533:VAL:HG21	0.41	2.51	4	1
1:A:510:LEU:C	1:A:510:LEU:CD1	0.41	2.89	5	1
1:A:514:ALA:HB2	1:A:545:SER:OG	0.41	2.15	5	1
2:C:73:LEU:HD23	2:C:73:LEU:C	0.41	2.36	5	1
2:B:16:GLU:OE2	2:B:18:GLU:OE2	0.41	2.37	3	1
2:B:1:MET:N	2:B:17:VAL:O	0.41	2.38	10	2
1:A:511:PRO:C	1:A:513:ALA:N	0.41	2.73	5	2
1:A:522:THR:O	1:A:526:ALA:HB2	0.41	2.16	10	1
2:C:12:THR:CG2	2:C:13:ILE:N	0.41	2.83	3	1
1:A:581:VAL:O	1:A:582:ASP:C	0.41	2.59	2	1
1:A:587:THR:HG1	2:B:68:HIS:CE1	0.41	2.34	9	1
2:C:44:ILE:HD12	2:C:70:VAL:HG21	0.41	1.92	9	1
1:A:497:PHE:O	1:A:498:ALA:C	0.41	2.58	4	2
2:C:11:LYS:NZ	2:C:34:GLU:OE2	0.41	2.45	2	1
2:C:55:THR:C	2:C:57:SER:N	0.41	2.73	2	1
2:C:18:GLU:C	2:C:20:SER:N	0.41	2.74	3	1
2:B:51:GLU:CD	2:B:51:GLU:N	0.41	2.74	6	1
1:A:608:TYR:CD1	1:A:608:TYR:N	0.41	2.89	7	1
2:C:7:THR:OG1	2:C:9:THR:OG1	0.41	2.38	7	1
1:A:491:LEU:HD23	1:A:491:LEU:C	0.41	2.35	7	1
1:A:566:LEU:H	1:A:566:LEU:HD12	0.41	1.76	1	1
2:B:73:LEU:O	2:B:74:ARG:O	0.41	2.39	1	1
1:A:580:GLN:OE1	1:A:580:GLN:O	0.41	2.39	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:509:LEU:N	1:A:509:LEU:HD12	0.41	2.30	6	1
1:A:541:ASP:O	1:A:545:SER:OG	0.41	2.33	1	1
2:B:28:ALA:O	2:B:32:ASP:OD2	0.40	2.39	7	1
1:A:568:LEU:N	1:A:568:LEU:HD12	0.40	2.30	5	1
1:A:545:SER:O	1:A:547:MET:N	0.40	2.55	1	1
2:C:42:ARG:NH1	2:C:49:GLN:CD	0.40	2.74	2	1
2:C:20:SER:O	2:C:21:ASP:C	0.40	2.60	6	1
1:A:495:ILE:HG22	1:A:495:ILE:O	0.40	2.16	8	1
2:B:46:ALA:C	2:B:48:LYS:N	0.40	2.74	8	1
1:A:530:LEU:C	1:A:530:LEU:CD2	0.40	2.90	9	1
1:A:502:ASN:OD1	1:A:503:ASP:OD1	0.40	2.40	10	1
2:B:60:ASN:ND2	2:B:60:ASN:N	0.40	2.68	10	1
2:B:28:ALA:O	2:B:32:ASP:OD1	0.40	2.39	6	1
2:C:7:THR:C	2:C:9:THR:H	0.40	2.20	1	1
1:A:496:ALA:C	1:A:498:ALA:H	0.40	2.19	5	1
2:B:57:SER:C	2:B:59:TYR:H	0.40	2.19	10	1
1:A:593:HIS:O	1:A:594:PRO:O	0.40	2.38	4	1
2:B:39:ASP:N	2:B:39:ASP:OD1	0.40	2.55	8	1
1:A:568:LEU:C	1:A:568:LEU:HD13	0.40	2.36	7	1
1:A:491:LEU:O	1:A:494:GLY:N	0.40	2.54	5	1
1:A:562:TRP:CE3	1:A:563:VAL:N	0.40	2.90	10	1
2:C:28:ALA:O	2:C:32:ASP:OD1	0.40	2.39	3	1
1:A:531:ALA:O	1:A:535:VAL:CA	0.40	2.70	4	1
1:A:506:LEU:CD1	1:A:506:LEU:N	0.40	2.84	6	1
2:C:60:ASN:O	2:C:61:ILE:C	0.40	2.60	6	1
1:A:568:LEU:N	1:A:568:LEU:CD1	0.40	2.84	8	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	113/131 (86%)	71±4 (63±3%)	31±4 (28±3%)	11±2 (9±2%)	2	11
2	B	74/76 (97%)	54±1 (73±1%)	16±1 (21±2%)	5±1 (6±1%)	3	21
2	C	74/76 (97%)	58±2 (78±2%)	13±2 (18±2%)	3±1 (4±2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2610/2830 (92%)	1828 (70%)	600 (23%)	182 (7%)	<b>3</b> <b>17</b>

All 68 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	C	35	GLY	10
2	B	35	GLY	10
2	B	54	ARG	10
1	A	516	THR	7
2	C	54	ARG	6
1	A	592	GLU	5
1	A	594	PRO	5
1	A	562	TRP	5
1	A	570	LEU	4
2	B	47	GLY	4
1	A	514	ALA	4
2	B	39	ASP	4
1	A	577	GLN	4
1	A	575	MET	4
2	B	46	ALA	4
1	A	515	SER	4
1	A	607	ALA	4
1	A	517	ASP	4
1	A	491	LEU	3
2	C	9	THR	3
1	A	569	ALA	3
1	A	500	SER	3
1	A	503	ASP	3
2	C	61	ILE	3
2	C	10	GLY	3
1	A	602	LEU	3
2	B	72	ARG	2
1	A	552	GLU	2
1	A	597	SER	2
1	A	536	GLY	2
2	B	34	GLU	2
1	A	499	GLY	2
2	B	75	GLY	2
2	C	39	ASP	2
1	A	519	PRO	2
1	A	576	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	561	ASP	2
2	C	74	ARG	2
1	A	518	LEU	2
2	B	74	ARG	2
1	A	578	GLY	2
1	A	568	LEU	2
1	A	573	LEU	2
1	A	502	ASN	2
2	C	34	GLU	1
2	B	8	LEU	1
1	A	596	THR	1
1	A	534	PHE	1
1	A	553	ARG	1
2	C	41	GLN	1
1	A	579	GLU	1
1	A	501	LYS	1
2	B	73	LEU	1
2	B	10	GLY	1
1	A	531	ALA	1
2	C	19	PRO	1
1	A	563	VAL	1
1	A	505	VAL	1
2	B	19	PRO	1
1	A	595	MET	1
1	A	591	ILE	1
1	A	520	ILE	1
1	A	593	HIS	1
2	B	45	PHE	1
1	A	564	ARG	1
1	A	566	LEU	1
1	A	537	THR	1
1	A	524	ALA	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	88/102 (86%)	83±2 (94±2%)	5±2 (6±2%)	27 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	68/68 (100%)	64±1 (94±2%)	4±1 (6±2%)	24 71
2	C	68/68 (100%)	65±1 (95±2%)	3±1 (5±2%)	33 78
All	All	2240/2380 (94%)	2109 (94%)	131 (6%)	28 74

All 51 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)
2	B	8	LEU	10
2	B	52	ASP	10
2	C	52	ASP	10
1	A	546	ILE	9
2	C	1	MET	6
2	B	20	SER	5
1	A	516	THR	5
2	C	20	SER	5
1	A	549	ASN	4
1	A	593	HIS	4
2	B	1	MET	3
2	B	68	HIS	3
1	A	518	LEU	3
1	A	515	SER	3
1	A	530	LEU	3
2	C	25	ASN	2
2	B	71	LEU	2
1	A	510	LEU	2
2	C	21	ASP	2
2	C	8	LEU	2
1	A	503	ASP	2
2	C	13	ILE	2
2	B	25	ASN	2
2	C	70	VAL	2
1	A	502	ASN	2
1	A	545	SER	2
2	B	58	ASP	2
2	B	39	ASP	1
1	A	532	HIS	1
2	C	31	GLN	1
2	B	65	SER	1
2	B	49	GLN	1
1	A	580	GLN	1

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Mol	Chain	Res	Type	Models (Total)
2	B	13	ILE	1
1	A	522	THR	1
1	A	505	VAL	1
2	C	68	HIS	1
1	A	561	ASP	1
2	B	14	THR	1
1	A	575	MET	1
1	A	595	MET	1
1	A	508	LEU	1
2	B	67	LEU	1
1	A	568	LEU	1
1	A	541	ASP	1
1	A	528	LEU	1
1	A	537	THR	1
2	C	60	ASN	1
1	A	582	ASP	1
1	A	553	ARG	1
2	B	54	ARG	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 carbohydrates in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 24% for the well-defined parts and 25% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2n3w\_cs.str

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

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1034
Number of shifts mapped to atoms	1034
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
$^{13}\text{C}_\alpha$	96	$-0.46 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	92	$0.22 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	63	$0.80 \pm 0.70$	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 24%, i.e. 767 atoms were assigned a chemical shift out of a possible 3181. 20 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	295/1307 (23%)	148/521 (28%)	89/530 (17%)	58/256 (23%)
Sidechain	448/1730 (26%)	265/999 (27%)	183/665 (28%)	0/66 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	24/144 (17%)	24/78 (31%)	0/61 (0%)	0/5 (0%)
Overall	767/3181 (24%)	437/1598 (27%)	272/1256 (22%)	58/327 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 25%, i.e. 833 atoms were assigned a chemical shift out of a possible 3365. 21 out of 51 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	319/1397 (23%)	160/557 (29%)	96/566 (17%)	63/274 (23%)
Sidechain	490/1824 (27%)	290/1052 (28%)	200/704 (28%)	0/68 (0%)
Aromatic	24/144 (17%)	24/78 (31%)	0/61 (0%)	0/5 (0%)
Overall	833/3365 (25%)	474/1687 (28%)	296/1331 (22%)	63/347 (18%)

#### 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:

