



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:25 PM GMT

PDB ID : 3K0F
Title : Crystal structure of the phosphorylation-site double mutant T426A/T432A of the KaiC circadian clock protein
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on : 2009-09-24
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

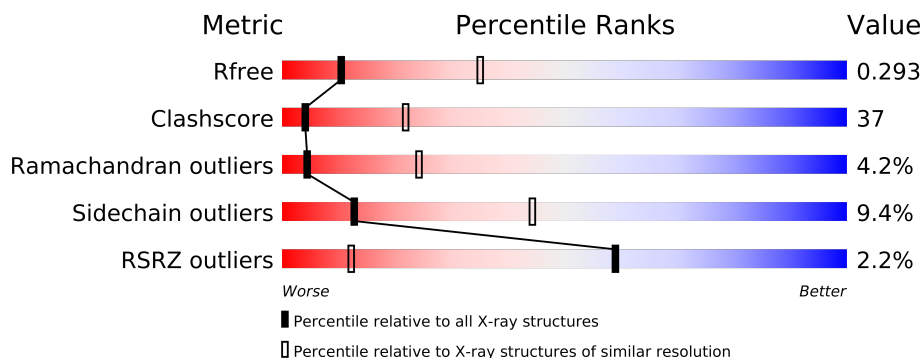
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	519	
2	B	519	
2	C	519	
2	D	519	
2	E	519	
2	F	519	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	B	521	-	X
3	MG	B	802	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	C	522	-	X
3	MG	C	803	-	X
3	MG	D	804	-	X
3	MG	F	806	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23930 atoms, of which 0 are hydrogen and 0 are deuterium.

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	S	0	0	0
			3981	2507	701	758	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	ALA	THR	ENGINEERED	UNP Q79PF4
A	432	ALA	THR	ENGINEERED	UNP Q79PF4

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	491	Total	C	N	O	P	S	0	0	0
			3870	2437	678	739	1	15			
2	C	488	Total	C	N	O	P	S	0	0	0
			3846	2423	674	733	1	15			
2	D	485	Total	C	N	O	P	S	0	0	0
			3822	2409	671	726	1	15			
2	E	492	Total	C	N	O	P	S	0	0	0
			3878	2443	679	740	1	15			
2	F	506	Total	C	N	O	P	S	0	0	0
			3985	2507	701	761	1	15			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	426	ALA	THR	ENGINEERED	UNP Q79PF4
B	432	ALA	THR	ENGINEERED	UNP Q79PF4
C	426	ALA	THR	ENGINEERED	UNP Q79PF4
C	432	ALA	THR	ENGINEERED	UNP Q79PF4
D	426	ALA	THR	ENGINEERED	UNP Q79PF4
D	432	ALA	THR	ENGINEERED	UNP Q79PF4

Continued on next page...

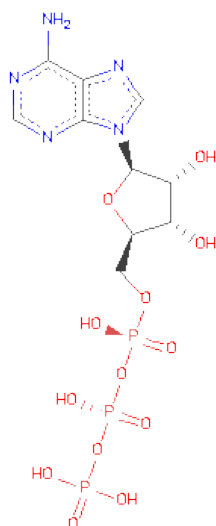
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	426	ALA	THR	ENGINEERED	UNP Q79PF4
E	432	ALA	THR	ENGINEERED	UNP Q79PF4
F	426	ALA	THR	ENGINEERED	UNP Q79PF4
F	432	ALA	THR	ENGINEERED	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	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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		
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.

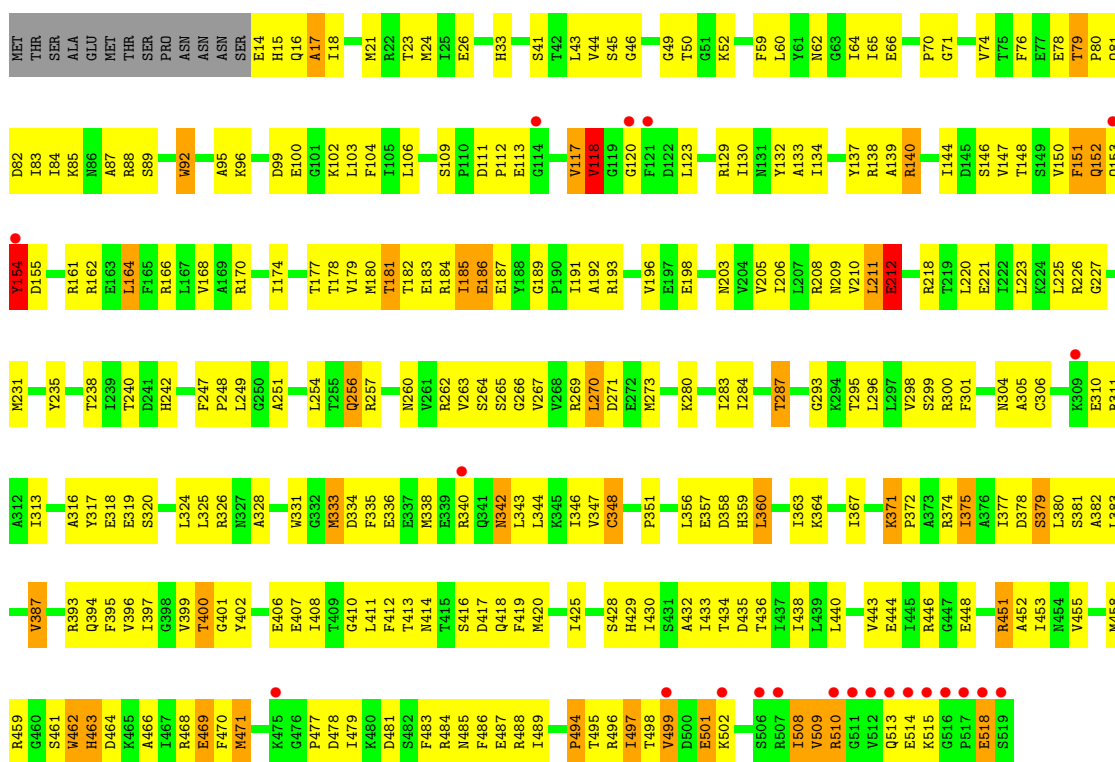
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	12	Total	O	0	0
			12	12		
5	C	23	Total	O	0	0
			23	23		
5	D	37	Total	O	0	0
			37	37		
5	E	34	Total	O	0	0
			34	34		
5	F	40	Total	O	0	0
			40	40		

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.

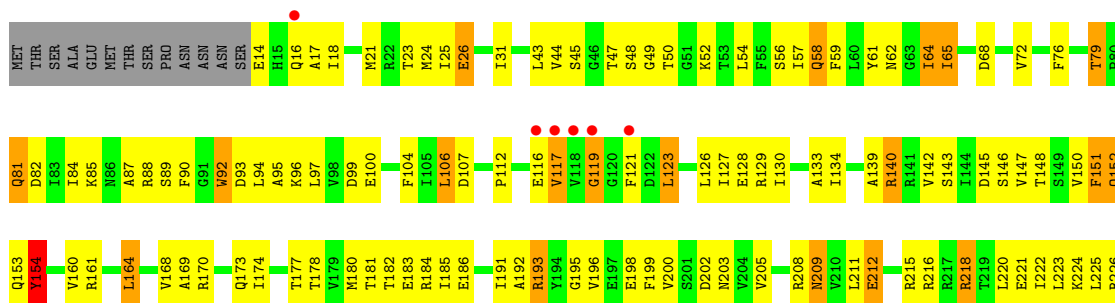
• Molecule 1: Circadian clock protein kinase KaiC

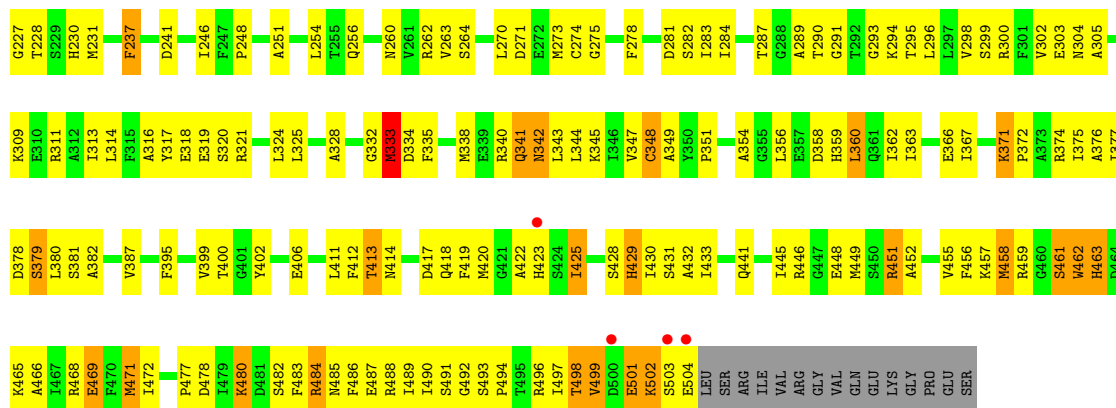
Chain A:



• Molecule 2: Circadian clock protein kinase KaiC

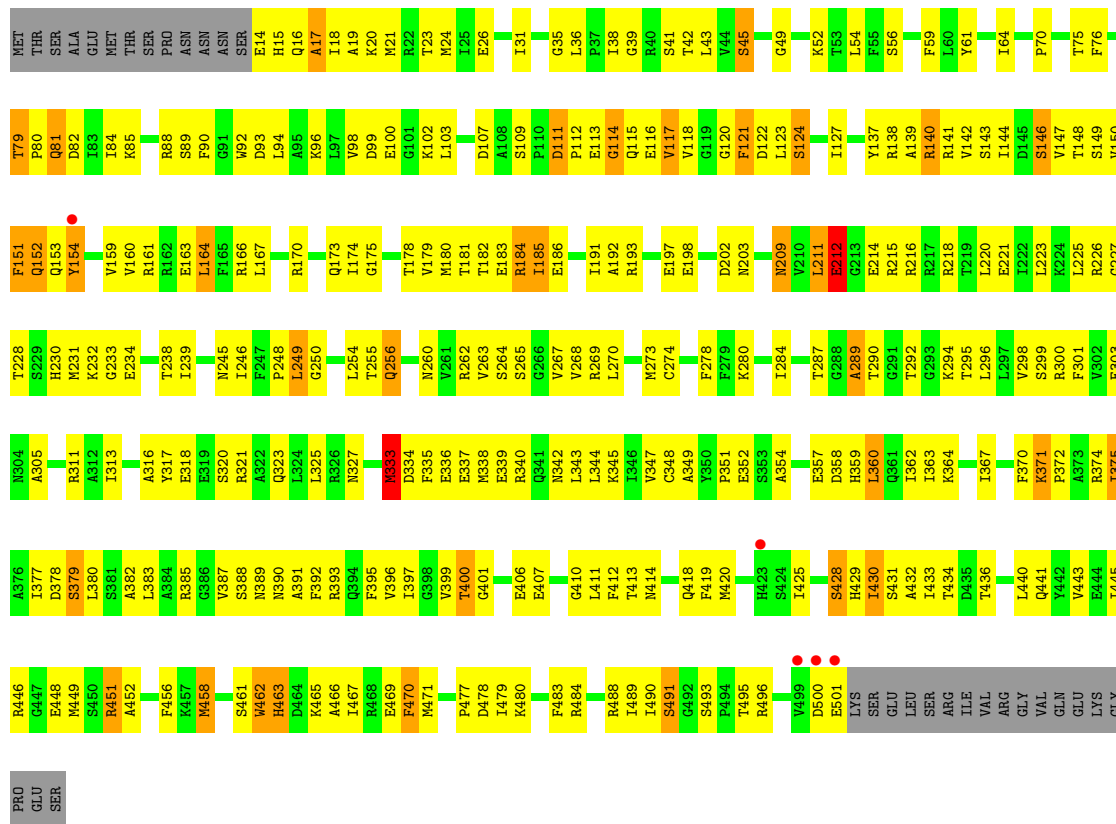
Chain B:





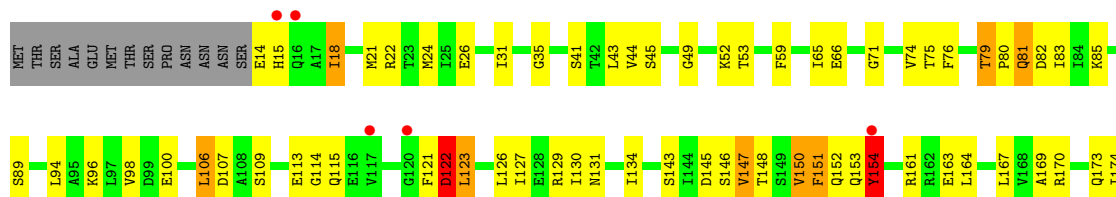
● Molecule 2: Circadian clock protein kinase KaiC

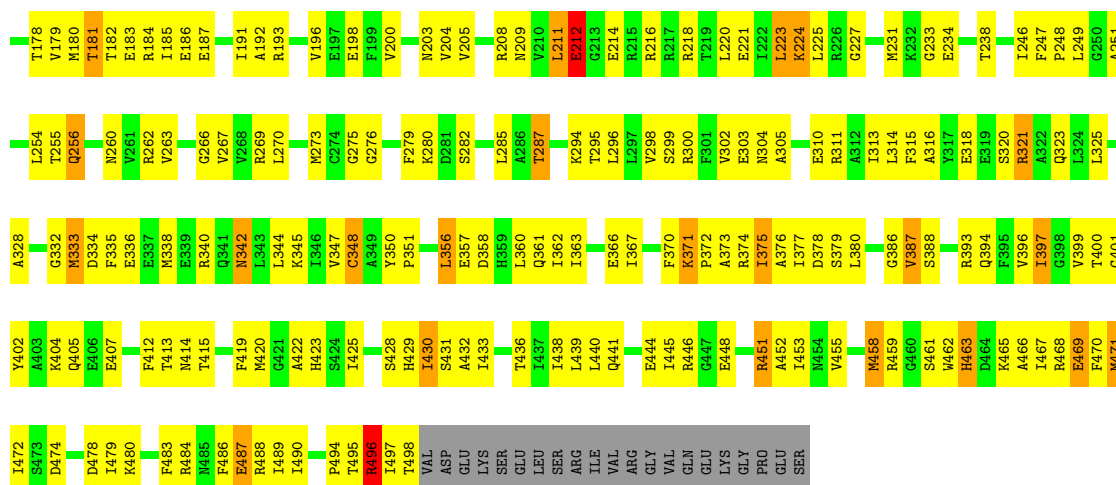
Chain C:



● Molecule 2: Circadian clock protein kinase KaiC

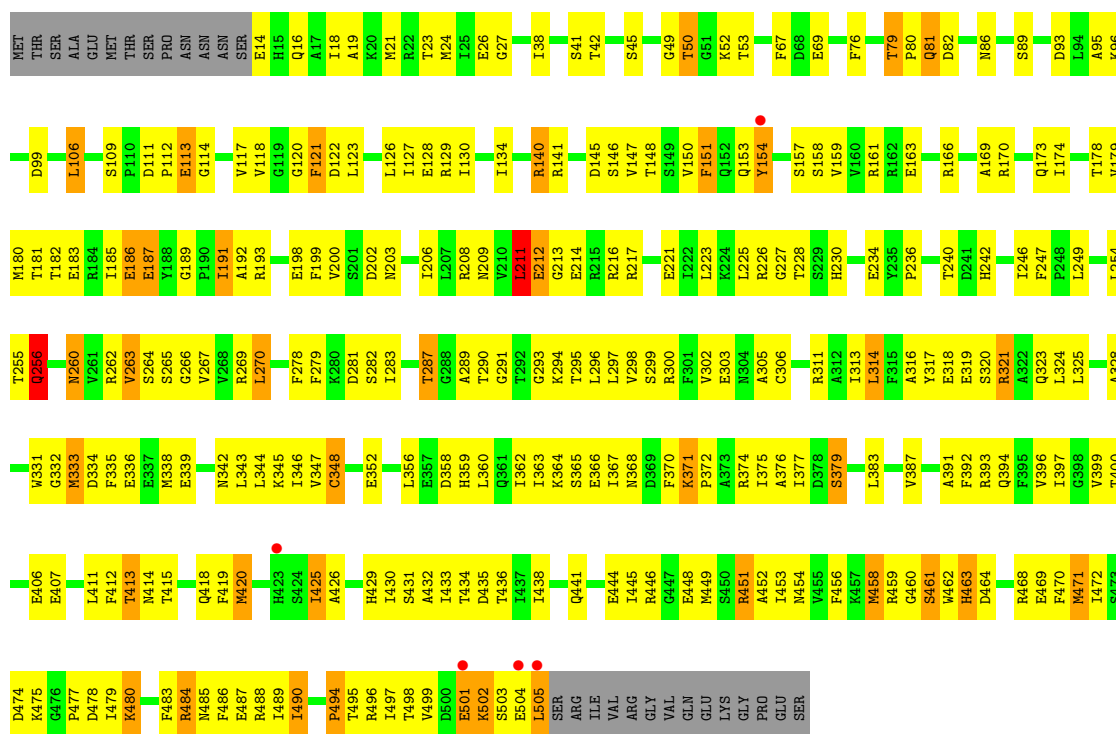
Chain D:





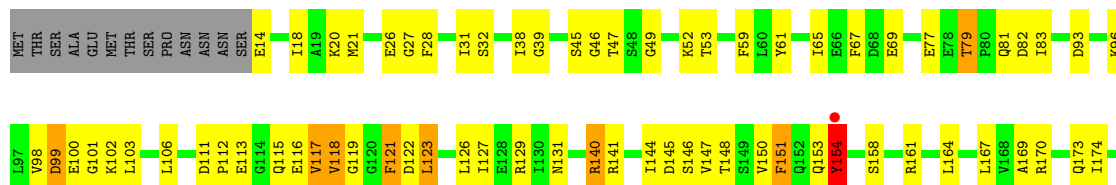
• Molecule 2: Circadian clock protein kinase KaiC

Chain E:



• Molecule 2: Circadian clock protein kinase KaiC

Chain F:



R468	E469	F470	M471	D478	I479	K480	F483	R484	N485	F486	I489	I490	S493	P494	T495	R496	I497	T498	V499	D500	E501	K502	S503	E504	L505	S506	R507	I508	V509	R510	G511	V512	Q513	E514	G515	P516	P517	E518	S519															
Y402	A403	K404	Q405	E406	E407	I408	T409	G410	L411	F412	T413	M414	T415	S416	D417	Q418	F419	M420	H423	S424	I425	A426	H429	I430	S431	A432	I433	T434	D435	T436	I437	L440	D441	V442	V443	E444	I445	R446	C447	E448	R451	A452	V455	F456	K457	M458	R459	G460	S461	M462	H463	A466	I467	
E336	E337	M338	E339	Q341	R340	N342	L343	L344	K345	M273	V347	G348	A349	E352	S353	A354	G355	L356	E357	D358	H359	L360	Q361	I362	I363	E366	I367	K371	P372	A373	R374	I375	A376	I377	D378	S379	L380	S381	A382	L383	A384	R385	G386	V387	S388	A391	F392	R393	V396	I397	G398	V399	T400	G401
R262	V263	S264	V267	V268	R269	L270	D271	E272	M273	C274	G277	F278	F279	K280	I283	I284	T287	G288	A289	G293	K294	T295	V298	S299	R300	F301	V302	E303	N304	A305	C306	E310	R311	A312	I313	L314	F315	A316	Y317	E318	E319	S320	R321	A322	Q323	L324	A251	L254	T255	Q256	V261			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.93Å 135.41Å 205.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 34.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.5 (30.00-3.00) 95.1 (34.88-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.288 0.238 , 0.293	Depositor DCC
R_{free} test set	7200 reflections (10.09%)	DCC
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.0	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74993 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23930	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/4047	0.65	0/5452
2	B	0.36	0/3924	0.63	0/5286
2	C	0.40	0/3900	0.64	0/5255
2	D	0.43	0/3876	0.68	0/5222
2	E	0.43	0/3932	0.68	1/5297 (0.0%)
2	F	0.41	0/4040	0.70	0/5441
All	All	0.40	0/23719	0.66	1/31953 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	213	GLY	N-CA-C	-5.22	100.04	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3981	0	3981	301	0
2	B	3870	0	3858	298	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3846	0	3834	285	0
2	D	3822	0	3815	310	0
2	E	3878	0	3869	300	0
2	F	3985	0	3980	345	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	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	7	0
4	B	62	0	24	8	0
4	C	62	0	24	5	0
4	D	62	0	24	3	0
4	E	62	0	24	8	0
4	F	62	0	24	7	0
5	A	21	0	0	7	0
5	B	12	0	0	3	0
5	C	23	0	0	2	0
5	D	37	0	0	6	0
5	E	34	0	0	12	0
5	F	40	0	0	10	0
All	All	23930	0	23481	1736	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

The worst 5 of 1736 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:106:LEU:HD11	2:F:129:ARG:CZ	1.82	1.09
1:A:396:VAL:HG11	1:A:430:ILE:HG21	1.30	1.09
1:A:379:SER:H	1:A:413:THR:HB	1.19	1.03
2:E:356:LEU:HD22	2:E:387:VAL:HG11	1.41	1.02
2:F:305:ALA:HB2	2:F:374:ARG:HD2	1.39	1.00

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	504/519 (97%)	427 (85%)	54 (11%)	23 (5%)	4	22
2	B	488/519 (94%)	411 (84%)	51 (10%)	26 (5%)	3	18
2	C	485/519 (93%)	420 (87%)	48 (10%)	17 (4%)	6	30
2	D	482/519 (93%)	424 (88%)	44 (9%)	14 (3%)	7	35
2	E	489/519 (94%)	416 (85%)	54 (11%)	19 (4%)	5	26
2	F	503/519 (97%)	422 (84%)	57 (11%)	24 (5%)	4	20
All	All	2951/3114 (95%)	2520 (85%)	308 (10%)	123 (4%)	4	24

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	117	VAL
1	A	154	TYR
1	A	333	MET
1	A	417	ASP

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%)	392 (91%)	38 (9%)	14	48
2	B	416/441 (94%)	375 (90%)	41 (10%)	11	40
2	C	413/441 (94%)	373 (90%)	40 (10%)	12	42
2	D	410/441 (93%)	372 (91%)	38 (9%)	13	45
2	E	417/441 (95%)	378 (91%)	39 (9%)	13	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	429/441 (97%)	389 (91%)	40 (9%)	13	45
All	All	2515/2647 (95%)	2279 (91%)	236 (9%)	13	44

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	360	LEU
2	D	187	GLU
2	F	302	VAL
2	C	400	THR
2	D	26	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	245	ASN
2	D	33	HIS
2	F	115	GLN
2	C	256	GLN
2	C	361	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

5 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
2	SEP	B	431	2	9,9,10	6.44	3 (33%)	10,12,14	1.20	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	C	431	2	9,9,10	5.60	2 (22%)	10,12,14	1.76	3 (30%)
2	SEP	D	431	2	9,9,10	6.86	5 (55%)	10,12,14	3.03	3 (30%)
2	SEP	E	431	2	9,9,10	5.95	4 (44%)	10,12,14	1.18	1 (10%)
2	SEP	F	431	2	9,9,10	5.14	4 (44%)	10,12,14	2.61	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
2	SEP	B	431	2	-	0/6/8/10	0/0/0/0
2	SEP	C	431	2	-	0/6/8/10	0/0/0/0
2	SEP	D	431	2	-	0/6/8/10	0/0/0/0
2	SEP	E	431	2	-	0/6/8/10	0/0/0/0
2	SEP	F	431	2	-	0/6/8/10	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	431	SEP	O-C	19.96	1.25	1.11
2	B	431	SEP	O-C	18.61	1.24	1.11
2	E	431	SEP	O-C	16.70	1.22	1.11
2	C	431	SEP	O-C	16.17	1.22	1.11
2	F	431	SEP	O-C	14.64	1.21	1.11

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	431	SEP	P-OG-CB	-6.94	98.13	118.19
2	D	431	SEP	P-OG-CB	-6.47	99.47	118.19
2	D	431	SEP	OG-CB-CA	6.10	117.33	108.69
2	F	431	SEP	OG-CB-CA	3.98	114.33	108.69
2	C	431	SEP	C-CA-N	3.39	117.21	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 9 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	33,33,33	1.19	2 (6%)	52,52,52	2.07	10 (19%)
4	ATP	A	903	3	33,33,33	1.13	3 (9%)	52,52,52	2.13	10 (19%)
4	ATP	B	901	3	33,33,33	1.12	2 (6%)	52,52,52	2.12	11 (21%)
4	ATP	B	903	3	33,33,33	1.18	3 (9%)	52,52,52	2.19	12 (23%)
4	ATP	C	901	3	33,33,33	1.18	3 (9%)	52,52,52	2.16	12 (23%)
4	ATP	C	903	3	33,33,33	1.05	1 (3%)	52,52,52	2.23	12 (23%)
4	ATP	D	901	3	33,33,33	1.13	3 (9%)	52,52,52	2.17	11 (21%)
4	ATP	D	903	-	33,33,33	1.17	2 (6%)	52,52,52	2.33	14 (26%)
4	ATP	E	901	3	33,33,33	1.15	2 (6%)	52,52,52	2.17	12 (23%)
4	ATP	E	903	-	33,33,33	1.25	3 (9%)	52,52,52	2.10	13 (25%)
4	ATP	F	901	3	33,33,33	1.15	3 (9%)	52,52,52	2.06	11 (21%)
4	ATP	F	903	-	33,33,33	1.08	2 (6%)	52,52,52	2.20	12 (23%)

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	-	0/22/38/38	0/1/3/3
4	ATP	A	903	3	-	0/22/38/38	0/1/3/3
4	ATP	B	901	3	-	0/22/38/38	0/1/3/3
4	ATP	B	903	3	-	0/22/38/38	0/1/3/3
4	ATP	C	901	3	-	0/22/38/38	0/1/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	C	903	3	-	0/22/38/38	0/1/3/3
4	ATP	D	901	3	-	0/22/38/38	0/1/3/3
4	ATP	D	903	-	-	0/22/38/38	0/1/3/3
4	ATP	E	901	3	-	0/22/38/38	0/1/3/3
4	ATP	E	903	-	-	0/22/38/38	0/1/3/3
4	ATP	F	901	3	-	0/22/38/38	0/1/3/3
4	ATP	F	903	-	-	0/22/38/38	0/1/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	901	ATP	C2-N3	3.73	1.39	1.32
4	E	903	ATP	C2-N3	3.67	1.39	1.32
4	E	901	ATP	C2-N3	3.63	1.39	1.32
4	B	903	ATP	C2-N3	3.60	1.39	1.32
4	D	901	ATP	C2-N3	3.41	1.38	1.32

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	903	ATP	N3-C2-N1	-11.34	119.23	128.71
4	B	901	ATP	N3-C2-N1	-10.66	119.80	128.71
4	C	903	ATP	N3-C2-N1	-10.56	119.88	128.71
4	A	903	ATP	N3-C2-N1	-10.53	119.90	128.71
4	E	901	ATP	N3-C2-N1	-10.49	119.94	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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	506/519 (97%)	0.09	22 (4%) 34 7	19, 74, 114, 146	0
2	B	491/519 (94%)	0.03	10 (2%) 62 12	31, 75, 116, 157	0
2	C	488/519 (94%)	-0.10	5 (1%) 79 22	29, 61, 114, 156	0
2	D	485/519 (93%)	-0.18	5 (1%) 79 22	17, 45, 100, 144	0
2	E	492/519 (94%)	-0.08	5 (1%) 79 22	10, 58, 105, 145	0
2	F	506/519 (97%)	0.05	19 (3%) 38 7	14, 73, 116, 135	0
All	All	2968/3114 (95%)	-0.03	66 (2%) 59 12	10, 64, 114, 157	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	517	PRO	5.0
1	A	518	GLU	5.0
1	A	517	PRO	4.8
2	F	518	GLU	4.1
1	A	120	GLY	3.8

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SEP	D	431	10/11	0.47	2.00	83,89,104,105	0
2	SEP	C	431	10/11	0.40	1.69	77,84,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SEP	F	431	10/11	0.46	1.60	73,82,88,88	0
2	SEP	E	431	10/11	0.29	0.33	71,78,90,91	0
2	SEP	B	431	10/11	0.29	-0.13	98,101,104,104	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	B	802	1/1	0.61	7.92	92,92,92,92	0
3	MG	B	521	1/1	0.42	3.33	33,33,33,33	0
3	MG	F	806	1/1	0.56	3.10	54,54,54,54	0
3	MG	C	803	1/1	0.36	2.48	16,16,16,16	0
3	MG	C	522	1/1	0.49	2.17	38,38,38,38	0
3	MG	D	804	1/1	0.44	2.16	17,17,17,17	0
4	ATP	F	903	31/31	0.28	1.55	30,37,41,44	0
3	MG	A	521	1/1	0.28	1.54	23,23,23,23	0
4	ATP	E	903	31/31	0.26	1.35	28,31,46,53	0
4	ATP	C	903	31/31	0.28	1.18	43,48,71,72	0
4	ATP	D	903	31/31	0.23	1.10	24,30,49,50	0
4	ATP	B	901	31/31	0.28	0.82	58,63,74,77	0
4	ATP	A	903	31/31	0.22	0.60	42,49,53,54	0
4	ATP	B	903	31/31	0.24	0.50	57,62,67,70	0
4	ATP	A	901	31/31	0.27	0.17	75,88,90,92	0
4	ATP	F	901	31/31	0.28	0.12	78,89,91,93	0
4	ATP	E	901	31/31	0.29	0.11	60,71,77,78	0
4	ATP	C	901	31/31	0.20	0.10	31,39,42,44	0
4	ATP	D	901	31/31	0.23	0.06	48,52,54,55	0
3	MG	E	805	1/1	0.26	-1.06	25,25,25,25	0
3	MG	A	801	1/1	0.24	-1.71	54,54,54,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.