



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 8, 2021 – 04:13 PM EST

PDB ID : 6X61
Title : Crystal structure of the N-terminal thioredoxin domain of SasA in complex with the N-terminal CI domain of KaiC from *Thermosynchococcus elongatus*
Authors : Swan, J.A.; Tripathi, S.M.; Partch, C.L.
Deposited on : 2020-05-27
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.24
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

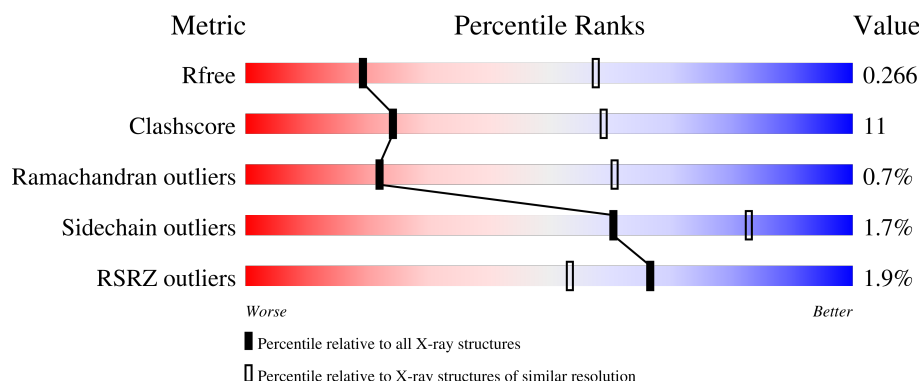
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	247	 69% 24% 6%
1	C	247	 73% 19% • 6%
1	E	247	 74% 18% • 6%
1	G	247	 65% 27% • 6%
1	I	247	 68% 23% • 7%

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Mol	Chain	Length	Quality of chain
1	K	247	<div><div></div><div>2%</div><div>69%</div><div>24%</div><div>6%</div></div>
2	B	108	<div><div></div><div>6%</div><div>60%</div><div>23%</div><div>•</div><div>16%</div></div>
2	D	108	<div><div></div><div>59%</div><div>25%</div><div>•</div><div>15%</div></div>
2	F	108	<div><div></div><div>%</div><div>61%</div><div>21%</div><div>•</div><div>17%</div></div>
2	H	108	<div><div></div><div>3%</div><div>61%</div><div>26%</div><div>13%</div></div>
2	J	108	<div><div></div><div>7%</div><div>58%</div><div>27%</div><div>•</div><div>14%</div></div>
2	L	108	<div><div></div><div>61%</div><div>25%</div><div>•</div><div>13%</div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15499 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1822	1165	309	345	3			
1	C	232	Total	C	N	O	S	0	0	0
			1831	1171	311	346	3			
1	E	231	Total	C	N	O	S	0	0	0
			1822	1165	309	345	3			
1	G	231	Total	C	N	O	S	0	0	0
			1819	1164	309	343	3			
1	I	230	Total	C	N	O	S	0	0	0
			1811	1158	308	342	3			
1	K	231	Total	C	N	O	S	0	0	0
			1822	1165	309	345	3			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ASP	-	expression tag	UNP Q79V60
A	10	TYR	-	expression tag	UNP Q79V60
A	11	LYS	-	expression tag	UNP Q79V60
A	12	ASP	-	expression tag	UNP Q79V60
A	13	ASP	-	expression tag	UNP Q79V60
A	14	ASP	-	expression tag	UNP Q79V60
A	15	ASP	-	expression tag	UNP Q79V60
A	16	LYS	-	expression tag	UNP Q79V60
A	41	ALA	ARG	engineered mutation	UNP Q79V60
A	173	ALA	LYS	engineered mutation	UNP Q79V60
A	248	ASP	-	expression tag	UNP Q79V60
A	249	TYR	-	expression tag	UNP Q79V60
A	250	LYS	-	expression tag	UNP Q79V60
A	251	ASP	-	expression tag	UNP Q79V60
A	252	ASP	-	expression tag	UNP Q79V60
A	253	ASP	-	expression tag	UNP Q79V60
A	254	ASP	-	expression tag	UNP Q79V60

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Chain	Residue	Modelled	Actual	Comment	Reference
A	255	LYS	-	expression tag	UNP Q79V60
C	9	ASP	-	expression tag	UNP Q79V60
C	10	TYR	-	expression tag	UNP Q79V60
C	11	LYS	-	expression tag	UNP Q79V60
C	12	ASP	-	expression tag	UNP Q79V60
C	13	ASP	-	expression tag	UNP Q79V60
C	14	ASP	-	expression tag	UNP Q79V60
C	15	ASP	-	expression tag	UNP Q79V60
C	16	LYS	-	expression tag	UNP Q79V60
C	41	ALA	ARG	engineered mutation	UNP Q79V60
C	173	ALA	LYS	engineered mutation	UNP Q79V60
C	248	ASP	-	expression tag	UNP Q79V60
C	249	TYR	-	expression tag	UNP Q79V60
C	250	LYS	-	expression tag	UNP Q79V60
C	251	ASP	-	expression tag	UNP Q79V60
C	252	ASP	-	expression tag	UNP Q79V60
C	253	ASP	-	expression tag	UNP Q79V60
C	254	ASP	-	expression tag	UNP Q79V60
C	255	LYS	-	expression tag	UNP Q79V60
E	9	ASP	-	expression tag	UNP Q79V60
E	10	TYR	-	expression tag	UNP Q79V60
E	11	LYS	-	expression tag	UNP Q79V60
E	12	ASP	-	expression tag	UNP Q79V60
E	13	ASP	-	expression tag	UNP Q79V60
E	14	ASP	-	expression tag	UNP Q79V60
E	15	ASP	-	expression tag	UNP Q79V60
E	16	LYS	-	expression tag	UNP Q79V60
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E	249	TYR	-	expression tag	UNP Q79V60
E	250	LYS	-	expression tag	UNP Q79V60
E	251	ASP	-	expression tag	UNP Q79V60
E	252	ASP	-	expression tag	UNP Q79V60
E	253	ASP	-	expression tag	UNP Q79V60
E	254	ASP	-	expression tag	UNP Q79V60
E	255	LYS	-	expression tag	UNP Q79V60
G	9	ASP	-	expression tag	UNP Q79V60
G	10	TYR	-	expression tag	UNP Q79V60
G	11	LYS	-	expression tag	UNP Q79V60
G	12	ASP	-	expression tag	UNP Q79V60
G	13	ASP	-	expression tag	UNP Q79V60

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Chain	Residue	Modelled	Actual	Comment	Reference
G	14	ASP	-	expression tag	UNP Q79V60
G	15	ASP	-	expression tag	UNP Q79V60
G	16	LYS	-	expression tag	UNP Q79V60
G	41	ALA	ARG	engineered mutation	UNP Q79V60
G	173	ALA	LYS	engineered mutation	UNP Q79V60
G	248	ASP	-	expression tag	UNP Q79V60
G	249	TYR	-	expression tag	UNP Q79V60
G	250	LYS	-	expression tag	UNP Q79V60
G	251	ASP	-	expression tag	UNP Q79V60
G	252	ASP	-	expression tag	UNP Q79V60
G	253	ASP	-	expression tag	UNP Q79V60
G	254	ASP	-	expression tag	UNP Q79V60
G	255	LYS	-	expression tag	UNP Q79V60
I	9	ASP	-	expression tag	UNP Q79V60
I	10	TYR	-	expression tag	UNP Q79V60
I	11	LYS	-	expression tag	UNP Q79V60
I	12	ASP	-	expression tag	UNP Q79V60
I	13	ASP	-	expression tag	UNP Q79V60
I	14	ASP	-	expression tag	UNP Q79V60
I	15	ASP	-	expression tag	UNP Q79V60
I	16	LYS	-	expression tag	UNP Q79V60
I	41	ALA	ARG	engineered mutation	UNP Q79V60
I	173	ALA	LYS	engineered mutation	UNP Q79V60
I	248	ASP	-	expression tag	UNP Q79V60
I	249	TYR	-	expression tag	UNP Q79V60
I	250	LYS	-	expression tag	UNP Q79V60
I	251	ASP	-	expression tag	UNP Q79V60
I	252	ASP	-	expression tag	UNP Q79V60
I	253	ASP	-	expression tag	UNP Q79V60
I	254	ASP	-	expression tag	UNP Q79V60
I	255	LYS	-	expression tag	UNP Q79V60
K	9	ASP	-	expression tag	UNP Q79V60
K	10	TYR	-	expression tag	UNP Q79V60
K	11	LYS	-	expression tag	UNP Q79V60
K	12	ASP	-	expression tag	UNP Q79V60
K	13	ASP	-	expression tag	UNP Q79V60
K	14	ASP	-	expression tag	UNP Q79V60
K	15	ASP	-	expression tag	UNP Q79V60
K	16	LYS	-	expression tag	UNP Q79V60
K	41	ALA	ARG	engineered mutation	UNP Q79V60
K	173	ALA	LYS	engineered mutation	UNP Q79V60
K	248	ASP	-	expression tag	UNP Q79V60

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Chain	Residue	Modelled	Actual	Comment	Reference
K	249	TYR	-	expression tag	UNP Q79V60
K	250	LYS	-	expression tag	UNP Q79V60
K	251	ASP	-	expression tag	UNP Q79V60
K	252	ASP	-	expression tag	UNP Q79V60
K	253	ASP	-	expression tag	UNP Q79V60
K	254	ASP	-	expression tag	UNP Q79V60
K	255	LYS	-	expression tag	UNP Q79V60

- Molecule 2 is a protein called Adaptive-response sensory-kinase SasA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	91	Total	C	N	O	0	0	0
			743	486	126	131			
2	D	92	Total	C	N	O	0	0	0
			754	492	130	132			
2	F	90	Total	C	N	O	0	0	0
			740	483	127	130			
2	H	94	Total	C	N	O	0	0	0
			773	505	131	137			
2	J	93	Total	C	N	O	0	0	0
			762	498	131	133			
2	L	94	Total	C	N	O	0	0	0
			770	502	132	136			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ASP	-	expression tag	UNP Q8DMT2
B	9	TYR	-	expression tag	UNP Q8DMT2
B	10	LYS	-	expression tag	UNP Q8DMT2
B	11	ASP	-	expression tag	UNP Q8DMT2
B	12	ASP	-	expression tag	UNP Q8DMT2
B	13	ASP	-	expression tag	UNP Q8DMT2
B	14	ASP	-	expression tag	UNP Q8DMT2
B	15	LYS	-	expression tag	UNP Q8DMT2
B	16	ALA	PRO	engineered mutation	UNP Q8DMT2
B	108	ASP	-	expression tag	UNP Q8DMT2
B	109	TYR	-	expression tag	UNP Q8DMT2
B	110	LYS	-	expression tag	UNP Q8DMT2
B	111	ASP	-	expression tag	UNP Q8DMT2
B	112	ASP	-	expression tag	UNP Q8DMT2
B	113	ASP	-	expression tag	UNP Q8DMT2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	114	ASP	-	expression tag	UNP Q8DMT2
B	115	LYS	-	expression tag	UNP Q8DMT2
D	8	ASP	-	expression tag	UNP Q8DMT2
D	9	TYR	-	expression tag	UNP Q8DMT2
D	10	LYS	-	expression tag	UNP Q8DMT2
D	11	ASP	-	expression tag	UNP Q8DMT2
D	12	ASP	-	expression tag	UNP Q8DMT2
D	13	ASP	-	expression tag	UNP Q8DMT2
D	14	ASP	-	expression tag	UNP Q8DMT2
D	15	LYS	-	expression tag	UNP Q8DMT2
D	16	ALA	PRO	engineered mutation	UNP Q8DMT2
D	108	ASP	-	expression tag	UNP Q8DMT2
D	109	TYR	-	expression tag	UNP Q8DMT2
D	110	LYS	-	expression tag	UNP Q8DMT2
D	111	ASP	-	expression tag	UNP Q8DMT2
D	112	ASP	-	expression tag	UNP Q8DMT2
D	113	ASP	-	expression tag	UNP Q8DMT2
D	114	ASP	-	expression tag	UNP Q8DMT2
D	115	LYS	-	expression tag	UNP Q8DMT2
F	8	ASP	-	expression tag	UNP Q8DMT2
F	9	TYR	-	expression tag	UNP Q8DMT2
F	10	LYS	-	expression tag	UNP Q8DMT2
F	11	ASP	-	expression tag	UNP Q8DMT2
F	12	ASP	-	expression tag	UNP Q8DMT2
F	13	ASP	-	expression tag	UNP Q8DMT2
F	14	ASP	-	expression tag	UNP Q8DMT2
F	15	LYS	-	expression tag	UNP Q8DMT2
F	16	ALA	PRO	engineered mutation	UNP Q8DMT2
F	108	ASP	-	expression tag	UNP Q8DMT2
F	109	TYR	-	expression tag	UNP Q8DMT2
F	110	LYS	-	expression tag	UNP Q8DMT2
F	111	ASP	-	expression tag	UNP Q8DMT2
F	112	ASP	-	expression tag	UNP Q8DMT2
F	113	ASP	-	expression tag	UNP Q8DMT2
F	114	ASP	-	expression tag	UNP Q8DMT2
F	115	LYS	-	expression tag	UNP Q8DMT2
H	8	ASP	-	expression tag	UNP Q8DMT2
H	9	TYR	-	expression tag	UNP Q8DMT2
H	10	LYS	-	expression tag	UNP Q8DMT2
H	11	ASP	-	expression tag	UNP Q8DMT2
H	12	ASP	-	expression tag	UNP Q8DMT2
H	13	ASP	-	expression tag	UNP Q8DMT2

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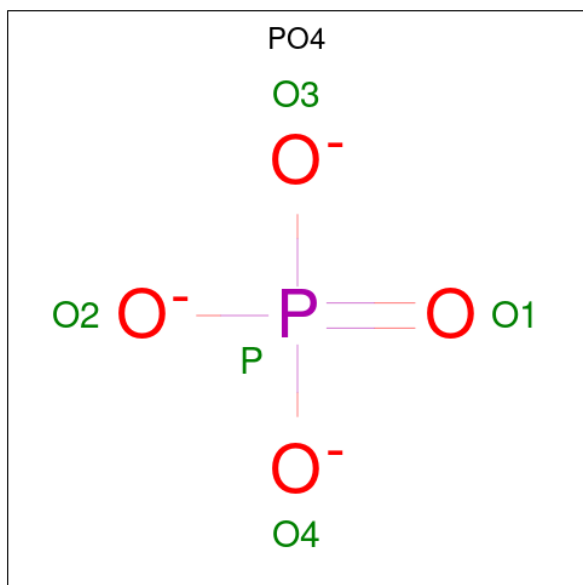
Chain	Residue	Modelled	Actual	Comment	Reference
H	14	ASP	-	expression tag	UNP Q8DMT2
H	15	LYS	-	expression tag	UNP Q8DMT2
H	16	ALA	PRO	engineered mutation	UNP Q8DMT2
H	108	ASP	-	expression tag	UNP Q8DMT2
H	109	TYR	-	expression tag	UNP Q8DMT2
H	110	LYS	-	expression tag	UNP Q8DMT2
H	111	ASP	-	expression tag	UNP Q8DMT2
H	112	ASP	-	expression tag	UNP Q8DMT2
H	113	ASP	-	expression tag	UNP Q8DMT2
H	114	ASP	-	expression tag	UNP Q8DMT2
H	115	LYS	-	expression tag	UNP Q8DMT2
J	8	ASP	-	expression tag	UNP Q8DMT2
J	9	TYR	-	expression tag	UNP Q8DMT2
J	10	LYS	-	expression tag	UNP Q8DMT2
J	11	ASP	-	expression tag	UNP Q8DMT2
J	12	ASP	-	expression tag	UNP Q8DMT2
J	13	ASP	-	expression tag	UNP Q8DMT2
J	14	ASP	-	expression tag	UNP Q8DMT2
J	15	LYS	-	expression tag	UNP Q8DMT2
J	16	ALA	PRO	engineered mutation	UNP Q8DMT2
J	108	ASP	-	expression tag	UNP Q8DMT2
J	109	TYR	-	expression tag	UNP Q8DMT2
J	110	LYS	-	expression tag	UNP Q8DMT2
J	111	ASP	-	expression tag	UNP Q8DMT2
J	112	ASP	-	expression tag	UNP Q8DMT2
J	113	ASP	-	expression tag	UNP Q8DMT2
J	114	ASP	-	expression tag	UNP Q8DMT2
J	115	LYS	-	expression tag	UNP Q8DMT2
L	8	ASP	-	expression tag	UNP Q8DMT2
L	9	TYR	-	expression tag	UNP Q8DMT2
L	10	LYS	-	expression tag	UNP Q8DMT2
L	11	ASP	-	expression tag	UNP Q8DMT2
L	12	ASP	-	expression tag	UNP Q8DMT2
L	13	ASP	-	expression tag	UNP Q8DMT2
L	14	ASP	-	expression tag	UNP Q8DMT2
L	15	LYS	-	expression tag	UNP Q8DMT2
L	16	ALA	PRO	engineered mutation	UNP Q8DMT2
L	108	ASP	-	expression tag	UNP Q8DMT2
L	109	TYR	-	expression tag	UNP Q8DMT2
L	110	LYS	-	expression tag	UNP Q8DMT2
L	111	ASP	-	expression tag	UNP Q8DMT2
L	112	ASP	-	expression tag	UNP Q8DMT2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	113	ASP	-	expression tag	UNP Q8DMT2
L	114	ASP	-	expression tag	UNP Q8DMT2
L	115	LYS	-	expression tag	UNP Q8DMT2

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

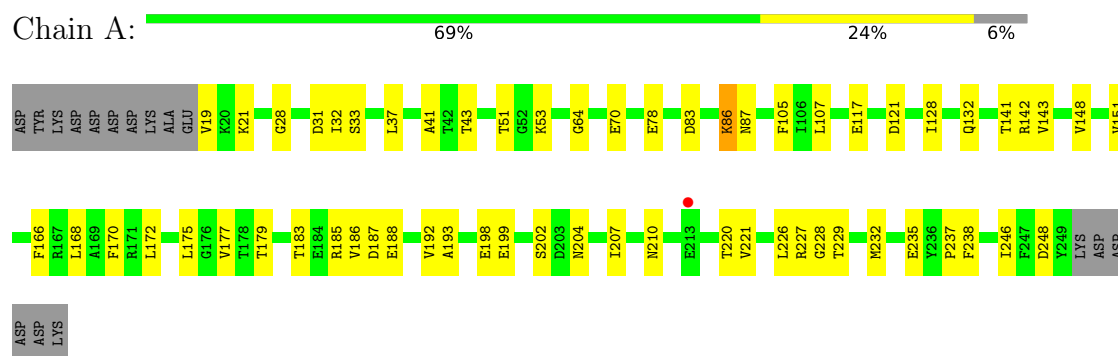


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		

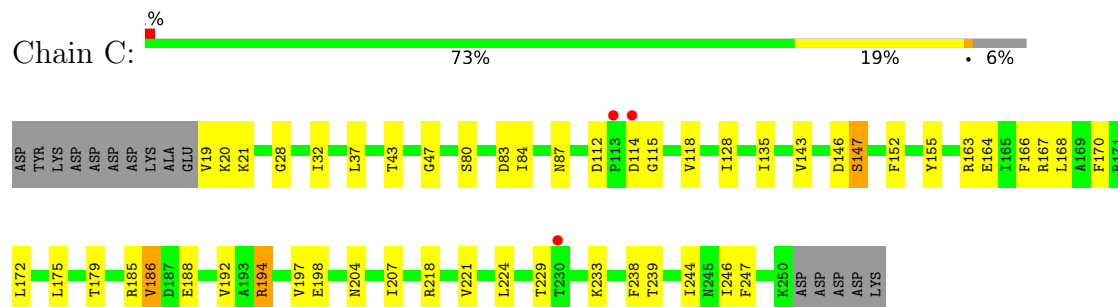
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

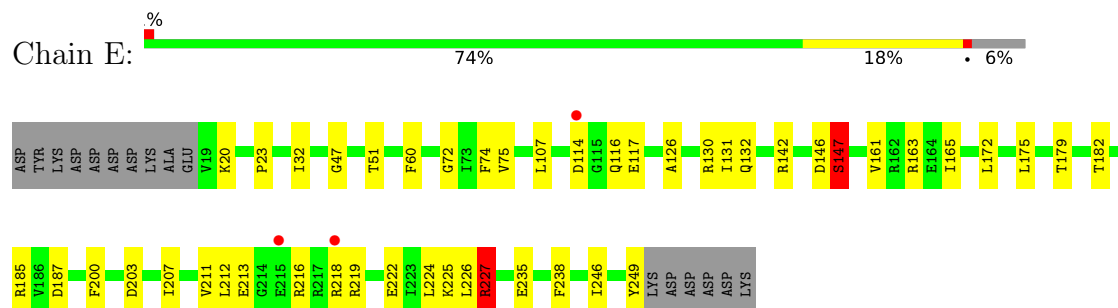
- Molecule 1: Circadian clock protein kinase KaiC



- Molecule 1: Circadian clock protein kinase KaiC



- Molecule 1: Circadian clock protein kinase KaiC

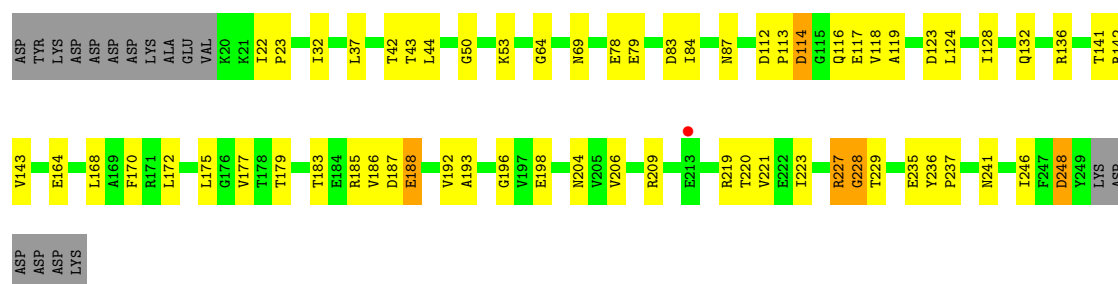


- Molecule 1: Circadian clock protein kinase KaiC



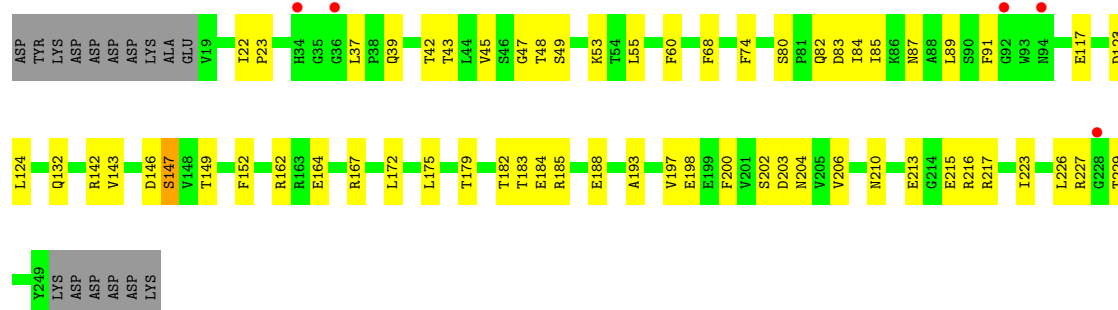
- Molecule 1: Circadian clock protein kinase KaiC

Chain I:  68% 23% 7%



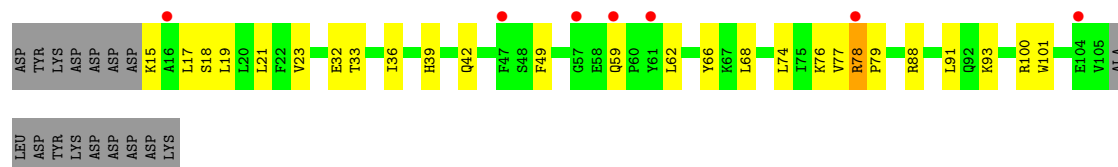
- Molecule 1: Circadian clock protein kinase KaiC

Chain K:  2% 69% 24% 6%

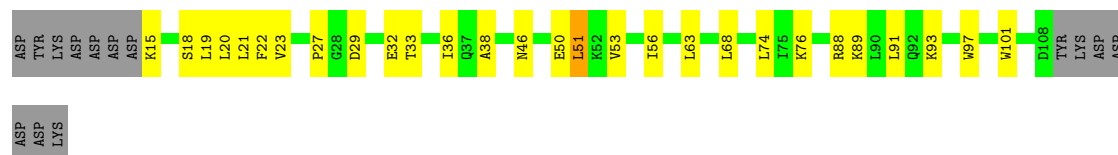


- Molecule 2: Adaptive-response sensory-kinase SasA

Chain B: 



- Molecule 2: Adaptive-response sensory-kinase SasA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.60Å 121.58Å 133.59Å 90.00° 108.78° 90.00°	Depositor
Resolution (Å)	49.05 – 3.20 49.05 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.05-3.20) 98.7 (49.05-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.222 , 0.265 0.222 , 0.266	Depositor DCC
R_{free} test set	2636 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15499	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.20% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.27	0/1856	0.48	0/2513
1	C	0.26	0/1865	0.51	0/2524
1	E	0.27	0/1856	0.48	0/2513
1	G	0.26	0/1853	0.48	0/2509
1	I	0.26	0/1845	0.48	0/2498
1	K	0.27	0/1856	0.51	0/2513
2	B	0.26	0/763	0.50	0/1040
2	D	0.26	0/774	0.49	0/1054
2	F	0.26	0/760	0.48	0/1036
2	H	0.27	0/794	0.47	0/1083
2	J	0.26	0/782	0.54	0/1065
2	L	0.26	0/790	0.48	0/1076
All	All	0.27	0/15794	0.49	0/21424

There are no bond length outliers.

There are no bond angle outliers.

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	1822	0	1821	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1831	0	1834	38	0
1	E	1822	0	1821	37	0
1	G	1819	0	1819	57	0
1	I	1811	0	1808	46	0
1	K	1822	0	1821	40	0
2	B	743	0	756	17	0
2	D	754	0	772	19	0
2	F	740	0	754	18	0
2	H	773	0	783	22	0
2	J	762	0	783	25	0
2	L	770	0	787	19	0
3	A	5	0	0	1	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	G	5	0	0	1	0
3	I	5	0	0	1	0
3	K	5	0	0	0	0
All	All	15499	0	15559	342	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 11.

The worst 5 of 342 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:K:172:LEU:HD13	1:K:179:THR:HG21	1.54	0.89
1:I:143:VAL:HB	1:I:179:THR:HG22	1.55	0.87
1:K:143:VAL:HB	1:K:179:THR:HG22	1.61	0.81
1:G:195:PHE:HA	1:G:198:GLU:HG2	1.61	0.80
1:G:135:ILE:HD12	1:G:177:VAL:HG11	1.65	0.79

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	229/247 (93%)	214 (93%)	15 (7%)	0	100	100
1	C	230/247 (93%)	211 (92%)	16 (7%)	3 (1%)	12	47
1	E	229/247 (93%)	211 (92%)	15 (7%)	3 (1%)	12	47
1	G	229/247 (93%)	213 (93%)	16 (7%)	0	100	100
1	I	228/247 (92%)	210 (92%)	14 (6%)	4 (2%)	8	41
1	K	229/247 (93%)	216 (94%)	12 (5%)	1 (0%)	34	69
2	B	89/108 (82%)	80 (90%)	8 (9%)	1 (1%)	14	51
2	D	90/108 (83%)	85 (94%)	5 (6%)	0	100	100
2	F	88/108 (82%)	83 (94%)	5 (6%)	0	100	100
2	H	92/108 (85%)	87 (95%)	5 (5%)	0	100	100
2	J	91/108 (84%)	87 (96%)	4 (4%)	0	100	100
2	L	92/108 (85%)	87 (95%)	4 (4%)	1 (1%)	14	51
All	All	1916/2130 (90%)	1784 (93%)	119 (6%)	13 (1%)	22	61

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	114	ASP
1	C	147	SER
1	E	114	ASP
1	I	228	GLY
2	L	51	LEU

5.3.2 Protein sidechains ⓘ

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	197/212 (93%)	194 (98%)	3 (2%)	65	85
1	C	198/212 (93%)	195 (98%)	3 (2%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	197/212 (93%)	194 (98%)	3 (2%)	65	85
1	G	196/212 (92%)	192 (98%)	4 (2%)	55	80
1	I	195/212 (92%)	190 (97%)	5 (3%)	46	76
1	K	197/212 (93%)	195 (99%)	2 (1%)	76	90
2	B	79/96 (82%)	77 (98%)	2 (2%)	47	77
2	D	80/96 (83%)	79 (99%)	1 (1%)	69	87
2	F	79/96 (82%)	78 (99%)	1 (1%)	69	87
2	H	82/96 (85%)	81 (99%)	1 (1%)	71	88
2	J	81/96 (84%)	79 (98%)	2 (2%)	47	77
2	L	82/96 (85%)	81 (99%)	1 (1%)	71	88
All	All	1663/1848 (90%)	1635 (98%)	28 (2%)	60	83

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	216	ARG
2	L	46	ASN
2	H	109	TYR
2	J	100	ARG
1	G	247	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	39	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	K	301	-	4,4,4	0.93	0	6,6,6	0.43	0
3	PO4	C	301	-	4,4,4	0.91	0	6,6,6	0.44	0
3	PO4	I	301	-	4,4,4	0.95	0	6,6,6	0.37	0
3	PO4	A	301	-	4,4,4	0.93	0	6,6,6	0.39	0
3	PO4	G	301	-	4,4,4	0.93	0	6,6,6	0.43	0
3	PO4	E	301	-	4,4,4	0.92	0	6,6,6	0.40	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	301	PO4	1	0
3	A	301	PO4	1	0
3	G	301	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	231/247 (93%)	-0.35	1 (0%) 92 89	29, 50, 89, 138	0
1	C	232/247 (93%)	-0.12	3 (1%) 77 65	29, 55, 87, 115	0
1	E	231/247 (93%)	-0.21	3 (1%) 77 65	24, 55, 95, 146	0
1	G	231/247 (93%)	-0.07	4 (1%) 70 57	28, 70, 111, 164	0
1	I	230/247 (93%)	-0.26	1 (0%) 92 89	35, 60, 96, 143	0
1	K	231/247 (93%)	0.01	5 (2%) 62 48	35, 62, 94, 118	0
2	B	91/108 (84%)	0.45	7 (7%) 13 7	38, 67, 112, 131	0
2	D	92/108 (85%)	-0.31	0 100 100	22, 40, 70, 82	0
2	F	90/108 (83%)	0.25	1 (1%) 80 69	27, 58, 95, 120	0
2	H	94/108 (87%)	-0.07	3 (3%) 47 31	30, 56, 85, 118	0
2	J	93/108 (86%)	0.41	8 (8%) 10 5	36, 68, 118, 147	0
2	L	94/108 (87%)	-0.31	0 100 100	28, 43, 72, 87	0
All	All	1940/2130 (91%)	-0.10	36 (1%) 66 53	22, 58, 100, 164	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	92	GLY	4.3
1	G	242	ASN	3.9
1	G	114	ASP	3.5
2	J	104	GLU	3.3
1	I	213	GLU	3.3

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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	G	301	5/5	0.96	0.11	55,61,65,65	0
3	PO4	I	301	5/5	0.96	0.15	32,48,56,57	0
3	PO4	A	301	5/5	0.97	0.18	27,40,45,50	0
3	PO4	E	301	5/5	0.97	0.10	23,27,41,44	0
3	PO4	K	301	5/5	0.97	0.13	30,43,49,50	0
3	PO4	C	301	5/5	0.99	0.12	37,46,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.