



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:32 PM GMT

PDB ID : 4IJM  
Title : Crystal structure of circadian clock protein KaiC A422V mutant  
Authors : Egli, M.; Pattanayek, R.  
Deposited on : 2012-12-21  
Resolution : 3.35 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.

---

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

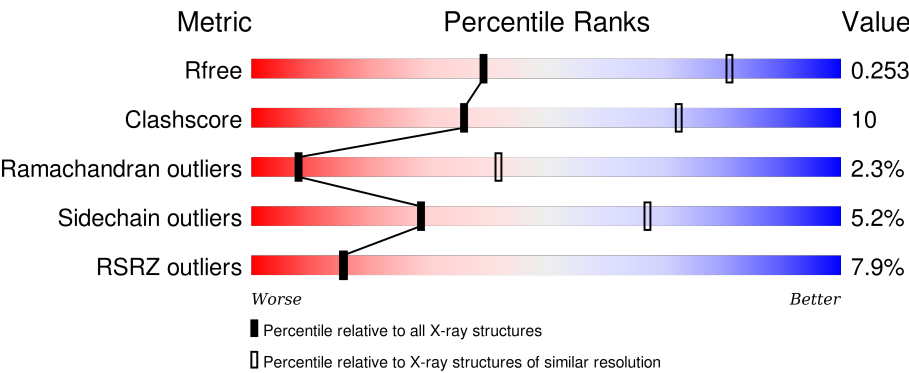
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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 <sub>free</sub>	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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 <=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	512	<div><div>13%</div><div><div></div><div>73%</div><div>23%</div><div>• •</div></div></div>
1	B	512	<div><div>8%</div><div><div></div><div>71%</div><div>23%</div><div>• •</div></div></div>
1	C	512	<div><div>5%</div><div><div></div><div>67%</div><div>25%</div><div>• 5%</div></div></div>
1	D	512	<div><div>5%</div><div><div></div><div>71%</div><div>21%</div><div>• 5%</div></div></div>
1	E	512	<div><div>5%</div><div><div></div><div>71%</div><div>23%</div><div>• •</div></div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	512	

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
4	PO4	B	605	-	-	-	X
4	PO4	D	604	-	-	-	X
4	PO4	E	605	-	-	-	X
4	PO4	F	603	-	-	-	X
4	PO4	F	604	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24219 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	2511	701	763	1	15			
1	B	489	Total	C	N	O	P	S	0	0	0
			3861	2433	676	736	1	15			
1	C	488	Total	C	N	O	P	S	0	0	0
			3852	2427	674	735	1	15			
1	D	485	Total	C	N	O	P	S	0	0	0
			3828	2413	671	728	1	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3884	2447	679	742	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3987	2509	701	761	1	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	VAL	ALA	ENGINEERED MUTATION	UNP Q79PF4
A	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	422	VAL	ALA	ENGINEERED MUTATION	UNP Q79PF4
B	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	422	VAL	ALA	ENGINEERED MUTATION	UNP Q79PF4
C	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	521	HIS	-	EXPRESSION TAG	UNP Q79PF4

*Continued on next page...*

*Continued from previous page...*

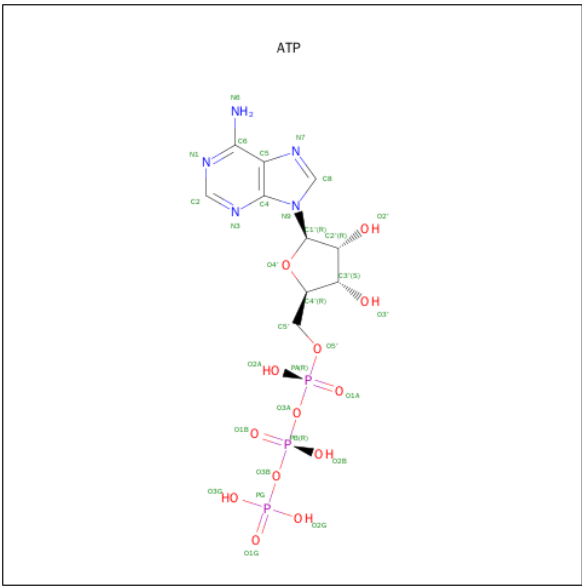
Chain	Residue	Modelled	Actual	Comment	Reference
C	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	422	VAL	ALA	ENGINEERED MUTATION	UNP Q79PF4
D	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	422	VAL	ALA	ENGINEERED MUTATION	UNP Q79PF4
E	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	422	VAL	ALA	ENGINEERED MUTATION	UNP Q79PF4
F	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	525	HIS	-	EXPRESSION TAG	UNP Q79PF4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	B	2	Total Mg 2 2	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	53	Total	O	0	0
			53	53		
5	C	83	Total	O	0	0
			83	83		
5	D	66	Total	O	0	0
			66	66		

*Continued on next page...*

*Continued from previous page...*

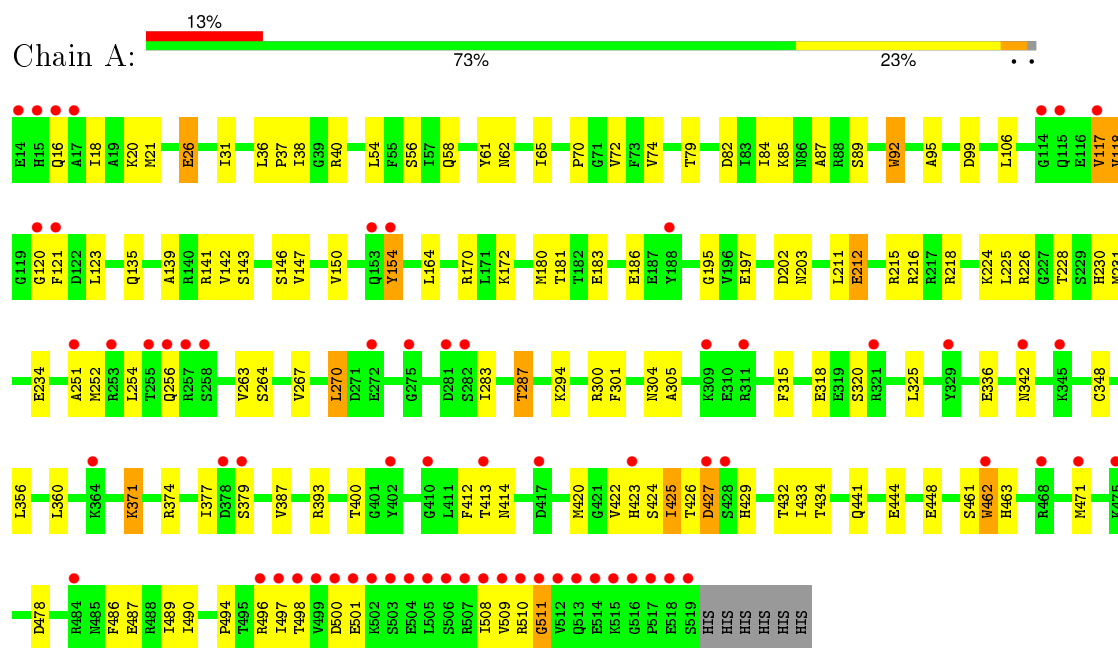
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	54	Total	O	0	0
			54	54		
5	F	67	Total	O	0	0
			67	67		



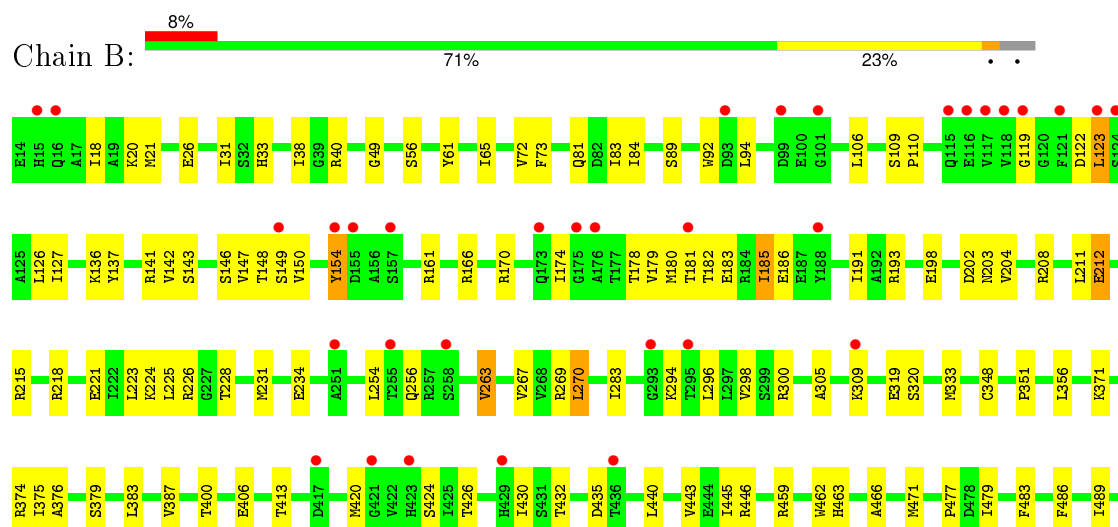
### 3 Residue-property plots

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.

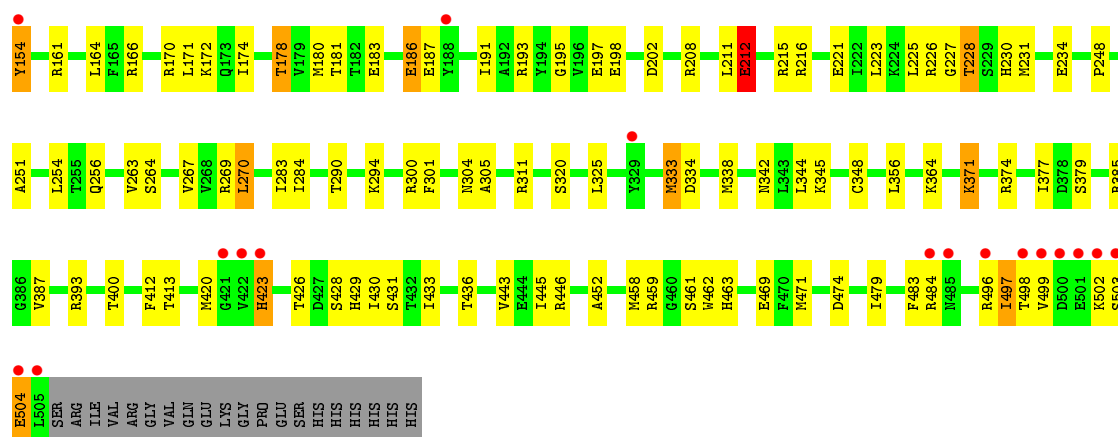
#### • Molecule 1: Circadian clock protein kinase KaiC



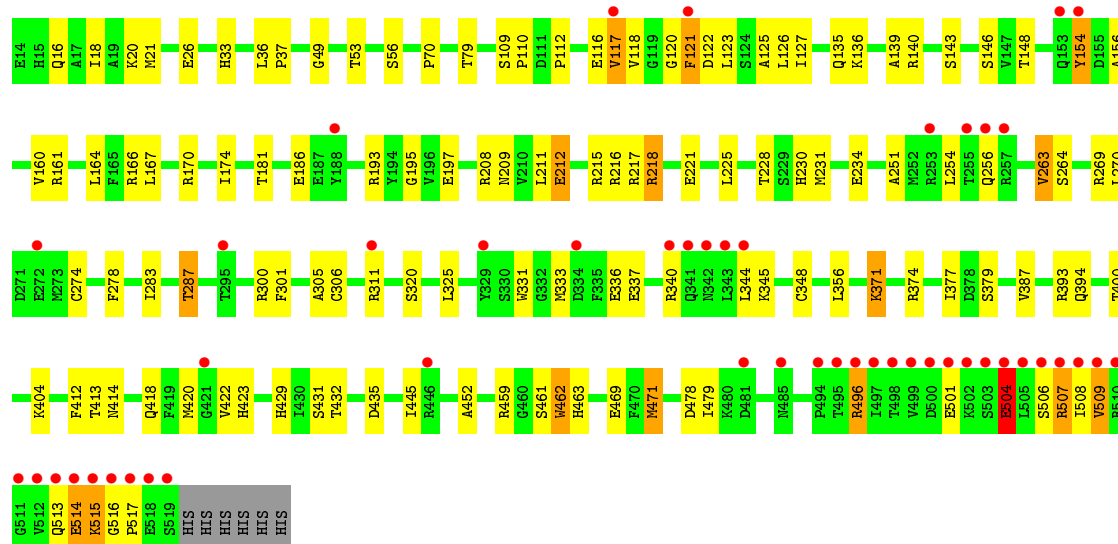
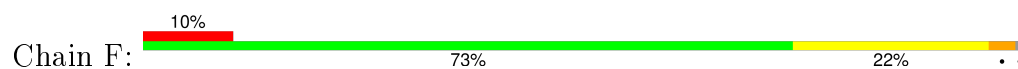
#### • Molecule 1: Circadian clock protein kinase KaiC







● Molecule 1: Circadian clock protein kinase KaiC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.36Å 134.47Å 203.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.35 29.96 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.96-3.35) 95.0 (29.96-3.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 3.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.217 , 0.261 0.213 , 0.253	Depositor DCC
$R_{free}$ test set	2544 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.6	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 57.4	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52369 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	24219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, PO4, 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	0.25	0/4045	0.41	2/5448 (0.0%)
1	B	0.25	0/3914	0.41	0/5273
1	C	0.22	0/3905	0.39	0/5262
1	D	0.22	0/3881	0.39	0/5229
1	E	0.23	0/3937	0.41	0/5304
1	F	0.22	0/4041	0.40	0/5443
All	All	0.23	0/23723	0.40	2/31959 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	MET	CA-CB-CG	-5.97	103.14	113.30
1	A	251	ALA	C-N-CA	-5.06	109.05	121.70

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	3991	0	3988	73	0
1	B	3861	0	3854	85	0
1	C	3852	0	3842	98	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3828	0	3823	79	0
1	E	3884	0	3877	86	0
1	F	3987	0	3983	74	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	93	0	36	6	0
3	B	62	0	24	2	0
3	C	62	0	24	3	0
3	D	62	0	24	0	0
3	E	62	0	24	1	0
3	F	31	0	12	1	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	1	0
5	A	74	0	0	8	0
5	B	53	0	0	5	0
5	C	83	0	0	5	0
5	D	66	0	0	1	0
5	E	54	0	0	9	0
5	F	67	0	0	4	0
All	All	24219	0	23511	453	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 10.

The worst 5 of 453 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:503:SER:HB3	1:E:504:GLU:HB2	1.29	1.12
1:B:499:VAL:C	1:B:501:GLU:HA	1.76	1.06
1:D:379:SER:H	1:D:413:THR:HB	1.41	0.83
1:F:379:SER:H	1:F:413:THR:HB	1.41	0.82
1:E:379:SER:H	1:E:413:THR:HB	1.43	0.82

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	503/512 (98%)	448 (89%)	39 (8%)	16 (3%)	5	34
1	B	486/512 (95%)	449 (92%)	28 (6%)	9 (2%)	10	46
1	C	485/512 (95%)	442 (91%)	31 (6%)	12 (2%)	7	40
1	D	482/512 (94%)	448 (93%)	27 (6%)	7 (2%)	13	51
1	E	489/512 (96%)	442 (90%)	37 (8%)	10 (2%)	9	45
1	F	503/512 (98%)	452 (90%)	37 (7%)	14 (3%)	6	37
All	All	2948/3072 (96%)	2681 (91%)	199 (7%)	68 (2%)	8	42

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ILE
1	C	17	ALA
1	C	117	VAL
1	E	463	HIS
1	F	154	TYR

### 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	432/438 (99%)	411 (95%)	21 (5%)	31	69
1	B	417/438 (95%)	395 (95%)	22 (5%)	28	66
1	C	416/438 (95%)	392 (94%)	24 (6%)	25	64

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	413/438 (94%)	394 (95%)	19 (5%)	33	71
1	E	420/438 (96%)	400 (95%)	20 (5%)	31	70
1	F	431/438 (98%)	405 (94%)	26 (6%)	24	62
All	All	2529/2628 (96%)	2397 (95%)	132 (5%)	29	67

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	333	MET
1	D	186	GLU
1	F	333	MET
1	C	371	LYS
1	D	26	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	16	GLN
1	F	245	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	8,10,11	1.51	1 (12%)	7,14,16	1.18	1 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	B	432	1	8,10,11	1.51	1 (12%)	7,14,16	1.17	1 (14%)
1	TPO	C	432	1	8,10,11	1.51	1 (12%)	7,14,16	1.18	1 (14%)
1	TPO	D	432	1	8,10,11	1.14	0	7,14,16	1.44	1 (14%)
1	TPO	E	432	1	8,10,11	1.09	0	7,14,16	1.26	1 (14%)
1	TPO	F	432	1	8,10,11	1.10	0	7,14,16	1.17	1 (14%)

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	-	1/8/11/13	0/0/0/0
1	TPO	B	432	1	-	0/8/11/13	0/0/0/0
1	TPO	C	432	1	-	0/8/11/13	0/0/0/0
1	TPO	D	432	1	-	0/8/11/13	0/0/0/0
1	TPO	E	432	1	-	0/8/11/13	0/0/0/0
1	TPO	F	432	1	-	0/8/11/13	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	432	TPO	P-O1P	3.07	1.61	1.51
1	A	432	TPO	P-O1P	3.10	1.61	1.51
1	B	432	TPO	P-O1P	3.13	1.61	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	432	TPO	CG2-CB-CA	-2.58	107.91	113.17
1	A	432	TPO	CG2-CB-CA	-2.17	108.75	113.17
1	E	432	TPO	CG2-CB-CA	-2.11	108.89	113.17
1	F	432	TPO	CG2-CB-CA	-2.06	108.97	113.17
1	B	432	TPO	CG2-CB-CA	-2.01	109.08	113.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	432	TPO	OG1-CB-CA-N

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 7 are monoatomic - leaving 20 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	$\# Z  > 2$
3	ATP	A	802	2	24,33,33	0.98	1 (4%)	31,52,52	1.80	5 (16%)
3	ATP	A	803	-	24,33,33	0.98	1 (4%)	31,52,52	1.92	5 (16%)
3	ATP	A	804	-	24,33,33	0.99	1 (4%)	31,52,52	1.90	5 (16%)
3	ATP	B	602	2	24,33,33	0.98	1 (4%)	31,52,52	1.77	5 (16%)
3	ATP	B	603	-	24,33,33	0.98	1 (4%)	31,52,52	1.95	6 (19%)
4	PO4	B	604	-	4,4,4	0.48	0	6,6,6	0.27	0
4	PO4	B	605	-	4,4,4	0.50	0	6,6,6	0.27	0
3	ATP	C	602	2	24,33,33	1.00	1 (4%)	31,52,52	1.90	6 (19%)
3	ATP	C	603	-	24,33,33	0.98	1 (4%)	31,52,52	1.85	6 (19%)
4	PO4	C	604	-	4,4,4	0.50	0	6,6,6	0.27	0
3	ATP	D	602	2	24,33,33	0.98	1 (4%)	31,52,52	1.88	5 (16%)
3	ATP	D	603	-	24,33,33	0.99	1 (4%)	31,52,52	1.87	5 (16%)
4	PO4	D	604	-	4,4,4	0.50	0	6,6,6	0.27	0
3	ATP	E	602	2	24,33,33	0.98	1 (4%)	31,52,52	1.85	5 (16%)
3	ATP	E	603	-	24,33,33	0.97	1 (4%)	31,52,52	1.89	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	E	604	-	4,4,4	0.49	0	6,6,6	0.27	0
4	PO4	E	605	-	4,4,4	0.49	0	6,6,6	0.27	0
3	ATP	F	602	2	24,33,33	0.99	1 (4%)	31,52,52	1.90	5 (16%)
4	PO4	F	603	-	4,4,4	0.50	0	6,6,6	0.27	0
4	PO4	F	604	-	4,4,4	0.49	0	6,6,6	0.27	0

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
3	ATP	A	802	2	-	0/18/38/38	0/3/3/3
3	ATP	A	803	-	-	0/18/38/38	0/3/3/3
3	ATP	A	804	-	-	0/18/38/38	0/3/3/3
3	ATP	B	602	2	-	0/18/38/38	0/3/3/3
3	ATP	B	603	-	-	0/18/38/38	0/3/3/3
4	PO4	B	604	-	-	0/0/0/0	0/0/0/0
4	PO4	B	605	-	-	0/0/0/0	0/0/0/0
3	ATP	C	602	2	-	0/18/38/38	0/3/3/3
3	ATP	C	603	-	-	0/18/38/38	0/3/3/3
4	PO4	C	604	-	-	0/0/0/0	0/0/0/0
3	ATP	D	602	2	-	0/18/38/38	0/3/3/3
3	ATP	D	603	-	-	0/18/38/38	0/3/3/3
4	PO4	D	604	-	-	0/0/0/0	0/0/0/0
3	ATP	E	602	2	-	0/18/38/38	0/3/3/3
3	ATP	E	603	-	-	0/18/38/38	0/3/3/3
4	PO4	E	604	-	-	0/0/0/0	0/0/0/0
4	PO4	E	605	-	-	0/0/0/0	0/0/0/0
3	ATP	F	602	2	-	0/18/38/38	0/3/3/3
4	PO4	F	603	-	-	0/0/0/0	0/0/0/0
4	PO4	F	604	-	-	0/0/0/0	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	603	ATP	C5-C4	3.11	1.47	1.40
3	B	603	ATP	C5-C4	3.11	1.47	1.40
3	E	602	ATP	C5-C4	3.13	1.47	1.40
3	B	602	ATP	C5-C4	3.14	1.47	1.40
3	A	804	ATP	C5-C4	3.15	1.47	1.40

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	ATP	N3-C2-N1	-6.79	123.70	128.89
3	E	602	ATP	N3-C2-N1	-6.74	123.74	128.89
3	A	803	ATP	N3-C2-N1	-6.71	123.76	128.89
3	C	603	ATP	N3-C2-N1	-6.66	123.79	128.89
3	B	602	ATP	N3-C2-N1	-6.66	123.79	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	ATP	2	0
3	A	803	ATP	3	0
3	A	804	ATP	1	0
3	B	603	ATP	2	0
3	C	602	ATP	1	0
3	C	603	ATP	2	0
3	E	602	ATP	1	0
3	F	602	ATP	1	0
4	F	604	PO4	1	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	505/512 (98%)	0.63	67 (13%) 4 4	27, 84, 140, 180	0
1	B	488/512 (95%)	0.50	40 (8%) 14 14	38, 84, 134, 171	0
1	C	487/512 (95%)	0.21	27 (5%) 29 28	29, 67, 120, 176	0
1	D	484/512 (94%)	0.11	24 (4%) 32 32	13, 50, 114, 144	0
1	E	491/512 (95%)	0.14	27 (5%) 29 28	8, 54, 120, 167	0
1	F	505/512 (98%)	0.33	49 (9%) 10 11	8, 66, 136, 181	0
All	All	2960/3072 (96%)	0.32	234 (7%) 15 16	8, 69, 130, 181	0

The worst 5 of 234 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	ARG	9.3
1	A	516	GLY	8.8
1	A	519	SER	8.6
1	D	120	GLY	8.4
1	F	516	GLY	7.9

### 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	F	432	11/12	0.83	0.26	-	46,73,98,100	0
1	TPO	D	432	11/12	0.85	0.31	-	38,55,98,100	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TPO	E	432	11/12	0.93	0.22	-	33,45,78,90	0
1	TPO	C	432	11/12	0.93	0.21	-	45,57,76,83	0
1	TPO	A	432	11/12	0.78	0.26	-	83,90,112,116	0
1	TPO	B	432	11/12	0.93	0.27	-	68,87,103,106	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	PO4	D	604	5/5	0.83	0.69	10.92	71,83,87,111	0
4	PO4	B	605	5/5	0.87	0.68	8.02	81,94,105,120	0
4	PO4	F	604	5/5	0.70	0.47	4.91	77,78,106,143	0
4	PO4	F	603	5/5	0.84	0.46	4.40	62,66,103,119	0
4	PO4	E	605	5/5	0.82	0.65	4.33	55,64,81,115	0
4	PO4	C	604	5/5	0.91	0.35	1.62	43,74,89,107	0
3	ATP	F	602	31/31	0.78	0.35	1.03	66,101,113,120	0
3	ATP	D	603	31/31	0.90	0.29	0.79	3,17,54,88	0
3	ATP	A	804	31/31	0.91	0.25	0.72	8,37,63,78	0
3	ATP	A	803	31/31	0.82	0.29	0.62	34,64,97,99	0
3	ATP	E	603	31/31	0.92	0.25	0.55	7,18,53,72	0
3	ATP	D	602	31/31	0.89	0.28	0.51	32,54,66,77	0
3	ATP	C	603	31/31	0.90	0.29	0.51	22,50,78,105	0
3	ATP	C	602	31/31	0.91	0.25	0.34	23,46,74,82	0
3	ATP	E	602	31/31	0.86	0.26	-0.08	38,79,94,95	0
3	ATP	A	802	31/31	0.86	0.28	-0.08	58,82,97,100	0
3	ATP	B	602	31/31	0.90	0.23	-0.18	52,66,86,93	0
3	ATP	B	603	31/31	0.86	0.28	-0.24	55,80,104,117	0
4	PO4	E	604	5/5	0.87	0.20	-1.26	112,123,141,148	0
2	MG	B	606	1/1	0.96	0.27	-	69,69,69,69	0
2	MG	A	801	1/1	0.93	0.30	-	82,82,82,82	0
2	MG	B	601	1/1	0.78	0.31	-	63,63,63,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	B	604	5/5	0.58	0.48	-	126,129,146,151	0
2	MG	C	601	1/1	0.72	0.27	-	43,43,43,43	0
2	MG	E	601	1/1	0.90	0.26	-	59,59,59,59	0
2	MG	F	601	1/1	0.59	0.55	-	85,85,85,85	0
2	MG	D	601	1/1	0.95	0.28	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.