



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:15 AM GMT

PDB ID : 3DVL  
Title : Crystal Structure of Full Length Circadian Clock Protein KaiC with Correct Geometry at Phosphorylation Sites  
Authors : Pattanayek, R.; Egli, M.  
Deposited on : 2008-07-18  
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.

---

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

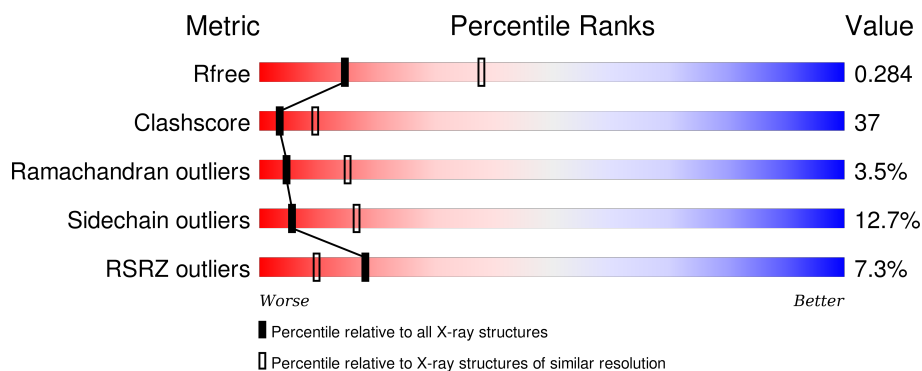
# 1 Overall quality at a glance ⓘ

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>42%</div> <div>10%</div> <div>• •</div> </div>
1	B	519	<div> <div>8%</div> <div>43%</div> <div>41%</div> <div>9%</div> <div>• 5%</div> </div>
1	C	519	<div> <div>5%</div> <div>47%</div> <div>36%</div> <div>11%</div> <div>• 6%</div> </div>
1	D	519	<div> <div>4%</div> <div>48%</div> <div>37%</div> <div>7%</div> <div>• 7%</div> </div>
1	E	519	<div> <div>6%</div> <div>46%</div> <div>38%</div> <div>11%</div> <div>5%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	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	TPO	A	432	-	-	X	-
1	SEP	B	431	-	-	X	-
1	TPO	B	432	X	-	X	-
1	SEP	C	431	-	-	X	-
1	TPO	D	432	X	-	-	-
1	TPO	E	432	X	-	-	-
1	TPO	F	432	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23870 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.

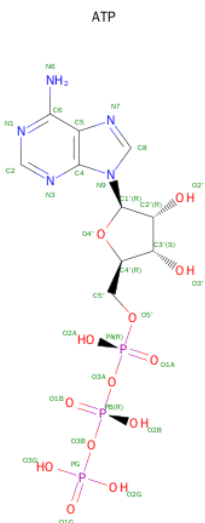
- Molecule 1 is a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3993	2509	701	766	2	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3878	2439	678	744	2	15			
1	C	488	Total	C	N	O	P	S	0	0	0
			3850	2425	674	735	1	15			
1	D	485	Total	C	N	O	P	S	0	0	0
			3826	2411	671	728	1	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
			3993	2509	701	766	2	15			

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

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

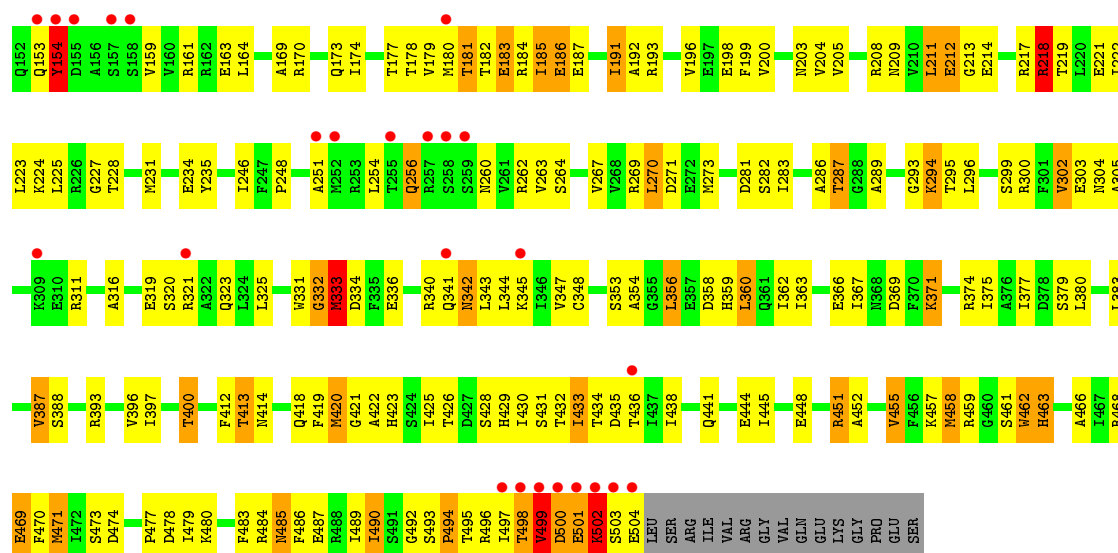
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



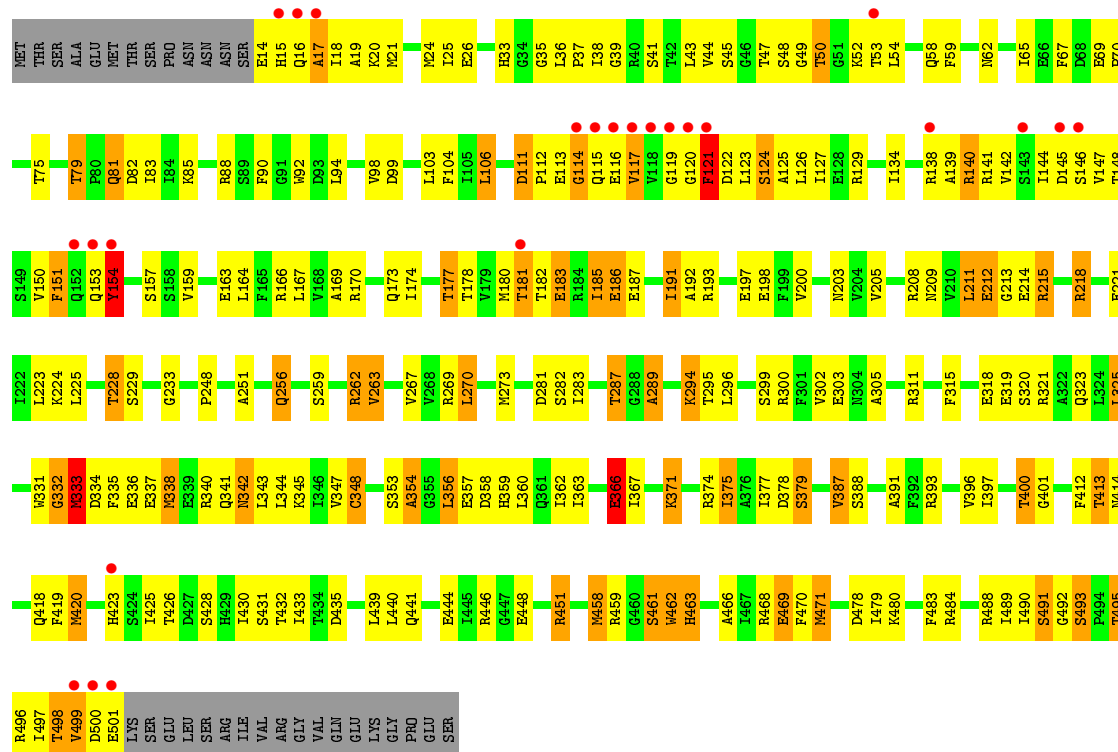
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	5	Total 5	O 5	0	0
4	C	7	Total 7	O 7	0	0
4	D	12	Total 12	O 12	0	0
4	E	10	Total 10	O 10	0	0
4	F	25	Total 25	O 25	0	0





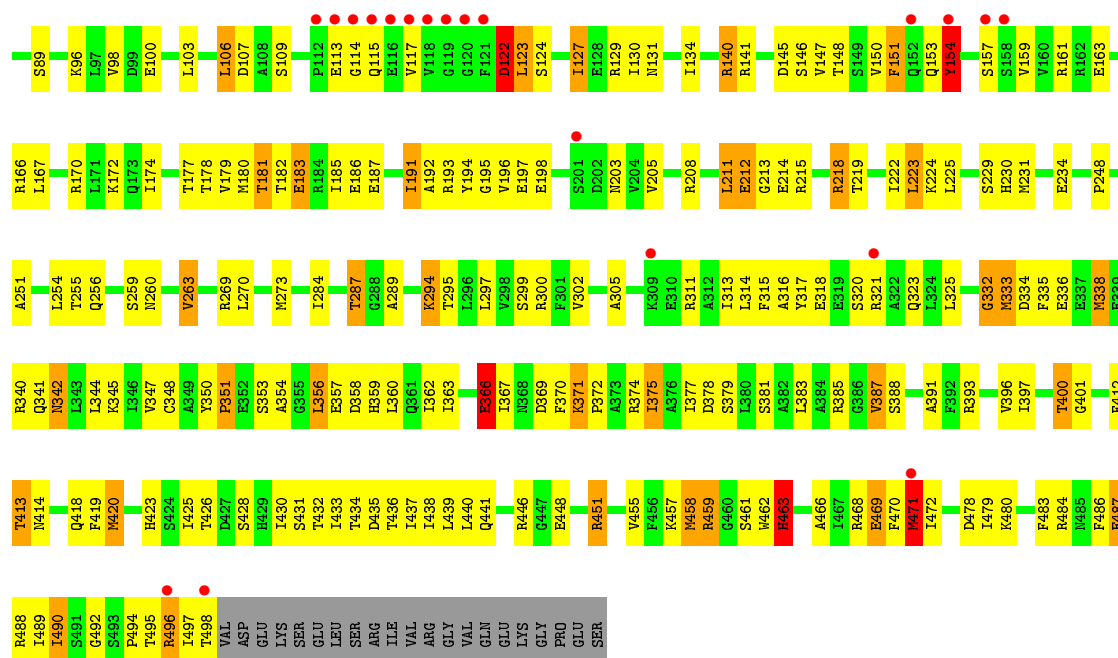
• Molecule 1: Circadian clock protein kinase kaiC



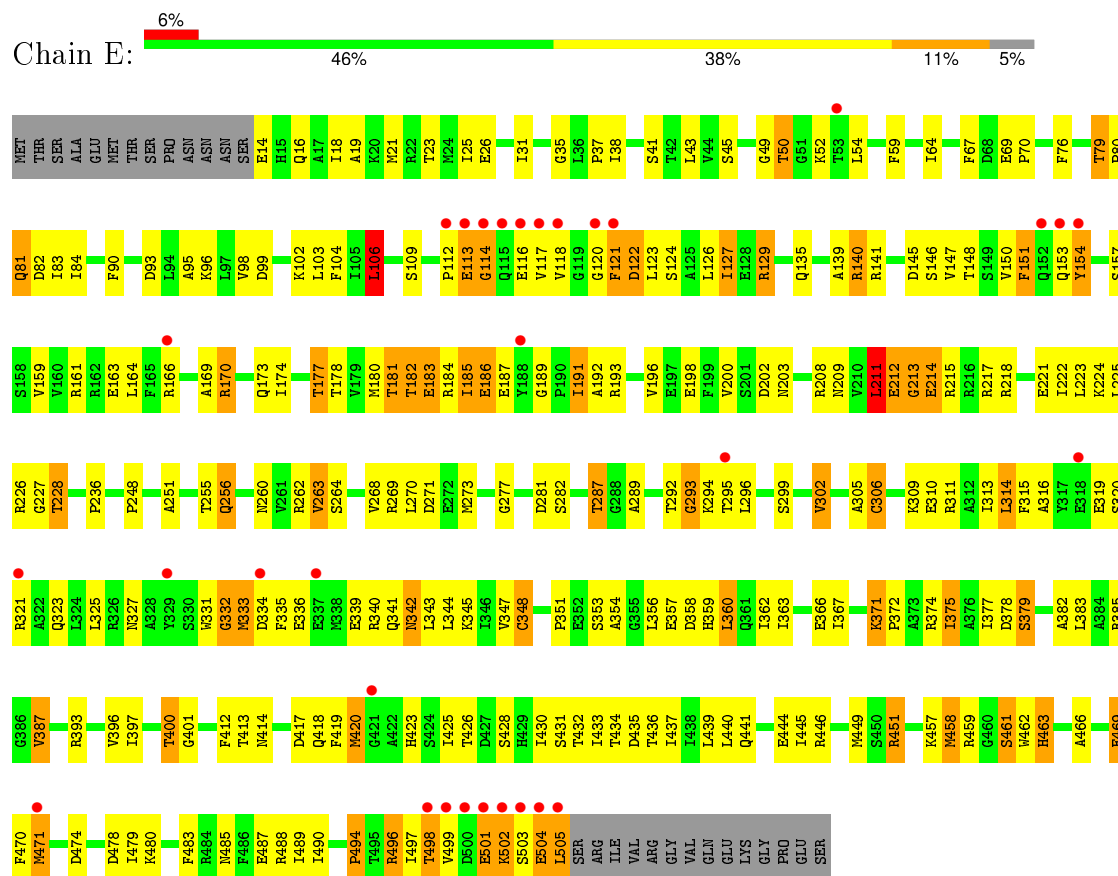
• Molecule 1: Circadian clock protein kinase kaiC







• Molecule 1: Circadian clock protein kinase kaiC



• Molecule 1: Circadian clock protein kinase kaiC



I467	S388	S320	T238	F165	I97	MET
R468		R321	I239	R166	V98	THR
E469	R393	A322		L167	E100	SER
F470		Q323	P248	V168		ALA
M471	V396	L324		A169		GLU
	I397	L325	A251	R170	L103	MET
D478	G398		R252	L171	F104	THR
I479	V399		R253	K172	T105	SER
K480	T400	W331	L254	Q173	L106	PRO
		T255	Q256	I174		ASN
F483	E406	G332	R257	T178	D111	ASN
R484	E407	M333		V179	P112	SER
M485	I408	D334		M180	E113	
F486		F335	N260	G114	G115	E14
	F412	E336		Q116		
I489	T413	E337	V263			
I490	M414	M338	T263	T182	V117	A19
		E339	S264	E183	V118	K20
S491	F419	R340	S265	R184	G119	M21
G492	M420	Q341	G266	I185	G120	R22
S493		M342		E186	F121	
P494		L343	R269	E187		
T495	H423	L344	L270		D122	T23
R496	S424	K345	M273	I191	L123	M24
I497	I425	I346	C274	A192	S124	
T498	T426	V347		R193	A125	E26
V499	D427	C348	F278	V196	L126	
D500	S428	A349		E197	I127	T31
E501	I430	Y350	I283	E198	E128	S32
K502	S431			F199	R129	R53
S503	T432	S353	T287	V200	I130	I38
E504	I433	A354	G288		M131	G39
L505	T434	G355	A289	N203	Y132	
S506	D435	L356				
R507	T436	E357	T292	R208	Y137	T42
I508	I437	D358	G293	N209	R138	L43
Y509	I438	H359	K294	V210	A139	V44
R510	L439	L360	T295	L211	R140	S45
G511	L440	Q361	L296	E212	R141	G46
V512		L362		G213		
Q513	V443	L363	S299	E214	I144	G49
E514	E444	E366	R300		D145	T50
K515	I445		F301	R217	S146	G51
G516	R446	L367	V302	R218	V147	K52
P517	G447		E303	T219	T148	T53
E518	E448	R371	A305	L220	S149	
S519		P372	C306	E221	V150	M62
		R374	A307	I222	F151	
	R451	L375	N308	L223	Q152	I65
	A452	A376		K224	Q153	
	V455	I377	R311	L225	V154	F76
	F456	D378	A312		D155	
	K457	S379	I313	S229	A156	T79
	M458	L380	F315	H230	S157	P80
	R459	S381	L314	M231	S158	Q81
	G460	L382	A316	E234	V159	D82
	S461	L383	Y317	T235	Y160	I83
	M462		E318	P236	R161	
	H463	V387	E319	L164	E162	D83
					E163	
					L164	K96

## 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)	89.6 (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, $R_{free}$	0.239 , 0.288 0.237 , 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 , 58.9	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	23870	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

### 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	0.96	3/4037 (0.1%)	1.00	3/5437 (0.1%)
1	B	0.83	2/3921 (0.1%)	0.95	5/5282 (0.1%)
1	C	0.87	2/3897 (0.1%)	0.95	2/5251 (0.0%)
1	D	1.00	4/3873 (0.1%)	1.01	2/5218 (0.0%)
1	E	1.01	5/3929 (0.1%)	1.03	5/5293 (0.1%)
1	F	1.00	5/4037 (0.1%)	1.02	4/5437 (0.1%)
All	All	0.95	21/23694 (0.1%)	0.99	21/31918 (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	B	1	0
1	D	1	0
1	E	1	0
1	F	1	0
All	All	4	0

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	366	GLU	CD-OE2	5.99	1.32	1.25
1	B	498	THR	CA-CB	5.92	1.68	1.53
1	F	366	GLU	CD-OE2	5.55	1.31	1.25
1	F	348	CYS	CB-SG	-5.54	1.72	1.81
1	A	366	GLU	CD-OE2	5.54	1.31	1.25

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	214	GLU	N-CA-C	-6.00	94.81	111.00
1	E	114	GLY	N-CA-C	5.96	128.00	113.10
1	A	516	GLY	N-CA-C	-5.92	98.29	113.10
1	B	218	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	116	GLU	N-CA-C	5.84	126.78	111.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	432	TPO	CB
1	D	432	TPO	CB
1	E	432	TPO	CB
1	F	432	TPO	CB

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	3993	0	3984	320	0
1	B	3878	0	3862	300	0
1	C	3850	0	3836	285	0
1	D	3826	0	3818	283	0
1	E	3886	0	3872	307	0
1	F	3993	0	3982	326	0
2	A	1	0	0	0	0
2	B	1	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	62	0	24	11	0
3	B	62	0	24	8	0
3	C	62	0	24	7	0
3	D	62	0	23	6	0
3	E	62	0	24	6	0
3	F	62	0	24	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	7	0	0	0	0
4	B	5	0	0	2	0
4	C	7	0	0	3	0
4	D	12	0	0	2	0
4	E	10	0	0	0	0
4	F	25	0	0	6	0
All	All	23870	0	23497	1727	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 37.

The worst 5 of 1727 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:F:115:GLN:CG	1:F:116:GLU:H	1.13	1.44
1:B:431:SEP:O	1:B:434:THR:HG22	1.38	1.19
1:D:431:SEP:O	1:D:432:TPO:HB	1.40	1.18
1:F:115:GLN:HG2	1:F:116:GLU:N	1.27	1.14
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.07	1.13

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%)	445 (89%)	35 (7%)	22 (4%)	3	10
1	B	487/519 (94%)	430 (88%)	45 (9%)	12 (2%)	7	24
1	C	484/519 (93%)	433 (90%)	32 (7%)	19 (4%)	4	12
1	D	481/519 (93%)	433 (90%)	37 (8%)	11 (2%)	8	26
1	E	488/519 (94%)	416 (85%)	53 (11%)	19 (4%)	4	12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	502/519 (97%)	442 (88%)	39 (8%)	21 (4%)	3	11
All	All	2944/3114 (94%)	2599 (88%)	241 (8%)	104 (4%)	4	15

5 of 104 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%)	372 (86%)	58 (14%)	5	14
1	B	417/442 (94%)	364 (87%)	53 (13%)	5	16
1	C	414/442 (94%)	357 (86%)	57 (14%)	4	13
1	D	411/442 (93%)	358 (87%)	53 (13%)	5	16
1	E	418/442 (95%)	368 (88%)	50 (12%)	6	19
1	F	430/442 (97%)	380 (88%)	50 (12%)	7	20
All	All	2520/2652 (95%)	2199 (87%)	321 (13%)	5	16

5 of 321 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	333	MET
1	D	154	TYR
1	F	287	THR
1	C	360	LEU
1	C	493	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	368	ASN
1	D	209	ASN
1	F	115	GLN
1	C	389	ASN
1	C	441	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	2.03	3 (37%)	8,12,14	3.65	2 (25%)
1	TPO	A	432	1	8,10,11	0.58	0	7,14,16	1.37	1 (14%)
1	SEP	B	431	1	8,9,10	1.92	1 (12%)	8,12,14	2.57	1 (12%)
1	TPO	B	432	1	8,10,11	0.48	0	7,14,16	1.42	1 (14%)
1	SEP	C	431	1	4,5,10	0.76	0	2,5,14	1.80	1 (50%)
1	TPO	C	432	1	8,10,11	1.29	1 (12%)	7,14,16	1.49	1 (14%)
1	SEP	D	431	1	4,5,10	1.52	1 (25%)	2,5,14	0.89	0
1	TPO	D	432	1	8,10,11	1.33	1 (12%)	7,14,16	1.96	3 (42%)
1	SEP	E	431	1	8,9,10	2.38	3 (37%)	8,12,14	2.78	3 (37%)
1	TPO	E	432	1	8,10,11	1.06	0	7,14,16	1.41	2 (28%)
1	SEP	F	431	1	8,9,10	1.92	3 (37%)	8,12,14	1.11	0
1	TPO	F	432	1	8,10,11	3.36	7 (87%)	7,14,16	5.63	4 (57%)

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	1/1/3/4	0/8/11/13	0/0/0/0
1	SEP	C	431	1	-	0/2/4/10	0/0/0/0
1	TPO	C	432	1	-	0/8/11/13	0/0/0/0
1	SEP	D	431	1	-	0/2/4/10	0/0/0/0
1	TPO	D	432	1	1/1/3/4	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	1/1/3/4	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	1/1/3/4	1/8/11/13	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	432	TPO	P-O2P	-6.02	1.33	1.54
1	F	432	TPO	CG2-CB	-3.64	1.42	1.51
1	F	432	TPO	P-O1P	-3.64	1.39	1.51
1	F	432	TPO	P-OG1	-2.81	1.51	1.60
1	F	432	TPO	CB-CA	-2.58	1.49	1.54

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	432	TPO	CG2-CB-CA	-9.27	94.31	113.17
1	A	431	SEP	OG-CB-CA	-7.86	101.57	108.27
1	E	431	SEP	OG-CB-CA	-5.58	103.52	108.27
1	F	432	TPO	OG1-P-O1P	-2.68	100.42	107.11
1	D	432	TPO	CG2-CB-CA	-2.67	107.73	113.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	432	TPO	CB
1	D	432	TPO	CB
1	B	432	TPO	CB
1	F	432	TPO	CB

All (1) torsion outliers are listed below:

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

There are no ring outliers.

11 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	431	SEP	5	0
1	A	432	TPO	6	0
1	B	431	SEP	6	0
1	B	432	TPO	8	0
1	C	431	SEP	4	0
1	C	432	TPO	5	0
1	D	431	SEP	2	0
1	D	432	TPO	3	0
1	E	431	SEP	2	0
1	E	432	TPO	5	0
1	F	431	SEP	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	$\# Z  > 2$
3	ATP	A	901	-	24,33,33	1.49	4 (16%)	31,52,52	2.61	7 (22%)
3	ATP	A	903	-	24,33,33	1.58	5 (20%)	31,52,52	2.62	8 (25%)
3	ATP	B	901	-	24,33,33	1.57	4 (16%)	31,52,52	2.69	7 (22%)
3	ATP	B	903	-	24,33,33	1.77	3 (12%)	31,52,52	2.98	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	C	901	-	24,33,33	1.50	4 (16%)	31,52,52	2.46	6 (19%)
3	ATP	C	903	-	24,33,33	1.31	2 (8%)	31,52,52	2.96	8 (25%)
3	ATP	D	901	-	24,33,33	1.54	4 (16%)	31,52,52	2.71	6 (19%)
3	ATP	D	903	-	24,33,33	1.72	4 (16%)	31,52,52	3.06	9 (29%)
3	ATP	E	901	-	24,33,33	1.56	3 (12%)	31,52,52	2.65	7 (22%)
3	ATP	E	903	-	24,33,33	1.73	8 (33%)	31,52,52	2.69	11 (35%)
3	ATP	F	901	-	24,33,33	1.66	5 (20%)	31,52,52	2.67	9 (29%)
3	ATP	F	903	-	24,33,33	1.52	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
3	ATP	A	901	-	-	0/18/38/38	0/3/3/3
3	ATP	A	903	-	-	0/18/38/38	0/3/3/3
3	ATP	B	901	-	-	0/18/38/38	0/3/3/3
3	ATP	B	903	-	-	0/18/38/38	0/3/3/3
3	ATP	C	901	-	-	0/18/38/38	0/3/3/3
3	ATP	C	903	-	-	0/18/38/38	0/3/3/3
3	ATP	D	901	-	-	0/18/38/38	0/3/3/3
3	ATP	D	903	-	-	0/18/38/38	0/3/3/3
3	ATP	E	901	-	-	0/18/38/38	0/3/3/3
3	ATP	E	903	-	-	0/18/38/38	0/3/3/3
3	ATP	F	901	-	-	0/18/38/38	0/3/3/3
3	ATP	F	903	-	-	0/18/38/38	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	903	ATP	O4'-C4'	-3.80	1.36	1.45
3	C	903	ATP	O4'-C4'	-3.36	1.37	1.45
3	C	901	ATP	PB-O1B	-3.16	1.39	1.51
3	D	903	ATP	PB-O1B	-3.07	1.39	1.51
3	D	903	ATP	PB-O2B	-3.05	1.41	1.54

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	903	ATP	N3-C2-N1	-12.58	119.26	128.89
3	D	901	ATP	N3-C2-N1	-12.34	119.44	128.89
3	B	901	ATP	N3-C2-N1	-12.34	119.45	128.89
3	B	903	ATP	N3-C2-N1	-12.32	119.46	128.89
3	D	903	ATP	N3-C2-N1	-12.21	119.55	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ATP	6	0
3	A	903	ATP	5	0
3	B	901	ATP	5	0
3	B	903	ATP	3	0
3	C	901	ATP	2	0
3	C	903	ATP	5	0
3	D	901	ATP	1	0
3	D	903	ATP	5	0
3	E	901	ATP	3	0
3	E	903	ATP	3	0
3	F	901	ATP	4	0
3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.46	60 (11%) 6 3	29, 76, 127, 154	0
1	B	489/519 (94%)	0.36	41 (8%) 14 6	24, 82, 128, 160	0
1	C	486/519 (93%)	0.11	24 (4%) 33 22	33, 73, 124, 160	0
1	D	483/519 (93%)	-0.09	23 (4%) 34 23	27, 58, 109, 160	0
1	E	490/519 (94%)	-0.01	31 (6%) 23 14	20, 60, 107, 155	0
1	F	504/519 (97%)	0.17	38 (7%) 17 9	20, 69, 114, 158	0
All	All	2956/3114 (94%)	0.17	217 (7%) 18 10	20, 71, 121, 160	0

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	117	VAL	8.6
1	E	505	LEU	8.3
1	D	121	PHE	8.1
1	F	516	GLY	7.9
1	B	117	VAL	7.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	TPO	C	432	11/12	0.65	0.35	-	10,19,77,79	0
1	TPO	A	432	11/12	0.73	0.33	-	19,19,19,19	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	0.75	0.27	-	17,18,22,23	0
1	TPO	D	432	11/12	0.80	0.27	-	19,19,19,19	0
1	SEP	E	431	10/11	0.57	0.37	-	13,56,60,60	0
1	SEP	D	431	6/11	0.79	0.25	-	57,63,68,70	0
1	SEP	C	431	6/11	0.80	0.34	-	75,79,81,84	0
1	SEP	B	431	10/11	0.78	0.29	-	29,81,86,88	0
1	SEP	A	431	10/11	0.78	0.33	-	17,78,80,83	0
1	SEP	F	431	10/11	0.68	0.36	-	13,79,83,83	0
1	TPO	B	432	11/12	0.76	0.31	-	29,29,29,29	0
1	TPO	F	432	11/12	0.79	0.30	-	16,20,74,75	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
2	MG	B	802	1/1	0.79	0.32	1.47	73,73,73,73	0
3	ATP	D	903	31/31	0.94	0.25	1.29	42,53,76,80	0
3	ATP	F	903	31/31	0.94	0.22	1.22	42,53,76,79	0
3	ATP	E	903	31/31	0.96	0.23	1.18	42,53,76,80	0
3	ATP	D	901	31/31	0.95	0.23	0.93	53,65,88,104	0
3	ATP	F	901	31/31	0.88	0.25	0.55	74,89,113,120	0
3	ATP	C	901	31/31	0.95	0.19	0.50	47,55,96,109	0
3	ATP	A	901	31/31	0.84	0.32	0.49	75,88,102,112	0
3	ATP	B	901	31/31	0.92	0.21	0.46	61,73,109,115	0
3	ATP	C	903	31/31	0.91	0.22	0.37	42,54,76,80	0
3	ATP	E	901	31/31	0.89	0.25	0.25	61,76,100,113	0
3	ATP	A	903	31/31	0.88	0.21	0.12	42,54,76,80	0
3	ATP	B	903	31/31	0.87	0.18	-0.61	43,54,76,80	0
2	MG	F	806	1/1	0.97	0.14	-	18,18,18,18	0
2	MG	C	803	1/1	0.90	0.12	-	18,18,18,18	0
2	MG	D	804	1/1	0.93	0.17	-	18,18,18,18	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
2	MG	E	805	1/1	0.86	0.11	-	18,18,18,18	0
2	MG	A	801	1/1	0.97	0.12	-	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.