



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:52 pm GMT

PDB ID : 1R8J
Title : Crystal Structure of Circadian Clock Protein KaiA from *Synechococcus elongatus*
Authors : Ye, S.; Vakonakis, I.; Sacchettini, J.C.; LiWang, A.C.
Deposited on : 2003-10-26
Resolution : 2.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

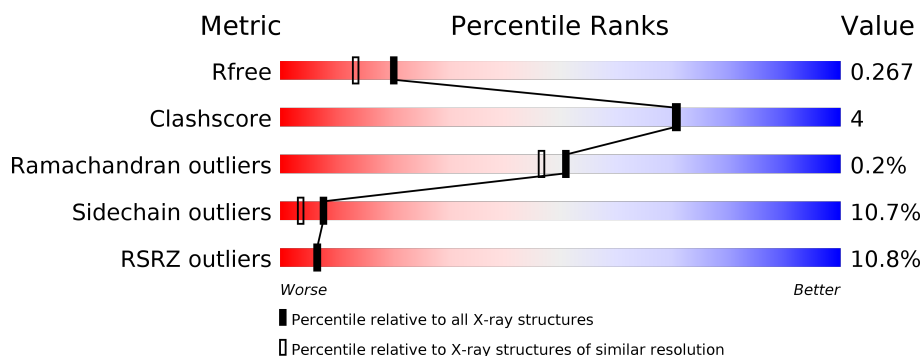
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.03 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	8396 (2.04-2.00)
Clashscore	112137	9678 (2.04-2.00)
Ramachandran outliers	110173	9566 (2.04-2.00)
Sidechain outliers	110143	9565 (2.04-2.00)
RSRZ outliers	101464	8490 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	289	 9% 77% 15% •• 6%
1	B	289	 11% 74% 15% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4577 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called KaiA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2197	1392	380	410	15			
1	B	264	Total	C	N	O	S	0	1	0
			2134	1353	370	398	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	-	CLONING ARTIFACT	UNP Q79PF6
A	-3	MET	-	CLONING ARTIFACT	UNP Q79PF6
A	-2	ALA	-	CLONING ARTIFACT	UNP Q79PF6
A	-1	ASP	-	CLONING ARTIFACT	UNP Q79PF6
A	0	ILE	-	CLONING ARTIFACT	UNP Q79PF6
A	1	VAL	-	CLONING ARTIFACT	UNP Q79PF6
B	-4	ALA	-	CLONING ARTIFACT	UNP Q79PF6
B	-3	MET	-	CLONING ARTIFACT	UNP Q79PF6
B	-2	ALA	-	CLONING ARTIFACT	UNP Q79PF6
B	-1	ASP	-	CLONING ARTIFACT	UNP Q79PF6
B	0	ILE	-	CLONING ARTIFACT	UNP Q79PF6
B	1	VAL	-	CLONING ARTIFACT	UNP Q79PF6

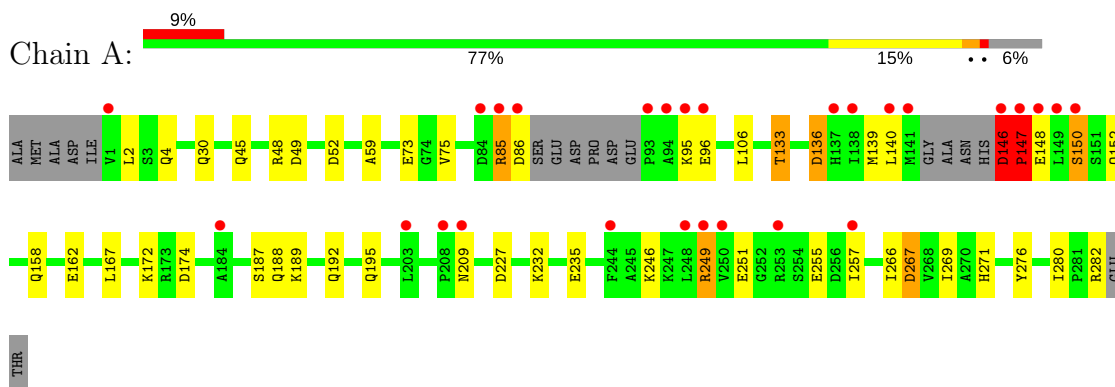
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	136	Total	O	0	0
			136	136		
2	B	110	Total	O	0	0
			110	110		

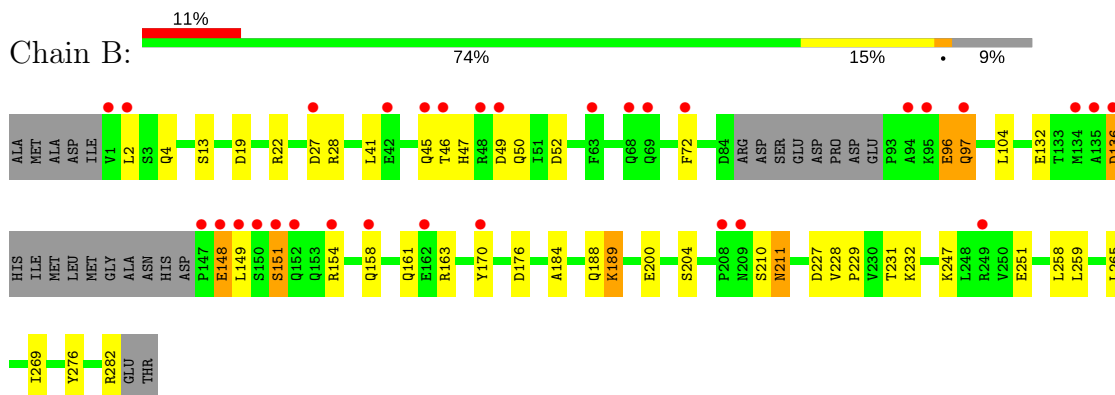
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: KaiA



• Molecule 1: KaiA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.11Å 125.82Å 56.82Å 90.00° 114.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.03 39.87 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.03) 98.9 (39.87-2.03)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.210 , 0.271 0.208 , 0.267	Depositor DCC
R_{free} test set	1901 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4577	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 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 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	0.46	0/2236	0.74	8/3027 (0.3%)
1	B	0.44	0/2177	0.70	7/2947 (0.2%)
All	All	0.45	0/4413	0.72	15/5974 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	267	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	136	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	27	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	146	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	227	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	49	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	174	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	49	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	136	ASP	CB-CG-OD2	5.62	123.35	118.30
1	A	86	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	227	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	19	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	52	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	52	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2197	0	2188	22	0
1	B	2134	0	2130	18	0
2	A	136	0	0	0	0
2	B	110	0	0	1	0
All	All	4577	0	4318	35	0

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 4.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLN:NE2	1:A:30:GLN:OE1	2.21	0.74
1:A:146:ASP:N	1:A:147:PRO:CD	2.53	0.71
1:B:96:GLU:HB2	1:B:97:GLN:HE21	1.57	0.69
1:B:204:SER:HB2	1:B:210:SER:HB2	1.75	0.67
1:B:148:GLU:HG3	1:B:149:LEU:N	2.11	0.65
1:B:184:ALA:O	1:B:188:GLN:HG2	1.99	0.62
1:A:192:GLN:HA	1:A:195:GLN:HE21	1.69	0.57
1:A:246:LYS:HA	1:A:249:ARG:HD2	1.88	0.54
1:A:276:TYR:HB3	1:B:276:TYR:HB3	1.93	0.51
1:B:229:PRO:HB2	1:B:231:THR:HG22	1.92	0.51
1:A:146:ASP:N	1:A:147:PRO:HD2	2.26	0.50
1:A:146:ASP:O	1:A:148:GLU:N	2.45	0.49
1:A:267:ASP:O	1:A:271:HIS:HD2	1.95	0.49
1:A:269:ILE:HG22	1:B:269:ILE:HG22	1.95	0.49
1:A:232:LYS:HA	1:A:235:GLU:HG2	1.95	0.48
1:A:266:ILE:HD13	1:B:265:LEU:HD23	1.96	0.48
1:B:228:VAL:CG1	1:B:232:LYS:HB2	2.43	0.47
1:B:204:SER:HB2	1:B:210:SER:CB	2.46	0.45
1:A:133:THR:OG1	1:A:136:ASP:HB2	2.17	0.45
1:A:147:PRO:HA	1:A:150:SER:HB2	1.99	0.45
1:B:229:PRO:HD2	1:B:232:LYS:HG3	1.98	0.45
1:A:59:ALA:HA	1:A:85:ARG:HB2	1.99	0.44
1:A:147:PRO:HA	1:A:150:SER:CB	2.47	0.44
1:A:280:ILE:HD12	1:B:170:TYR:CE1	2.52	0.44
1:A:147:PRO:N	1:A:150:SER:HB2	2.33	0.44
1:A:73:GLU:HG3	1:A:75:VAL:HG23	2.00	0.44
1:B:151:SER:OG	1:B:154:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLU:HB2	1:B:97:GLN:H	1.47	0.43
1:B:96:GLU:HB2	1:B:97:GLN:NE2	2.29	0.43
1:A:146:ASP:N	1:A:147:PRO:HD3	2.32	0.43
1:B:47:HIS:HB3	1:B:50:GLN:HB2	1.99	0.43
1:A:45:GLN:HG2	1:A:48:ARG:HH21	1.84	0.41
1:A:95:LYS:HG2	1:B:211:ASN:HD21	1.85	0.41
1:B:189:LYS:NZ	2:B:357:HOH:O	2.54	0.41
1:A:146:ASP:N	1:A:146:ASP:OD2	2.54	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	266/289 (92%)	257 (97%)	8 (3%)	1 (0%)	38	31
1	B	259/289 (90%)	250 (96%)	9 (4%)	0	100	100
All	All	525/578 (91%)	507 (97%)	17 (3%)	1 (0%)	51	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	242/255 (95%)	218 (90%)	24 (10%)	9	5
1	B	235/255 (92%)	207 (88%)	28 (12%)	6	3
All	All	477/510 (94%)	425 (89%)	52 (11%)	8	3

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	85	ARG
1	A	96	GLU
1	A	106	LEU
1	A	133	THR
1	A	139	MET
1	A	140	LEU
1	A	146	ASP
1	A	147	PRO
1	A	150	SER
1	A	152	GLN
1	A	158	GLN
1	A	162	GLU
1	A	167	LEU
1	A	172	LYS
1	A	187	SER
1	A	188	GLN
1	A	189	LYS
1	A	209	ASN
1	A	249	ARG
1	A	251	GLU
1	A	255	GLU
1	A	257	ILE
1	A	282	ARG
1	B	2	LEU
1	B	4	GLN
1	B	13	SER
1	B	22[A]	ARG
1	B	22[B]	ARG
1	B	28	ARG
1	B	41	LEU
1	B	45	GLN
1	B	46	THR
1	B	72	PHE
1	B	96	GLU

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Mol	Chain	Res	Type
1	B	97	GLN
1	B	104	LEU
1	B	132	GLU
1	B	136	ASP
1	B	148	GLU
1	B	151	SER
1	B	158	GLN
1	B	161	GLN
1	B	163	ARG
1	B	189	LYS
1	B	200	GLU
1	B	211	ASN
1	B	247	LYS
1	B	251	GLU
1	B	258	LEU
1	B	259	LEU
1	B	282	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	21	GLN
1	A	137	HIS
1	A	181	ASN
1	A	195	GLN
1	A	211	ASN
1	A	271	HIS
1	B	18	GLN
1	B	45	GLN
1	B	97	GLN
1	B	113	GLN
1	B	152	GLN
1	B	161	GLN
1	B	181	ASN
1	B	195	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	272/289 (94%)	0.46	27 (9%) 8 8	17, 33, 68, 77	0
1	B	264/289 (91%)	0.68	31 (11%) 5 5	20, 39, 66, 76	0
All	All	536/578 (92%)	0.57	58 (10%) 6 7	17, 36, 68, 77	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	ALA	8.2
1	B	97	GLN	5.6
1	A	1	VAL	5.6
1	B	149	LEU	5.5
1	A	86	ASP	5.5
1	A	250	VAL	5.4
1	A	137	HIS	5.2
1	A	93	PRO	5.1
1	A	146	ASP	5.0
1	B	72	PHE	5.0
1	B	95	LYS	4.8
1	A	95	LYS	4.7
1	A	141	MET	4.4
1	A	138	ILE	4.3
1	A	84	ASP	4.3
1	A	209	ASN	4.3
1	B	45	GLN	4.2
1	A	147	PRO	4.2
1	B	150	SER	4.0
1	A	244	PHE	3.9
1	A	96	GLU	3.9
1	B	158	GLN	3.6
1	B	1	VAL	3.5
1	A	208	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	27	ASP	3.4
1	B	209	ASN	3.4
1	B	69	GLN	3.3
1	B	151	SER	3.1
1	B	152	GLN	3.1
1	A	85	ARG	3.1
1	B	135	ALA	3.0
1	B	68	GLN	3.0
1	A	257	ILE	2.9
1	B	136	ASP	2.9
1	B	162	GLU	2.9
1	B	208	PRO	2.9
1	A	140	LEU	2.8
1	A	248	LEU	2.8
1	B	63	PHE	2.8
1	B	46	THR	2.8
1	B	148	GLU	2.7
1	A	184	ALA	2.7
1	A	149	LEU	2.7
1	A	249	ARG	2.7
1	A	148	GLU	2.6
1	B	170	TYR	2.6
1	A	203	LEU	2.3
1	B	154	ARG	2.3
1	B	2	LEU	2.3
1	B	49	ASP	2.2
1	B	48	ARG	2.2
1	A	253	ARG	2.2
1	B	42	GLU	2.2
1	A	150	SER	2.2
1	B	134	MET	2.1
1	B	147	PRO	2.1
1	B	249	ARG	2.0
1	B	94	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.