



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:53 pm GMT

PDB ID : 3K09  
Title : Crystal structure of the phosphorylation-site mutant S431D of the KaiC circadian clock protein  
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.  
Deposited on : 2009-09-24  
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](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	:	1.7.2 (RC1), CSD as538be (2017)
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)	:	trunk28620

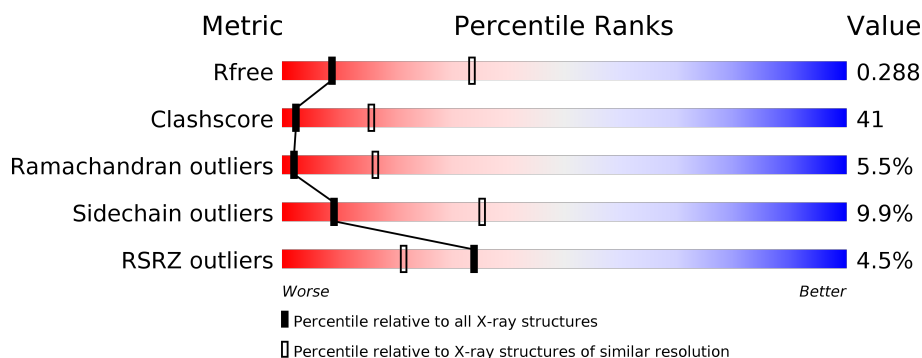
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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>9%</div> <div>40%</div> <div>49%</div> <div>8%</div> <div>• •</div> </div>
1	B	519	<div> <div>4%</div> <div>37%</div> <div>48%</div> <div>9%</div> <div>• 5%</div> </div>
1	E	519	<div> <div>2%</div> <div>37%</div> <div>49%</div> <div>9%</div> <div>5%</div> </div>
2	C	519	<div> <div>3%</div> <div>36%</div> <div>50%</div> <div>8%</div> <div>6%</div> </div>
2	D	519	<div> <div>3%</div> <div>37%</div> <div>48%</div> <div>7%</div> <div>• 7%</div> </div>
2	F	519	<div> <div>5%</div> <div>39%</div> <div>49%</div> <div>9%</div> <div>• •</div> </div>

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
3	MG	A	701	-	-	-	X
3	MG	A	702	-	-	-	X
3	MG	A	802	-	-	-	X
3	MG	B	701	-	-	-	X
3	MG	C	701	-	-	-	X
3	MG	D	702	-	-	-	X
3	MG	E	520	-	-	-	X
3	MG	E	701	-	-	-	X
3	MG	F	701	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23855 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
			3991	2510	701	764	1	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3876	2440	678	742	1	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3884	2446	679	743	1	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ASP	SER	ENGINEERED	UNP Q79PF4
B	431	ASP	SER	ENGINEERED	UNP Q79PF4
E	431	ASP	SER	ENGINEERED	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	S		0	0	0
			3848	2426	674	733	15				
2	D	485	Total	C	N	O	S		0	0	0
			3824	2412	671	726	15				
2	F	506	Total	C	N	O	S		0	0	0
			3987	2510	701	761	15				

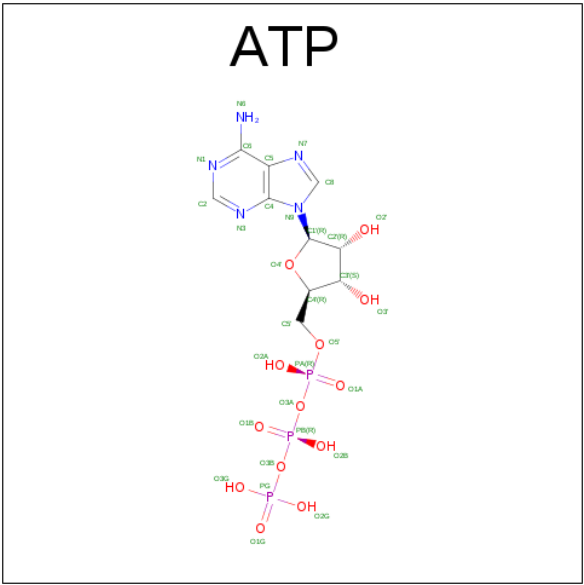
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	431	ASP	SER	ENGINEERED	UNP Q79PF4
D	431	ASP	SER	ENGINEERED	UNP Q79PF4
F	431	ASP	SER	ENGINEERED	UNP Q79PF4

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	Mg	0	0
			3	3		
3	E	4	Total	Mg	0	0
			4	4		
3	B	1	Total	Mg	0	0
			1	1		
3	C	4	Total	Mg	0	0
			4	4		
3	A	5	Total	Mg	0	0
			5	5		
3	F	3	Total	Mg	0	0
			3	3		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

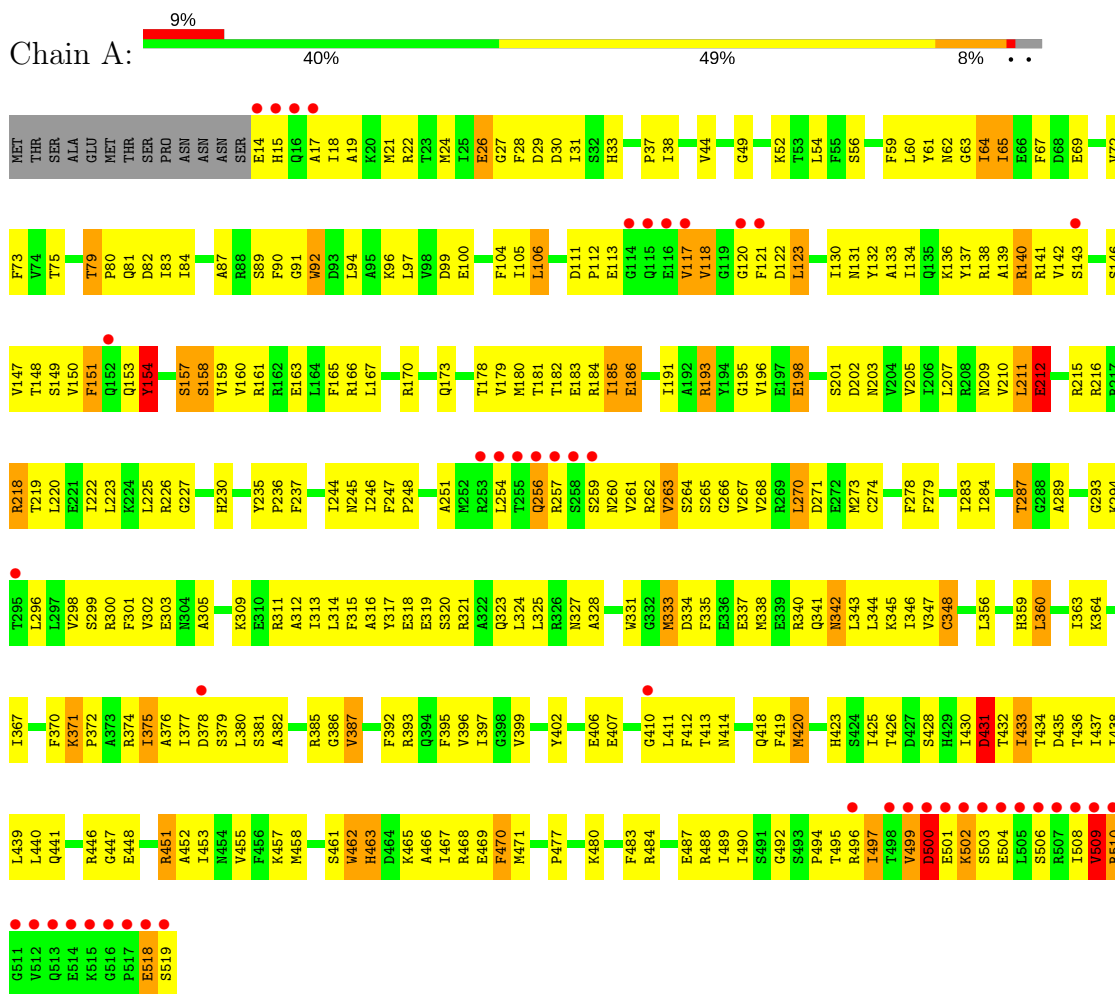
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	5	Total	O	0	0
			5	5		
5	C	5	Total	O	0	0
			5	5		
5	D	10	Total	O	0	0
			10	10		
5	E	7	Total	O	0	0
			7	7		
5	F	19	Total	O	0	0
			19	19		

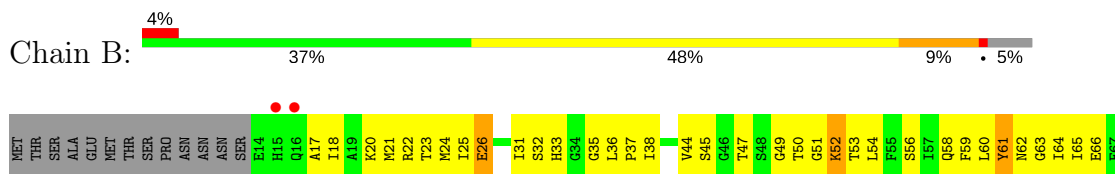
### 3 Residue-property plots [i](#)

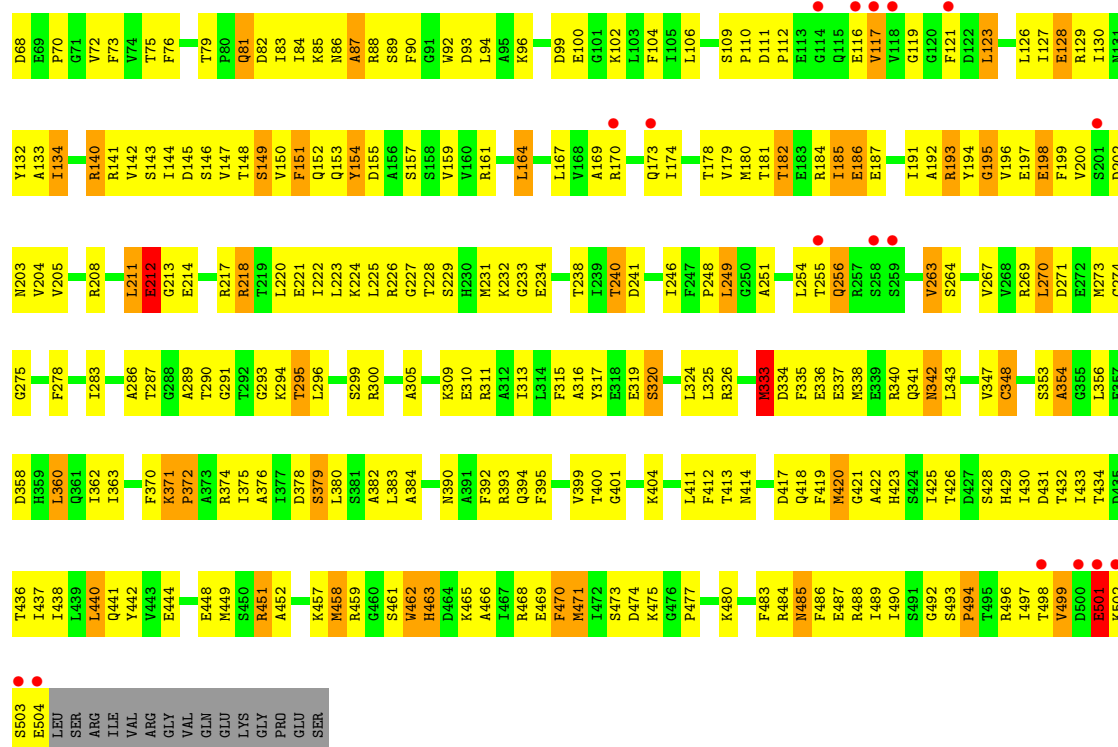
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Circadian clock protein kinase kaiC

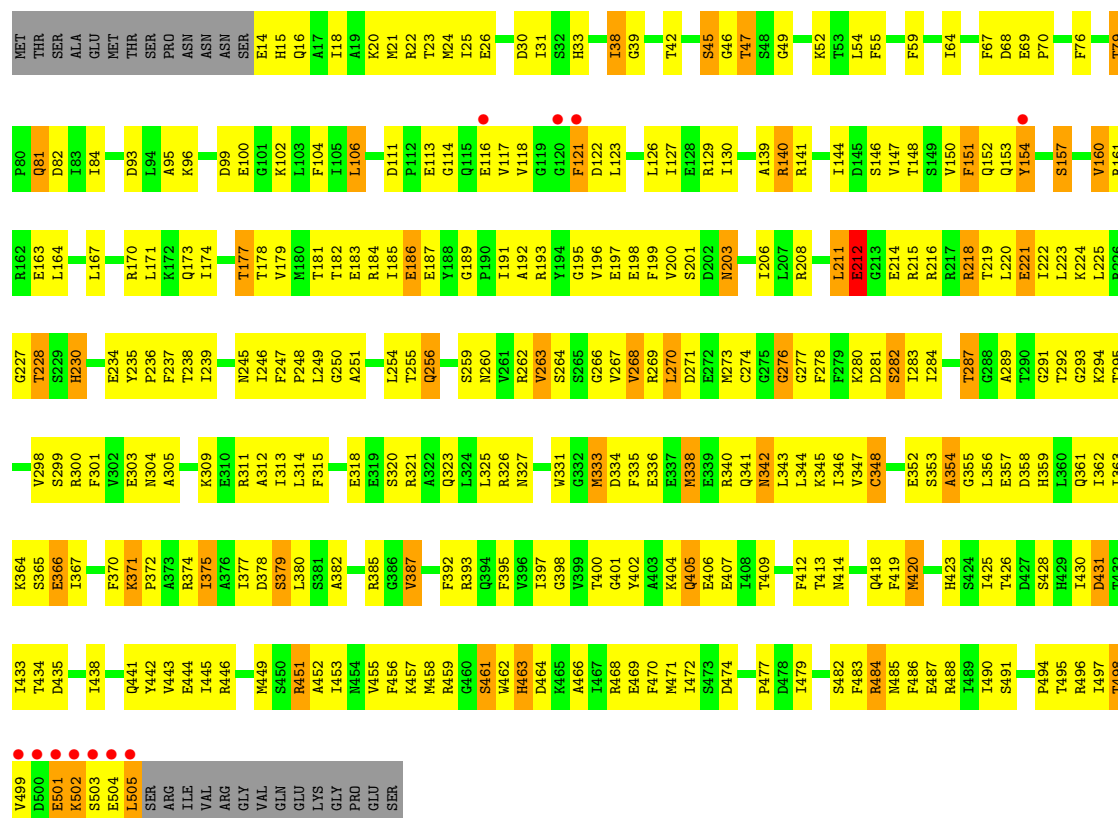


#### • Molecule 1: Circadian clock protein kinase kaiC



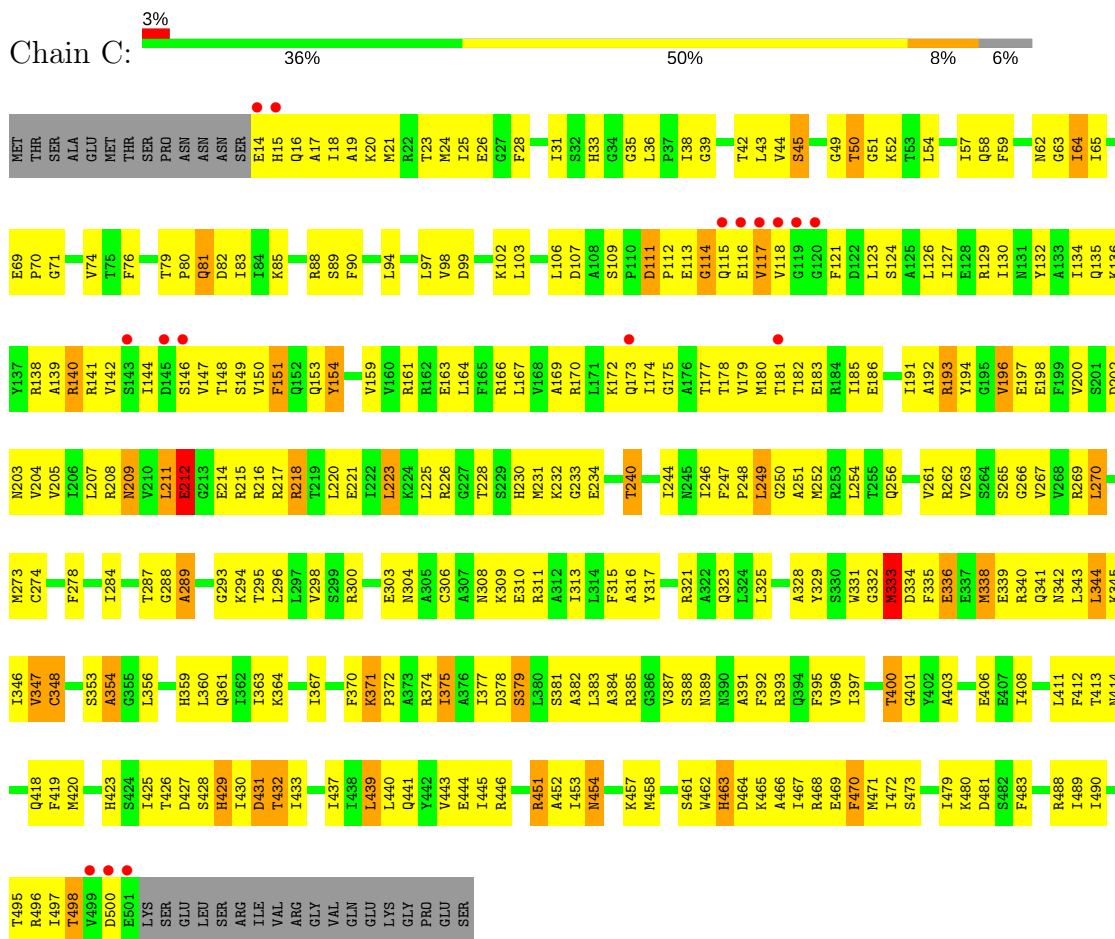


● Molecule 1: Circadian clock protein kinase kaiC

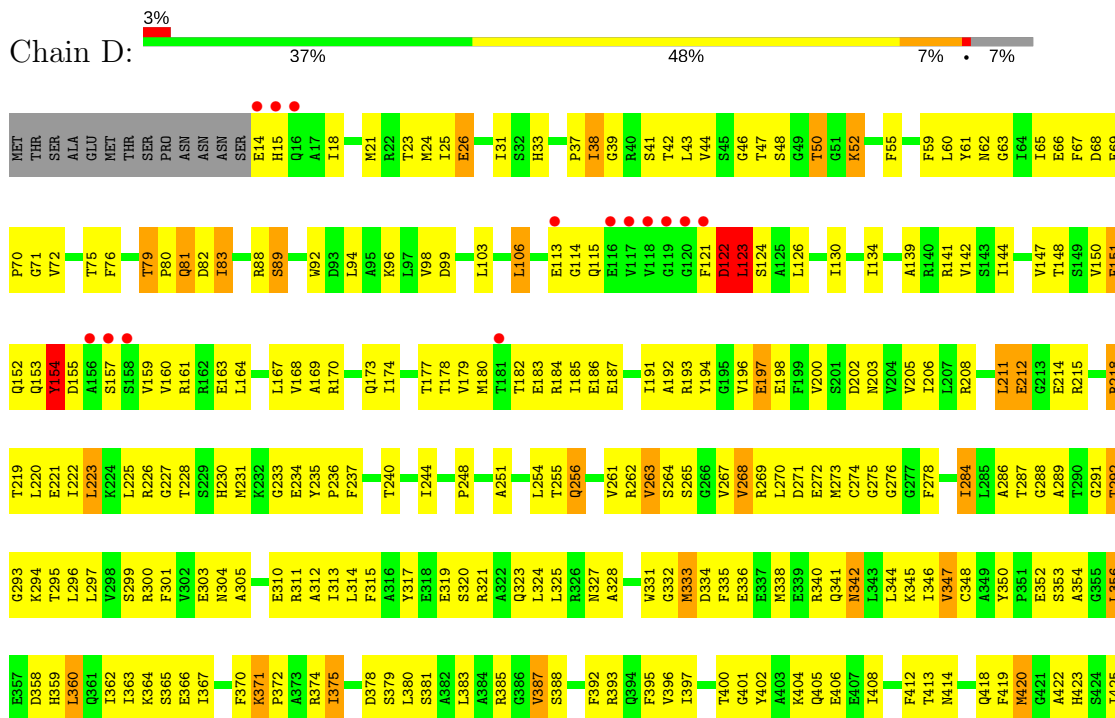


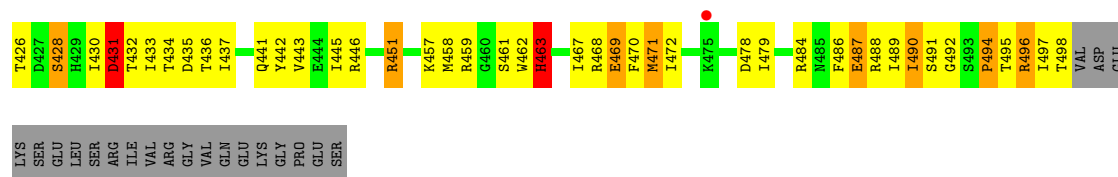


• Molecule 2: Circadian clock protein kinase kaiC



• Molecule 2: Circadian clock protein kinase kaiC





• 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, $\alpha$ , $\beta$ , $\gamma$	132.50Å 135.83Å 204.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.98 – 3.19	Depositor EDS
% Data completeness (in resolution range)	81.4 (30.00-3.20) 90.1 (29.98-3.19)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.296 0.237 , 0.288	Depositor DCC
$R_{free}$ test set	5684 reflections (10.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.9	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 65.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MG, ATP

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	0.43	0/4045	0.70	0/5448
1	B	0.41	0/3929	0.66	0/5293
1	E	0.49	0/3937	0.72	1/5304 (0.0%)
2	C	0.44	0/3913	0.68	0/5275
2	D	0.47	0/3889	0.72	0/5242
2	F	0.47	0/4053	0.72	0/5461
All	All	0.45	0/23766	0.70	1/32023 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	380	LEU	N-CA-C	-5.39	96.44	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3991	0	3984	337	0
1	B	3876	0	3861	326	0
1	E	3884	0	3873	337	0
2	C	3848	0	3838	337	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3824	0	3819	332	0
2	F	3987	0	3984	384	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
3	E	4	0	0	0	0
3	F	3	0	0	0	0
4	A	62	0	24	5	0
4	B	62	0	24	7	0
4	C	62	0	24	4	0
4	D	62	0	24	6	0
4	E	62	0	24	6	0
4	F	62	0	24	9	0
5	A	7	0	0	1	0
5	B	5	0	0	2	0
5	C	5	0	0	1	0
5	D	10	0	0	2	0
5	E	7	0	0	1	0
5	F	19	0	0	4	0
All	All	23855	0	23503	1939	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 41.

The worst 5 of 1939 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:E:305:ALA:HB2	1:E:374:ARG:HD2	1.16	1.14
1:A:14:GLU:HG3	1:A:15:HIS:H	1.13	1.13
2:F:115:GLN:HG2	2:F:116:GLU:N	1.56	1.13
2:F:115:GLN:HG2	2:F:116:GLU:H	0.97	1.10
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.14	1.08

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	503/519 (97%)	389 (77%)	83 (16%)	31 (6%)	2	13
1	B	488/519 (94%)	383 (78%)	71 (14%)	34 (7%)	1	9
1	E	489/519 (94%)	396 (81%)	66 (14%)	27 (6%)	2	16
2	C	486/519 (94%)	394 (81%)	69 (14%)	23 (5%)	3	20
2	D	483/519 (93%)	396 (82%)	68 (14%)	19 (4%)	3	25
2	F	504/519 (97%)	411 (82%)	65 (13%)	28 (6%)	2	16
All	All	2953/3114 (95%)	2369 (80%)	422 (14%)	162 (6%)	2	16

5 of 162 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	VAL
1	A	154	TYR
1	A	157	SER
1	A	387	VAL
1	A	420	MET

### 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	431/443 (97%)	387 (90%)	44 (10%)	8	34
1	B	418/443 (94%)	381 (91%)	37 (9%)	11	41
1	E	419/443 (95%)	373 (89%)	46 (11%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	416/444 (94%)	380 (91%)	36 (9%)	12	42
2	D	413/444 (93%)	372 (90%)	41 (10%)	9	35
2	F	432/444 (97%)	386 (89%)	46 (11%)	8	32
All	All	2529/2661 (95%)	2279 (90%)	250 (10%)	9	35

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	454	ASN
2	D	270	LEU
2	F	321	ARG
2	C	500	ASP
2	D	123	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	414	ASN
2	D	323	GLN
2	F	368	ASN
2	C	429	HIS
2	D	33	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	TPO	A	432	1	9,10,11	1.49	1 (11%)	10,14,16	1.19	1 (10%)
1	TPO	B	432	1	9,10,11	1.33	1 (11%)	10,14,16	1.49	1 (10%)
1	TPO	E	432	1	9,10,11	1.35	2 (22%)	10,14,16	1.25	2 (20%)

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	TPO	A	432	1	-	0/8/11/13	0/0/0/0
1	TPO	B	432	1	-	0/8/11/13	0/0/0/0
1	TPO	E	432	1	-	0/8/11/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	432	TPO	CB-CA	-2.25	1.50	1.53
1	E	432	TPO	P-OG1	-2.08	1.55	1.59
1	B	432	TPO	CA-C	3.23	1.54	1.50
1	A	432	TPO	CA-C	3.61	1.55	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	TPO	CG2-CB-CA	-3.48	106.77	113.22
1	A	432	TPO	CG2-CB-CA	-3.00	107.65	113.22
1	E	432	TPO	CG2-CB-CA	-2.50	108.58	113.22
1	E	432	TPO	O-C-CA	-2.06	120.34	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	432	TPO	2	0
1	B	432	TPO	2	0



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 20 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	27,33,33	1.28	2 (7%)	25,52,52	2.46	4 (16%)
4	ATP	A	903	3	27,33,33	1.15	3 (11%)	25,52,52	2.49	5 (20%)
4	ATP	B	901	-	27,33,33	1.19	4 (14%)	25,52,52	2.47	5 (20%)
4	ATP	B	903	3	27,33,33	1.25	3 (11%)	25,52,52	2.54	5 (20%)
4	ATP	C	901	3	27,33,33	1.21	2 (7%)	25,52,52	2.49	6 (24%)
4	ATP	C	903	3	27,33,33	1.33	4 (14%)	25,52,52	2.52	4 (16%)
4	ATP	D	901	3	27,33,33	1.24	3 (11%)	25,52,52	2.43	5 (20%)
4	ATP	D	903	3	27,33,33	1.35	4 (14%)	25,52,52	2.59	4 (16%)
4	ATP	E	901	3	27,33,33	1.27	1 (3%)	25,52,52	2.55	4 (16%)
4	ATP	E	903	3	27,33,33	1.23	3 (11%)	25,52,52	2.63	5 (20%)
4	ATP	F	901	3	27,33,33	1.30	2 (7%)	25,52,52	2.44	5 (20%)
4	ATP	F	903	3	27,33,33	1.24	1 (3%)	25,52,52	2.48	4 (16%)

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	3	-	0/18/38/38	0/3/3/3
4	ATP	B	901	-	-	0/18/38/38	0/3/3/3
4	ATP	B	903	3	-	0/18/38/38	0/3/3/3
4	ATP	C	901	3	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	C	903	3	-	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	3	-	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	3	-	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	3	-	0/18/38/38	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	903	ATP	C2'-C1'	-2.73	1.49	1.53
4	E	903	ATP	C8-N7	-2.08	1.30	1.34
4	C	903	ATP	C2-N1	2.00	1.37	1.33
4	C	903	ATP	PG-O3B	2.01	1.63	1.60
4	C	901	ATP	O4'-C1'	2.04	1.44	1.41

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	903	ATP	N3-C2-N1	-10.75	119.49	128.86
4	E	903	ATP	N3-C2-N1	-10.60	119.63	128.86
4	B	901	ATP	N3-C2-N1	-10.41	119.79	128.86
4	E	901	ATP	N3-C2-N1	-10.39	119.81	128.86
4	C	903	ATP	N3-C2-N1	-10.36	119.84	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	ATP	1	0
4	A	903	ATP	4	0
4	B	901	ATP	4	0
4	B	903	ATP	3	0
4	C	901	ATP	3	0
4	C	903	ATP	1	0
4	D	901	ATP	4	0
4	D	903	ATP	2	0
4	E	901	ATP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	903	ATP	2	0
4	F	901	ATP	5	0
4	F	903	ATP	4	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	505/519 (97%)	0.15	45 (8%) 10 6	30, 83, 129, 159	0
1	B	490/519 (94%)	0.05	19 (3%) 40 26	43, 85, 130, 165	0
1	E	491/519 (94%)	-0.19	11 (2%) 62 48	8, 65, 118, 160	0
2	C	488/519 (94%)	-0.08	16 (3%) 47 31	25, 73, 127, 169	0
2	D	485/519 (93%)	-0.26	15 (3%) 49 33	17, 60, 115, 158	0
2	F	506/519 (97%)	-0.05	27 (5%) 27 15	11, 73, 125, 146	0
All	All	2965/3114 (95%)	-0.06	133 (4%) 34 21	8, 73, 126, 169	0

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	517	PRO	7.2
1	A	519	SER	6.8
2	F	500	ASP	6.4
1	A	518	GLU	6.3
2	C	500	ASP	6.2

### 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	TPO	E	432	11/12	0.94	0.19	-	61,68,76,76	0
1	TPO	B	432	11/12	0.77	0.34	-	84,94,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TPO	A	432	11/12	0.84	0.21	-	82,90,97,97	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
3	MG	E	701	1/1	0.97	0.95	21.73	91,91,91,91	0
3	MG	A	702	1/1	0.67	0.63	9.04	90,90,90,90	0
3	MG	C	701	1/1	0.81	1.19	7.58	112,112,112,112	0
3	MG	B	701	1/1	0.97	0.61	6.11	69,69,69,69	0
3	MG	E	520	1/1	0.96	0.33	5.67	42,42,42,42	0
3	MG	D	702	1/1	0.98	0.70	4.60	90,90,90,90	0
3	MG	F	701	1/1	0.97	0.39	3.40	60,60,60,60	0
3	MG	A	701	1/1	0.97	0.50	3.19	75,75,75,75	0
3	MG	E	702	1/1	0.93	0.35	1.84	18,18,18,18	0
3	MG	A	520	1/1	0.97	0.40	1.73	113,113,113,113	0
3	MG	F	702	1/1	0.97	0.22	1.65	19,19,19,19	0
3	MG	A	802	1/1	0.98	0.43	1.31	44,44,44,44	0
4	ATP	E	903	31/31	0.93	0.23	1.31	24,31,51,52	0
4	ATP	D	903	31/31	0.91	0.27	1.10	36,41,61,63	0
4	ATP	D	901	31/31	0.94	0.24	0.83	58,63,70,70	0
4	ATP	A	903	31/31	0.89	0.25	0.78	57,60,67,68	0
4	ATP	B	903	31/31	0.90	0.24	0.75	62,69,79,80	0
4	ATP	F	903	31/31	0.94	0.20	0.59	27,33,45,47	0
4	ATP	B	901	31/31	0.92	0.24	0.55	62,71,84,84	0
4	ATP	F	901	31/31	0.88	0.28	0.49	93,98,104,104	0
4	ATP	C	901	31/31	0.93	0.19	0.27	47,54,68,69	0
4	ATP	C	903	31/31	0.92	0.21	0.12	45,49,77,80	0
4	ATP	E	901	31/31	0.90	0.24	0.01	68,74,77,77	0
4	ATP	A	901	31/31	0.88	0.26	-0.17	72,82,84,84	0
3	MG	C	802	1/1	0.97	0.08	-1.87	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	D	801	1/1	0.98	0.08	-2.02	26,26,26,26	0
3	MG	E	801	1/1	0.71	0.20	-2.59	25,25,25,25	0
3	MG	D	520	1/1	0.83	0.37	-	25,25,25,25	0
3	MG	C	801	1/1	0.76	0.40	-	28,28,28,28	0
3	MG	F	801	1/1	0.98	0.35	-	40,40,40,40	0
3	MG	C	702	1/1	0.88	1.16	-	104,104,104,104	0
3	MG	A	801	1/1	0.84	0.22	-	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.