Full wwPDB NMR Structure Validation Report (i)

Jun 16, 2024 – 08:35 PM EDT

PDB ID	:	5JYV
BMRB ID	:	30093
Title	:	NMR structure of foldswitch-stablized KaiB in complex with pseudo receiver domain of CikA from Thermosynechococcus elongatus
Authors	:	Tseng, R.D.; LiWang, A.L.
Deposited on	:	2016-05-15

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:

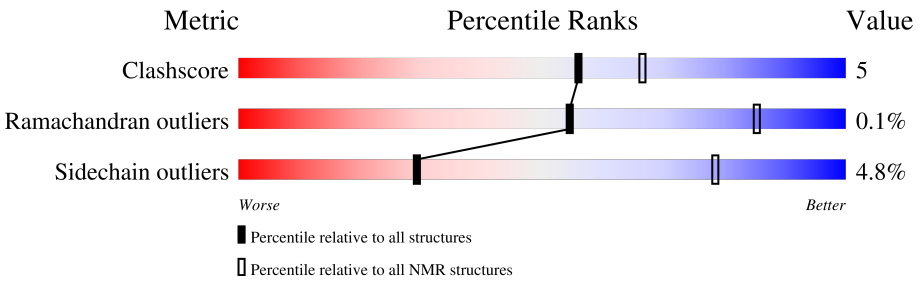
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 87%.

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	117	74% 14% 12%
2	B	106	79% 8% 13%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 9 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:614-A:692, A:699-A:722, B:6-B:97 (195)	0.99	9

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3558 atoms, of which 1823 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Two-component sensor histidine kinase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	117	1831	580	924	147	177	3	0

- Molecule 2 is a protein called Circadian clock protein KaiB.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	106	1727	532	899	142	153	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ALA	TYR	engineered mutation	UNP Q79V61
B	29	ALA	ASN	engineered mutation	UNP Q79V61
B	89	ALA	GLY	engineered mutation	UNP Q79V61
B	91	ARG	ASP	engineered mutation	UNP Q79V61
B	94	ALA	TYR	engineered mutation	UNP Q79V61
B	100	TYR	-	expression tag	UNP Q79V61
B	101	LYS	-	expression tag	UNP Q79V61
B	102	ASP	-	expression tag	UNP Q79V61
B	103	ASP	-	expression tag	UNP Q79V61
B	104	ASP	-	expression tag	UNP Q79V61
B	105	ASP	-	expression tag	UNP Q79V61
B	106	LYS	-	expression tag	UNP Q79V61

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: Two-component sensor histidine kinase

Chain A: 74% 14% 12%

E613 I616 L633 T634 T635 Y638 Q639 V640 I641 W642 L643 L654 T655 V659 L660 L686 F689 S693 K694 G695 N696 Y697 Q698 L706 P707 I708 S723 L724 A725 T726 S727 A728 Q729

• Molecule 2: Circadian clock protein KaiB

Chain B: 79% 8% 13%

M1 A2 P3 L4 R5 K6 L12 L25 I31 F36 N50 P51 Q52 R83 G98 D99 Y100 K101 D102 D103 D104 D105 K106

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: Two-component sensor histidine kinase

Chain A: 74% 12% • 12%

E613 S620 T634 T635 Y638 L654 T655 P656 I657 A658 V659 L660 L661 A662 L686 F689 G692 S693 K694 G695 N696 Y697 Q698 P705 L721 T722 S723 L724 A725 T726 S727 A728 Q729

• Molecule 2: Circadian clock protein KaiB

Chain B: 71% 13% • 13%

M1 A2 P3 L4 R5 K6 T7 N17 T18 P19 N20 L25 I31 L32 E33 K37 V44 K49 N50 L53 P63 P71 P72 L80 R83 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.2 Score per residue for model 2

- Molecule 1: Two-component sensor histidine kinase

Chain A: 72% 15% • 12%

E613 I616 L633 T634 Y638 Q639 V640 L643 L652 T655 L660 L661 F665 V674 I688 F689 I690 S693 K694 G695 N696 Y697 Q698 G699 L706 P707 I708 V717 S723 L724 A725 T726 S727 A728 Q729

- Molecule 2: Circadian clock protein KaiB

Chain B: 62% 25% 13%

M1 A2 P3 L4 R5 K6 T7 A8 V9 L10 K11 V14 N17 I31 L32 E33 K34 E35 F36 K37 K43 L48 K49 N50 P51 Q52 P63 T64 L65 A66 R83 L87 R91 L92 L93 A94 E95 E96 I97 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.3 Score per residue for model 3

- Molecule 1: Two-component sensor histidine kinase

Chain A: 71% 17% 12%

E613 I616 V617 L633 T634 T635 Y638 I641 W642 L643 E647 L654 T655 P656 L660 V674 D675 Q676 L686 K687 I688 F689 S693 K694 G695 N696 Y697 Q698 L706 P707 S723 L724 A725 T726 S727 A728 Q729

- Molecule 2: Circadian clock protein KaiB

Chain B: 72% 15% 13%

M1 A2 P3 L4 R5 Y13 I31 L32 E33 K34 V39 Y40 A41 L42 N50 P51 Q52 P63 K67 V73 R83 V86 A94 I97 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.4 Score per residue for model 4

- Molecule 1: Two-component sensor histidine kinase

Chain A: 69% 18% • 12%

E613 I616 V617 T625 T634 Y638 Q639 V640 L643 L654 T655 P656 I657 A658 V659 L660 V674 L686 K687 I688 L691 G692 S693 K694 G695 N696 Y697 Q698 R702 L706 P707 I708 F713 L721 T722 S723 L724 A725 T726 S727 A728 Q729

- Molecule 2: Circadian clock protein KaiB

Chain B: 69% 16% • 13%

M1 A2 P3 L4 R5 V9 L10 K11 L12 A15 V22 L25 K26 I31 A41 L48 K49 N50 P51 Q52 L53 A66 K67 P70 R83 E84 K85 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.5 Score per residue for model 5

- Molecule 1: Two-component sensor histidine kinase

Chain A: 73% 15% 12%

E613 I616 L633 T634 T635 Y638 Q639 V640 I641 L654 V659 L660 Q676 Q679 R680 L686 F689 S693 K694 G695 N696 Y697 Q698 L706 P707 I708 L721 T722 S723 L724 A725 T726 S727 A728 Q729

- Molecule 2: Circadian clock protein KaiB

Chain B: 71% 16% 13%

M1 A2 P3 L4 R5 K6 K11 L12 Y13 L28 I31 L32 F36 N50 P51 Q52 L53 P63 T64 L65 A66 R83 L87 R91 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.6 Score per residue for model 6

- Molecule 1: Two-component sensor histidine kinase

Chain A: 74% 13% • 12%

E613 L618 V619 S620 L633 Q639 V640 I641 W642 L654 T655 V659 F665 D675 R678 L686 S693 K694 G695 N696 Y697 Q698 L706 P707 S723 L724 A725 T726 S727 A728 Q729

- Molecule 2: Circadian clock protein KaiB

Chain B: 81% 6% 13%

M1 A2 P3 L4 R5 L10 V39 Y40 N50 P51 Q52 L65 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.7 Score per residue for model 7

- Molecule 1: Two-component sensor histidine kinase

Chain A: 67% 21% • 12%

E613 I616 L633 T634 T635 Y638 Q639 V640 I641 W642 L643 R650 L651 L652 A653 L654 T655 P656 I657 A658 V659 L660 F665 V674 L686 K687 I688 F689 S693 K694 G695 N696 Y697 Q698 L706 P707 I708 V717 L721 T722 S723 L724 A725 T726 S727 A728 Q729

- Molecule 2: Circadian clock protein KaiB

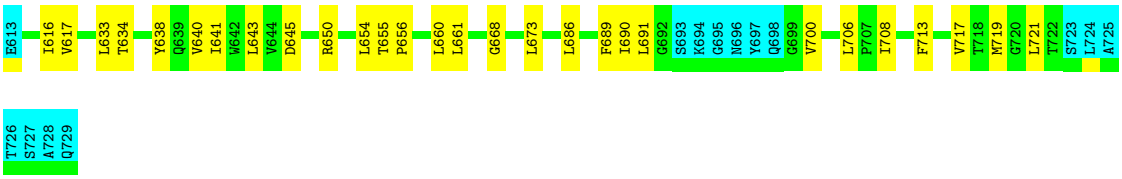
Chain B: 70% 17% 13%

M1 A2 P3 L4 R5 L10 K11 L12 N30 I31 L32 E33 G38 V39 Y40 A41 L42 K43 N50 P51 Q52 L65 A66 K67 V68 V73 V86 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.8 Score per residue for model 8

- Molecule 1: Two-component sensor histidine kinase

Chain A: 64% 24% 12%



- Molecule 2: Circadian clock protein KaiB

Chain B: 70% 17% 13%

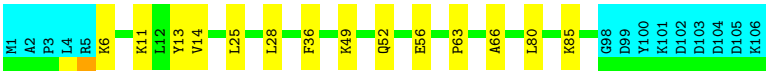
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Two-component sensor histidine kinase

Chain A: 70% 18% 12%

- Molecule 2: Circadian clock protein KaiB

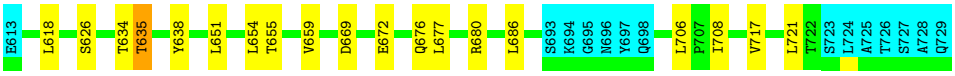
Chain B: 74% 13% 13%



4.2.10 Score per residue for model 10

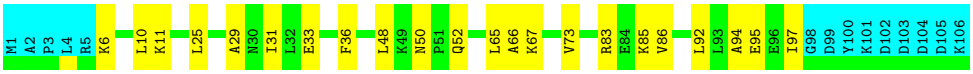
- Molecule 1: Two-component sensor histidine kinase

Chain A: 72% 15% • 12%



- Molecule 2: Circadian clock protein KaiB

Chain B: 66% 21% 13%



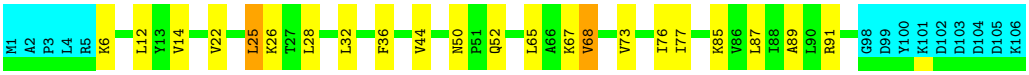
4.2.11 Score per residue for model 11

- Molecule 1: Two-component sensor histidine kinase

Chain A: 67% 21% 12%

- Molecule 2: Circadian clock protein KaiB

Chain B: 66% 19% • 13%



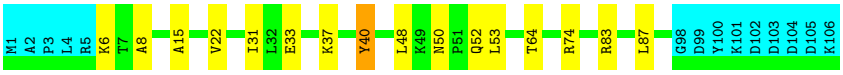
4.2.12 Score per residue for model 12

- Molecule 1: Two-component sensor histidine kinase

Chain A: 77% 11% 12%

- Molecule 2: Circadian clock protein KaiB

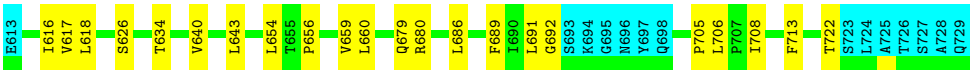
Chain B: 72% 14% • 13%



4.2.13 Score per residue for model 13

- Molecule 1: Two-component sensor histidine kinase

Chain A: 69% 19% 12%



- Molecule 2: Circadian clock protein KaiB

Chain B: 64% 22% • 13%

M1 A2 P3 L4 R5 K6 L12 Y13 V14 A24 L25 L28 E33 F36 K37 G38 V47 L48 A54 I59 T62 P63 T64 L69 P70 R74 L80 R83 V86 E96 I97 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.14 Score per residue for model 14

• Molecule 1: Two-component sensor histidine kinase

Chain A: 65% 22% • 12%

E613 G614 R615 I616 L633 T634 T635 Y638 Q639 V640 I641 V644 L652 A653 L654 V659 L660 L661 F665 V674 R680 E684 Q685 L686 K687 I688 F689 S693 K694 G695 N696 Y697 Q698 R702 L706 P707 V717 T718 M719 G720 L721 T722 S723 L724 A725 T726 S727 A728 Q729

• Molecule 2: Circadian clock protein KaiB

Chain B: 77% 9% 13%

M1 A2 P3 L4 R5 K6 A15 I31 K34 E35 F36 L48 K49 V68 V73 R83 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.15 Score per residue for model 15

• Molecule 1: Two-component sensor histidine kinase

Chain A: 79% 9% 12%

E613 V617 L618 T634 Y638 I641 L654 T655 P656 V659 L686 S693 K694 G695 N696 Y697 Q698 T718 S723 L724 A725 T726 S727 A728 Q729

• Molecule 2: Circadian clock protein KaiB

Chain B: 75% 11% 13%

M1 A2 P3 L4 R5 L12 V22 L25 K26 E33 F36 K37 Q52 E56 T64 L65 I76 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.16 Score per residue for model 16

• Molecule 1: Two-component sensor histidine kinase

Chain A: 71% 16% • 12%

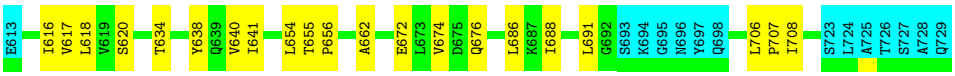
• Molecule 2: Circadian clock protein KaiB

Chain B:

4.2.17 Score per residue for model 17

• Molecule 1: Two-component sensor histidine kinase

Chain A:



• Molecule 2: Circadian clock protein KaiB

Chain B:

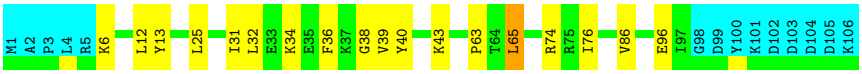
4.2.18 Score per residue for model 18

• Molecule 1: Two-component sensor histidine kinase

Chain A:

• Molecule 2: Circadian clock protein KaiB

Chain B:



4.2.19 Score per residue for model 19

• Molecule 1: Two-component sensor histidine kinase

Chain A: 66% 21% • 12%

E613 G614 R615 L618 V619 T625 C630 S631 I632 L633 T634 T635 Y638 Q639 V640 I641 W642 L643 R650 L654 T655 V659 L660 V674 L686 K687 I688 F689 S693 K694 G695 N696 Y697 Q698 L706 P707 I708 V717 L721 T722 S723 L724 A725 T726 S727 A728 Q729

• Molecule 2: Circadian clock protein KaiB

Chain B: 74% 13% 13%

M1 A2 P3 L4 R5 K6 T7 A8 V9 L10 K11 L12 L25 I31 L32 Y40 A41 N50 P51 Q52 T62 L65 R83 G98 D99 Y100 K101 D102 D103 D104 D105 K106

4.2.20 Score per residue for model 20

• Molecule 1: Two-component sensor histidine kinase

Chain A: 68% 18% • 12%

E613 I616 V619 T625 I629 L633 T634 Y638 Q639 V640 D645 L654 V659 L660 D669 E672 R678 L686 F689 S693 K694 G695 N696 Y697 Q698 Y703 I704 P705 L706 P707 I708 M719 S723 L724 A725 T726 S727 A728 Q729

• Molecule 2: Circadian clock protein KaiB

Chain B: 74% 13% 13%

M1 A2 P3 L4 R5 K6 T7 L12 L25 I31 L32 E33 F36 K37 K67 P70 I77 R83 E84 K85 A94 I97 G98 D99 Y100 K101 D102 D103 D104 D105 K106

5 Refinement protocol and experimental data overview (i)

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

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
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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	2637
Number of shifts mapped to atoms	2637
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	803	826	826	10±3
2	B	714	794	794	7±3
All	All	30340	32400	32400	325

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:634:THR:HA	1:A:638:TYR:O	0.71	1.85	1	16
1:A:634:THR:OG1	2:B:7:THR:HG21	0.71	1.86	1	1
2:B:25:LEU:HD11	2:B:44:VAL:HG21	0.70	1.63	1	2
1:A:706:LEU:HD23	1:A:708:ILE:HG23	0.70	1.64	13	10
2:B:15:ALA:HB1	2:B:48:LEU:HB2	0.67	1.66	4	3
2:B:8:ALA:HB3	2:B:40:TYR:HB3	0.67	1.65	12	2
1:A:641:ILE:HG21	1:A:654:LEU:HD13	0.65	1.67	14	12
2:B:93:LEU:O	2:B:96:GLU:HG2	0.65	1.90	2	2
2:B:76:ILE:HD13	2:B:89:ALA:HB1	0.64	1.70	11	1
2:B:50:ASN:OD1	2:B:53:LEU:HG	0.64	1.92	17	5
1:A:654:LEU:HD11	2:B:25:LEU:HD12	0.64	1.70	1	1
2:B:32:LEU:HD11	2:B:90:LEU:HG	0.63	1.70	8	1
1:A:659:VAL:HG23	1:A:686:LEU:HD11	0.62	1.69	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:616:ILE:HG21	1:A:633:LEU:HD13	0.62	1.71	11	3
1:A:669:ASP:O	1:A:672:GLU:HG2	0.61	1.96	18	4
1:A:660:LEU:HD23	1:A:689:PHE:HB2	0.61	1.72	13	13
2:B:54:ALA:HA	2:B:59:ILE:HD12	0.61	1.72	13	1
2:B:31:ILE:HD11	2:B:83:ARG:HG3	0.60	1.73	5	9
2:B:14:VAL:HG12	2:B:63:PRO:HB3	0.60	1.72	13	3
1:A:654:LEU:HD11	2:B:25:LEU:HD23	0.60	1.73	4	1
2:B:11:LYS:HB2	2:B:66:ALA:HB3	0.60	1.74	16	7
2:B:32:LEU:HB3	2:B:40:TYR:CE2	0.60	2.31	8	1
1:A:674:VAL:HG22	1:A:688:ILE:HG21	0.60	1.72	7	5
1:A:617:VAL:HG22	1:A:656:PRO:HG3	0.59	1.74	16	2
2:B:50:ASN:OD1	2:B:52:GLN:HG2	0.59	1.97	6	8
2:B:28:LEU:HD11	2:B:80:LEU:HD12	0.59	1.73	9	1
1:A:717:VAL:O	1:A:721:LEU:HG	0.59	1.97	14	5
1:A:706:LEU:HD12	1:A:707:PRO:HA	0.59	1.75	20	2
1:A:674:VAL:HG13	1:A:688:ILE:HD13	0.58	1.75	19	2
2:B:27:THR:HG23	2:B:83:ARG:HG3	0.58	1.75	17	1
1:A:616:ILE:HB	1:A:640:VAL:HG22	0.58	1.75	20	2
1:A:692:GLY:O	1:A:705:PRO:HA	0.57	2.00	13	2
2:B:33:GLU:O	2:B:37:LYS:HB2	0.56	2.00	15	4
1:A:654:LEU:HD21	2:B:25:LEU:HD12	0.56	1.77	20	1
1:A:626:SER:HA	1:A:642:TRP:CZ3	0.56	2.36	9	2
1:A:653:ALA:HB2	2:B:22:VAL:HG13	0.56	1.78	16	3
1:A:652:LEU:HA	1:A:655:THR:HG23	0.55	1.78	7	2
2:B:9:VAL:HG11	2:B:43:LYS:HE2	0.55	1.79	2	1
2:B:83:ARG:HA	2:B:86:VAL:HG12	0.55	1.79	10	3
1:A:634:THR:HB	2:B:7:THR:HG21	0.54	1.79	20	3
2:B:67:LYS:CB	2:B:73:VAL:HB	0.53	2.33	11	1
2:B:92:LEU:O	2:B:95:GLU:HG2	0.53	2.03	10	1
1:A:618:LEU:HD22	1:A:642:TRP:CH2	0.53	2.39	9	2
2:B:69:LEU:HD12	2:B:70:PRO:HA	0.53	1.80	13	1
1:A:654:LEU:HD21	2:B:25:LEU:HB3	0.53	1.80	13	3
1:A:633:LEU:HD11	1:A:717:VAL:HG11	0.52	1.81	7	1
1:A:661:LEU:HB2	1:A:690:ILE:HG22	0.52	1.80	8	2
1:A:690:ILE:HG12	1:A:700:VAL:HG11	0.51	1.82	8	1
1:A:617:VAL:HG23	1:A:656:PRO:HB3	0.51	1.80	8	7
1:A:659:VAL:HG13	1:A:686:LEU:HD11	0.51	1.80	9	4
2:B:94:ALA:O	2:B:97:ILE:HG22	0.51	2.05	17	5
1:A:634:THR:O	2:B:38:GLY:HA2	0.51	2.06	13	3
2:B:33:GLU:O	2:B:37:LYS:HB3	0.51	2.06	8	4
1:A:691:LEU:HD21	1:A:708:ILE:HD12	0.51	1.82	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:658:ALA:HB2	1:A:721:LEU:HD21	0.50	1.83	4	1
2:B:12:LEU:CD2	2:B:65:LEU:HG	0.50	2.36	11	1
1:A:625:THR:O	1:A:629:ILE:HB	0.50	2.06	11	2
1:A:643:LEU:HD13	1:A:650:ARG:HB3	0.50	1.83	11	1
2:B:67:LYS:O	2:B:73:VAL:HA	0.50	2.07	3	2
1:A:620:SER:HB2	1:A:662:ALA:HB3	0.49	1.84	1	1
2:B:67:LYS:HE2	2:B:70:PRO:O	0.49	2.07	4	2
2:B:22:VAL:O	2:B:26:LYS:HG3	0.49	2.07	15	3
2:B:10:LEU:HG	2:B:65:LEU:HD21	0.49	1.84	6	2
1:A:651:LEU:HD13	1:A:677:LEU:HD21	0.49	1.83	10	2
1:A:619:VAL:HG12	1:A:645:ASP:HB3	0.49	1.84	20	1
1:A:641:ILE:HD13	1:A:654:LEU:HD13	0.49	1.84	18	1
2:B:63:PRO:HB2	2:B:80:LEU:HD12	0.48	1.84	1	1
1:A:639:GLN:HE21	2:B:32:LEU:HD22	0.48	1.68	16	1
1:A:616:ILE:O	1:A:640:VAL:HA	0.48	2.07	9	11
1:A:706:LEU:HA	1:A:707:PRO:C	0.48	2.29	3	5
2:B:32:LEU:HD12	2:B:36:PHE:HB2	0.48	1.85	11	4
2:B:65:LEU:HD22	2:B:76:ILE:HD12	0.48	1.86	15	1
2:B:18:THR:HB	2:B:20:ASN:OD1	0.48	2.08	1	1
2:B:29:ALA:O	2:B:33:GLU:HG2	0.47	2.09	10	1
2:B:34:LYS:O	2:B:37:LYS:HG2	0.47	2.09	8	1
2:B:32:LEU:HD11	2:B:40:TYR:HB2	0.47	1.85	17	1
1:A:620:SER:HB3	1:A:642:TRP:CH2	0.47	2.44	6	1
1:A:618:LEU:HD13	1:A:629:ILE:HG21	0.46	1.87	16	2
1:A:620:SER:HB3	1:A:662:ALA:HB3	0.46	1.87	17	1
1:A:633:LEU:HD21	1:A:717:VAL:HG11	0.46	1.88	2	1
1:A:618:LEU:HD21	1:A:626:SER:HA	0.46	1.87	13	2
2:B:25:LEU:HD11	2:B:44:VAL:CG2	0.46	2.37	1	2
2:B:39:VAL:HG23	2:B:40:TYR:CD1	0.46	2.46	6	2
1:A:706:LEU:CD1	1:A:707:PRO:HA	0.46	2.38	6	1
1:A:676:GLN:O	1:A:680:ARG:HG2	0.46	2.11	5	2
2:B:13:TYR:O	2:B:63:PRO:HA	0.45	2.11	9	4
2:B:30:ASN:O	2:B:33:GLU:HG2	0.45	2.11	7	1
2:B:31:ILE:HD11	2:B:86:VAL:HG13	0.45	1.89	10	2
1:A:645:ASP:OD2	1:A:668:GLY:HA3	0.45	2.11	8	1
2:B:9:VAL:HG12	2:B:41:ALA:HB3	0.45	1.88	4	1
1:A:675:ASP:O	1:A:678:ARG:HG2	0.45	2.11	6	3
1:A:654:LEU:HD11	2:B:25:LEU:HD22	0.45	1.87	10	2
1:A:617:VAL:HG12	1:A:641:ILE:HB	0.45	1.88	16	1
1:A:674:VAL:HG11	1:A:699:GLY:HA3	0.45	1.89	2	1
2:B:36:PHE:CE2	2:B:94:ALA:HB2	0.45	2.47	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:65:LEU:HD11	2:B:76:ILE:HD12	0.45	1.88	18	1
2:B:24:ALA:HB1	2:B:80:LEU:HD23	0.44	1.87	13	1
1:A:660:LEU:HD13	1:A:713:PHE:HZ	0.44	1.72	9	2
2:B:39:VAL:HG13	2:B:40:TYR:HD1	0.44	1.73	7	2
2:B:12:LEU:HD22	2:B:28:LEU:HD22	0.44	1.90	13	1
2:B:50:ASN:OD1	2:B:52:GLN:HB3	0.43	2.13	4	3
1:A:657:ILE:HD12	1:A:721:LEU:HD11	0.43	1.89	1	1
1:A:691:LEU:HD11	1:A:713:PHE:HE1	0.43	1.73	4	4
2:B:10:LEU:HG	2:B:65:LEU:HD11	0.43	1.90	7	1
2:B:68:VAL:HA	2:B:73:VAL:HG12	0.43	1.90	14	2
1:A:705:PRO:O	1:A:708:ILE:HG22	0.43	2.13	20	1
1:A:633:LEU:HB2	1:A:640:VAL:HG21	0.43	1.91	6	3
1:A:656:PRO:HD2	1:A:686:LEU:HD11	0.43	1.91	12	1
2:B:28:LEU:HD13	2:B:80:LEU:HD11	0.43	1.91	13	1
2:B:71:PRO:HA	2:B:72:PRO:C	0.43	2.34	1	2
2:B:31:ILE:CD1	2:B:86:VAL:HG13	0.43	2.44	3	2
2:B:29:ALA:O	2:B:33:GLU:HB2	0.43	2.13	8	1
1:A:617:VAL:CG2	1:A:656:PRO:HG3	0.43	2.44	16	1
1:A:629:ILE:HD11	1:A:708:ILE:HD11	0.43	1.91	20	1
2:B:67:LYS:O	2:B:73:VAL:HG13	0.42	2.14	8	1
2:B:52:GLN:O	2:B:56:GLU:HG2	0.42	2.14	9	2
2:B:47:VAL:HG21	2:B:62:THR:HG21	0.42	1.90	13	1
1:A:615:ARG:HA	1:A:639:GLN:O	0.42	2.15	19	1
1:A:643:LEU:HD21	1:A:654:LEU:HD12	0.42	1.89	19	1
1:A:645:ASP:OD1	1:A:673:LEU:HD11	0.42	2.13	8	1
1:A:657:ILE:O	1:A:686:LEU:HA	0.42	2.15	7	1
2:B:87:LEU:O	2:B:91:ARG:HB2	0.42	2.14	2	1
1:A:631:SER:O	1:A:635:THR:HG22	0.41	2.15	16	2
1:A:656:PRO:O	1:A:686:LEU:HD12	0.41	2.16	3	1
2:B:83:ARG:HA	2:B:86:VAL:CG1	0.41	2.46	13	1
1:A:672:GLU:HG3	1:A:676:GLN:OE1	0.41	2.15	17	1
1:A:630:CYS:SG	2:B:41:ALA:HB1	0.41	2.56	19	1
2:B:87:LEU:O	2:B:91:ARG:HG2	0.41	2.16	5	2
1:A:652:LEU:HD21	1:A:680:ARG:HG3	0.41	1.92	14	1
2:B:28:LEU:HA	2:B:86:VAL:HG11	0.40	1.93	16	1
1:A:674:VAL:HG13	1:A:688:ILE:CD1	0.40	2.45	19	1
2:B:10:LEU:HB3	2:B:65:LEU:HD11	0.40	1.94	10	1
1:A:643:LEU:HD11	1:A:650:ARG:HB3	0.40	1.92	18	1
1:A:629:ILE:HD11	1:A:708:ILE:HD13	0.40	1.94	11	1
1:A:618:LEU:HD12	1:A:660:LEU:O	0.40	2.17	19	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	103/117 (88%)	101±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
2	B	92/106 (87%)	91±1 (98±1%)	1±1 (1±1%)	0±0 (0±0%)	54	85
All	All	3900/4460 (87%)	3830 (98%)	68 (2%)	2 (0%)	54	85

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	17	ASN	1
2	B	68	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	91/102 (89%)	87±2 (96±2%)	4±2 (4±2%)	32	81
2	B	79/91 (87%)	75±2 (95±2%)	4±2 (5±2%)	26	75
All	All	3400/3860 (88%)	3236 (95%)	164 (5%)	29	78

All 58 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	655	THR	14
2	B	6	LYS	11
2	B	12	LEU	9
1	A	643	LEU	8
2	B	36	PHE	7

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Mol	Chain	Res	Type	Models (Total)
1	A	665	PHE	6
2	B	64	THR	5
1	A	686	LEU	5
2	B	85	LYS	5
1	A	719	MET	5
2	B	25	LEU	4
2	B	49	LYS	4
2	B	34	LYS	4
1	A	625	THR	4
2	B	48	LEU	3
1	A	635	THR	3
2	B	32	LEU	3
2	B	42	LEU	3
2	B	28	LEU	3
1	A	618	LEU	3
1	A	639	GLN	3
1	A	650	ARG	3
2	B	77	ILE	3
2	B	74	ARG	3
1	A	633	LEU	3
1	A	721	LEU	2
2	B	17	ASN	2
1	A	702	ARG	2
1	A	679	GLN	2
2	B	43	LYS	2
1	A	680	ARG	2
1	A	629	ILE	2
1	A	634	THR	1
1	A	722	THR	1
2	B	18	THR	1
1	A	647	GLU	1
1	A	676	GLN	1
2	B	67	LYS	1
2	B	80	LEU	1
1	A	691	LEU	1
2	B	14	VAL	1
2	B	68	VAL	1
1	A	651	LEU	1
2	B	40	TYR	1
2	B	87	LEU	1
2	B	96	GLU	1
1	A	615	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	644	VAL	1
1	A	661	LEU	1
1	A	718	THR	1
1	A	716	GLN	1
2	B	39	VAL	1
2	B	69	LEU	1
2	B	83	ARG	1
2	B	65	LEU	1
1	A	619	VAL	1
2	B	62	THR	1
1	A	678	ARG	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)

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 (i)

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *final_complex_renumber.txt*

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	2637
Number of shifts mapped to atoms	2637
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	217	-0.07 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	204	0.06 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	213	0.08 ± 0.07	None needed (< 0.5 ppm)
^{15}N	199	0.28 ± 0.29	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 87%, i.e. 2422 atoms were assigned a chemical shift out of a possible 2770. 0 out of 51 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	950/961 (99%)	384/388 (99%)	387/390 (99%)	179/183 (98%)
Sidechain	1470/1705 (86%)	1004/1123 (89%)	466/528 (88%)	0/54 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	2/104 (2%)	1/50 (2%)	0/52 (0%)	1/2 (50%)
Overall	2422/2770 (87%)	1389/1561 (89%)	853/970 (88%)	180/239 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 2637 atoms were assigned a chemical shift out of a possible 3117. 0 out of 53 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1055/1101 (96%)	426/445 (96%)	430/446 (96%)	199/210 (95%)
Sidechain	1580/1894 (83%)	1078/1242 (87%)	502/589 (85%)	0/63 (0%)
Aromatic	2/122 (2%)	1/58 (2%)	0/62 (0%)	1/2 (50%)
Overall	2637/3117 (85%)	1505/1745 (86%)	932/1097 (85%)	200/275 (73%)

7.1.4 Statistically unusual chemical shifts (i)

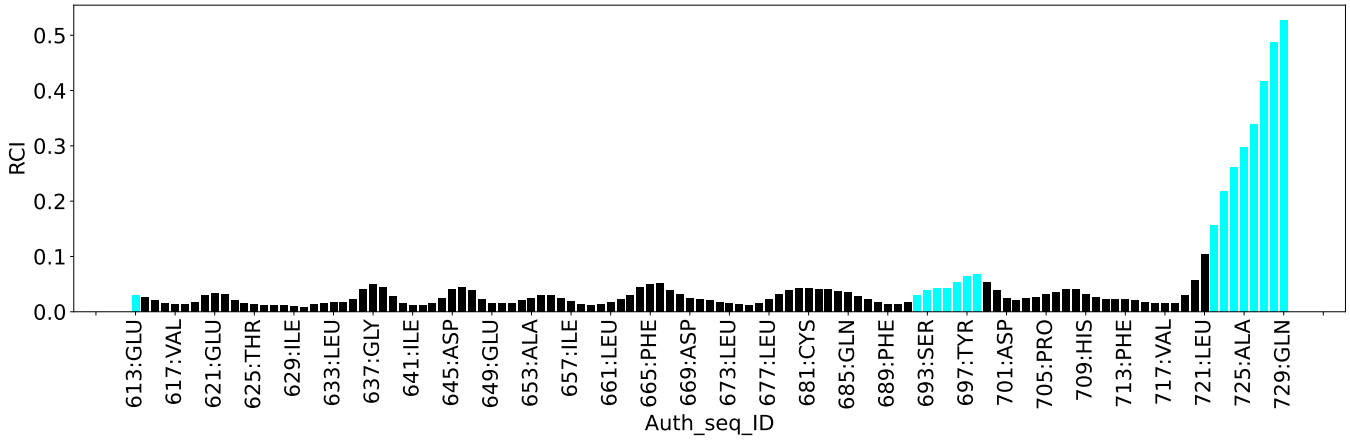
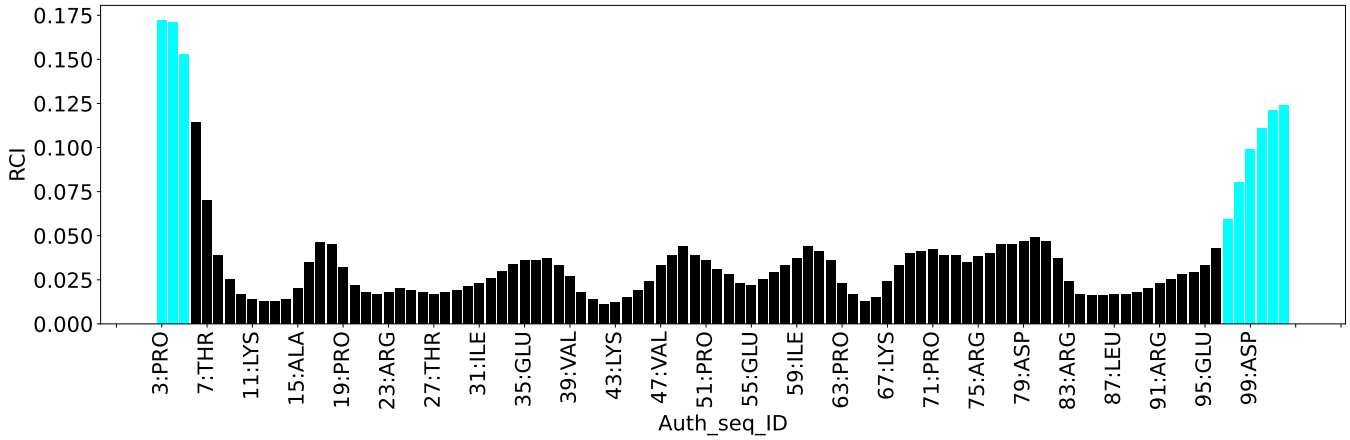
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	626	SER	HB2	1.17	2.61 – 5.13	-10.7

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:



Random coil index (RCI) for chain B: