



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:10 PM UTC

PDB ID : 7DTA / pdb_00007dta
BMRB ID : 36404
Title : Solution structure of the C-clamp domain from human HDBP1 in complex with DNA
Authors : Duan, B.; Xia, B.
Deposited on : 2021-01-04

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

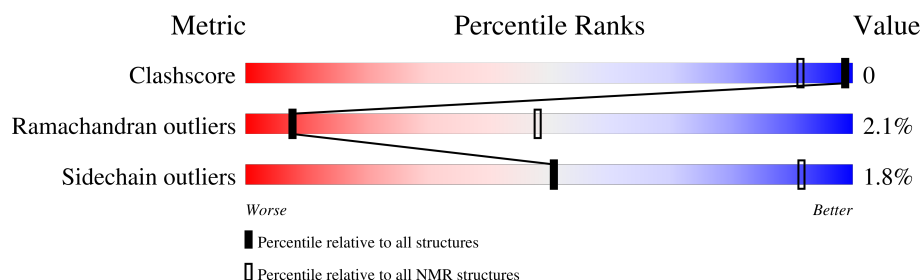
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 62%.

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	33	
2	B	11	
3	C	11	

2 Ensemble composition and analysis

This entry contains 20 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:359-A:382 (24)	0.24	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 and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1253 atoms, of which 528 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SLC2A4 regulator.

Mol	Chain	Residues	Atoms						Trace
1	A	33	Total	C	H	N	O	S	0
			557	173	278	56	45	5	

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms						Trace
2	B	11	Total	C	H	N	O	P	0
			349	107	125	43	64	10	

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3').

Mol	Chain	Residues	Atoms						Trace
3	C	11	Total	C	H	N	O	P	0
			346	106	125	41	64	10	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

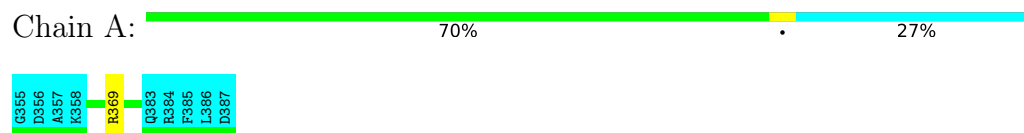
Mol	Chain	Residues	Atoms	
4	A	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

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: SLC2A4 regulator

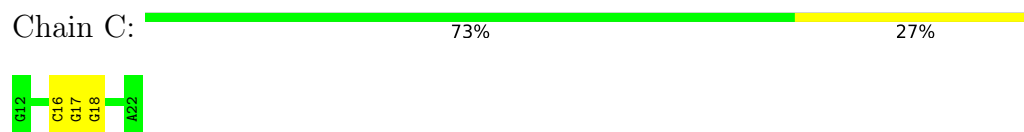


- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')



There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

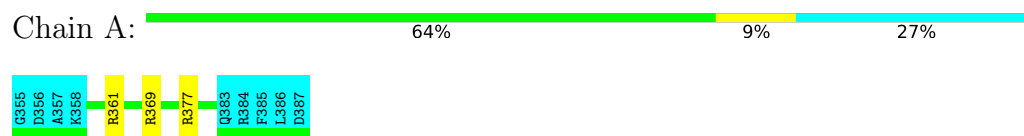


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: SLC2A4 regulator



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  91% 9%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C:  73% 27%



4.2.2 Score per residue for model 2

- Molecule 1: SLC2A4 regulator

Chain A:  67% 6% 27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  73% 27%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

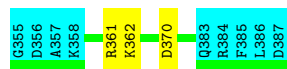
Chain C:  73% 27%



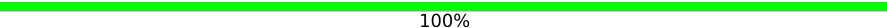
4.2.3 Score per residue for model 3

- Molecule 1: SLC2A4 regulator

Chain A:  64% 9% 27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C: 



4.2.4 Score per residue for model 4

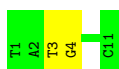
- Molecule 1: SLC2A4 regulator

Chain A: 



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B: 



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C: 



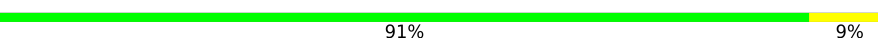
4.2.5 Score per residue for model 5

- Molecule 1: SLC2A4 regulator

Chain A: 

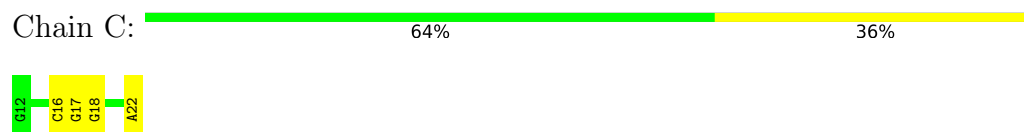


- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B: 



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')



4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: SLC2A4 regulator

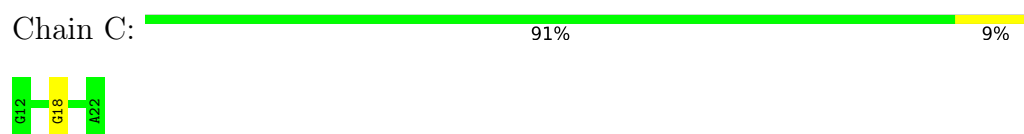


- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')



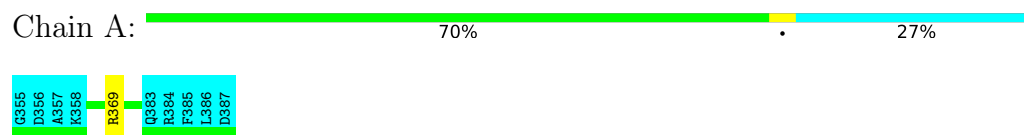
There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')



4.2.7 Score per residue for model 7

- Molecule 1: SLC2A4 regulator

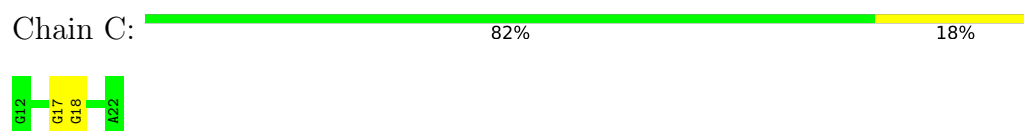


- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')



There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')



4.2.8 Score per residue for model 8

- Molecule 1: SLC2A4 regulator

Chain A:  67% 6% 27%



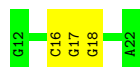
- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  82% 18%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C:  73% 27%



4.2.9 Score per residue for model 9

- Molecule 1: SLC2A4 regulator

Chain A:  64% 6% 27%

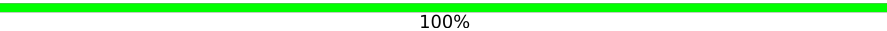


- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  91% 9%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C:  100%

There are no outlier residues in this chain.

4.2.10 Score per residue for model 10

- Molecule 1: SLC2A4 regulator

Chain A:  67% 6% 27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  91% 9%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

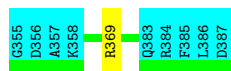
Chain C:  82% 18%



4.2.11 Score per residue for model 11

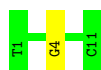
- Molecule 1: SLC2A4 regulator

Chain A:  70% 27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  91% 9%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C:  91% 9%



4.2.12 Score per residue for model 12

- Molecule 1: SLC2A4 regulator

Chain A:  70% 27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B: 91% 9%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C: 100%

There are no outlier residues in this chain.

4.2.13 Score per residue for model 13

- Molecule 1: SLC2A4 regulator

Chain A: 70% . 27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B: 100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

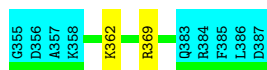
Chain C: 73% 27%



4.2.14 Score per residue for model 14

- Molecule 1: SLC2A4 regulator

Chain A: 67% 6% 27%

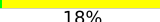


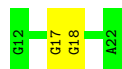
- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C:  82%  18%



4.2.15 Score per residue for model 15

- Molecule 1: SLC2A4 regulator

Chain A:  67%  6%  27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C:  91%  9%



4.2.16 Score per residue for model 16

- Molecule 1: SLC2A4 regulator

Chain A:  64%  6%  27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  91%  9%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C:  100%

There are no outlier residues in this chain.

4.2.17 Score per residue for model 17

- Molecule 1: SLC2A4 regulator

Chain A:  67% 6% 27%



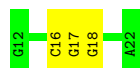
- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  82% 18%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C:  73% 27%



4.2.18 Score per residue for model 18

- Molecule 1: SLC2A4 regulator

Chain A:  70% 27%



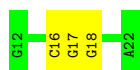
- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B:  73% 27%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

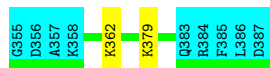
Chain C:  73% 27%



4.2.19 Score per residue for model 19

- Molecule 1: SLC2A4 regulator

Chain A: 67% 6% 27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B: 100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C: 73% 27%



4.2.20 Score per residue for model 20

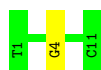
- Molecule 1: SLC2A4 regulator

Chain A: 64% 9% 27%



- Molecule 2: DNA (5'-D(*TP*AP*TP*GP*CP*CP*GP*GP*GP*AP*C)-3')

Chain B: 91% 9%



- Molecule 3: DNA (5'-D(*GP*TP*CP*CP*CP*GP*GP*CP*AP*TP*A)-3')

Chain C: 73% 27%



5 Refinement protocol and experimental data overview

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

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
CYANA	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	611
Number of shifts mapped to atoms	611
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	62%

6 Model quality

6.1 Standard geometry

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

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	1.01±0.02	0±0/210 (0.0± 0.0%)	1.54±0.04	1±1/279 (0.3± 0.2%)
2	B	0.80±0.01	0±0/251 (0.0± 0.0%)	1.22±0.02	0±0/386 (0.0± 0.0%)
3	C	0.79±0.02	0±0/247 (0.0± 0.0%)	1.24±0.02	0±0/379 (0.0± 0.0%)
All	All	0.86	0/14160 (0.0%)	1.32	14/20880 (0.1%)

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	0.6±0.7
2	B	0.0±0.0	0.9±0.9
3	C	0.0±0.0	2.0±1.2
All	All	0	71

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
1	A	369	ARG	NE-CZ-NH2	6.46	125.01	119.20	16	4
1	A	370	ASP	CA-CB-CG	5.69	118.29	112.60	3	2
1	A	377	ARG	NE-CZ-NH1	5.58	127.08	121.50	1	8

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)
3	C	18	DG	Sidechain	15
3	C	17	DG	Sidechain	12
3	C	16	DC	Sidechain	10
1	A	361	ARG	Sidechain	9
2	B	6	DC	Sidechain	7
2	B	4	DG	Sidechain	5
2	B	3	DT	Sidechain	3
2	B	5	DC	Sidechain	3
3	C	22	DA	Sidechain	2
1	A	369	ARG	Sidechain	2
2	B	2	DA	Sidechain	1
3	C	21	DT	Sidechain	1
3	C	19	DC	Sidechain	1

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	205	208	208	0±0
2	B	224	125	125	0±0
3	C	221	125	125	0±0
All	All	13020	9160	9160	3

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:362:LYS:HE3	2:B:3:DT:H4'	0.46	1.86	8	1
1:A:379:LYS:HE2	3:C:16:DC:C5	0.46	2.46	2	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	24/33 (73%)	22±1 (91±3%)	2±1 (7±3%)	0±0 (2±2%)	8	48
All	All	480/660 (73%)	435 (91%)	35 (7%)	10 (2%)	8	48

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	369	ARG	10

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	21/28 (75%)	20±5 (93±22%)	0±0 (2±2%)	52	92
All	All	399/560 (71%)	392 (98%)	7 (2%)	51	91

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	362	LYS	7

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](#)

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

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 62% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	611
Number of shifts mapped to atoms	611
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	33	-0.51 ± 0.56	None needed (imprecise)
$^{13}\text{C}_\beta$	31	0.62 ± 0.25	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	33	0.49 ± 0.84	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 62%, i.e. 496 atoms were assigned a chemical shift out of a possible 796. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	97/121 (80%)	49/49 (100%)	24/48 (50%)	24/24 (100%)
Sidechain	169/203 (83%)	113/129 (88%)	52/58 (90%)	4/16 (25%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	32/33 (97%)	16/16 (100%)	14/15 (93%)	2/2 (100%)
Sugar	148/264 (56%)	148/154 (96%)	0/110 (0%)	0/0 (—%)
Base	50/175 (29%)	50/109 (46%)	0/37 (0%)	0/29 (0%)
Overall	496/796 (62%)	376/457 (82%)	90/268 (34%)	30/71 (42%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 65%, i.e. 598 atoms were assigned a chemical shift out of a possible 921. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	133/167 (80%)	67/68 (99%)	33/66 (50%)	33/33 (100%)
Sidechain	225/272 (83%)	151/172 (88%)	69/79 (87%)	5/21 (24%)
Aromatic	42/43 (98%)	21/21 (100%)	19/20 (95%)	2/2 (100%)
Sugar	148/264 (56%)	148/154 (96%)	0/110 (0%)	0/0 (—%)
Base	50/175 (29%)	50/109 (46%)	0/37 (0%)	0/29 (0%)
Overall	598/921 (65%)	437/524 (83%)	121/312 (39%)	40/85 (47%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	369	ARG	HA	1.70	2.06 – 6.51	-5.8
1	A	384	ARG	HG2	0.08	0.26 – 2.87	-5.7
1	C	14	DC	H6	6.07	6.12 – 8.81	-5.2

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:

