Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 12:15 AM EDT

PDB ID	:	2LT7
BMRB ID	:	18462
Title	:	Solution NMR structure of Kaiso zinc finger DNA binding domain in complex with Kaiso binding site DNA
Authors	:	Buck-Koehntop, B.A.; Stanfield, R.L.; Ekiert, D.C.; Martinez-Yamout, M.A.; Dyson, H.; Wilson, I.A.; Wright, P.E.
Deposited on	:	2012-05-15

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 (i) 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 (i)) were used in the production of this report:

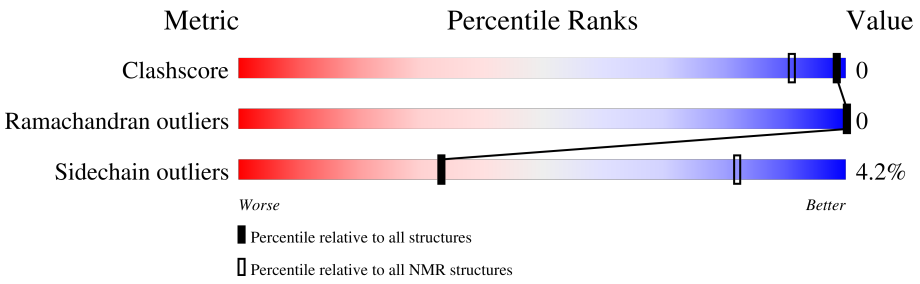
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	133	74% 8% • 17%
2	D	19	84% 16%
3	E	19	74% 21% 5%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 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:482-A:573, A:583-A:600 (110)	0.53	4

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 3 single-model clusters were found.

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

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3435 atoms, of which 1532 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcriptional regulator Kaiso.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	133	2232	712	1105	212	193	10	0

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	D	19	597	184	214	68	113	18	0

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
3	E	19	603	186	213	75	111	18	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
4	A	3	3	3

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: Transcriptional regulator Kaiso

Chain A: 74% 8% • 17%

A472 N473 K474 R475 M476 K477 V478 K479 H480 D481 Y484 Y493 R501 V504 R510 R511 N514 R537 R549 S574 Q575 D576 P577 S578 G579 D580 S581 K582 R595 L600 S601 D602 R603 S604

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

Chain D: 84% 16%

G1 C7 C8 T9 G19

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

Chain E: 74% 21% 5%

C20 T26 G27 G28 C29 A30 G31 C38

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: Transcriptional regulator Kaiso

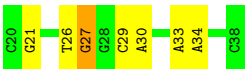
Chain A: 74% 7% • 17%

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

Chain D:

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

Chain E:



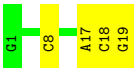
4.2.2 Score per residue for model 2

• Molecule 1: Transcriptional regulator Kaiso

Chain A:

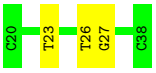
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

Chain E:



4.2.3 Score per residue for model 3

• Molecule 1: Transcriptional regulator Kaiso

Chain A: 74% 8% • 17%

A472 N473 K474 R475 M476 K477 V478 K479 H480 D481 Y484 Y493 R501 V504 R510 N514 R549 Y562 M565 S574 Q575 D576 P577 S578 G579 D580 S581 K582 R595 Y599 L600 S601 D602 R603 S604

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

Chain D: 84% 16%

G1 C4 C7 C8 T9 G19

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

Chain E: 68% 32%

C20 T26 G27 G28 C29 A30 A33 A34 C38

4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Transcriptional regulator Kaiso

Chain A: 71% 9% • 17%

A472 N473 K474 R475 M476 K477 V478 K479 H480 D481 Y484 Y493 R501 V504 R510 R511 N514 Y536 R537 H543 R549 C552 S574 Q575 D576 P577 S578 G579 D580 S581 K582 R590 R595 L600 S601 D602 R603 S604

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

Chain D: 84% 16%

G1 C7 C8 T9 G10 C11 G19

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

Chain E: 74% 21% 5%

C20 T23 T26 G27 G31 G32 A33 C38

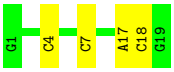
4.2.5 Score per residue for model 5

• Molecule 1: Transcriptional regulator Kaiso

Chain A:

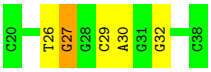
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

Chain E:



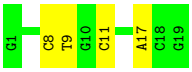
4.2.6 Score per residue for model 6

• Molecule 1: Transcriptional regulator Kaiso

Chain A:

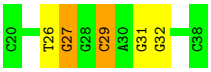
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

Chain E:



4.2.7 Score per residue for model 7

• Molecule 1: Transcriptional regulator Kaiso

Chain A: 71% 10% • 17%

A472 N473 K474 R475 M476 K477 V478 K479 H480 D481 Y484 R491 V492 Y493 Y503 V504 R510 R511 N514 Y536 R537 R548 R549 S574 Q575 D576 P577 S578 G579 D580 S581 K582 L586 R595 L600 S601 D602 R603 S604

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

Chain D: 84% 16%

G1 C8 A16 A17 C18 G19

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

Chain E: 74% 21% 5%

C20 A24 T25 T26 G27 G28 C29 A30 C38

4.2.8 Score per residue for model 8

• Molecule 1: Transcriptional regulator Kaiso

Chain A: 72% 10% • 17%

A472 N473 K474 R475 M476 K477 V478 K479 H480 D481 Y484 R491 V492 Y493 R501 V504 R510 R511 N514 Y536 R537 R549 S574 Q575 D576 P577 S578 G579 D580 S581 K582 R585 R595 L600 S601 D602 R603 S604

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

Chain D: 84% 16%

G1 T9 A17 C18 G19

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

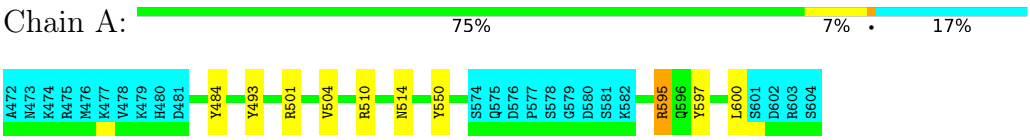
Chain E: 74% 21% 5%

C20 T23 T26 G27 A30 G31 G32 C38

4.2.9 Score per residue for model 9

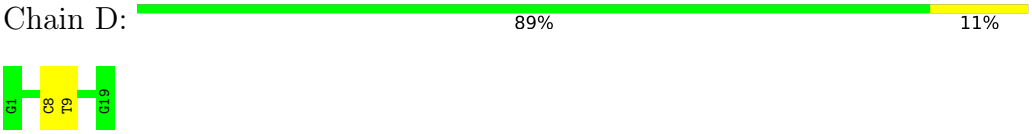
• Molecule 1: Transcriptional regulator Kaiso

Chain A:



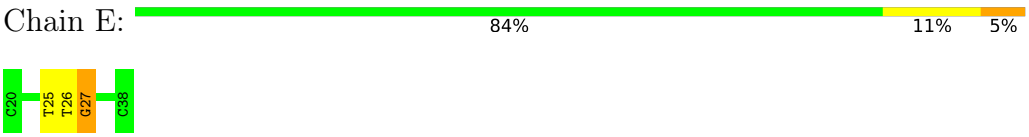
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

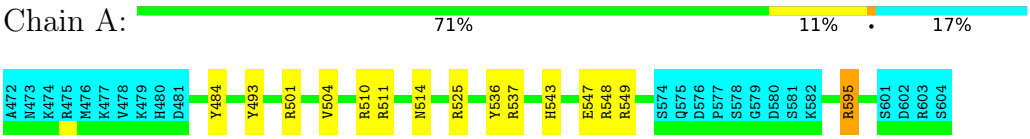
Chain E:



4.2.10 Score per residue for model 10

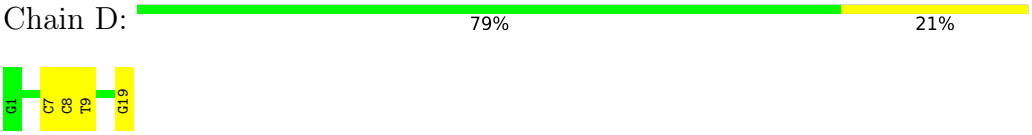
• Molecule 1: Transcriptional regulator Kaiso

Chain A:



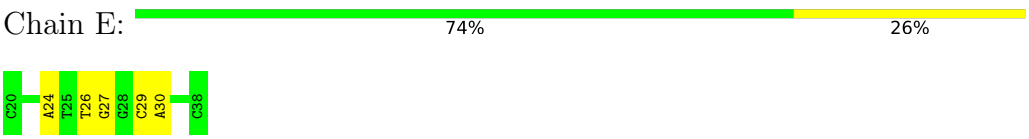
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

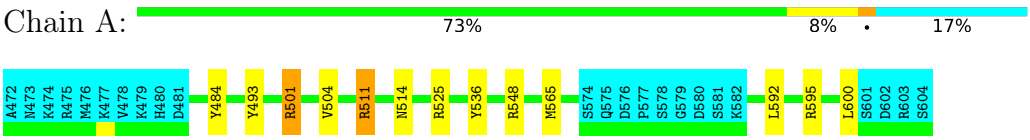
Chain E:



4.2.11 Score per residue for model 11

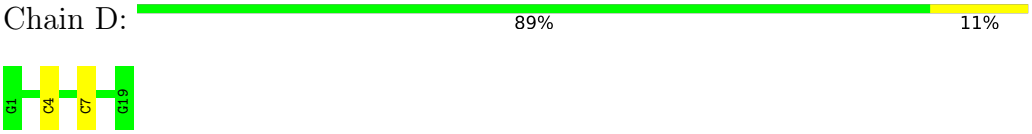
• Molecule 1: Transcriptional regulator Kaiso

Chain A:



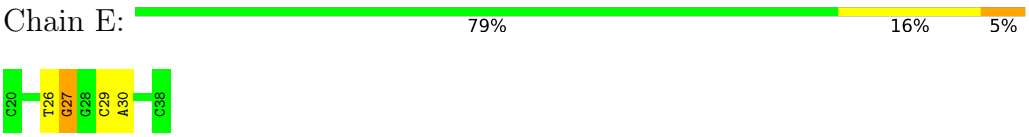
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

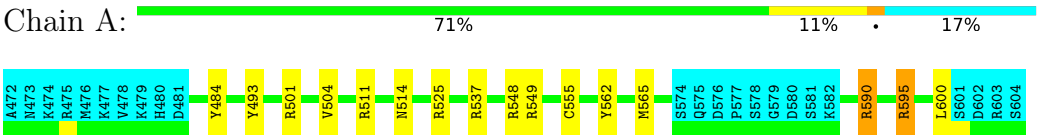
Chain E:



4.2.12 Score per residue for model 12

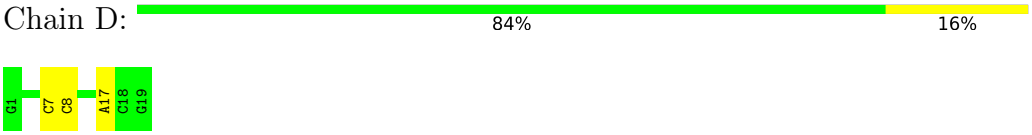
• Molecule 1: Transcriptional regulator Kaiso

Chain A:



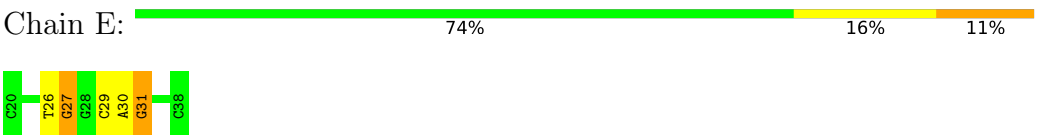
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

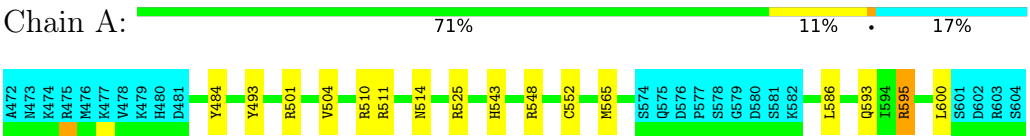
Chain E:



4.2.13 Score per residue for model 13

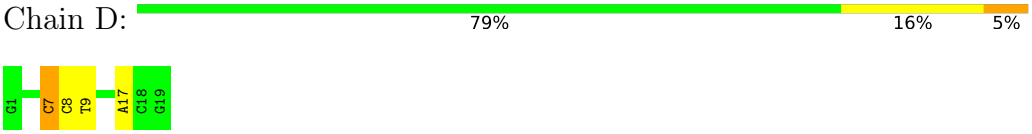
• Molecule 1: Transcriptional regulator Kaiso

Chain A:



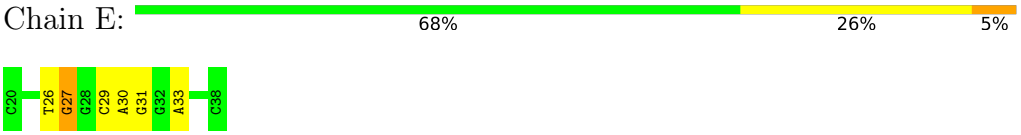
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

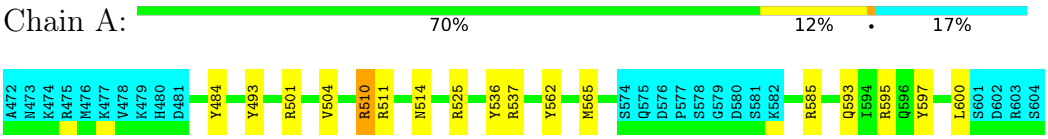
Chain E:



4.2.14 Score per residue for model 14

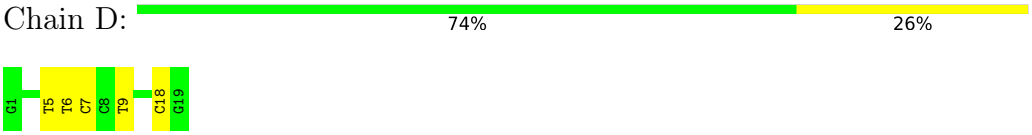
• Molecule 1: Transcriptional regulator Kaiso

Chain A:



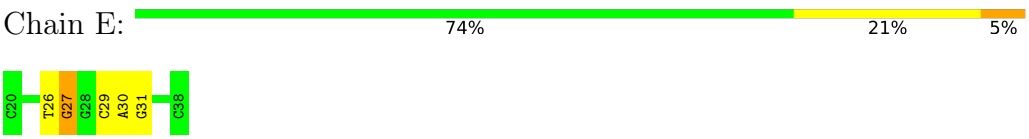
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

Chain E:



4.2.15 Score per residue for model 15

• Molecule 1: Transcriptional regulator Kaiso

Chain A: 71% 10% • 17%

A472 N473 K474 R475 M476 K477 V478 K479 H480 D481 Y484 R491 Y492 Y493 R501 V504 R510 R511 N514 Y536 R537 R548 S574 Q575 D576 P577 S578 G579 D580 S581 K582 R590 Q593 I594 R595 Q596 Y597 L600 S601 D602 R603 S604

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

Chain D: 79% 21%

G1 C8 C11 C12 A17 C18 G19

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

Chain E: 84% 11% 5%

C20 T26 G27 A30 C38

4.2.16 Score per residue for model 16

• Molecule 1: Transcriptional regulator Kaiso

Chain A: 73% 8% • 17%

A472 N473 K474 R475 M476 K477 V478 K479 H480 D481 Y484 Y493 R501 S502 Y503 V504 R510 R511 N514 R537 R548 R549 Y550 S574 Q575 D576 P577 S578 G579 D580 S581 K582 R595 S601 D602 R603 S604

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

Chain D: 84% 11% 5%

G1 C7 C8 A17 C18 G19

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

Chain E: 68% 32%

C20 T26 G27 G28 C29 A30 G31 G32 A33 C38

4.2.17 Score per residue for model 17

• Molecule 1: Transcriptional regulator Kaiso

Chain A: 70% 10% • 17%

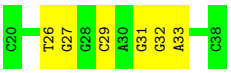
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D: 100%

There are no outlier residues in this chain.

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

Chain E: 68% 32%



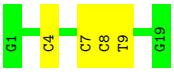
4.2.18 Score per residue for model 18

• Molecule 1: Transcriptional regulator Kaiso

Chain A: 69% 12% • 17%

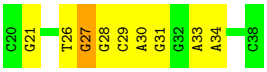
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D: 79% 21%



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

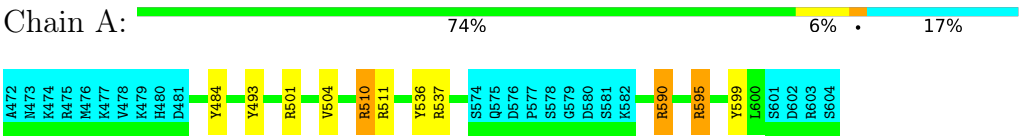
Chain E: 53% 42% 5%



4.2.19 Score per residue for model 19

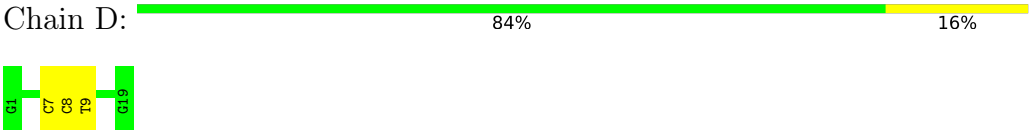
• Molecule 1: Transcriptional regulator Kaiso

Chain A:



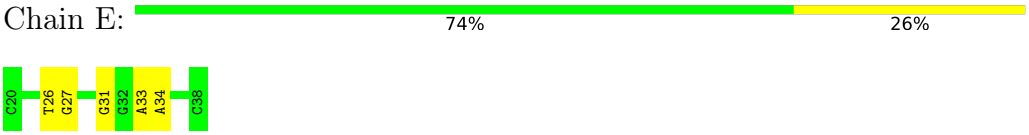
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

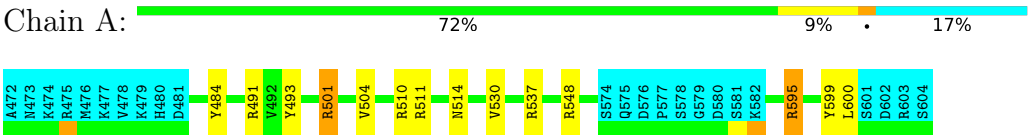
Chain E:



4.2.20 Score per residue for model 20

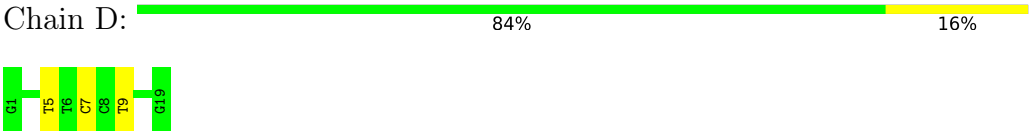
• Molecule 1: Transcriptional regulator Kaiso

Chain A:



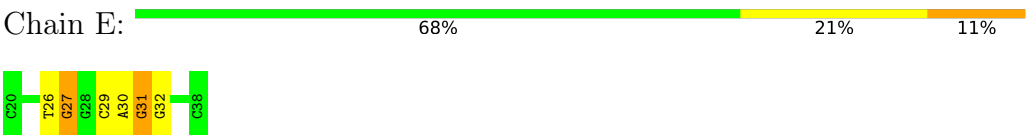
• Molecule 2: DNA (5'-D(*GP*TP*GP*CP*TP*TP*CP*CP*TP*GP*CP*CP*AP*AP*TP*AP*AP*CP*G)-3')

Chain D:



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

Chain E:



5 Refinement protocol and experimental data overview (i)

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
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	2061
Number of shifts mapped to atoms	2061
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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

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	0.88±0.01	0±0/979 (0.0± 0.0%)	1.08±0.04	10±2/1320 (0.8± 0.2%)
2	D	1.61±0.02	0±0/428 (0.0± 0.1%)	1.43±0.01	2±1/658 (0.3± 0.2%)
3	E	1.57±0.02	0±0/438 (0.0± 0.0%)	1.42±0.02	3±1/675 (0.4± 0.1%)
All	All	1.26	2/36900 (0.0%)	1.27	306/53060 (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	A	0.0±0.0	3.4±1.1
2	D	0.0±0.0	1.3±1.1
3	E	0.0±0.0	4.1±1.3
All	All	0	175

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
3	E	31	DG	P-O5'	5.22	1.65	1.59	12	1
2	D	6	DT	C5-C7	5.13	1.53	1.50	14	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	501	ARG	NE-CZ-NH1	14.18	127.39	120.30	12	19
1	A	511	ARG	NE-CZ-NH1	11.45	126.03	120.30	11	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	510	ARG	NE-CZ-NH1	10.30	125.45	120.30	16	17
1	A	549	ARG	NE-CZ-NH1	8.82	124.71	120.30	3	10
1	A	511	ARG	NE-CZ-NH2	-8.55	116.02	120.30	10	11
1	A	493	TYR	CB-CG-CD2	-8.49	115.90	121.00	5	20
1	A	585	ARG	NE-CZ-NH1	7.68	124.14	120.30	6	4
1	A	549	ARG	NE-CZ-NH2	-7.61	116.50	120.30	3	3
1	A	491	ARG	NE-CZ-NH1	7.54	124.07	120.30	5	7
1	A	590	ARG	NE-CZ-NH2	-7.30	116.65	120.30	15	3
1	A	536	TYR	CB-CG-CD2	-7.11	116.73	121.00	2	10
1	A	595	ARG	NE-CZ-NH1	7.10	123.85	120.30	1	17
1	A	548	ARG	NE-CZ-NH1	6.94	123.77	120.30	12	9
2	D	9	DT	C1'-O4'-C4'	-6.87	103.23	110.10	18	12
3	E	27	DG	C1'-O4'-C4'	-6.84	103.26	110.10	6	20
1	A	501	ARG	NE-CZ-NH2	6.80	123.70	120.30	16	2
3	E	27	DG	C3'-C2'-C1'	-6.51	94.68	102.50	6	17
1	A	590	ARG	NE-CZ-NH1	6.49	123.55	120.30	15	6
3	E	31	DG	C1'-O4'-C4'	-6.49	103.61	110.10	4	7
1	A	595	ARG	NE-CZ-NH2	-6.44	117.08	120.30	6	6
3	E	29	DC	O4'-C4'-C3'	6.40	109.84	106.00	1	4
1	A	504	VAL	CA-CB-CG1	6.30	120.35	110.90	4	20
1	A	537	ARG	NE-CZ-NH2	6.17	123.39	120.30	18	1
1	A	537	ARG	NE-CZ-NH1	6.14	123.37	120.30	18	5
2	D	7	DC	O4'-C4'-C3'	6.06	109.64	106.00	1	12
2	D	17	DA	O4'-C4'-C3'	5.98	109.59	106.00	16	4
1	A	501	ARG	NH1-CZ-NH2	-5.85	112.97	119.40	16	4
2	D	5	DT	O4'-C4'-C3'	5.80	109.48	106.00	20	2
1	A	493	TYR	CB-CG-CD1	5.78	124.47	121.00	5	1
1	A	525	ARG	NE-CZ-NH1	5.74	123.17	120.30	14	5
1	A	530	VAL	CG1-CB-CG2	-5.67	101.83	110.90	20	1
1	A	511	ARG	NH1-CZ-NH2	-5.65	113.19	119.40	15	2
1	A	537	ARG	NH1-CZ-NH2	-5.61	113.23	119.40	18	1
3	E	26	DT	C1'-O4'-C4'	-5.49	104.61	110.10	4	1
1	A	525	ARG	CD-NE-CZ	5.44	131.21	123.60	1	1
2	D	9	DT	C3'-C2'-C1'	-5.33	96.11	102.50	20	5
2	D	18	DC	O4'-C4'-C3'	5.31	109.19	106.00	14	2
2	D	8	DC	O4'-C4'-C3'	5.31	109.19	106.00	10	3
2	D	4	DC	O4'-C4'-C3'	5.29	109.17	106.00	11	4
3	E	31	DG	P-O3'-C3'	5.21	125.95	119.70	18	1
2	D	16	DA	O4'-C4'-C3'	5.20	109.12	106.00	7	1
3	E	24	DA	C1'-O4'-C4'	-5.20	104.90	110.10	10	1
1	A	537	ARG	CA-CB-CG	5.17	124.78	113.40	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	599	TYR	CA-CB-CG	5.12	123.12	113.40	18	1
1	A	537	ARG	CB-CG-CD	5.07	124.79	111.60	2	1
3	E	25	DT	O4'-C4'-C3'	5.05	109.03	106.00	9	1
3	E	28	DG	P-O5'-C5'	5.03	128.94	120.90	18	1
3	E	33	DA	O4'-C4'-C3'	5.02	109.01	106.00	17	1
1	A	590	ARG	CD-NE-CZ	5.02	130.63	123.60	2	1
3	E	26	DT	O4'-C4'-C3'	5.01	109.01	106.00	7	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	484	TYR	Sidechain	20
3	E	26	DT	Sidechain	19
1	A	595	ARG	Sidechain	17
3	E	30	DA	Sidechain	14
3	E	27	DG	Sidechain	13
3	E	29	DC	Sidechain	11
2	D	8	DC	Sidechain	8
3	E	33	DA	Sidechain	7
2	D	17	DA	Sidechain	6
1	A	501	ARG	Sidechain	5
1	A	503	TYR	Sidechain	5
1	A	597	TYR	Sidechain	5
3	E	32	DG	Sidechain	5
3	E	34	DA	Sidechain	4
1	A	599	TYR	Sidechain	4
2	D	18	DC	Sidechain	3
2	D	19	DG	Sidechain	3
3	E	23	DT	Sidechain	3
1	A	562	TYR	Sidechain	3
2	D	11	DC	Sidechain	3
1	A	537	ARG	Sidechain	3
3	E	31	DG	Sidechain	3
3	E	21	DG	Sidechain	2
1	A	511	ARG	Sidechain	2
1	A	550	TYR	Sidechain	2
2	D	7	DC	Sidechain	2
1	A	544	HIS	Sidechain	1
3	E	24	DA	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
2	D	12	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	949	932	929	0±0
4	A	3	0	0	0±0
All	All	34500	27180	27210	5

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:552:CYS:HG	4:A:703:ZN:ZN	0.96	0.70	4	3
1:A:524:CYS:HG	4:A:702:ZN:ZN	0.87	0.60	2	1
1:A:555:CYS:HG	4:A:703:ZN:ZN	0.55	0.36	12	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	A	110/133 (83%)	108±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
All	All	2200/2660 (83%)	2154 (98%)	46 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	104/125 (83%)	100±1 (96±1%)	4±1 (4±1%)	33	82
All	All	2080/2500 (83%)	1992 (96%)	88 (4%)	33	82

All 17 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	514	ASN	19
1	A	600	LEU	17
1	A	537	ARG	14
1	A	510	ARG	7
1	A	565	MET	7
1	A	543	HIS	4
1	A	590	ARG	4
1	A	586	LEU	3
1	A	593	GLN	3
1	A	560	ILE	2
1	A	592	LEU	2
1	A	525	ARG	1
1	A	529	LYS	1
1	A	547	GLU	1
1	A	548	ARG	1
1	A	549	ARG	1
1	A	589	CYS	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 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 (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_KBS*

7.1.1 Bookkeeping (i)

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	2061
Number of shifts mapped to atoms	2061
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	133	-0.18 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	127	1.14 ± 0.18	Should be checked
$^{13}C'$	127	-0.45 ± 0.12	None needed (< 0.5 ppm)
^{15}N	126	0.21 ± 0.43	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 1784 atoms were assigned a chemical shift out of a possible 2398. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	541/547 (99%)	217/220 (99%)	217/220 (99%)	107/107 (100%)
Sidechain	746/867 (86%)	513/562 (91%)	218/259 (84%)	15/46 (33%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	195/232 (84%)	90/110 (82%)	86/103 (83%)	19/19 (100%)
Sugar	213/456 (47%)	213/266 (80%)	0/190 (0%)	0/0 (—%)
Base	89/296 (30%)	89/182 (49%)	0/66 (0%)	0/48 (0%)
Overall	1784/2398 (74%)	1122/1340 (84%)	521/838 (62%)	141/220 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 2034 atoms were assigned a chemical shift out of a possible 2692. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	646/661 (98%)	260/266 (98%)	260/266 (98%)	126/129 (98%)
Sidechain	885/1039 (85%)	607/669 (91%)	261/312 (84%)	17/58 (29%)
Aromatic	201/240 (84%)	92/114 (81%)	88/105 (84%)	21/21 (100%)
Sugar	213/456 (47%)	213/266 (80%)	0/190 (0%)	0/0 (—%)
Base	89/296 (30%)	89/182 (49%)	0/66 (0%)	0/48 (0%)
Overall	2034/2692 (76%)	1261/1497 (84%)	609/939 (65%)	164/256 (64%)

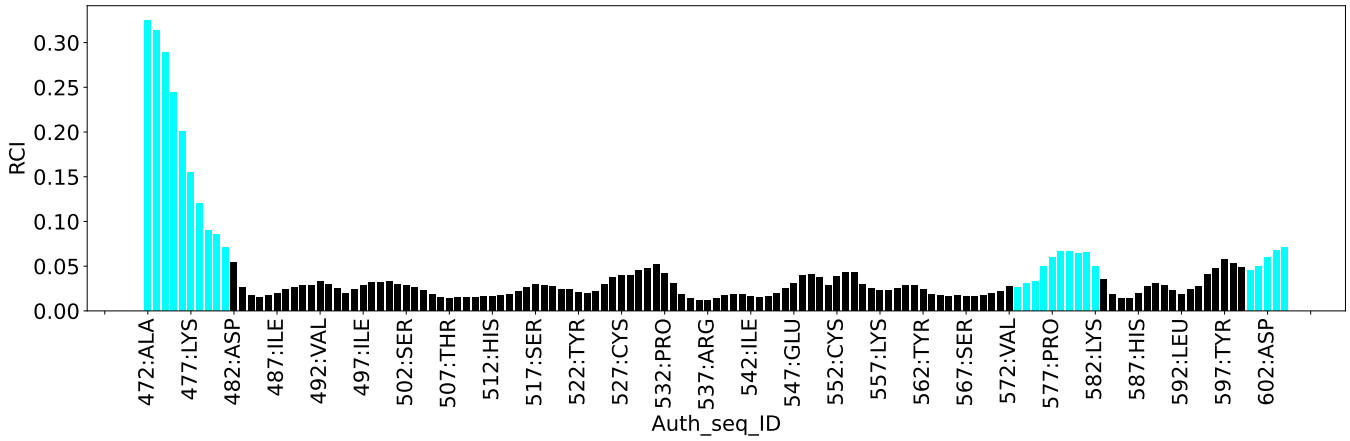
7.1.4 Statistically unusual chemical shifts (i)

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
2	A	503	TYR	CE2	133.06	111.68 – 124.17	12.1
2	A	503	TYR	CE1	133.06	111.24 – 124.66	11.3
2	A	550	TYR	CE2	131.42	111.68 – 124.17	10.8
2	A	550	TYR	CE1	131.42	111.24 – 124.66	10.0
2	A	562	TYR	CD1	121.57	125.84 – 139.60	-8.1
2	A	562	TYR	CD2	121.57	125.28 – 140.14	-7.5
2	A	533	LEU	HB2	-0.20	-0.07 – 3.30	-5.4
2	A	540	HIS	CD2	137.28	103.95 – 136.66	5.2
2	A	503	TYR	HE1	7.82	5.59 – 7.82	5.0

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: