



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:17 AM GMT

PDB ID : 2GBL  
Title : Crystal Structure of Full Length Circadian Clock Protein KaiC with Phosphorylation Sites  
Authors : Pattanayek, R.; Williams, D.R.; Pattanayek, S.; Xu, Y.; Mori, T.; Johnson, C.H.; Stewart, P.L.; Egli, M.  
Deposited on : 2006-03-10  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

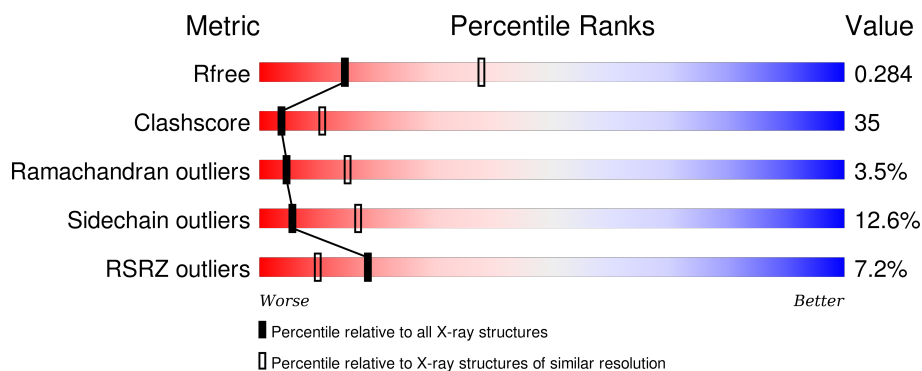
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	519	<div> <div>12%</div> <div>45%</div> <div>40%</div> <div>10%</div> <div>• •</div> </div>
1	B	519	<div> <div>7%</div> <div>42%</div> <div>42%</div> <div>9%</div> <div>• 5%</div> </div>
1	E	519	<div> <div>6%</div> <div>45%</div> <div>39%</div> <div>10%</div> <div>• 5%</div> </div>
1	F	519	<div> <div>7%</div> <div>45%</div> <div>41%</div> <div>10%</div> <div>• •</div> </div>
2	C	519	<div> <div>5%</div> <div>46%</div> <div>36%</div> <div>11%</div> <div>• 6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	519	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	431	-	-	X	-
1	SEP	B	431	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23872 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	506	Total	C	N	O	P	S	0	0	0
			3994	2509	701	767	2	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3878	2439	678	744	2	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3886	2445	679	745	2	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3994	2509	701	767	2	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
A	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
B	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
B	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
E	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
E	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
F	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
F	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4

- Molecule 2 is a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	488	Total	C	N	O	P	S	0	0	0
			3850	2425	674	735	1	15			
2	D	485	Total	C	N	O	P	S	0	0	0
			3826	2411	671	728	1	15			

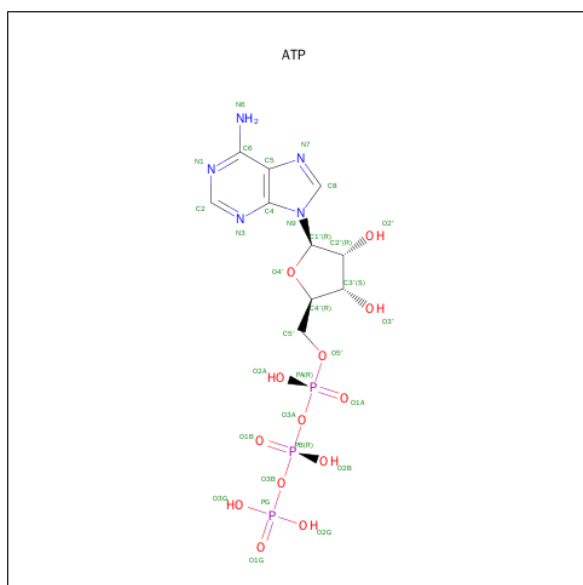
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
D	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

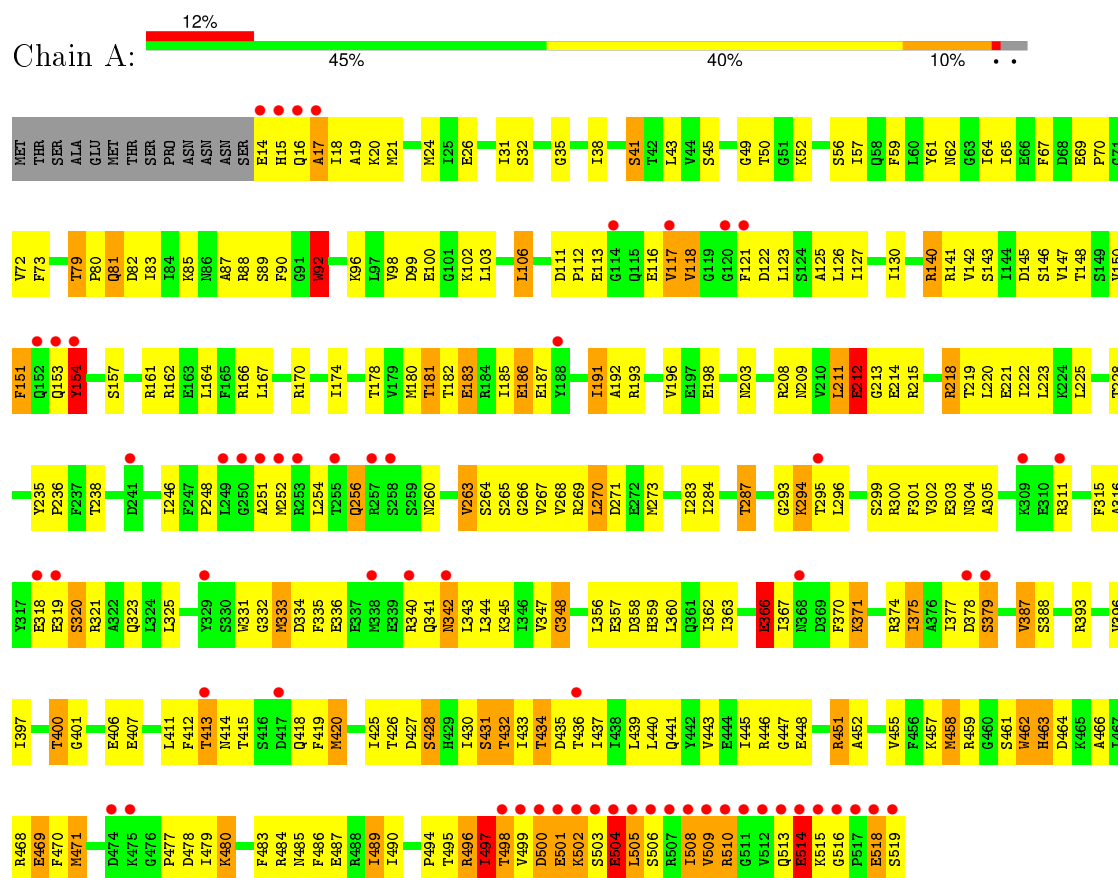
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	5	Total	O	0	0
			5	5		
5	C	7	Total	O	0	0
			7	7		
5	D	13	Total	O	0	0
			13	13		
5	E	10	Total	O	0	0
			10	10		
5	F	23	Total	O	0	0
			23	23		

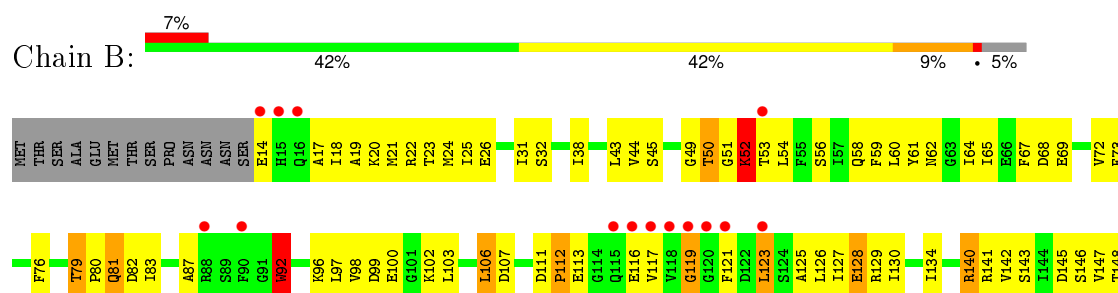
### 3 Residue-property plots

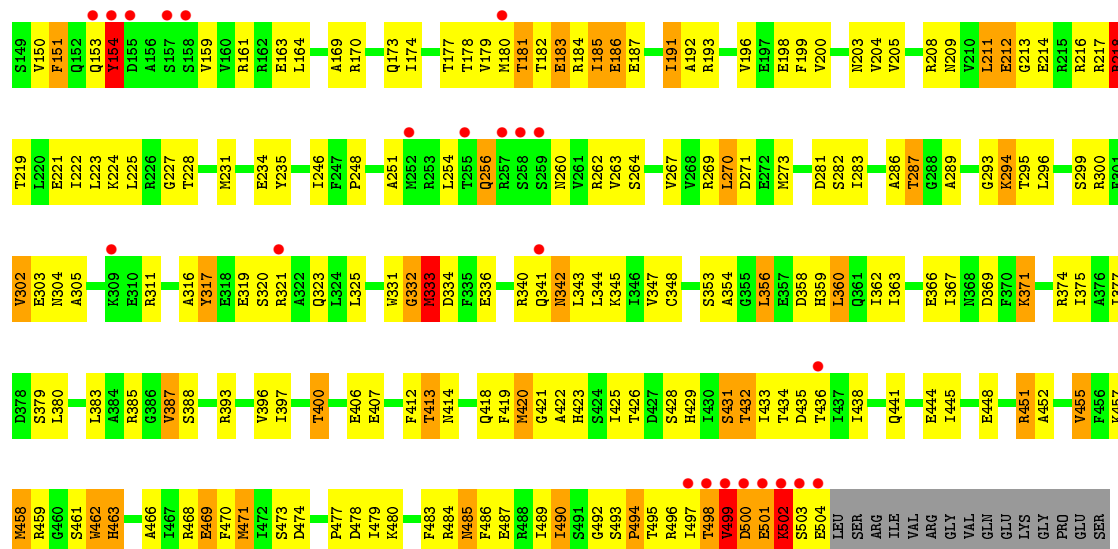
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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*

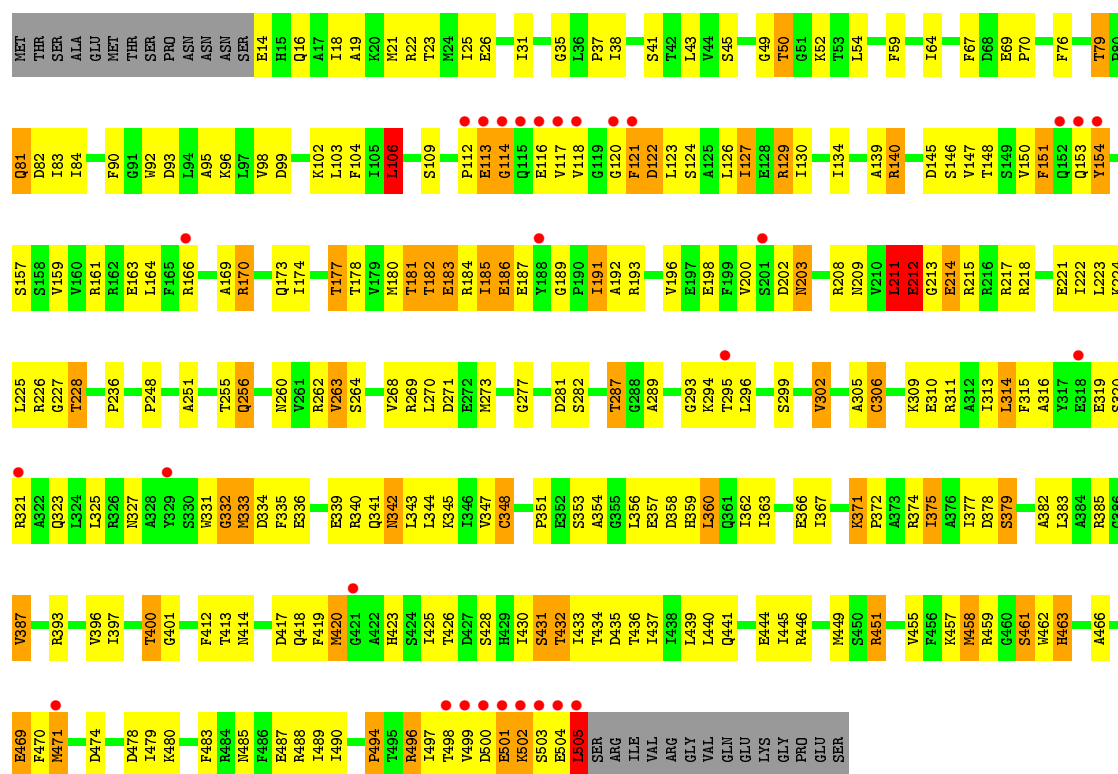
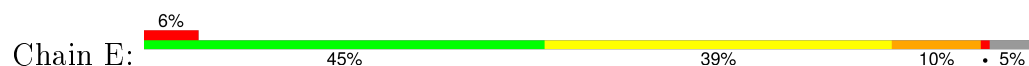


- Molecule 1: Circadian clock protein kinase *kaiC*





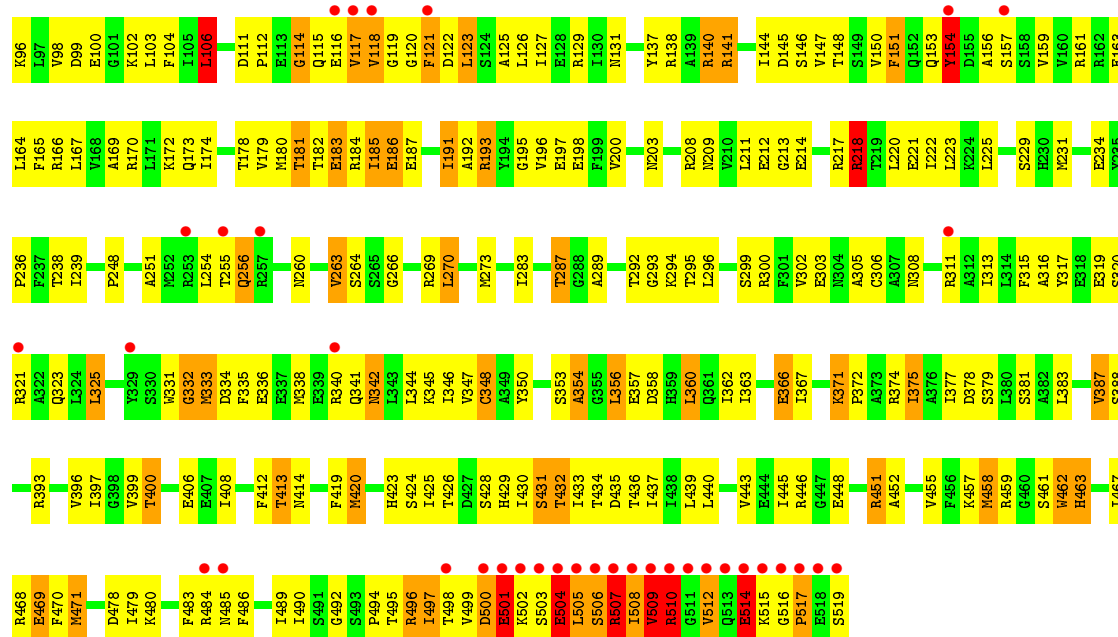
• Molecule 1: Circadian clock protein kinase kaiC



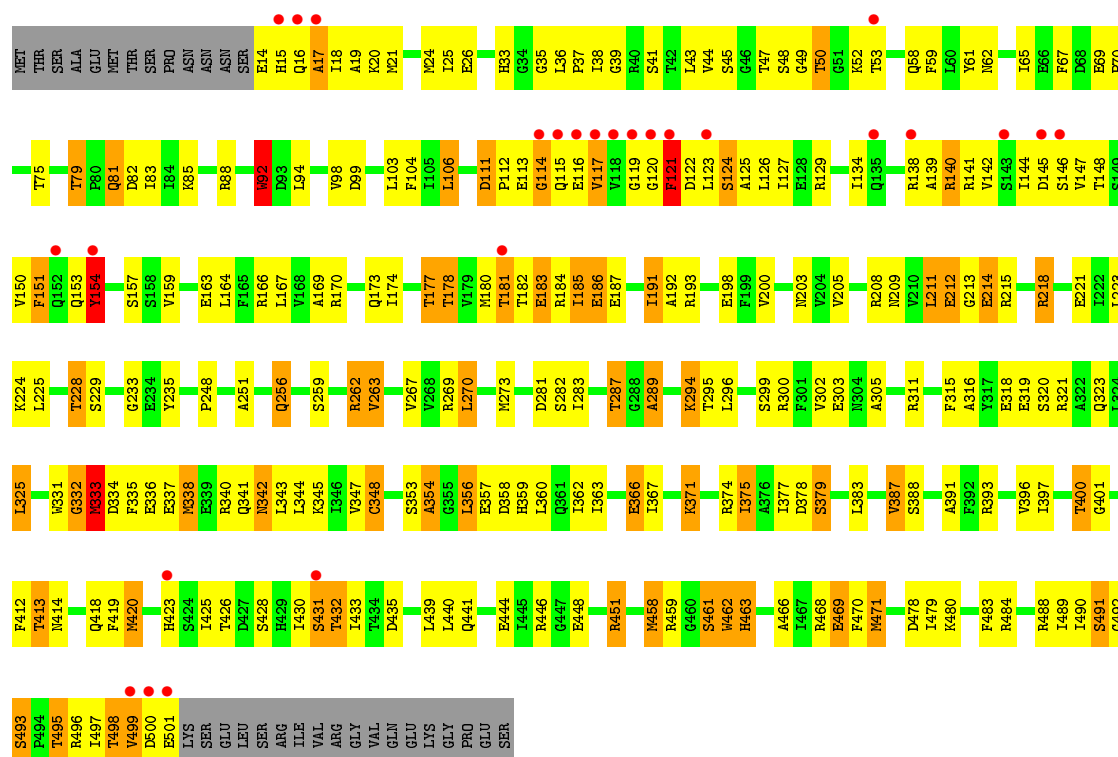
• Molecule 1: Circadian clock protein kinase kaiC







• Molecule 2: Circadian clock protein kinase kaiC



• Molecule 2: Circadian clock protein kinase kaiC





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.87Å 135.58Å 204.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.73 – 2.83	Depositor EDS
% Data completeness (in resolution range)	0.8 (30.00-2.80) 89.7 (29.73-2.83)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.230 , 0.290 0.232 , 0.284	Depositor DCC
$R_{free}$ test set	4041 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 67.9	EDS
Estimated twinning fraction	0.013 for k,h,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 87615 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: TPO, MG, ATP, SEP

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	1.00	9/4038 (0.2%)	1.00	3/5437 (0.1%)
1	B	0.89	6/3921 (0.2%)	0.97	8/5282 (0.2%)
1	E	1.06	8/3929 (0.2%)	1.07	9/5293 (0.2%)
1	F	1.02	7/4038 (0.2%)	1.04	9/5437 (0.2%)
2	C	0.91	6/3903 (0.2%)	0.97	4/5259 (0.1%)
2	D	1.03	7/3879 (0.2%)	1.05	7/5226 (0.1%)
All	All	0.99	43/23708 (0.2%)	1.02	40/31934 (0.1%)

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 outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	E	0	2
1	F	0	3
2	C	0	2
2	D	0	2
All	All	0	14

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	TRP	CE3-CZ3	13.50	1.61	1.38
1	A	92	TRP	CE3-CZ3	12.25	1.59	1.38
1	E	92	TRP	CG-CD1	-10.83	1.21	1.36
1	F	92	TRP	CG-CD1	-10.41	1.22	1.36
1	E	92	TRP	CB-CG	-9.45	1.33	1.50

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	216	ARG	NE-CZ-NH1	-10.39	115.10	120.30
1	F	114	GLY	N-CA-C	7.92	132.90	113.10
2	C	213	GLY	N-CA-C	-7.41	94.57	113.10
1	E	500	ASP	CB-CG-OD2	7.16	124.74	118.30
2	D	226	ARG	NE-CZ-NH1	-6.79	116.91	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	SEP	Mainchain
1	A	432	TPO	Mainchain
1	B	317	TYR	Sidechain
1	B	431	SEP	Mainchain
1	B	432	TPO	Mainchain

## 5.2 Too-close contacts

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	3994	0	3984	299	0
1	B	3878	0	3862	295	0
1	E	3886	0	3872	282	0
1	F	3994	0	3984	322	0
2	C	3850	0	3837	282	0
2	D	3826	0	3818	275	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	62	0	24	11	0
4	B	62	0	24	8	0
4	C	62	0	24	7	0
4	D	62	0	23	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	62	0	24	6	0
4	F	62	0	24	7	0
5	A	8	0	0	0	0
5	B	5	0	0	2	0
5	C	7	0	0	2	0
5	D	13	0	0	2	0
5	E	10	0	0	0	0
5	F	23	0	0	6	0
All	All	23872	0	23500	1663	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 35.

The worst 5 of 1663 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:B:426:THR:HB	1:B:431:SEP:O3P	1.37	1.22
2:D:147:VAL:HG11	2:D:180:MET:HE3	1.24	1.20
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.07	1.15
1:A:14:GLU:HG3	1:A:15:HIS:H	1.08	1.11
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.29	1.11

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	502/519 (97%)	442 (88%)	39 (8%)	21 (4%)	3	11
1	B	487/519 (94%)	431 (88%)	44 (9%)	12 (2%)	7	24
1	E	488/519 (94%)	422 (86%)	49 (10%)	17 (4%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	502/519 (97%)	443 (88%)	38 (8%)	21 (4%)	3	11
2	C	485/519 (93%)	436 (90%)	30 (6%)	19 (4%)	4	12
2	D	482/519 (93%)	433 (90%)	37 (8%)	12 (2%)	7	24
All	All	2946/3114 (95%)	2607 (88%)	237 (8%)	102 (4%)	4	15

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	154	TYR
1	A	211	LEU
1	A	333	MET
1	A	387	VAL

### 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	430/442 (97%)	373 (87%)	57 (13%)	5	14
1	B	417/442 (94%)	364 (87%)	53 (13%)	5	16
1	E	418/442 (95%)	368 (88%)	50 (12%)	6	19
1	F	430/442 (97%)	381 (89%)	49 (11%)	7	21
2	C	415/443 (94%)	358 (86%)	57 (14%)	4	13
2	D	412/443 (93%)	360 (87%)	52 (13%)	5	17
All	All	2522/2654 (95%)	2204 (87%)	318 (13%)	5	17

5 of 318 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	325	LEU
2	D	154	TYR
1	F	287	THR
2	C	360	LEU

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Mol	Chain	Res	Type
2	C	491	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	323	GLN
2	D	81	GLN
1	F	115	GLN
2	C	368	ASN
2	C	414	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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
1	SEP	A	431	1	8,9,10	5.79	4 (50%)	8,12,14	4.81	5 (62%)
1	TPO	A	432	1	8,10,11	5.77	5 (62%)	7,14,16	2.54	3 (42%)
1	SEP	B	431	1	8,9,10	5.63	4 (50%)	8,12,14	4.04	5 (62%)
1	TPO	B	432	1	8,10,11	5.98	5 (62%)	7,14,16	2.32	4 (57%)
2	TPO	C	432	2	8,10,11	6.16	5 (62%)	7,14,16	3.57	4 (57%)
2	TPO	D	432	2	8,10,11	5.28	6 (75%)	7,14,16	3.16	3 (42%)
1	SEP	E	431	1	8,9,10	5.84	5 (62%)	8,12,14	2.59	6 (75%)
1	TPO	E	432	1	8,10,11	5.08	6 (75%)	7,14,16	2.72	3 (42%)
1	SEP	F	431	1	8,9,10	5.85	5 (62%)	8,12,14	3.54	3 (37%)
1	TPO	F	432	1	8,10,11	5.68	6 (75%)	7,14,16	3.11	6 (85%)



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	431	1	-	0/6/8/10	0/0/0/0
1	TPO	A	432	1	-	0/8/11/13	0/0/0/0
1	SEP	B	431	1	-	0/6/8/10	0/0/0/0
1	TPO	B	432	1	-	0/8/11/13	0/0/0/0
2	TPO	C	432	2	-	0/8/11/13	0/0/0/0
2	TPO	D	432	2	-	0/8/11/13	0/0/0/0
1	SEP	E	431	1	-	0/6/8/10	0/0/0/0
1	TPO	E	432	1	-	0/8/11/13	0/0/0/0
1	SEP	F	431	1	-	0/6/8/10	0/0/0/0
1	TPO	F	432	1	-	0/8/11/13	0/0/0/0

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	432	TPO	CB-CA	-5.15	1.44	1.54
1	F	432	TPO	CB-CA	-2.59	1.49	1.54
1	F	432	TPO	CA-N	2.06	1.54	1.47
2	D	432	TPO	CB-CA	2.22	1.58	1.54
1	F	431	SEP	CB-CA	2.25	1.59	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	432	TPO	C-CA-N	-6.90	95.41	109.83
2	C	432	TPO	C-CA-N	-6.15	96.98	109.83
1	F	431	SEP	O-C-CA	-5.81	110.37	125.49
1	A	431	SEP	O-C-CA	-5.79	110.41	125.49
2	C	432	TPO	O-C-CA	-5.51	110.90	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	431	SEP	4	0
1	A	432	TPO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	431	SEP	5	0
1	B	432	TPO	2	0
2	C	432	TPO	2	0
2	D	432	TPO	3	0
1	E	431	SEP	1	0
1	E	432	TPO	1	0
1	F	431	SEP	2	0
1	F	432	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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
4	ATP	A	901	3	24,33,33	1.49	4 (16%)	31,52,52	2.61	7 (22%)
4	ATP	A	903	-	24,33,33	1.58	5 (20%)	31,52,52	2.62	8 (25%)
4	ATP	B	901	3	24,33,33	1.49	5 (20%)	31,52,52	2.70	7 (22%)
4	ATP	B	903	-	24,33,33	1.73	3 (12%)	31,52,52	3.06	12 (38%)
4	ATP	C	901	3	24,33,33	1.45	4 (16%)	31,52,52	2.56	8 (25%)
4	ATP	C	903	-	24,33,33	1.24	2 (8%)	31,52,52	2.90	8 (25%)
4	ATP	D	901	3	24,33,33	1.51	5 (20%)	31,52,52	2.67	6 (19%)
4	ATP	D	903	-	24,33,33	1.73	5 (20%)	31,52,52	3.08	11 (35%)
4	ATP	E	901	3	24,33,33	1.55	3 (12%)	31,52,52	2.73	6 (19%)
4	ATP	E	903	-	24,33,33	1.66	9 (37%)	31,52,52	2.87	10 (32%)
4	ATP	F	901	3	24,33,33	1.50	5 (20%)	31,52,52	2.67	7 (22%)
4	ATP	F	903	-	24,33,33	1.40	4 (16%)	31,52,52	2.73	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	901	3	-	0/18/38/38	0/3/3/3
4	ATP	A	903	-	-	0/18/38/38	0/3/3/3
4	ATP	B	901	3	-	0/18/38/38	0/3/3/3
4	ATP	B	903	-	-	0/18/38/38	0/3/3/3
4	ATP	C	901	3	-	0/18/38/38	0/3/3/3
4	ATP	C	903	-	-	0/18/38/38	0/3/3/3
4	ATP	D	901	3	-	0/18/38/38	0/3/3/3
4	ATP	D	903	-	-	0/18/38/38	0/3/3/3
4	ATP	E	901	3	-	0/18/38/38	0/3/3/3
4	ATP	E	903	-	-	0/18/38/38	0/3/3/3
4	ATP	F	901	3	-	0/18/38/38	0/3/3/3
4	ATP	F	903	-	-	0/18/38/38	0/3/3/3

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	903	ATP	O4'-C4'	-3.96	1.35	1.45
4	C	901	ATP	PB-O1B	-3.35	1.38	1.51
4	C	903	ATP	O4'-C4'	-3.29	1.37	1.45
4	D	903	ATP	PB-O2B	-3.12	1.41	1.54
4	D	903	ATP	PB-O1B	-3.11	1.39	1.51

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	ATP	N3-C2-N1	-12.95	118.98	128.89
4	B	901	ATP	N3-C2-N1	-12.42	119.38	128.89
4	C	903	ATP	N3-C2-N1	-12.40	119.40	128.89
4	E	901	ATP	N3-C2-N1	-12.27	119.50	128.89
4	D	901	ATP	N3-C2-N1	-12.19	119.56	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	ATP	6	0
4	A	903	ATP	5	0
4	B	901	ATP	5	0
4	B	903	ATP	3	0
4	C	901	ATP	2	0
4	C	903	ATP	5	0
4	D	901	ATP	2	0
4	D	903	ATP	5	0
4	E	901	ATP	4	0
4	E	903	ATP	2	0
4	F	901	ATP	4	0
4	F	903	ATP	3	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	504/519 (97%)	0.43	60 (11%) 6 3	30, 77, 128, 155	0
1	B	489/519 (94%)	0.33	37 (7%) 17 9	41, 83, 129, 161	0
1	E	490/519 (94%)	-0.04	29 (5%) 26 16	21, 61, 107, 156	0
1	F	504/519 (97%)	0.16	36 (7%) 19 10	21, 69, 115, 159	0
2	C	487/519 (93%)	0.08	26 (5%) 30 20	34, 73, 125, 161	0
2	D	484/519 (93%)	-0.10	25 (5%) 31 20	27, 59, 110, 161	0
All	All	2958/3114 (94%)	0.15	213 (7%) 18 10	21, 71, 122, 161	0

The worst 5 of 213 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	PRO	8.1
1	F	117	VAL	8.1
1	B	117	VAL	7.9
2	D	121	PHE	7.7
1	E	503	SER	7.6

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	B	431	10/11	0.80	0.30	-	4,82,87,88	0
1	SEP	A	431	10/11	0.78	0.30	-	4,79,81,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TPO	B	432	11/12	0.85	0.27	-	3,19,83,84	0
1	TPO	F	432	11/12	0.76	0.32	-	3,10,75,76	0
2	TPO	D	432	11/12	0.77	0.31	-	3,9,61,64	0
2	TPO	C	432	11/12	0.76	0.27	-	3,10,78,79	0
1	TPO	A	432	11/12	0.80	0.28	-	3,19,82,83	0
1	TPO	E	432	11/12	0.83	0.22	-	3,10,59,61	0
1	SEP	F	431	10/11	0.62	0.38	-	4,80,83,83	0
1	SEP	E	431	10/11	0.71	0.33	-	4,57,60,61	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ATP	D	903	31/31	0.94	0.25	1.32	42,54,77,81	0
4	ATP	E	903	31/31	0.96	0.23	1.18	42,54,77,80	0
4	ATP	F	903	31/31	0.94	0.22	1.14	42,54,76,80	0
3	MG	B	802	1/1	0.81	0.29	1.03	73,73,73,73	0
4	ATP	D	901	31/31	0.95	0.23	0.93	53,66,89,104	0
4	ATP	B	901	31/31	0.92	0.22	0.60	62,73,109,116	0
4	ATP	F	901	31/31	0.88	0.25	0.55	74,90,114,121	0
4	ATP	C	901	31/31	0.95	0.19	0.49	48,55,97,110	0
4	ATP	A	901	31/31	0.84	0.32	0.48	75,89,103,112	0
4	ATP	E	901	31/31	0.90	0.24	0.23	61,77,101,113	0
4	ATP	C	903	31/31	0.92	0.22	0.23	43,54,77,81	0
4	ATP	A	903	31/31	0.88	0.22	0.16	42,54,76,81	0
4	ATP	B	903	31/31	0.89	0.18	-0.55	43,54,77,81	0
3	MG	E	805	1/1	0.98	0.08	-	19,19,19,19	0
3	MG	D	804	1/1	0.91	0.17	-	19,19,19,19	0
3	MG	F	806	1/1	0.98	0.13	-	19,19,19,19	0
3	MG	C	803	1/1	0.89	0.12	-	19,19,19,19	0
3	MG	A	801	1/1	0.96	0.12	-	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.