



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:04 PM UTC

PDB ID : 6Y3L / pdb_00006y3l
BMRB ID : 28016
Title : NMR solution structure of the hazelnut allergen Cor a 1.0404
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Deposited on : 2020-02-18

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

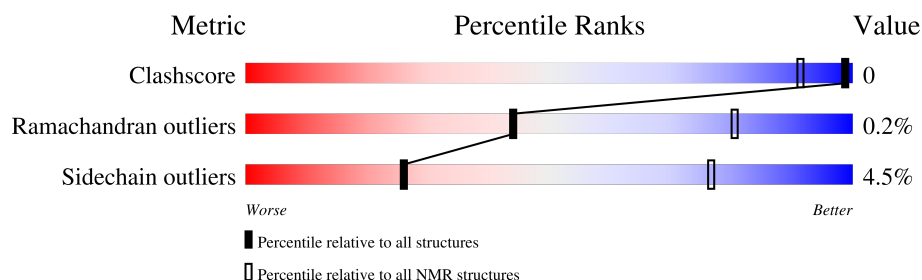
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

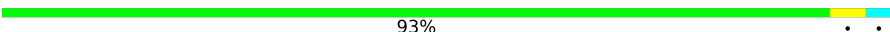
The overall completeness of chemical shifts assignment is 84%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	160	 93% . .

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 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:2-A:59, A:64-A:160 (155)	0.49	16

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

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

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

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2449 atoms, of which 1217 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major allergen variant Cor a 1.0404.

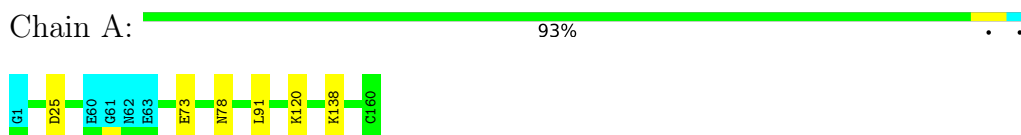
Mol	Chain	Residues	Atoms						Trace
1	A	160	Total	C	H	N	O	S	0
			2449	792	1217	202	234	4	

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: Major allergen variant Cor a 1.0404

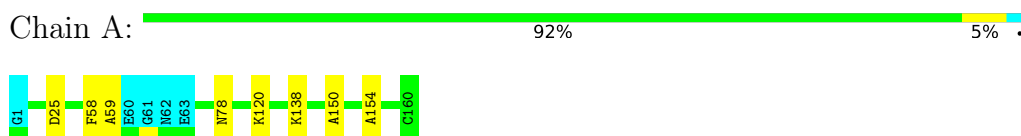


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

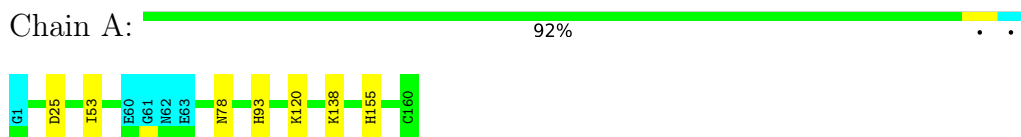
4.2.1 Score per residue for model 1

- Molecule 1: Major allergen variant Cor a 1.0404



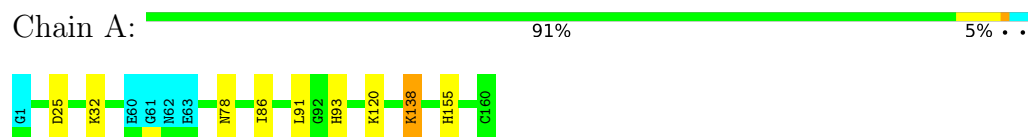
4.2.2 Score per residue for model 2

- Molecule 1: Major allergen variant Cor a 1.0404



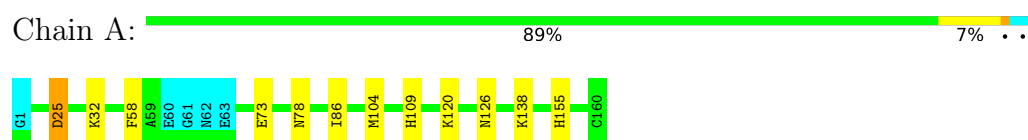
4.2.3 Score per residue for model 3

- Molecule 1: Major allergen variant Cor a 1.0404



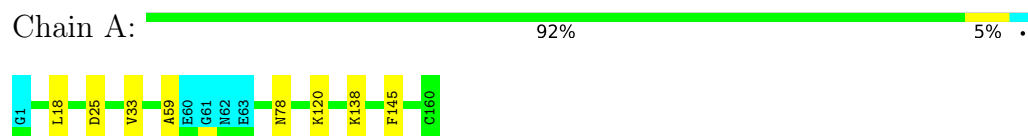
4.2.4 Score per residue for model 4

- Molecule 1: Major allergen variant Cor a 1.0404



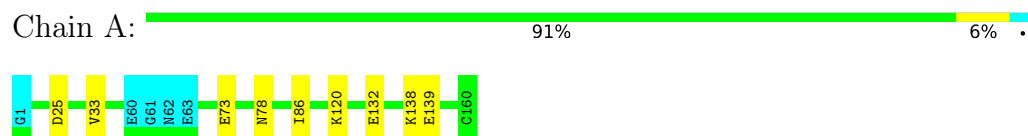
4.2.5 Score per residue for model 5

- Molecule 1: Major allergen variant Cor a 1.0404



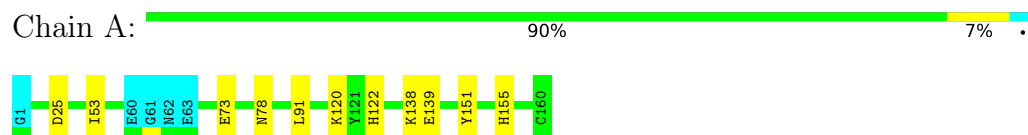
4.2.6 Score per residue for model 6

- Molecule 1: Major allergen variant Cor a 1.0404



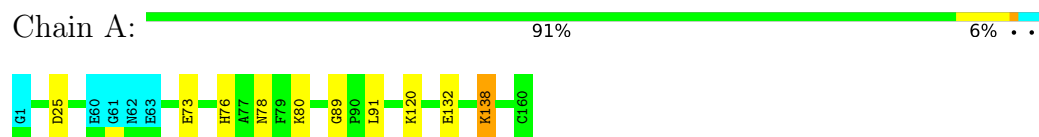
4.2.7 Score per residue for model 7

- Molecule 1: Major allergen variant Cor a 1.0404



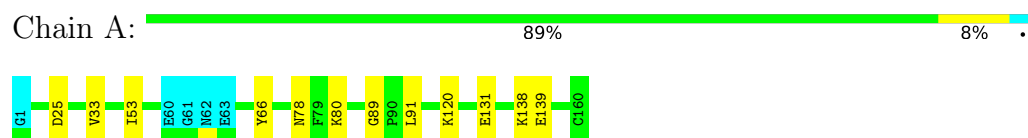
4.2.8 Score per residue for model 8

- Molecule 1: Major allergen variant Cor a 1.0404



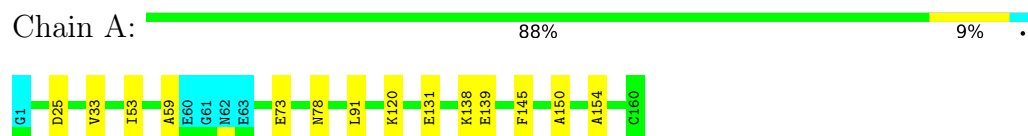
4.2.9 Score per residue for model 9

- Molecule 1: Major allergen variant Cor a 1.0404



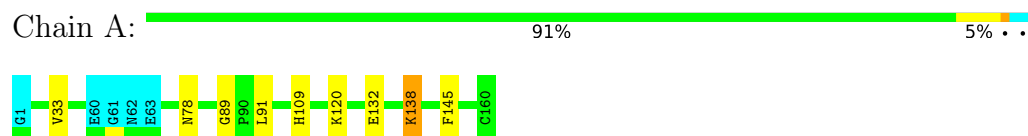
4.2.10 Score per residue for model 10

- Molecule 1: Major allergen variant Cor a 1.0404



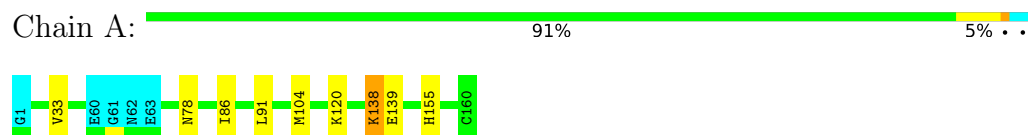
4.2.11 Score per residue for model 11

- Molecule 1: Major allergen variant Cor a 1.0404



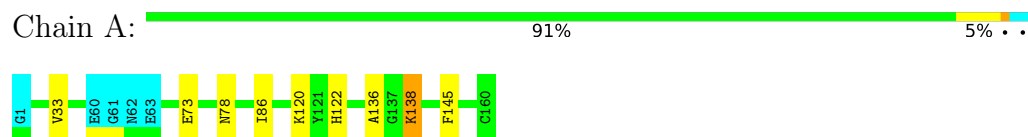
4.2.12 Score per residue for model 12

- Molecule 1: Major allergen variant Cor a 1.0404



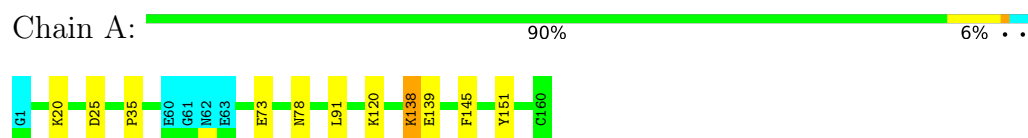
4.2.13 Score per residue for model 13

- Molecule 1: Major allergen variant Cor a 1.0404



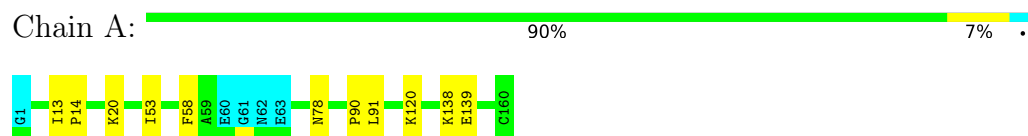
4.2.14 Score per residue for model 14

- Molecule 1: Major allergen variant Cor a 1.0404



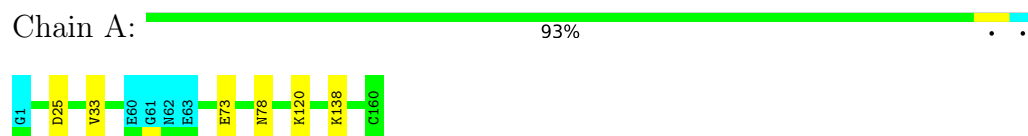
4.2.15 Score per residue for model 15

- Molecule 1: Major allergen variant Cor a 1.0404



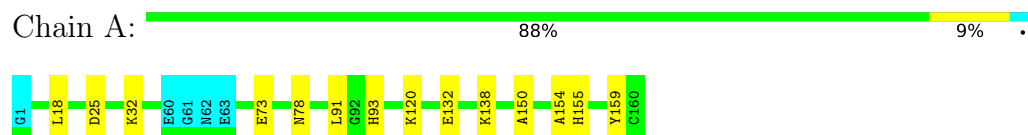
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Major allergen variant Cor a 1.0404



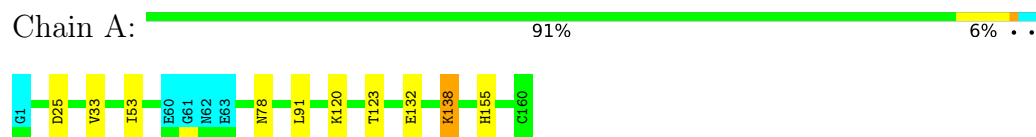
4.2.17 Score per residue for model 17

- Molecule 1: Major allergen variant Cor a 1.0404



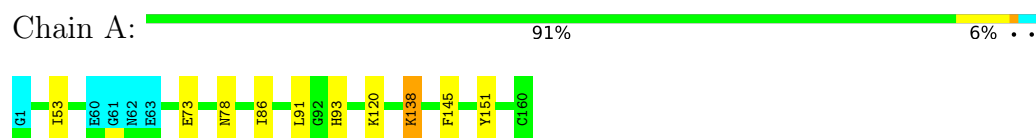
4.2.18 Score per residue for model 18

- Molecule 1: Major allergen variant Cor a 1.0404



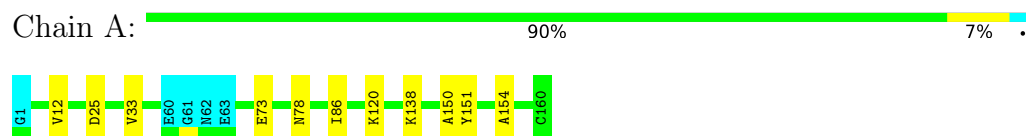
4.2.19 Score per residue for model 19

- Molecule 1: Major allergen variant Cor a 1.0404



4.2.20 Score per residue for model 20

- Molecule 1: Major allergen variant Cor a 1.0404



5 Refinement protocol and experimental data overview

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

Of the 40 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 calculation	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1742
Number of shifts mapped to atoms	1742
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality

6.1 Standard geometry

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	A	0.83±0.01	0±0/1229 (0.0± 0.0%)	1.41±0.02	4±1/1658 (0.3± 0.1%)
All	All	0.83	1/24580 (0.0%)	1.41	85/33160 (0.3%)

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	1.1±0.9
All	All	0	22

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	14	PRO	CA-C	5.33	1.54	1.51	15	1

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
1	A	58	PHE	CA-CB-CG	6.62	120.42	113.80	4	3
1	A	155	HIS	CB-CG-CD2	-5.97	123.44	131.20	4	7
1	A	13	ILE	CA-C-N	5.73	123.84	119.66	15	1
1	A	13	ILE	C-N-CA	5.73	123.84	119.66	15	1
1	A	25	ASP	CA-C-N	5.68	128.17	120.44	1	14
1	A	25	ASP	C-N-CA	5.68	128.17	120.44	1	14
1	A	20	LYS	CA-C-N	5.59	128.24	120.63	15	2
1	A	20	LYS	C-N-CA	5.59	128.24	120.63	15	2
1	A	25	ASP	CA-CB-CG	5.59	118.19	112.60	18	2
1	A	145	PHE	CA-CB-CG	5.53	119.33	113.80	14	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	138	LYS	CA-CB-CG	5.49	125.08	114.10	8	8
1	A	151	TYR	CA-C-N	5.48	127.89	120.65	19	1
1	A	151	TYR	C-N-CA	5.48	127.89	120.65	19	1
1	A	59	ALA	N-CA-C	5.43	117.31	110.24	1	2
1	A	93	HIS	CB-CG-CD2	-5.36	124.24	131.20	19	4
1	A	89	GLY	CA-C-N	5.34	125.00	119.56	8	3
1	A	89	GLY	C-N-CA	5.34	125.00	119.56	8	3
1	A	18	LEU	CA-C-N	5.28	127.62	120.65	17	2
1	A	18	LEU	C-N-CA	5.28	127.62	120.65	17	2
1	A	122	HIS	CB-CG-CD2	-5.25	124.37	131.20	7	2
1	A	109	HIS	CB-CG-CD2	-5.24	124.39	131.20	4	2
1	A	76	HIS	CB-CG-CD2	-5.15	124.50	131.20	8	1
1	A	136	ALA	CA-C-N	5.05	125.55	119.94	13	1
1	A	136	ALA	C-N-CA	5.05	125.55	119.94	13	1

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)
1	A	91	LEU	Peptide	12
1	A	139	GLU	Peptide	7
1	A	151	TYR	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	A	1198	1191	1191	0±1
All	All	23960	23820	23820	6

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ALA:O	1:A:154:ALA:HB3	0.41	2.15	1	4
1:A:131:GLU:H	1:A:131:GLU:CD	0.41	2.23	9	2

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	154/160 (96%)	148±2 (96±1%)	6±2 (4±1%)	0±0 (0±0%)	44	80
All	All	3080/3200 (96%)	2955 (96%)	120 (4%)	5 (0%)	44	80

All 5 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	126	ASN	1
1	A	59	ALA	1
1	A	35	PRO	1
1	A	159	TYR	1
1	A	12	VAL	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	124/127 (98%)	118±1 (95±1%)	6±1 (5±1%)	26	77
All	All	2480/2540 (98%)	2368 (95%)	112 (5%)	26	77

All 15 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	78	ASN	20
1	A	120	LYS	20
1	A	138	LYS	20
1	A	73	GLU	11
1	A	33	VAL	10
1	A	53	ILE	7
1	A	86	ILE	7
1	A	132	GLU	5
1	A	32	LYS	3
1	A	25	ASP	2
1	A	104	MET	2
1	A	80	LYS	2
1	A	66	TYR	1
1	A	90	PRO	1
1	A	123	THR	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 oligosaccharides 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 [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 84% for the well-defined parts and 83% 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	1742
Number of shifts mapped to atoms	1742
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
$^{13}\text{C}_\alpha$	145	-0.23 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	134	-0.17 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	144	-0.13 ± 0.13	None needed (< 0.5 ppm)
^{15}N	132	0.31 ± 0.35	None needed (< 0.5 ppm)

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 84%, i.e. 1737 atoms were assigned a chemical shift out of a possible 2058. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	704/770 (91%)	284/314 (90%)	288/310 (93%)	132/146 (90%)
Sidechain	919/1082 (85%)	616/708 (87%)	295/347 (85%)	8/27 (30%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	114/206 (55%)	53/100 (53%)	51/94 (54%)	10/12 (83%)
Overall	1737/2058 (84%)	953/1122 (85%)	634/751 (84%)	150/185 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1742 atoms were assigned a chemical shift out of a possible 2106. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	705/797 (88%)	284/326 (87%)	289/320 (90%)	132/151 (87%)
Sidechain	923/1103 (84%)	618/720 (86%)	296/355 (83%)	9/28 (32%)
Aromatic	114/206 (55%)	53/100 (53%)	51/94 (54%)	10/12 (83%)
Overall	1742/2106 (83%)	955/1146 (83%)	636/769 (83%)	151/191 (79%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

