wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:36 PM GMT

PDB ID	:	1U9I
Title	:	Crystal Structure of Circadian Clock Protein KaiC with Phosphorylation Sites
Authors	:	Xu, Y.; Mori, T.; Pattanayek, R.; Pattanayek, S.; Egli, M.; Johnson, C.H.
Deposited on	:	2004-08-09
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

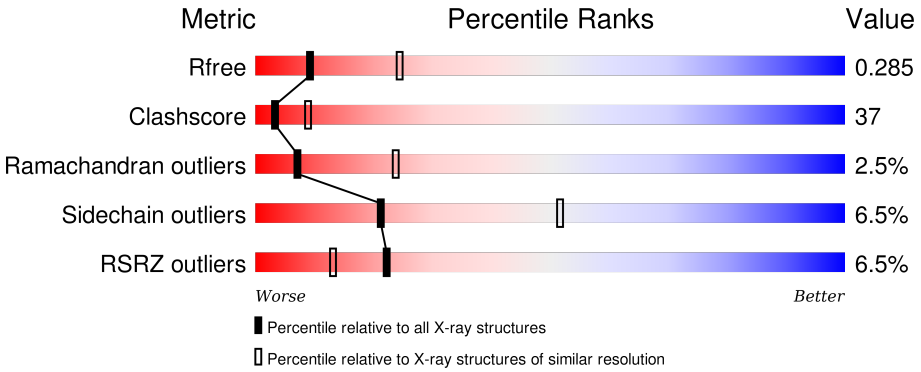
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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 >=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	519	9% 48% 40% 5% 7%
1	B	519	7% 47% 41% 5% 7%
1	E	519	6% 47% 40% 6% 7%
1	F	519	4% 43% 43% 6% 7%
2	C	519	5% 42% 44% 7% 7%

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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	B	431	-	-	X	-
1	SEP	E	431	-	-	X	-
1	SEP	F	431	-	-	X	-
3	MG	B	520	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23375 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 KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	P	S	0	0	0
			3823	2407	670	729	2	15			
1	B	484	Total	C	N	O	P	S	0	0	0
			3823	2407	670	729	2	15			
1	E	484	Total	C	N	O	P	S	0	0	0
			3823	2407	670	729	2	15			
1	F	484	Total	C	N	O	P	S	0	0	0
			3823	2407	670	729	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 KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	484	Total	C	N	O	P	S	0	0	0
			3819	2407	670	726	1	15			
2	D	484	Total	C	N	O	P	S	0	0	0
			3819	2407	670	726	1	15			

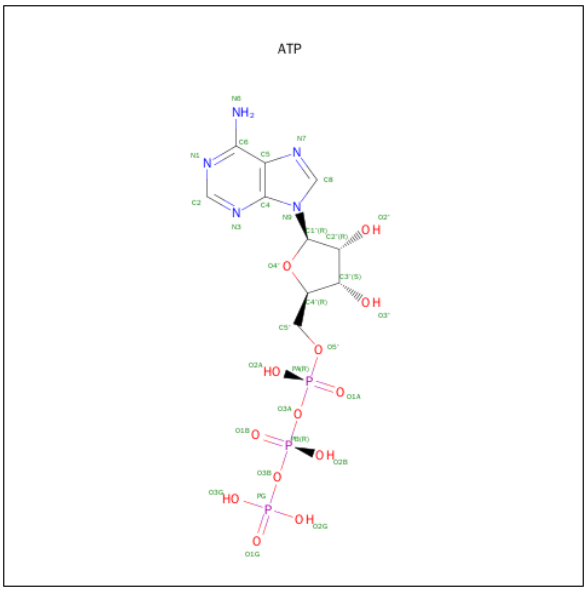
There are 2 discrepancies between the modelled and reference sequences:

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: $C_{10}H_{16}N_5O_{13}P_3$).



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

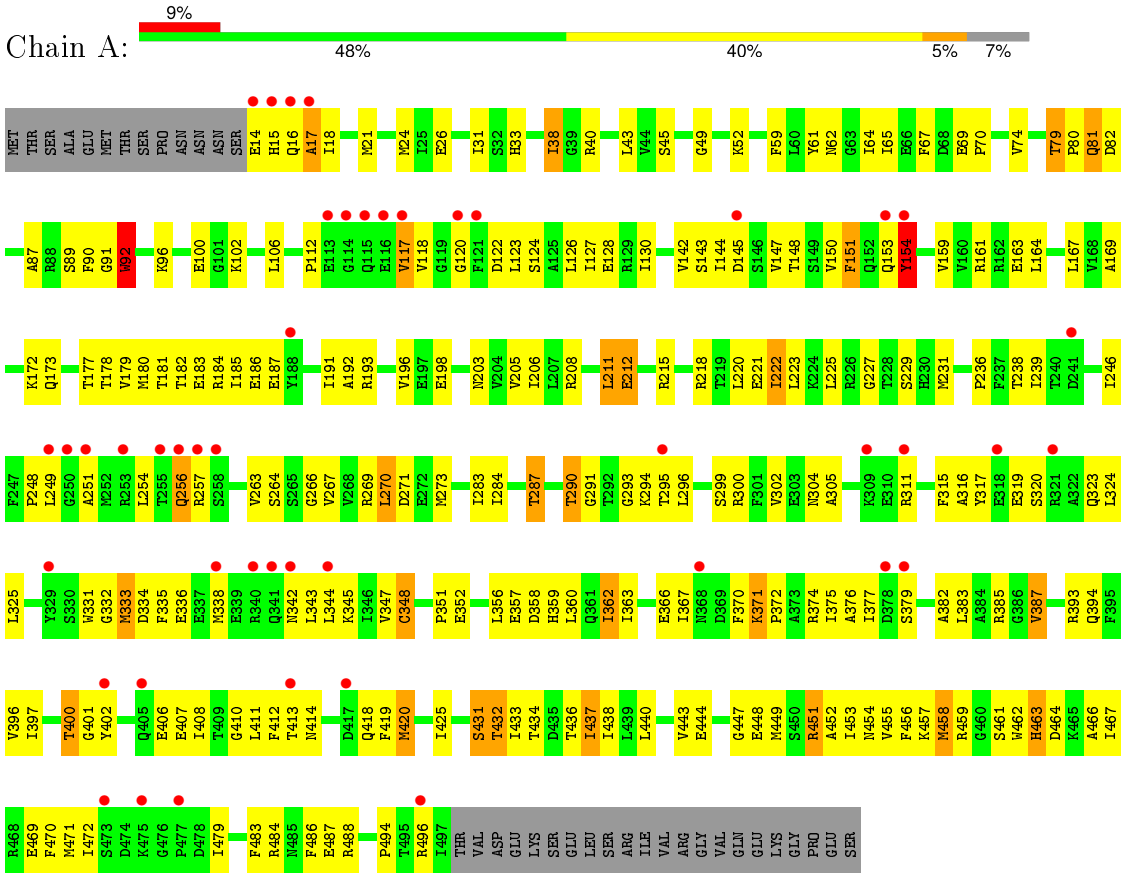
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	5	Total	O	0	0
			5	5		
5	C	7	Total	O	0	0
			7	7		
5	D	13	Total	O	0	0
			13	13		
5	E	10	Total	O	0	0
			10	10		
5	F	24	Total	O	0	0
			24	24		

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 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.

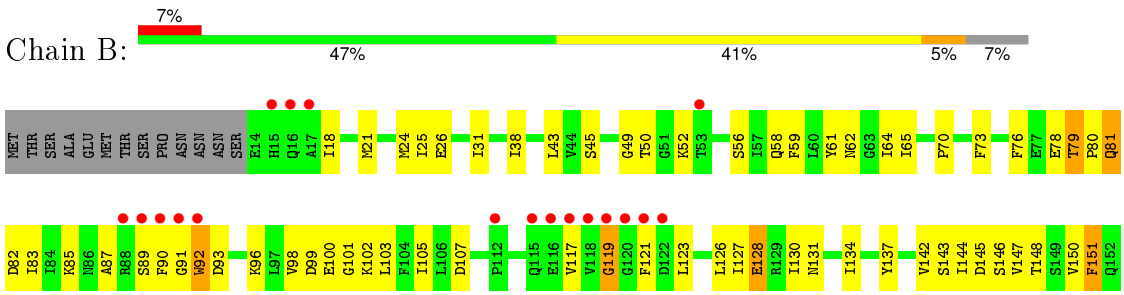
- Molecule 1: KaiC

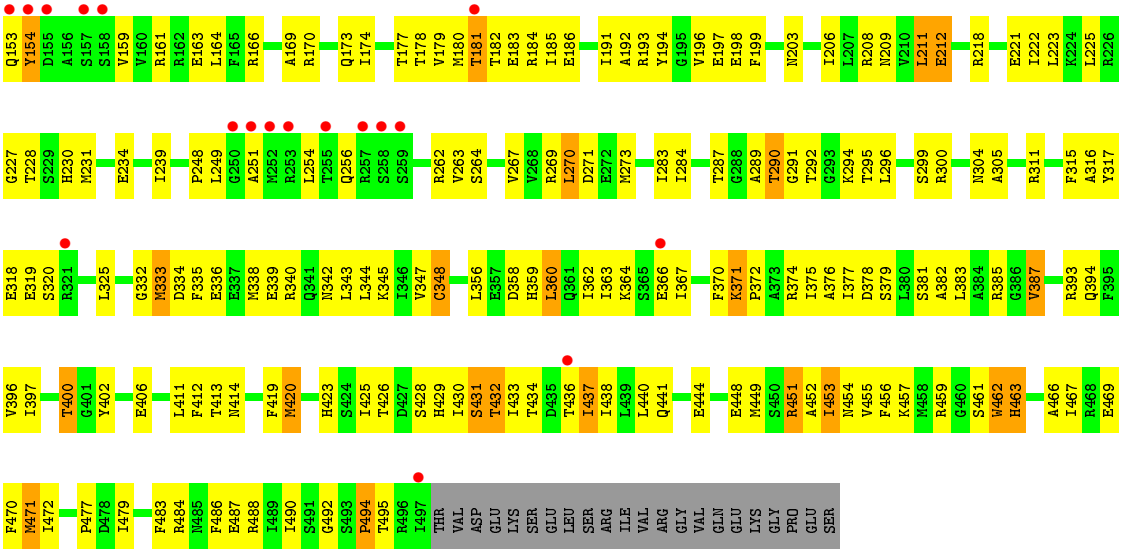
Chain A:



- Molecule 1: KaiC

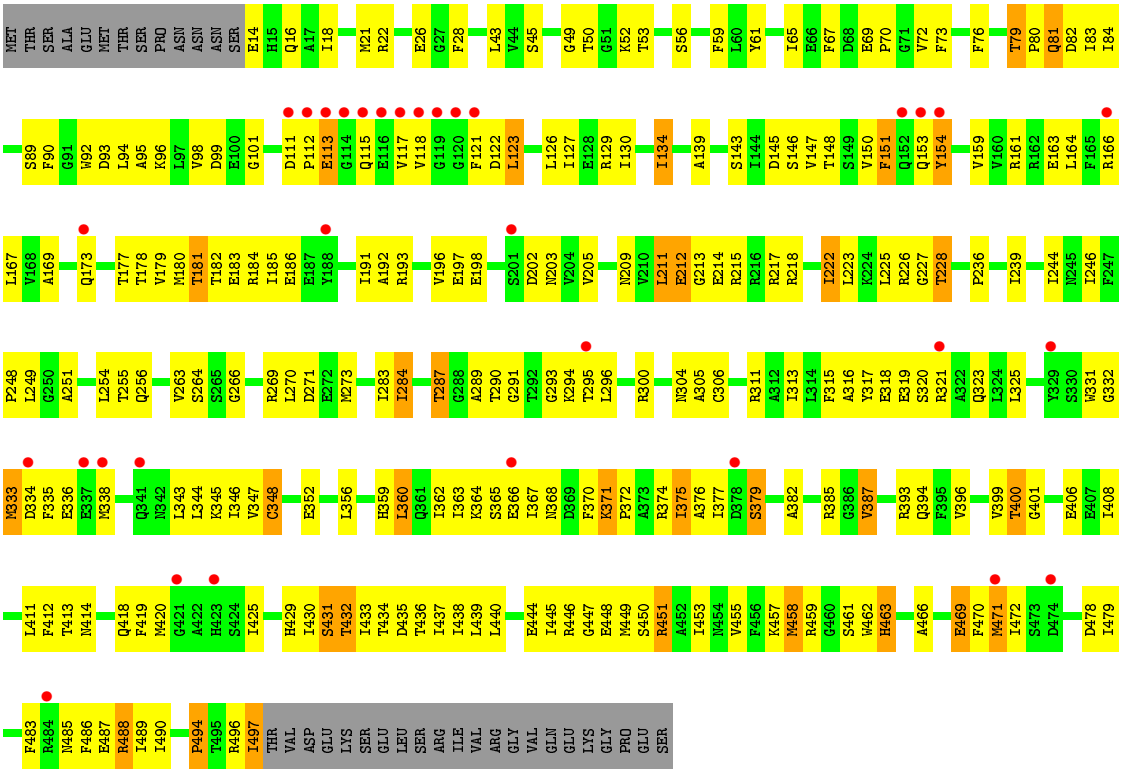
Chain B:





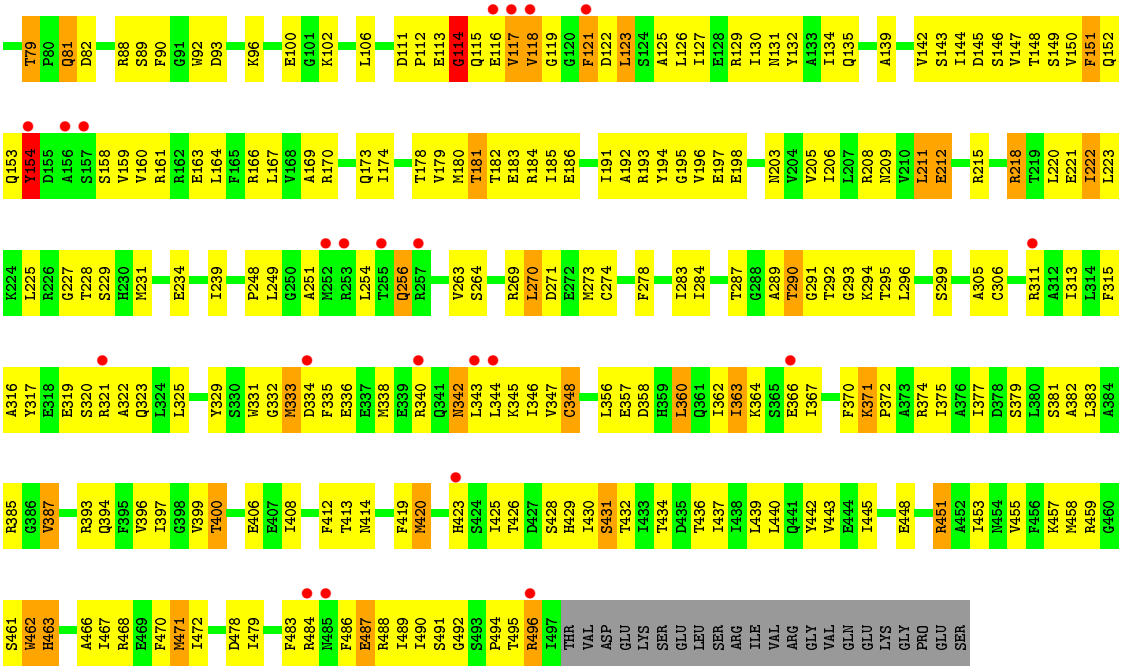
- Molecule 1: KaiC

Chain E:



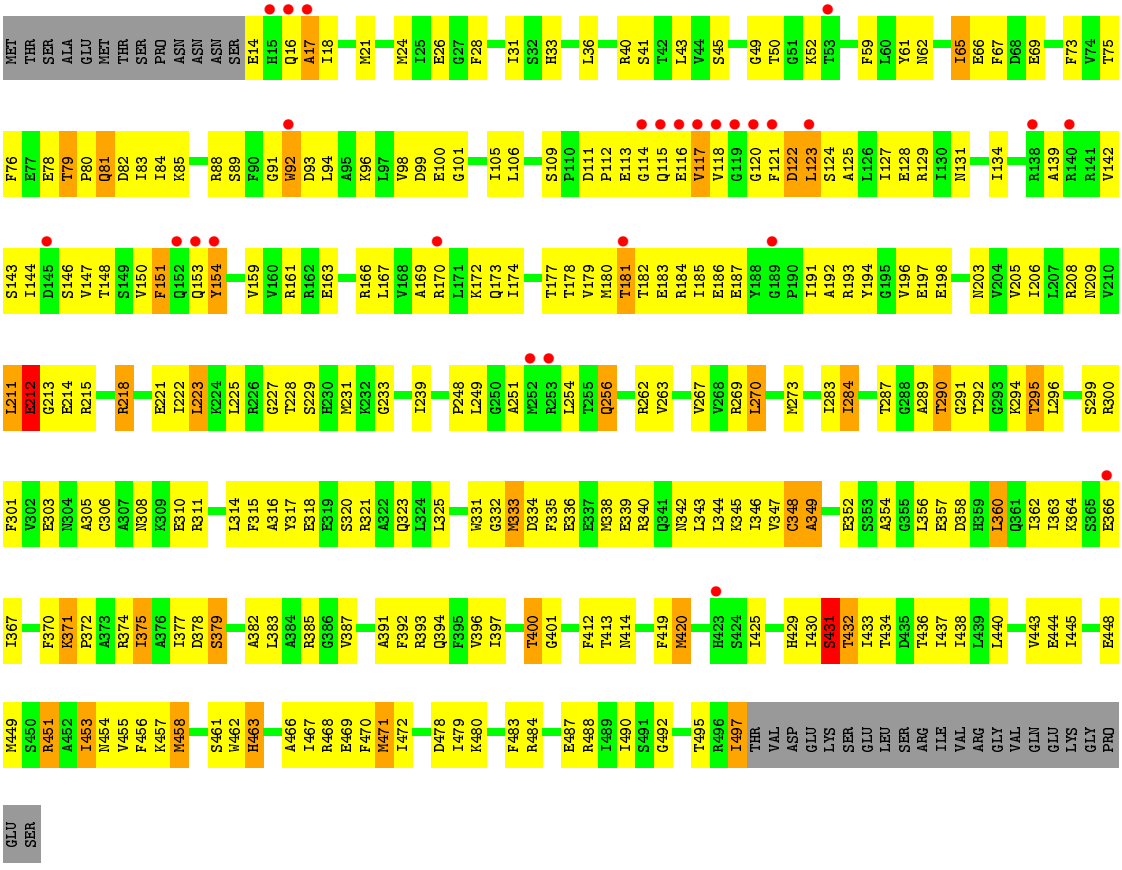
- Molecule 1: KaiC

Chain F:



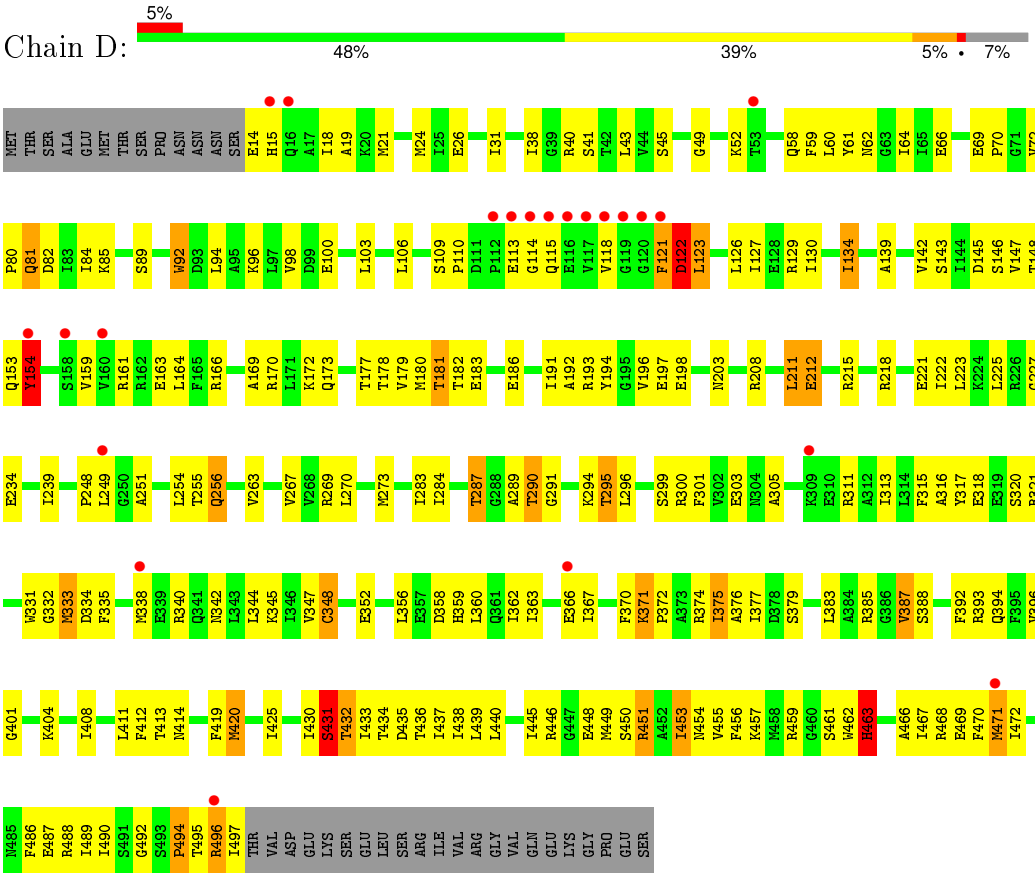
• Molecule 2: KaiC

Chain C:



• Molecule 2: KaiC

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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)	(Not available) (30.00-2.80) 89.7 (29.73-2.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.290 0.253 , 0.285	Depositor DCC
R_{free} test set	4041 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.8	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 87615 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23375	wwPDB-VP
Average B, all atoms (Å^2)	75.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.48	3/3866 (0.1%)	0.65	3/5208 (0.1%)
1	B	0.39	0/3866	0.62	0/5208
1	E	0.42	0/3866	0.65	1/5208 (0.0%)
1	F	0.40	0/3866	0.64	1/5208 (0.0%)
2	C	0.42	2/3872 (0.1%)	0.64	3/5216 (0.1%)
2	D	0.43	1/3872 (0.0%)	0.67	3/5216 (0.1%)
All	All	0.43	6/23208 (0.0%)	0.65	11/31264 (0.0%)

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	2
1	E	0	2
1	F	0	1
2	C	0	2
2	D	0	2
All	All	0	11

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	TRP	CB-CG	12.20	1.72	1.50
1	A	92	TRP	CA-CB	9.80	1.75	1.53
1	A	92	TRP	CG-CD2	-6.71	1.32	1.43
2	C	92	TRP	CG-CD1	-6.26	1.27	1.36
2	C	92	TRP	CA-CB	-5.38	1.42	1.53

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	92	TRP	CA-CB-CG	8.38	129.62	113.70
2	C	213	GLY	N-CA-C	-6.51	96.83	113.10
1	A	92	TRP	CB-CG-CD1	6.44	135.38	127.00
1	E	213	GLY	N-CA-C	-6.33	97.27	113.10
2	D	92	TRP	CB-CG-CD1	5.86	134.62	127.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	SEP	Mainchain
1	A	432	TPO	Mainchain
1	B	431	SEP	Mainchain
1	B	432	TPO	Mainchain
2	C	431	SER	Mainchain

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	3823	0	3811	283	1
1	B	3823	0	3812	296	1
1	E	3823	0	3811	294	0
1	F	3823	0	3810	347	0
2	C	3819	0	3813	305	0
2	D	3819	0	3813	320	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	8	0
4	B	62	0	24	8	0
4	C	62	0	24	12	0
4	D	62	0	24	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	62	0	24	8	0
4	F	62	0	24	7	0
5	A	8	0	0	0	0
5	B	5	0	0	0	0
5	C	7	0	0	2	0
5	D	13	0	0	1	0
5	E	10	0	0	2	0
5	F	24	0	0	5	0
All	All	23375	0	23014	1719	1

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 37.

The worst 5 of 1719 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TRP:CB	1:A:92:TRP:CA	1.75	1.60
1:E:429:HIS:HA	1:E:431:SEP:O1P	1.46	1.14
1:B:431:SEP:H	1:B:431:SEP:P	1.69	1.14
1:F:313:ILE:HB	1:F:375:ILE:CD1	1.78	1.14
1:B:284:ILE:HD12	1:B:436:THR:HB	1.31	1.13

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:NH1	1:B:137:TYR:OH[3_755]	2.15	0.05

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	480/519 (92%)	438 (91%)	31 (6%)	11 (2%)	8 26
1	B	480/519 (92%)	430 (90%)	41 (8%)	9 (2%)	10 32
1	E	480/519 (92%)	434 (90%)	31 (6%)	15 (3%)	5 17
1	F	480/519 (92%)	436 (91%)	34 (7%)	10 (2%)	9 29
2	C	481/519 (93%)	431 (90%)	35 (7%)	15 (3%)	5 17
2	D	481/519 (93%)	437 (91%)	32 (7%)	12 (2%)	7 24
All	All	2882/3114 (92%)	2606 (90%)	204 (7%)	72 (2%)	7 24

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	117	VAL
1	A	154	TYR
1	A	211	LEU
1	A	333	MET

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	410/442 (93%)	383 (93%)	27 (7%)	21 51
1	B	410/442 (93%)	388 (95%)	22 (5%)	27 60
1	E	410/442 (93%)	384 (94%)	26 (6%)	22 53
1	F	410/442 (93%)	380 (93%)	30 (7%)	17 44
2	C	411/443 (93%)	385 (94%)	26 (6%)	22 53
2	D	411/443 (93%)	382 (93%)	29 (7%)	18 46
All	All	2462/2654 (93%)	2302 (94%)	160 (6%)	21 52

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	458	MET

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Mol	Chain	Res	Type
2	D	270	LEU
1	F	290	THR
2	C	497	ILE
2	D	134	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	414	ASN
2	D	368	ASN
1	F	209	ASN
2	D	81	GLN
2	D	414	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1.69	1 (12%)	8,12,14	1.39	1 (12%)
1	TPO	A	432	1	8,10,11	0.89	0	7,14,16	1.32	1 (14%)
1	SEP	B	431	1	8,9,10	1.83	2 (25%)	8,12,14	1.82	2 (25%)
1	TPO	B	432	1	8,10,11	1.04	0	7,14,16	1.27	1 (14%)
2	TPO	C	432	2	8,10,11	3.37	4 (50%)	7,14,16	4.35	3 (42%)
2	TPO	D	432	2	8,10,11	3.46	2 (25%)	7,14,16	3.82	3 (42%)
1	SEP	E	431	1	8,9,10	2.38	3 (37%)	8,12,14	1.99	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	TPO	E	432	1	8,10,11	1.30	2 (25%)	7,14,16	2.20	2 (28%)
1	SEP	F	431	1	8,9,10	1.00	0	8,12,14	1.32	2 (25%)
1	TPO	F	432	1	8,10,11	3.53	2 (25%)	7,14,16	1.06	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
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 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	432	TPO	CB-CA	-7.31	1.40	1.54
1	F	432	TPO	CG2-CB	-6.32	1.36	1.51
2	C	432	TPO	CG2-CB	-2.45	1.45	1.51
1	E	432	TPO	CB-CA	-2.05	1.50	1.54
2	C	432	TPO	O-C	2.09	1.29	1.19

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	432	TPO	C-CA-N	-8.51	92.05	109.83
2	D	432	TPO	C-CA-N	-8.20	92.69	109.83
2	C	432	TPO	O-C-CA	-6.88	107.28	125.44
2	D	432	TPO	O-C-CA	-4.87	112.58	125.44
1	E	432	TPO	O-C-CA	-4.45	113.69	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	431	SEP	2	0
1	A	432	TPO	2	0
1	B	431	SEP	13	0
1	B	432	TPO	2	0
2	C	432	TPO	5	0
2	D	432	TPO	3	0
1	E	431	SEP	4	0
1	E	432	TPO	2	0
1	F	431	SEP	5	0
1	F	432	TPO	2	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	521	3	24,33,33	1.33	4 (16%)	31,52,52	2.85	10 (32%)
4	ATP	A	522	-	24,33,33	1.29	3 (12%)	31,52,52	2.58	6 (19%)
4	ATP	B	521	3	24,33,33	1.34	3 (12%)	31,52,52	2.88	8 (25%)
4	ATP	B	522	-	24,33,33	1.29	3 (12%)	31,52,52	2.59	6 (19%)
4	ATP	C	521	3	24,33,33	1.37	4 (16%)	31,52,52	2.80	7 (22%)
4	ATP	C	522	-	24,33,33	1.11	1 (4%)	31,52,52	2.60	5 (16%)
4	ATP	D	521	3	24,33,33	1.38	4 (16%)	31,52,52	2.85	7 (22%)
4	ATP	D	522	-	24,33,33	1.27	2 (8%)	31,52,52	2.66	5 (16%)
4	ATP	E	601	3	24,33,33	1.36	4 (16%)	31,52,52	2.86	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ATP	E	603	-	24,33,33	1.17	1 (4%)	31,52,52	2.60	5 (16%)
4	ATP	F	701	3	24,33,33	1.37	3 (12%)	31,52,52	2.84	9 (29%)
4	ATP	F	703	-	24,33,33	1.25	2 (8%)	31,52,52	2.58	5 (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	521	3	-	0/18/38/38	0/3/3/3
4	ATP	A	522	-	-	0/18/38/38	0/3/3/3
4	ATP	B	521	3	-	0/18/38/38	0/3/3/3
4	ATP	B	522	-	-	0/18/38/38	0/3/3/3
4	ATP	C	521	3	-	0/18/38/38	0/3/3/3
4	ATP	C	522	-	-	0/18/38/38	0/3/3/3
4	ATP	D	521	3	-	0/18/38/38	0/3/3/3
4	ATP	D	522	-	-	0/18/38/38	0/3/3/3
4	ATP	E	601	3	-	0/18/38/38	0/3/3/3
4	ATP	E	603	-	-	0/18/38/38	0/3/3/3
4	ATP	F	701	3	-	0/18/38/38	0/3/3/3
4	ATP	F	703	-	-	0/18/38/38	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	521	ATP	O2'-C2'	-2.42	1.37	1.43
4	E	601	ATP	O2'-C2'	-2.16	1.37	1.43
4	D	522	ATP	O4'-C4'	-2.10	1.40	1.45
4	C	521	ATP	O2'-C2'	-2.04	1.38	1.43
4	A	521	ATP	O2'-C2'	-2.00	1.38	1.43

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	521	ATP	N3-C2-N1	-11.80	119.86	128.89
4	D	522	ATP	N3-C2-N1	-11.64	119.98	128.89
4	C	522	ATP	N3-C2-N1	-11.59	120.02	128.89
4	E	601	ATP	N3-C2-N1	-11.59	120.02	128.89
4	A	521	ATP	N3-C2-N1	-11.52	120.07	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	521	ATP	5	0
4	A	522	ATP	3	0
4	B	521	ATP	4	0
4	B	522	ATP	4	0
4	C	521	ATP	8	0
4	C	522	ATP	4	0
4	D	521	ATP	8	0
4	D	522	ATP	3	0
4	E	601	ATP	4	0
4	E	603	ATP	4	0
4	F	701	ATP	4	0
4	F	703	ATP	3	0

5.7 Other polymers

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, 95^{th} 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	482/519 (92%)	0.37	46 (9%)	10	5	32, 78, 130, 157	0
1	B	482/519 (92%)	0.46	36 (7%)	17	9	43, 85, 131, 163	0
1	E	482/519 (92%)	0.03	32 (6%)	22	13	23, 62, 109, 158	0
1	F	482/519 (92%)	0.12	22 (4%)	36	25	23, 71, 117, 161	0
2	C	483/519 (93%)	0.23	27 (5%)	28	18	36, 75, 126, 163	0
2	D	483/519 (93%)	0.03	24 (4%)	32	21	29, 60, 112, 163	0
All	All	2894/3114 (92%)	0.21	187 (6%)	22	13	23, 73, 124, 163	0

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	118	VAL	10.2
1	B	118	VAL	8.9
1	B	116	GLU	8.3
1	B	117	VAL	7.3
1	A	121	PHE	7.3

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^{th} 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^2)	Q<0.9
1	TPO	B	432	11/12	0.69	0.40	-	5,21,85,86	0
2	TPO	D	432	11/12	0.65	0.39	-	5,11,63,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	TPO	F	432	11/12	0.59	0.43	-	5,12,77,78	0
1	TPO	A	432	11/12	0.67	0.43	-	5,21,84,85	0
2	TPO	C	432	11/12	0.68	0.41	-	5,12,80,81	0
1	TPO	E	432	11/12	0.72	0.34	-	5,12,61,63	0
1	SEP	E	431	10/11	0.57	0.41	-	6,59,62,63	0
1	SEP	F	431	10/11	0.65	0.42	-	6,82,85,85	0
1	SEP	A	431	10/11	0.68	0.41	-	6,81,83,86	0
1	SEP	B	431	10/11	0.65	0.43	-	6,84,89,90	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^{th} 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^2)	Q<0.9
3	MG	B	520	1/1	0.61	0.36	2.86	75,75,75,75	0
4	ATP	D	522	31/31	0.89	0.28	1.86	44,56,79,83	0
4	ATP	F	703	31/31	0.90	0.23	1.27	44,56,78,82	0
4	ATP	E	603	31/31	0.94	0.24	1.21	44,56,78,82	0
4	ATP	F	701	31/31	0.85	0.28	1.02	76,92,116,123	0
4	ATP	D	521	31/31	0.93	0.25	0.90	55,68,91,106	0
4	ATP	B	521	31/31	0.90	0.23	0.72	64,75,111,118	0
4	ATP	A	522	31/31	0.84	0.25	0.52	44,56,78,83	0
4	ATP	C	521	31/31	0.92	0.19	0.32	50,57,99,112	0
4	ATP	C	522	31/31	0.88	0.24	0.28	45,56,79,83	0
4	ATP	A	521	31/31	0.86	0.28	0.12	77,91,105,114	0
4	ATP	E	601	31/31	0.90	0.24	-0.00	63,79,103,115	0
4	ATP	B	522	31/31	0.84	0.22	-0.09	45,56,79,83	0
3	MG	F	520	1/1	0.52	0.31	-	21,21,21,21	0
3	MG	D	520	1/1	0.68	0.24	-	21,21,21,21	0
3	MG	C	520	1/1	0.97	0.10	-	21,21,21,21	0
3	MG	A	520	1/1	0.86	0.15	-	21,21,21,21	0
3	MG	E	520	1/1	0.77	0.22	-	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.