



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 05:23 PM UTC

PDB ID : 5LXK / pdb_00005lxk
BMRB ID : 34046
Title : NMR structure of the C-terminal domain of the Bacteriophage T5 decoration protein pb10.
Authors : Vernhes, E.; Gilquin, B.; Cuniasse, P.; Boulanger, P.; Zinn-Justin, S.
Deposited on : 2016-09-22

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

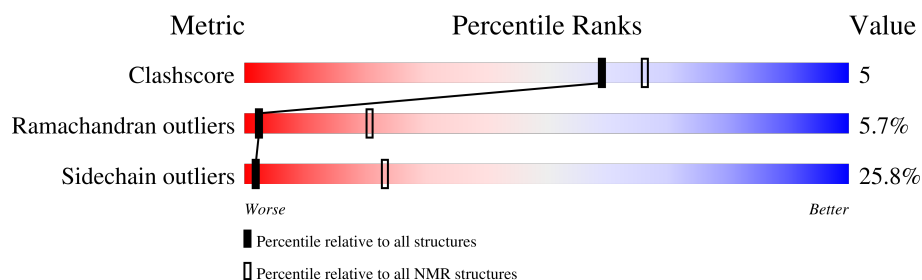
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 95%.

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	101	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:79-A:156 (78)	0.50	7

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1334 atoms, of which 659 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Decoration protein.

Mol	Chain	Residues	Atoms						Trace
1	A	96	Total	C	H	N	O	S	0
			1334	417	659	107	149	2	

There are 9 discrepancies between the modelled and reference sequences:

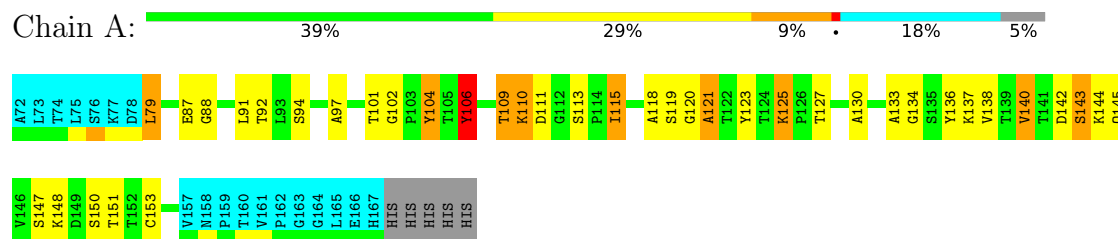
Chain	Residue	Modelled	Actual	Comment	Reference
A	72	ALA	-	expression tag	UNP Q6QGD6
A	165	LEU	-	expression tag	UNP Q6QGD6
A	166	GLU	-	expression tag	UNP Q6QGD6
A	167	HIS	-	expression tag	UNP Q6QGD6
A	168	HIS	-	expression tag	UNP Q6QGD6
A	169	HIS	-	expression tag	UNP Q6QGD6
A	170	HIS	-	expression tag	UNP Q6QGD6
A	171	HIS	-	expression tag	UNP Q6QGD6
A	172	HIS	-	expression tag	UNP Q6QGD6

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: Decoration protein

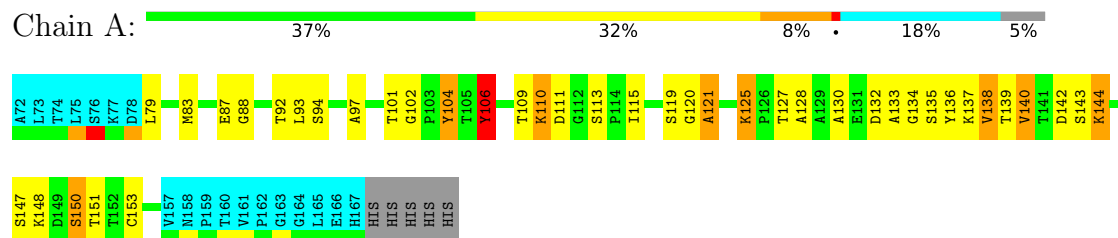


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

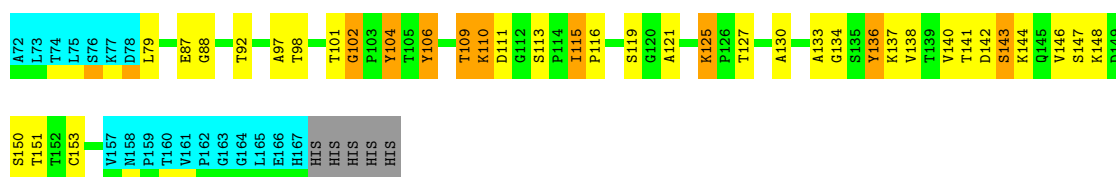
- Molecule 1: Decoration protein



4.2.2 Score per residue for model 2

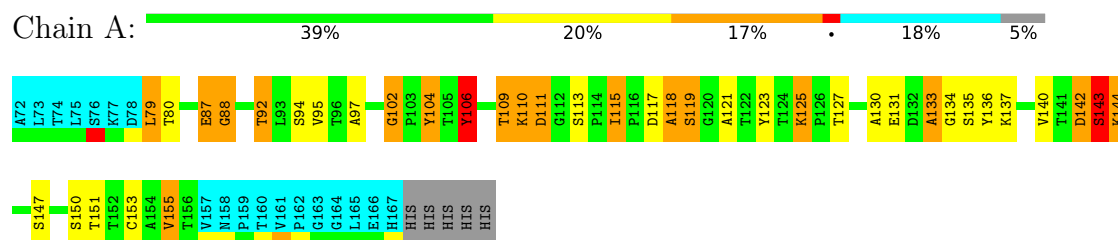
- Molecule 1: Decoration protein





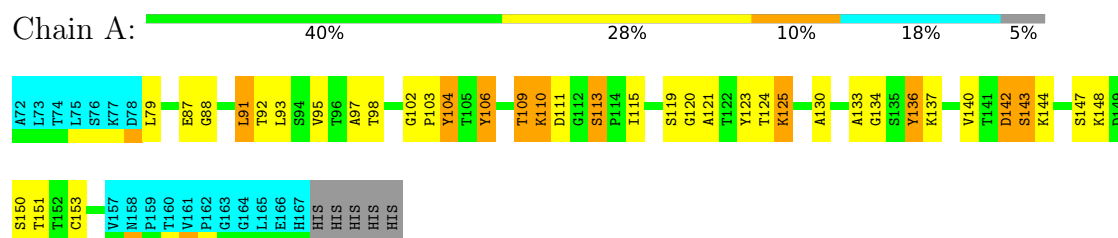
4.2.3 Score per residue for model 3

- Molecule 1: Decoration protein



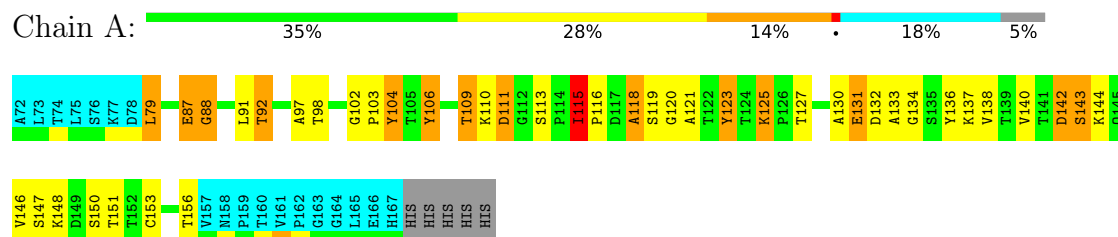
4.2.4 Score per residue for model 4

- Molecule 1: Decoration protein



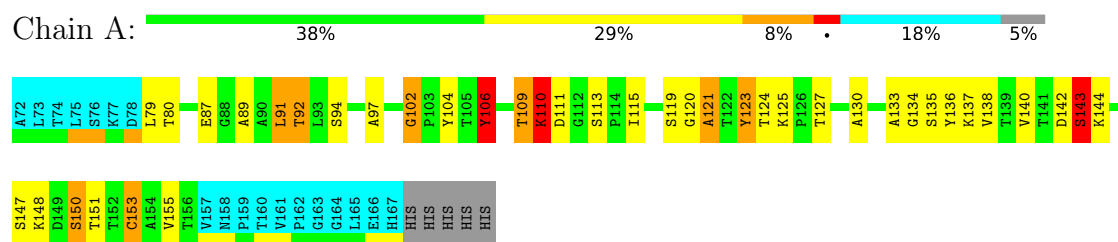
4.2.5 Score per residue for model 5

- Molecule 1: Decoration protein



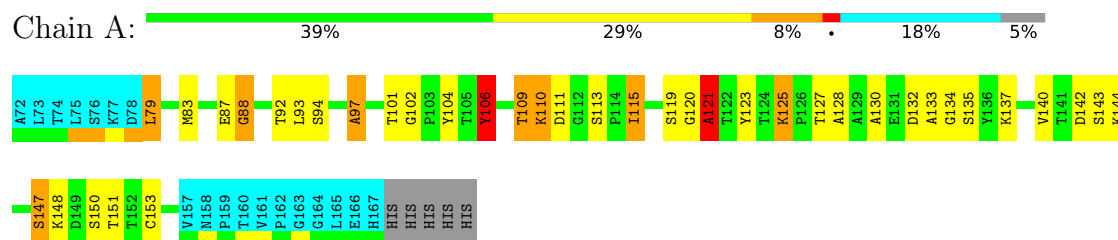
4.2.6 Score per residue for model 6

- Molecule 1: Decoration protein



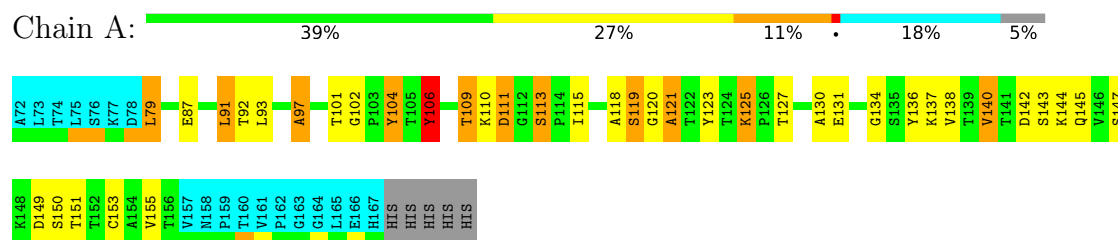
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Decoration protein



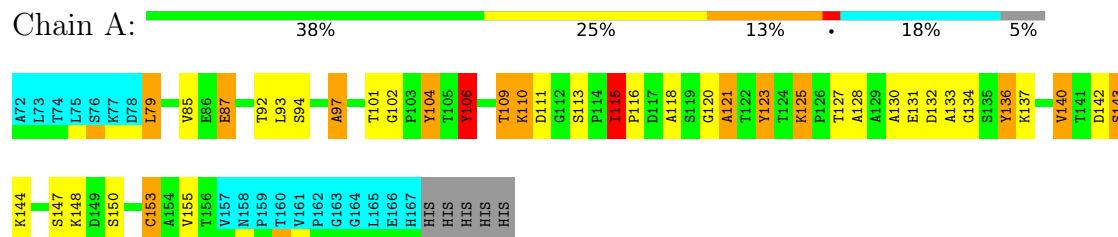
4.2.8 Score per residue for model 8

- Molecule 1: Decoration protein



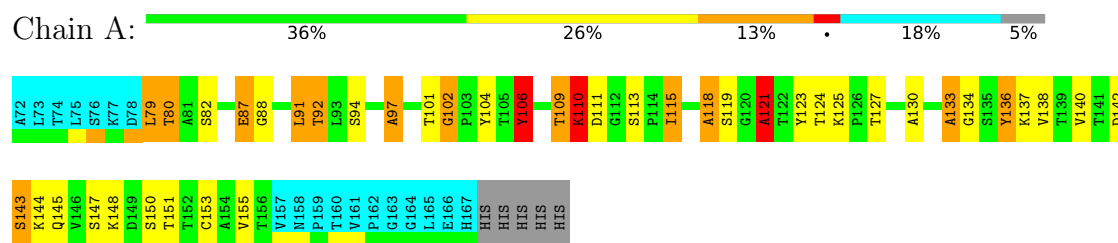
4.2.9 Score per residue for model 9

- Molecule 1: Decoration protein



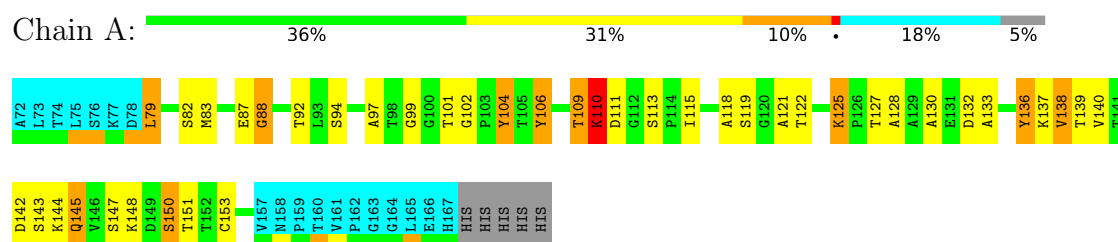
4.2.10 Score per residue for model 10

- Molecule 1: Decoration protein



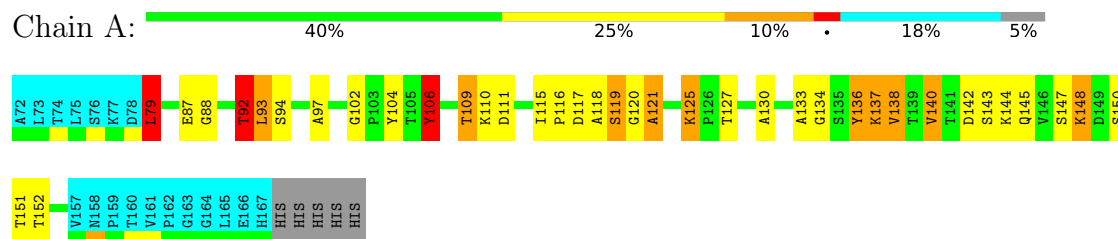
4.2.11 Score per residue for model 11

- Molecule 1: Decoration protein



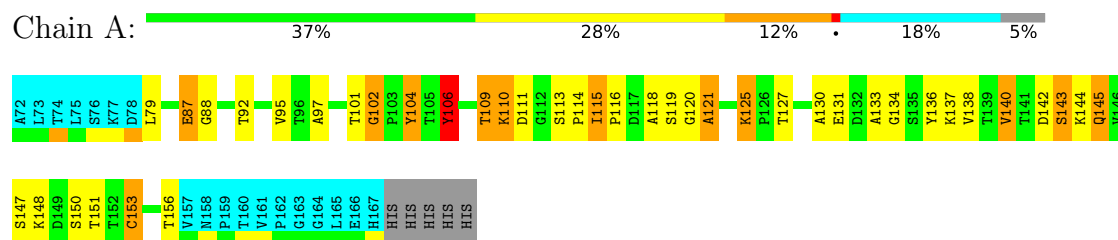
4.2.12 Score per residue for model 12

- Molecule 1: Decoration protein



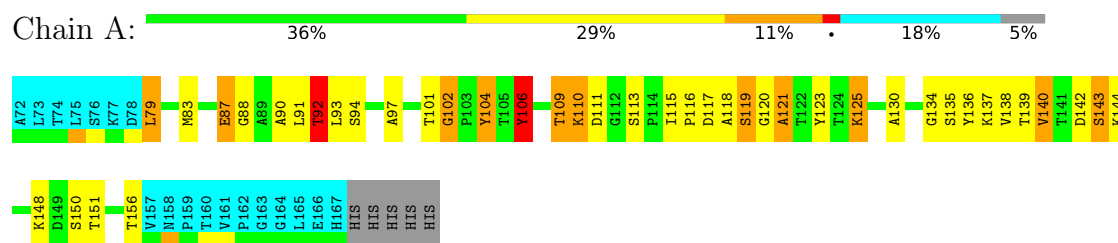
4.2.13 Score per residue for model 13

- Molecule 1: Decoration protein



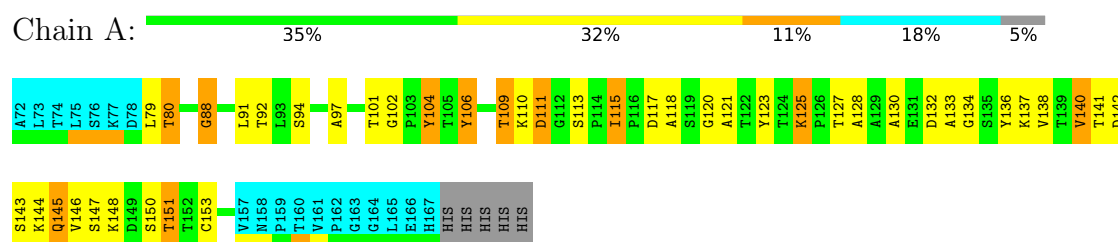
4.2.14 Score per residue for model 14

- Molecule 1: Decoration protein



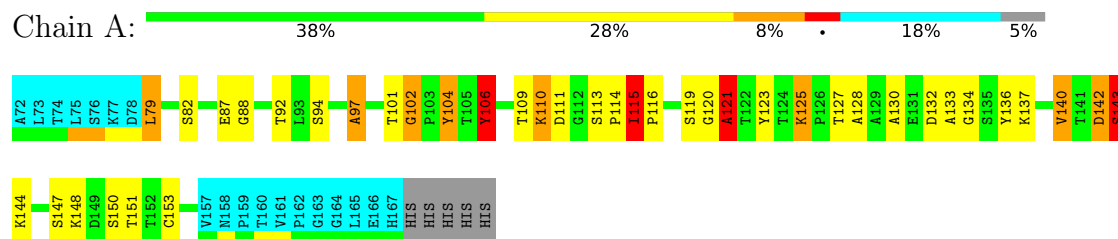
4.2.15 Score per residue for model 15

- Molecule 1: Decoration protein



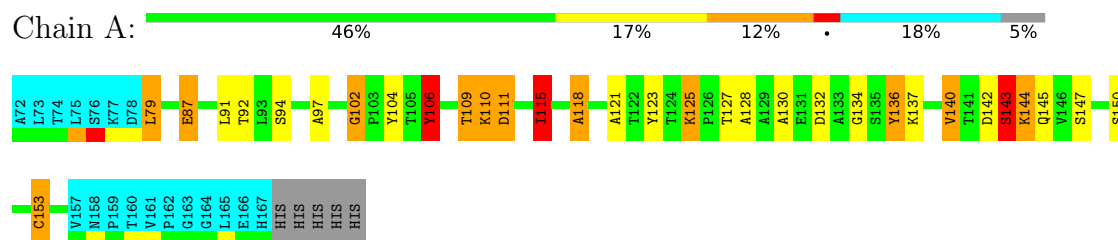
4.2.16 Score per residue for model 16

- Molecule 1: Decoration protein



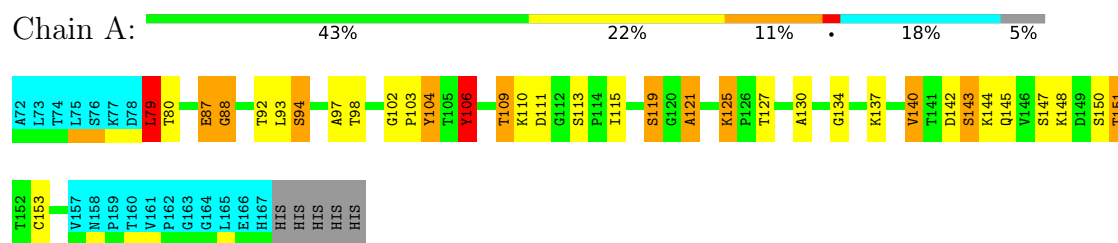
4.2.17 Score per residue for model 17

- Molecule 1: Decoration protein



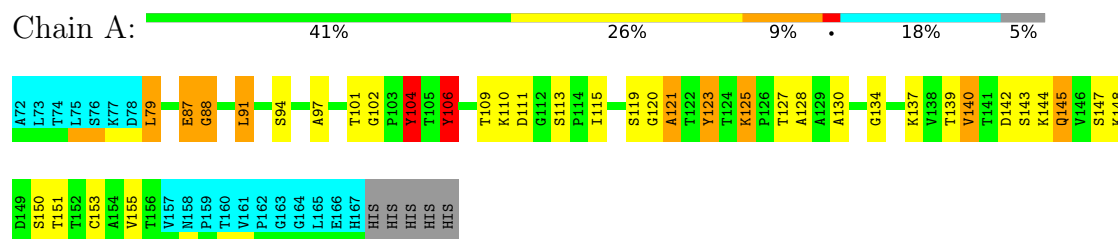
4.2.18 Score per residue for model 18

- Molecule 1: Decoration protein



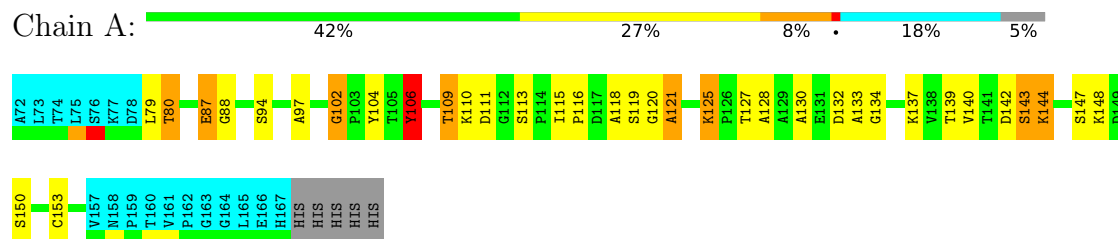
4.2.19 Score per residue for model 19

- Molecule 1: Decoration protein



4.2.20 Score per residue for model 20

- Molecule 1: Decoration protein



5 Refinement protocol and experimental data overview

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

Of the 200 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
INCA	structure calculation	
CNS	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	1054
Number of shifts mapped to atoms	1054
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%

6 Model quality i

6.1 Standard geometry i

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	1.41±0.03	1±1/556 (0.1± 0.2%)	2.48±0.04	44±4/764 (5.7± 0.5%)
All	All	1.41	14/11120 (0.1%)	2.48	876/15280 (5.7%)

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	1.0±0.0	2.8±0.9
All	All	20	56

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	153	CYS	CA-CB	5.52	1.60	1.53	13	3
1	A	111	ASP	CA-C	-5.38	1.45	1.53	9	5
1	A	87	GLU	N-CA	5.34	1.52	1.46	10	3
1	A	134	GLY	CA-C	-5.10	1.45	1.52	17	2
1	A	132	ASP	C-N	5.05	1.40	1.33	5	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	150	SER	CA-C-N	12.81	140.10	120.75	20	20
1	A	150	SER	C-N-CA	12.81	140.10	120.75	20	20
1	A	97	ALA	N-CA-C	11.85	127.60	109.23	11	20
1	A	111	ASP	N-CA-CB	11.00	127.35	111.62	5	20
1	A	111	ASP	CA-C-O	-10.73	109.47	122.03	3	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	111	ASP	O-C-N	10.23	135.35	122.57	14	20
1	A	104	TYR	N-CA-C	9.65	125.45	110.20	5	20
1	A	106	TYR	N-CA-C	9.47	123.25	109.14	7	20
1	A	113	SER	CA-C-N	8.92	128.68	119.76	16	17
1	A	113	SER	C-N-CA	8.92	128.68	119.76	16	17
1	A	79	LEU	N-CA-C	8.85	121.00	111.36	5	3
1	A	144	LYS	CA-C-N	8.79	134.58	122.19	12	20
1	A	144	LYS	C-N-CA	8.79	134.58	122.19	12	20
1	A	119	SER	N-CA-CB	-8.41	97.91	110.60	20	5
1	A	111	ASP	N-CA-C	8.40	122.73	111.30	3	20
1	A	142	ASP	CA-C-N	8.32	137.43	121.54	1	20
1	A	142	ASP	C-N-CA	8.32	137.43	121.54	1	20
1	A	133	ALA	N-CA-C	8.25	122.34	109.96	11	14
1	A	113	SER	N-CA-C	8.25	123.02	109.58	8	15
1	A	91	LEU	N-CA-CB	-8.15	97.77	110.65	8	1
1	A	102	GLY	CA-C-N	8.14	129.23	120.11	4	20
1	A	102	GLY	C-N-CA	8.14	129.23	120.11	4	20
1	A	134	GLY	CA-C-N	-8.03	111.91	123.00	19	19
1	A	134	GLY	C-N-CA	-8.03	111.91	123.00	19	19
1	A	109	THR	N-CA-CB	7.86	123.56	111.46	14	17
1	A	125	LYS	N-CA-CB	7.83	123.37	110.05	11	4
1	A	94	SER	CA-C-N	7.64	133.64	123.17	1	13
1	A	94	SER	C-N-CA	7.64	133.64	123.17	1	13
1	A	151	THR	N-CA-C	7.62	120.15	110.24	3	15
1	A	115	ILE	CA-C-N	7.43	127.78	119.32	15	7
1	A	115	ILE	C-N-CA	7.43	127.78	119.32	15	7
1	A	118	ALA	CA-C-N	7.40	133.63	122.23	20	4
1	A	118	ALA	C-N-CA	7.40	133.63	122.23	20	4
1	A	97	ALA	CA-C-N	7.39	134.37	122.10	20	19
1	A	97	ALA	C-N-CA	7.39	134.37	122.10	20	19
1	A	130	ALA	N-CA-C	7.30	120.17	111.33	4	20
1	A	155	VAL	CB-CA-C	7.13	120.26	110.99	3	1
1	A	111	ASP	CA-CB-CG	7.04	119.64	112.60	19	20
1	A	101	THR	CA-C-O	-6.96	113.09	120.40	2	11
1	A	125	LYS	CA-C-N	6.93	126.64	119.64	2	18
1	A	125	LYS	C-N-CA	6.93	126.64	119.64	2	18
1	A	150	SER	CB-CA-C	6.91	122.58	109.37	19	5
1	A	87	GLU	N-CA-CB	6.85	119.73	109.19	6	11
1	A	103	PRO	CA-C-N	6.82	131.17	121.42	18	3
1	A	103	PRO	C-N-CA	6.82	131.17	121.42	18	3
1	A	111	ASP	CA-C-N	6.78	133.15	122.51	13	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	111	ASP	C-N-CA	6.78	133.15	122.51	13	20
1	A	118	ALA	N-CA-C	6.64	119.39	110.35	12	2
1	A	87	GLU	N-CA-C	6.64	120.47	110.64	2	14
1	A	79	LEU	O-C-N	-6.41	114.39	122.27	16	4
1	A	131	GLU	CA-C-N	6.33	132.21	121.14	8	5
1	A	131	GLU	C-N-CA	6.33	132.21	121.14	8	5
1	A	92	THR	N-CA-C	-6.32	99.42	109.59	15	4
1	A	145	GLN	CB-CA-C	6.22	120.08	111.63	13	8
1	A	113	SER	CB-CA-C	6.21	118.22	108.84	3	5
1	A	92	THR	CA-CB-CG2	6.07	120.81	110.50	12	3
1	A	121	ALA	N-CA-CB	6.06	120.74	110.49	12	11
1	A	150	SER	O-C-N	6.04	131.05	123.19	16	5
1	A	80	THR	N-CA-C	-6.01	97.99	110.80	15	6
1	A	82	SER	N-CA-C	5.95	117.75	107.93	16	2
1	A	142	ASP	N-CA-CB	5.91	120.48	110.49	3	13
1	A	113	SER	O-C-N	-5.87	116.75	121.80	14	3
1	A	114	PRO	O-C-N	-5.82	116.12	123.10	16	1
1	A	138	VAL	CA-C-N	5.79	131.33	123.11	8	9
1	A	138	VAL	C-N-CA	5.79	131.33	123.11	8	9
1	A	143	SER	N-CA-C	5.79	123.14	110.80	5	8
1	A	109	THR	CA-C-N	-5.77	114.41	123.13	16	1
1	A	109	THR	C-N-CA	-5.77	114.41	123.13	16	1
1	A	117	ASP	CA-C-N	5.75	129.44	120.75	12	2
1	A	117	ASP	C-N-CA	5.75	129.44	120.75	12	2
1	A	94	SER	N-CA-C	5.72	118.78	108.48	18	1
1	A	79	LEU	N-CA-CB	-5.66	101.78	110.16	5	2
1	A	110	LYS	CA-C-N	5.65	130.43	122.46	17	1
1	A	110	LYS	C-N-CA	5.65	130.43	122.46	17	1
1	A	142	ASP	CA-CB-CG	5.62	118.22	112.60	18	3
1	A	101	THR	CA-C-N	5.59	130.65	121.87	16	5
1	A	101	THR	C-N-CA	5.59	130.65	121.87	16	5
1	A	147	SER	CA-C-N	5.58	132.19	122.81	7	1
1	A	147	SER	C-N-CA	5.58	132.19	122.81	7	1
1	A	110	LYS	CA-CB-CG	5.49	125.08	114.10	16	1
1	A	110	LYS	N-CA-CB	-5.47	101.96	110.87	17	1
1	A	115	ILE	CA-CB-CG1	5.46	119.69	110.40	5	4
1	A	149	ASP	CA-CB-CG	5.45	118.05	112.60	8	1
1	A	98	THR	N-CA-C	-5.45	100.64	108.60	5	3
1	A	79	LEU	CA-C-N	5.45	132.14	122.45	19	1
1	A	79	LEU	C-N-CA	5.45	132.14	122.45	19	1
1	A	80	THR	CA-CB-CG2	5.43	119.72	110.50	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	135	SER	N-CA-CB	5.42	119.08	110.57	3	2
1	A	150	SER	N-CA-CB	5.42	119.41	110.69	8	1
1	A	122	THR	CB-CA-C	5.40	118.90	111.23	11	1
1	A	135	SER	CA-C-N	5.39	130.16	122.72	1	2
1	A	135	SER	C-N-CA	5.39	130.16	122.72	1	2
1	A	82	SER	CB-CA-C	-5.34	104.80	111.43	10	2
1	A	118	ALA	N-CA-CB	5.34	119.52	110.49	17	1
1	A	130	ALA	CA-C-N	5.34	129.14	120.60	16	1
1	A	130	ALA	C-N-CA	5.34	129.14	120.60	16	1
1	A	91	LEU	N-CA-C	5.33	117.58	108.90	10	2
1	A	148	LYS	N-CA-C	-5.30	101.25	109.72	12	1
1	A	138	VAL	N-CA-C	5.28	116.26	108.45	13	1
1	A	87	GLU	CA-C-O	5.22	125.78	120.88	4	3
1	A	144	LYS	N-CA-C	-5.19	106.62	113.17	9	1
1	A	151	THR	CA-C-N	5.19	129.75	121.66	2	2
1	A	151	THR	C-N-CA	5.19	129.75	121.66	2	2
1	A	90	ALA	N-CA-C	5.18	117.19	108.96	14	1
1	A	93	LEU	N-CA-C	-5.17	98.97	108.02	12	1
1	A	80	THR	N-CA-CB	5.13	119.16	110.49	20	1
1	A	99	GLY	CA-C-N	5.13	128.54	121.26	11	1
1	A	99	GLY	C-N-CA	5.13	128.54	121.26	11	1
1	A	114	PRO	CB-CA-C	-5.08	104.56	111.12	13	1
1	A	146	VAL	CA-C-N	5.06	129.13	122.30	5	1
1	A	146	VAL	C-N-CA	5.06	129.13	122.30	5	1
1	A	85	VAL	CA-C-N	5.05	128.04	120.87	9	1
1	A	85	VAL	C-N-CA	5.05	128.04	120.87	9	1
1	A	135	SER	CB-CA-C	5.03	118.43	109.72	6	1
1	A	124	THR	CA-C-N	5.01	129.82	122.66	6	1
1	A	124	THR	C-N-CA	5.01	129.82	122.66	6	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	111	ASP	CA	20

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	106	TYR	Sidechain	20
1	A	110	LYS	Peptide	13

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	123	TYR	Sidechain	11
1	A	136	TYR	Sidechain	9
1	A	104	TYR	Sidechain	3

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	546	528	528	5±2
All	All	10920	10560	10560	99

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:LEU:HD21	1:A:136:TYR:CZ	0.68	2.23	8	1
1:A:110:LYS:HG2	1:A:115:ILE:HG22	0.67	1.66	17	1
1:A:91:LEU:HD21	1:A:128:ALA:HB2	0.65	1.68	19	1
1:A:128:ALA:HB1	1:A:132:ASP:CB	0.57	2.27	15	8
1:A:79:LEU:O	1:A:92:THR:HG22	0.56	2.01	12	3
1:A:138:VAL:HG13	1:A:150:SER:HB2	0.56	1.77	1	1
1:A:93:LEU:HD11	1:A:136:TYR:CD2	0.53	2.38	12	1
1:A:93:LEU:HD21	1:A:136:TYR:CD2	0.53	2.38	4	1
1:A:138:VAL:HG13	1:A:150:SER:OG	0.53	2.04	11	1
1:A:93:LEU:HD11	1:A:136:TYR:CD1	0.51	2.40	1	1
1:A:115:ILE:HD11	1:A:118:ALA:HB2	0.50	1.81	10	2
1:A:102:GLY:H	1:A:143:SER:HB3	0.50	1.66	16	9
1:A:97:ALA:HB3	1:A:121:ALA:HB2	0.49	1.85	10	5
1:A:88:GLY:HA2	1:A:127:THR:HG23	0.48	1.84	11	9
1:A:110:LYS:HD3	1:A:136:TYR:CE2	0.47	2.44	6	1
1:A:79:LEU:HD22	1:A:94:SER:H	0.47	1.69	18	1
1:A:110:LYS:HD2	1:A:136:TYR:CZ	0.47	2.44	11	5
1:A:138:VAL:HG13	1:A:140:VAL:HG22	0.47	1.87	12	1
1:A:91:LEU:HD21	1:A:128:ALA:CB	0.46	2.38	19	1
1:A:91:LEU:HD12	1:A:153:CYS:SG	0.46	2.49	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:LEU:HD23	1:A:136:TYR:CZ	0.46	2.46	4	2
1:A:91:LEU:HD23	1:A:136:TYR:CE1	0.46	2.45	17	1
1:A:104:TYR:HB3	1:A:140:VAL:HG12	0.45	1.89	15	9
1:A:106:TYR:HB3	1:A:140:VAL:HG13	0.45	1.88	17	1
1:A:104:TYR:CE2	1:A:142:ASP:CG	0.45	2.95	5	2
1:A:115:ILE:HB	1:A:116:PRO:CD	0.45	2.42	16	1
1:A:79:LEU:HD13	1:A:153:CYS:SG	0.45	2.52	3	1
1:A:106:TYR:CD1	1:A:106:TYR:N	0.44	2.85	16	7
1:A:115:ILE:HB	1:A:116:PRO:HD2	0.44	1.89	5	2
1:A:106:TYR:CD2	1:A:106:TYR:N	0.44	2.86	14	2
1:A:110:LYS:NZ	1:A:136:TYR:CZ	0.43	2.86	10	1
1:A:91:LEU:O	1:A:124:THR:HG23	0.43	2.12	4	2
1:A:110:LYS:CB	1:A:136:TYR:HA	0.43	2.43	2	3
1:A:104:TYR:CE1	1:A:142:ASP:CG	0.43	2.96	4	2
1:A:137:LYS:HE2	1:A:152:THR:HG22	0.43	1.90	12	1
1:A:79:LEU:HB3	1:A:93:LEU:HA	0.43	1.91	18	1
1:A:141:THR:HG23	1:A:146:VAL:C	0.42	2.39	2	2
1:A:91:LEU:HG	1:A:136:TYR:CE2	0.42	2.49	6	1
1:A:79:LEU:HG	1:A:94:SER:H	0.41	1.75	17	1
1:A:79:LEU:H	1:A:79:LEU:HD12	0.41	1.75	3	1
1:A:115:ILE:CD1	1:A:118:ALA:HB2	0.40	2.46	3	1
1:A:80:THR:HB	1:A:153:CYS:SG	0.40	2.56	10	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	78/101 (77%)	63±1 (81±2%)	10±2 (13±2%)	4±1 (6±1%)	2	21
All	All	1560/2020 (77%)	1268 (81%)	203 (13%)	89 (6%)	2	21

All 8 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	121	ALA	20
1	A	143	SER	20
1	A	120	GLY	14
1	A	88	GLY	14
1	A	119	SER	7
1	A	118	ALA	7
1	A	116	PRO	5
1	A	117	ASP	2

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/79 (75%)	44±2 (74±3%)	15±2 (26±3%)	2	23
All	All	1180/1580 (75%)	875 (74%)	305 (26%)	2	23

All 33 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	79	LEU	20
1	A	115	ILE	20
1	A	125	LYS	20
1	A	137	LYS	20
1	A	140	VAL	20
1	A	109	THR	19
1	A	147	SER	19
1	A	92	THR	17
1	A	148	LYS	17
1	A	153	CYS	16
1	A	106	TYR	15
1	A	110	LYS	10
1	A	119	SER	10
1	A	87	GLU	10
1	A	127	THR	9
1	A	155	VAL	6
1	A	123	TYR	6
1	A	139	THR	5

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Mol	Chain	Res	Type	Models (Total)
1	A	111	ASP	5
1	A	91	LEU	5
1	A	145	GLN	5
1	A	83	MET	4
1	A	144	LYS	4
1	A	93	LEU	4
1	A	151	THR	4
1	A	95	VAL	3
1	A	156	THR	3
1	A	113	SER	2
1	A	138	VAL	2
1	A	80	THR	2
1	A	131	GLU	1
1	A	150	SER	1
1	A	98	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 95% for the well-defined parts and 94% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *c72_depchim_renum.bmrB*

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	1054
Number of shifts mapped to atoms	1054
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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	0.20 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	87	0.07 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	94	0.48 ± 0.17	None needed (< 0.5 ppm)
^{15}N	88	-1.22 ± 0.33	Should be applied

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 95%, i.e. 846 atoms were assigned a chemical shift out of a possible 894. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	384/389 (99%)	155/159 (97%)	155/156 (99%)	74/74 (100%)
Sidechain	418/457 (91%)	285/303 (94%)	132/148 (89%)	1/6 (17%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	44/48 (92%)	22/22 (100%)	21/25 (84%)	1/1 (100%)
Overall	846/894 (95%)	462/484 (95%)	308/329 (94%)	76/81 (94%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 1054 atoms were assigned a chemical shift out of a possible 1119. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	467/477 (98%)	189/195 (97%)	190/192 (99%)	88/90 (98%)
Sidechain	543/587 (93%)	371/389 (95%)	170/190 (89%)	2/8 (25%)
Aromatic	44/55 (80%)	22/26 (85%)	21/27 (78%)	1/2 (50%)
Overall	1054/1119 (94%)	582/610 (95%)	381/409 (93%)	91/100 (91%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	123	TYR	HB3	0.59	0.93 – 4.76	-5.9
1	A	123	TYR	HB2	1.06	1.09 – 4.72	-5.1

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:

