



# wwPDB NMR Structure Validation Summary Report ⓘ

Nov 2, 2024 – 01:00 PM EDT

PDB ID : 6N13  
Title : UbCH7-Ub Complex with R0RBR Parkin and phosphoubiquitin  
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This is a wwPDB NMR Structure Validation Summary 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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.39

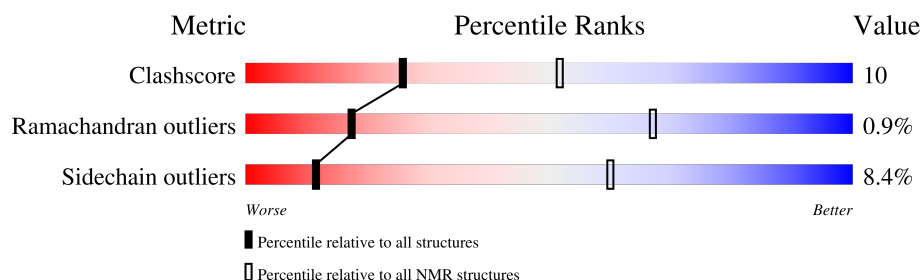
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 5%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	B	322	
2	D	76	
3	C	156	
4	A	76	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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	B:144-B:337, B:389-B:465, C:501-C:654, A:1-A:64, A:66-A:70 (494)	0.64	8
2	D:701-D:771 (71)	0.36	3

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6
2	3, 8
3	7, 10
Single-model clusters	1; 9

### 3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6124 atoms, of which 1146 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	322	Total	C	H	N	O	S	0
			3070	1548	567	454	462	39	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	347	CYS	GLN	engineered mutation	UNP O60260

- Molecule 2 is a protein called ubiquitin.

Mol	Chain	Residues	Atoms						Trace
2	D	76	Total	C	H	N	O	S	0
			746	378	145	105	117	1	

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 L3.

Mol	Chain	Residues	Atoms						Trace
3	C	154	Total	C	H	N	O	S	0
			1551	807	290	218	233	3	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	499	GLY	-	expression tag	UNP P68036
C	500	HIS	-	expression tag	UNP P68036
C	517	SER	CYS	engineered mutation	UNP P68036
C	586	LYS	CYS	engineered mutation	UNP P68036
C	637	SER	CYS	engineered mutation	UNP P68036

- Molecule 4 is a protein called phosphoubiquitin.

Mol	Chain	Residues	Atoms							Trace
4	A	76	Total	C	H	N	O	P	S	0
			749	378	144	105	120	1	1	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

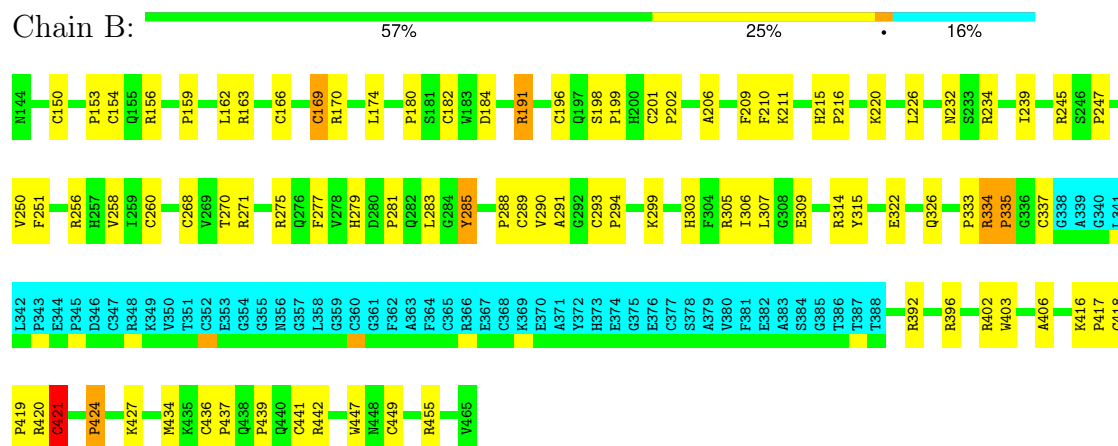
Mol	Chain	Residues	Atoms	
5	B	8	Total	Zn
			8	8

## 4 Residue-property plots

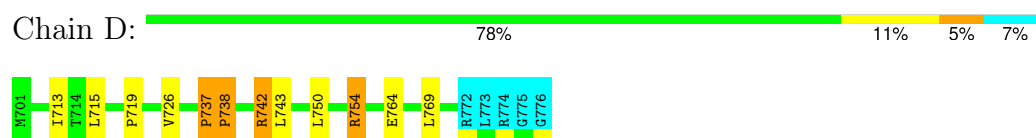
### 4.1 Average score per residue in the NMR ensemble

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.

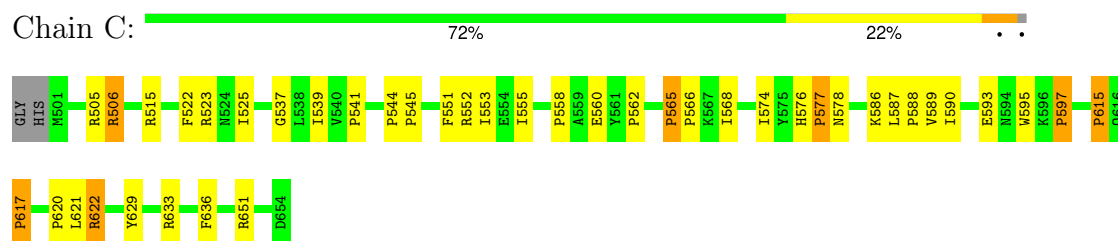
- Molecule 1: E3 ubiquitin-protein ligase parkin



- Molecule 2: ubiquitin



- Molecule 3: Ubiquitin-conjugating enzyme E2 L3



- Molecule 4: phosphoubiquitin

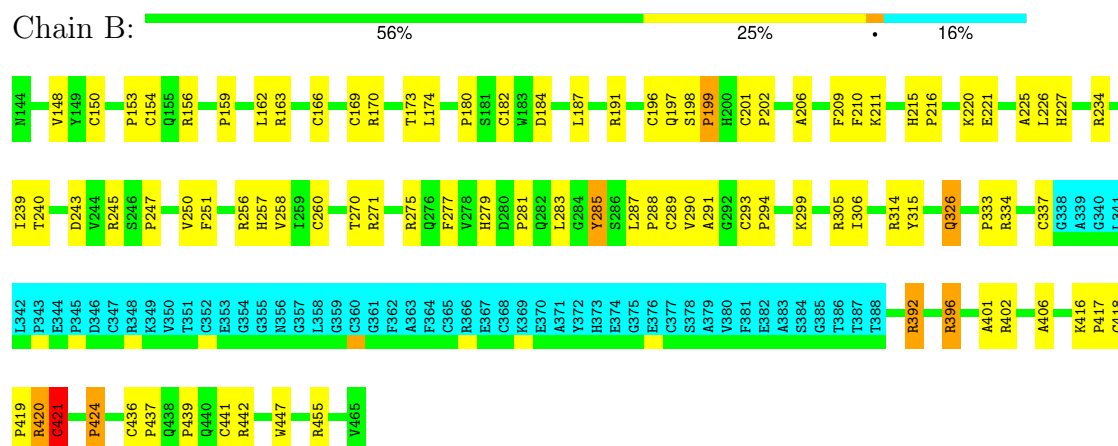




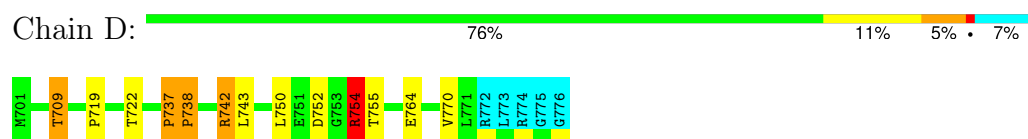
## 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

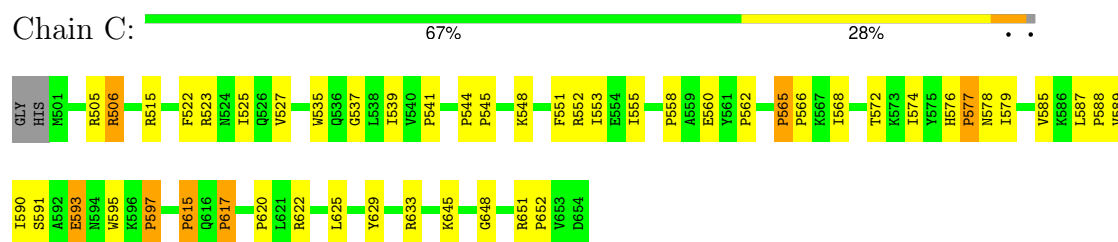
- Molecule 1: E3 ubiquitin-protein ligase parkin



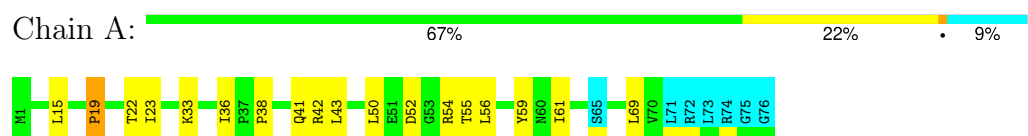
- Molecule 2: ubiquitin



- Molecule 3: Ubiquitin-conjugating enzyme E2 L3



- Molecule 4: phosphoubiquitin



## 5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 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
HADDOCK	structure calculation	
PyMOL	geometry optimization	2.0.0

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	398
Number of shifts mapped to atoms	398
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	5%



## 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, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	0.46±0.02	0±0/2197 ( 0.0± 0.0%)	1.16±0.03	21±1/2980 ( 0.7± 0.0%)
2	D	0.43±0.02	0±0/570 ( 0.0± 0.0%)	0.93±0.04	2±0/770 ( 0.3± 0.1%)
3	C	0.46±0.02	0±0/1292 ( 0.0± 0.0%)	1.10±0.03	9±1/1743 ( 0.5± 0.0%)
4	A	0.42±0.02	0±0/555 ( 0.0± 0.0%)	0.96±0.05	2±0/748 ( 0.3± 0.0%)
All	All	0.45	2/46140 ( 0.0%)	1.10	345/62410 ( 0.6%)

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	B	0.0±0.0	3.2±1.1
2	D	0.0±0.0	0.8±0.6
3	C	0.0±0.0	1.7±0.8
4	A	0.0±0.0	0.1±0.3
All	All	0	58

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	436	CYS	CB-SG	-7.29	1.69	1.82	2	2

5 of 45 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	436	CYS	CA-CB-SG	18.66	147.60	114.00	2	2
1	B	421	CYS	CA-CB-SG	9.89	131.81	114.00	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	54	ARG	NE-CZ-NH1	8.48	124.54	120.30	4	10
1	B	256	ARG	NE-CZ-NH1	8.29	124.44	120.30	7	10
3	C	622	ARG	NE-CZ-NH1	8.13	124.37	120.30	1	10

There are no chirality outliers.

5 of 19 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	285	TYR	Sidechain	9
1	B	315	TYR	Sidechain	9
3	C	506	ARG	Sidechain	9
2	D	754	ARG	Sidechain	7
1	B	392	ARG	Sidechain	3

## 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	B	2140	491	2049	54±9
2	D	563	130	583	10±6
3	C	1261	290	1274	22±5
4	A	549	127	570	9±2
5	B	8	0	0	10±2
All	All	45210	10380	44758	900

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 10.

5 of 320 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:201:CYS:HG	5:B:504:ZN:ZN	0.95	0.69	7	9
1:B:250:VAL:HG22	1:B:258:VAL:HG12	0.92	1.40	7	10
1:B:436:CYS:HG	5:B:507:ZN:ZN	0.89	0.75	6	10
3:C:548:LYS:HB3	3:C:645:LYS:HE2	0.87	1.46	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:217:THR:HB	1:B:221:GLU:HG2	0.86	1.42	6	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	B	269/322 (84%)	234±4 (87±2%)	30±4 (11±2%)	5±1 (2±0%)	10	54
2	D	70/76 (92%)	68±2 (97±3%)	2±2 (3±3%)	0±0 (0±0%)	100	100
3	C	152/156 (97%)	140±2 (92±1%)	11±2 (7±1%)	1±0 (0±0%)	32	76
4	A	68/76 (89%)	65±2 (96±2%)	3±2 (4±2%)	0±0 (0±0%)	50	84
All	All	5590/6300 (89%)	5073 (91%)	464 (8%)	53 (1%)	17	67

5 of 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	406	ALA	10
1	B	421	CYS	10
1	B	424	PRO	7
1	B	328	GLY	4
1	B	335	PRO	4

### 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	B	241/278 (87%)	220±1 (91±1%)	21±1 (9±1%)	11	59
2	D	65/68 (96%)	61±1 (94±1%)	4±1 (6±1%)	17	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	138/139 (99%)	123±1 (89±1%)	15±1 (11±1%)	8	53
4	A	63/67 (94%)	60±1 (95±1%)	3±1 (5±1%)	23	76
All	All	5070/5520 (92%)	4643 (92%)	427 (8%)	11	60

5 of 70 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	B	153	PRO	10
1	B	159	PRO	10
1	B	202	PRO	10
1	B	220	LYS	10
1	B	247	PRO	10

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	SEP	A	65	4	8,9,10	1.02±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
4	SEP	A	65	4	7,12,14	2.89±0.20	3±0 (42±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SEP	A	65	4	-	0±0,6,8,10	-

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	65	SEP	OG-CB-CA	6.84	114.80	108.14	2	10
4	A	65	SEP	OG-P-O1P	3.22	115.13	106.44	10	10
4	A	65	SEP	O2P-P-OG	2.79	113.94	106.67	3	10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 5% for the well-defined parts and 5% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_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	398
Number of shifts mapped to atoms	398
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
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	205	$0.54 \pm 0.38$	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 5%, i.e. 387 atoms were assigned a chemical shift out of a possible 7777. 0 out of 77 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	387/2779 (14%)	187/1122 (17%)	0/1130 (0%)	200/527 (38%)
Sidechain	0/4458 (0%)	0/2876 (0%)	0/1389 (0%)	0/193 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/540 (0%)	0/268 (0%)	0/245 (0%)	0/27 (0%)
Overall	387/7777 (5%)	187/4266 (4%)	0/2764 (0%)	200/747 (27%)

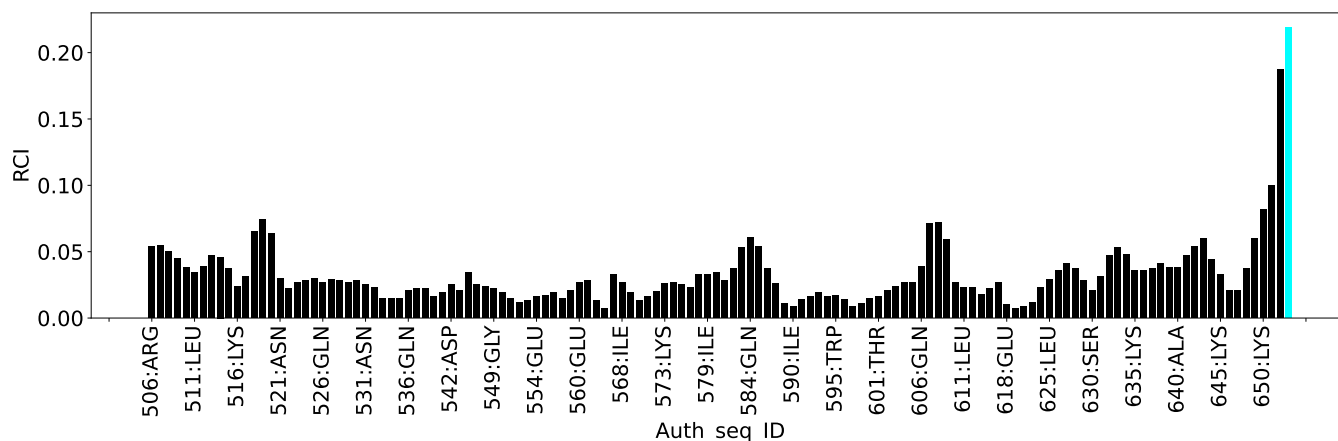
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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

Random coil index (RCI) for chain C:



Random coil index (RCI) for chain D:



