



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:10 PM GMT

PDB ID : 3S1A
Title : Crystal structure of the phosphorylation-site double mutant S431E/T432E of the KaiC circadian clock protein
Authors : Pattanayek, R.; Williams, D.W.; Rossi, G.; Weigand, S.; Mori, T.; Johnson, C.H.; Stewart, P.L.; Egli, M.
Deposited on : 2011-05-14
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>

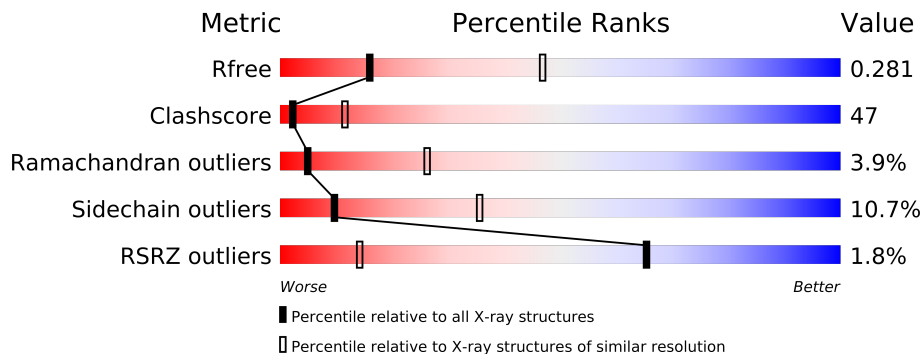
The following versions of software and data (see [references](#)) were used in the production of this report:

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	525	
1	F	525	
2	B	525	
2	C	525	
2	D	525	
2	E	525	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	526	-	X
4	MG	A	701	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	MG	C	702	-	X
4	MG	D	701	-	X
4	MG	D	702	-	X
4	MG	D	801	-	X
4	MG	F	702	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23898 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	P	S	0	0	0
			3994	2512	701	765	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3994	2512	701	765	1	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
A	432	GLU	THR	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
F	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
F	432	GLU	THR	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 a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	491	Total	C	N	O	S		0	0	0
			3875	2442	678	740	15				
2	C	488	Total	C	N	O	S		0	0	0
			3851	2428	674	734	15				

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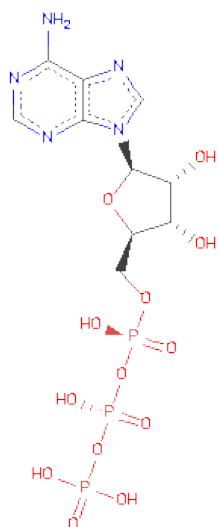
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	485	Total	C	N	O	S	0	0	0
			3827	2414	671	727	15			
2	E	492	Total	C	N	O	S	0	0	0
			3883	2448	679	741	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
B	432	GLU	THR	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	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
C	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
C	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
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	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
D	432	GLU	THR	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	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
E	432	GLU	THR	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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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	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		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	4	Total 4 Mg 4	0	0
4	E	2	Total 2 Mg 2	0	0
4	B	4	Total 4 Mg 4	0	0
4	C	4	Total 4 Mg 4	0	0
4	A	4	Total 4 Mg 4	0	0
4	F	3	Total 3 Mg 3	0	0

- Molecule 5 is water.

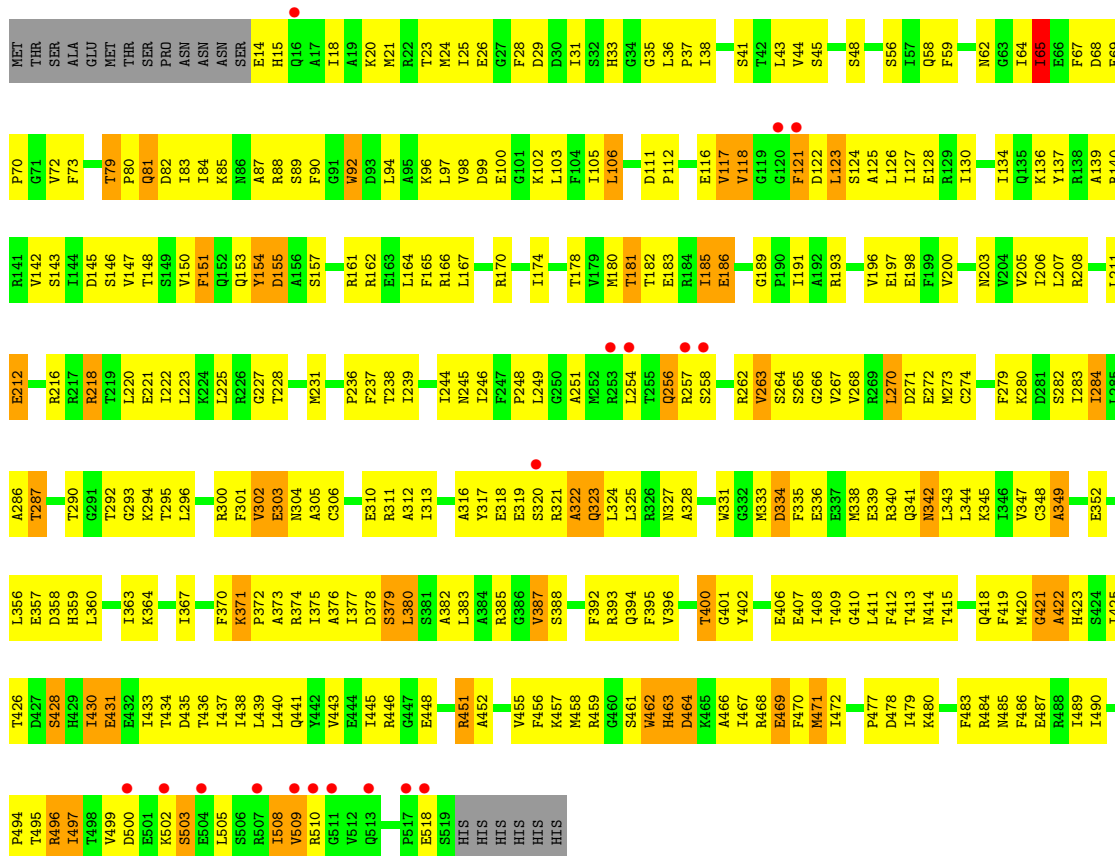
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total 5 O 5	0	0
5	B	6	Total 6 O 6	0	0
5	C	10	Total 10 O 10	0	0
5	D	32	Total 32 O 32	0	0
5	E	16	Total 16 O 16	0	0
5	F	12	Total 12 O 12	0	0

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.

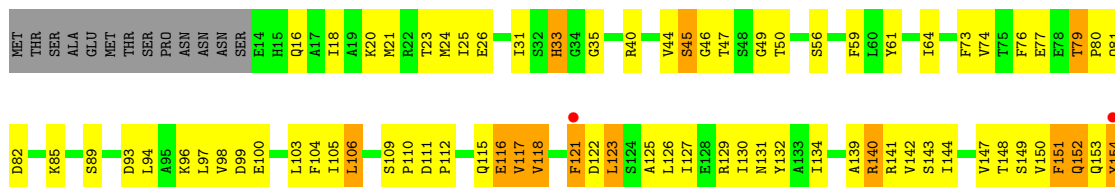
- Molecule 1: Circadian clock protein kinase *kaiC*

Chain A: 



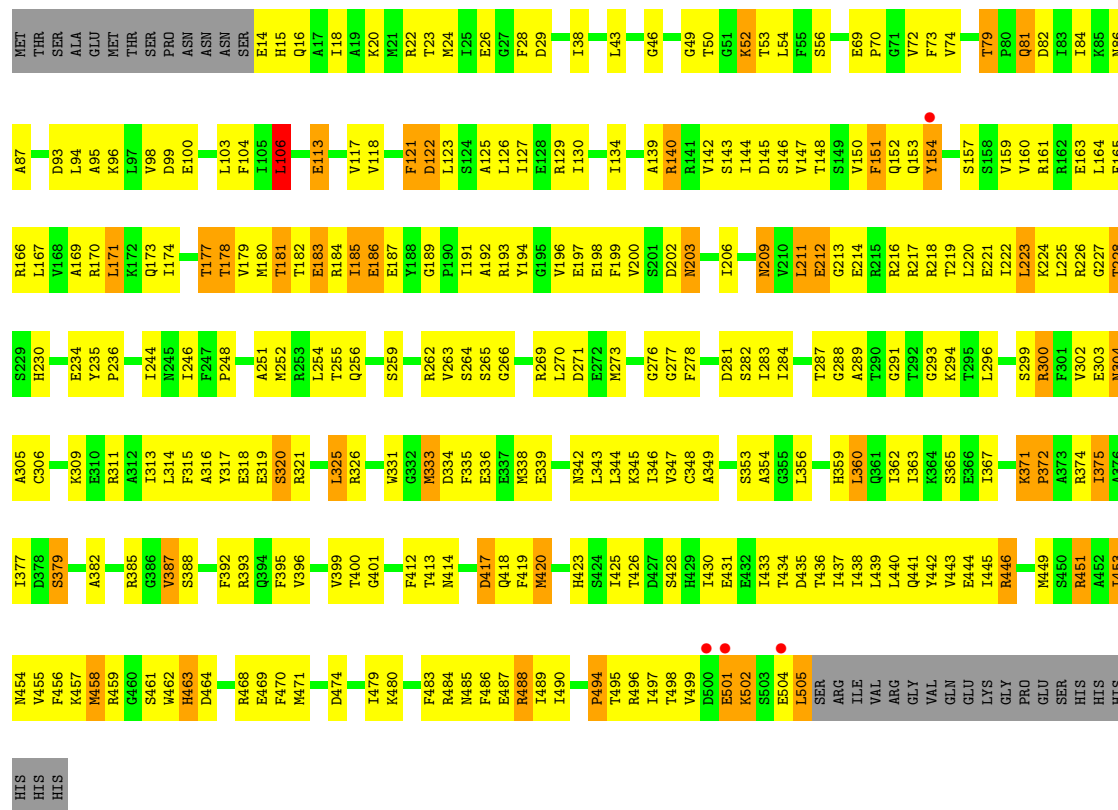
- Molecule 1: Circadian clock protein kinase *kaiC*

Chain F: 





Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.67Å 135.49Å 204.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 3.00 16.96 – 2.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (17.00-3.00) 92.3 (16.96-2.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.87Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.288 0.239 , 0.281	Depositor DCC
R_{free} test set	6459 reflections (10.06%)	DCC
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.2	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 81280 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23898	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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	0.43	0/4049	0.72	1/5453 (0.0%)
1	F	0.46	0/4049	0.73	0/5453
2	B	0.40	0/3940	0.67	0/5309
2	C	0.41	0/3916	0.69	1/5278 (0.0%)
2	D	0.50	0/3892	0.73	0/5245
2	E	0.49	0/3948	0.75	2/5320 (0.0%)
All	All	0.45	0/23794	0.72	4/32058 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	213	GLY	N-CA-C	-5.96	98.21	113.10
2	E	106	LEU	CA-CB-CG	5.81	128.67	115.30
2	C	213	GLY	N-CA-C	-5.28	99.90	113.10
1	A	380	LEU	N-CA-C	-5.23	96.88	111.00

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	3994	0	3985	444	0
1	F	3994	0	3983	405	0
2	B	3875	0	3863	437	0
2	C	3851	0	3839	382	0
2	D	3827	0	3819	358	0
2	E	3883	0	3875	351	0
3	A	62	0	24	7	0
3	B	62	0	24	8	0
3	C	62	0	24	5	0
3	D	62	0	24	6	0
3	E	62	0	24	11	0
3	F	62	0	24	6	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
5	A	5	0	0	0	0
5	B	6	0	0	1	0
5	C	10	0	0	2	0
5	D	32	0	0	13	0
5	E	16	0	0	0	0
5	F	12	0	0	1	0
All	All	23898	0	23508	2227	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 47.

The worst 5 of 2227 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:VAL:HG12	1:A:463:HIS:CD2	1.63	1.30
1:A:320:SEP:HB2	2:B:254:LEU:O	1.42	1.17
1:A:254:LEU:CD2	1:F:320:SEP:HA	1.74	1.16
1:A:321:ARG:O	1:A:324:LEU:HB2	1.45	1.14
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.10	1.14

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	503/525 (96%)	406 (81%)	76 (15%)	21 (4%)	4	24
1	F	503/525 (96%)	422 (84%)	61 (12%)	20 (4%)	5	25
2	B	489/525 (93%)	389 (80%)	82 (17%)	18 (4%)	5	28
2	C	486/525 (93%)	419 (86%)	45 (9%)	22 (4%)	4	22
2	D	483/525 (92%)	415 (86%)	52 (11%)	16 (3%)	6	32
2	E	490/525 (93%)	402 (82%)	69 (14%)	19 (4%)	5	26
All	All	2954/3150 (94%)	2453 (83%)	385 (13%)	116 (4%)	5	26

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	TYR
1	A	334	ASP
1	A	462	TRP
1	A	463	HIS
1	A	503	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/449 (96%)	389 (90%)	42 (10%)	12	42
1	F	431/449 (96%)	383 (89%)	48 (11%)	9	34
2	B	419/450 (93%)	370 (88%)	49 (12%)	8	31
2	C	416/450 (92%)	374 (90%)	42 (10%)	11	39
2	D	413/450 (92%)	367 (89%)	46 (11%)	9	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	420/450 (93%)	377 (90%)	43 (10%)	11	38
All	All	2530/2698 (94%)	2260 (89%)	270 (11%)	10	35

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	375	ILE
2	D	223	LEU
1	F	321	ARG
2	C	453	ILE
2	D	121	PHE

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

Mol	Chain	Res	Type
2	C	256	GLN
2	C	429	HIS
1	F	260	ASN
2	C	260	ASN
2	C	368	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	320	1	9,9,10	5.98	3 (33%)	10,12,14	3.00	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	F	320	1	9,9,10	5.92	4 (44%)	10,12,14	2.69	5 (50%)

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	320	1	-	0/6/8/10	0/0/0/0
1	SEP	F	320	1	-	0/6/8/10	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	SEP	O-C	16.88	1.23	1.11
1	F	320	SEP	O-C	16.82	1.23	1.11
1	A	320	SEP	P-O1P	4.44	1.66	1.51
1	F	320	SEP	P-O1P	4.11	1.65	1.51
1	A	320	SEP	CA-C	3.40	1.54	1.48

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	SEP	C-CA-N	-6.65	107.18	113.83
1	F	320	SEP	P-OG-CB	-4.95	103.89	118.19
1	A	320	SEP	P-OG-CB	-4.71	104.56	118.19
1	F	320	SEP	OG-CB-CA	-4.12	102.85	108.69
1	F	320	SEP	O3P-P-OG	3.88	117.36	106.65

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 33 ligands modelled in this entry, 21 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	4	33,33,33	1.13	3 (9%)	52,52,52	2.11	11 (21%)
3	ATP	A	903	4	33,33,33	1.24	4 (12%)	52,52,52	2.06	10 (19%)
3	ATP	B	901	4	33,33,33	1.15	4 (12%)	52,52,52	2.06	10 (19%)
3	ATP	B	903	4	33,33,33	1.17	4 (12%)	52,52,52	2.09	10 (19%)
3	ATP	C	901	4	33,33,33	1.18	2 (6%)	52,52,52	2.16	12 (23%)
3	ATP	C	903	4	33,33,33	1.13	3 (9%)	52,52,52	2.25	10 (19%)
3	ATP	D	901	4	33,33,33	1.15	3 (9%)	52,52,52	2.21	12 (23%)
3	ATP	D	903	4	33,33,33	1.13	3 (9%)	52,52,52	2.22	13 (25%)
3	ATP	E	901	4	33,33,33	1.19	3 (9%)	52,52,52	2.17	14 (26%)
3	ATP	E	903	-	33,33,33	1.13	2 (6%)	52,52,52	2.11	12 (23%)
3	ATP	F	901	4	33,33,33	1.13	3 (9%)	52,52,52	2.08	13 (25%)
3	ATP	F	903	4	33,33,33	1.24	3 (9%)	52,52,52	2.15	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
3	ATP	A	901	4	-	0/22/38/38	0/1/3/3
3	ATP	A	903	4	-	0/22/38/38	0/1/3/3
3	ATP	B	901	4	-	0/22/38/38	0/1/3/3
3	ATP	B	903	4	-	0/22/38/38	0/1/3/3
3	ATP	C	901	4	-	0/22/38/38	0/1/3/3
3	ATP	C	903	4	-	0/22/38/38	0/1/3/3
3	ATP	D	901	4	-	0/22/38/38	0/1/3/3
3	ATP	D	903	4	-	0/22/38/38	0/1/3/3
3	ATP	E	901	4	-	0/22/38/38	0/1/3/3
3	ATP	E	903	-	-	0/22/38/38	0/1/3/3
3	ATP	F	901	4	-	0/22/38/38	0/1/3/3
3	ATP	F	903	4	-	0/22/38/38	0/1/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	903	ATP	C2-N3	3.87	1.39	1.32
3	C	901	ATP	C2-N3	3.58	1.39	1.32
3	E	901	ATP	C2-N3	3.44	1.39	1.32
3	A	901	ATP	C2-N3	3.40	1.38	1.32
3	F	901	ATP	C2-N3	3.35	1.38	1.32

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ATP	N3-C2-N1	-10.79	119.69	128.71
3	C	903	ATP	N3-C2-N1	-10.76	119.71	128.71
3	C	901	ATP	N3-C2-N1	-10.46	119.97	128.71
3	B	903	ATP	N3-C2-N1	-10.34	120.06	128.71
3	B	901	ATP	N3-C2-N1	-10.32	120.08	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	506/525 (96%)	0.07	18 (3%)	41 8	31, 77, 121, 154	0
1	F	506/525 (96%)	-0.10	11 (2%)	59 12	18, 66, 113, 145	0
2	B	491/525 (93%)	0.04	10 (2%)	62 12	43, 82, 126, 158	0
2	C	488/525 (92%)	-0.13	5 (1%)	79 22	30, 69, 122, 160	0
2	D	485/525 (92%)	-0.25	7 (1%)	72 18	20, 53, 106, 152	0
2	E	492/525 (93%)	-0.19	4 (0%)	83 26	15, 59, 104, 148	0
All	All	2968/3150 (94%)	-0.09	55 (1%)	65 13	15, 69, 117, 160	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	507	ARG	3.9
2	D	118	VAL	3.7
1	F	516	GLY	3.6
1	A	120	GLY	3.3
1	A	257	ARG	3.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
1	SEP	A	320	10/11	0.54	0.95	49,59,66,68	0
1	SEP	F	320	10/11	0.37	0.24	45,57,63,66	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(Å ²)	Q<0.9
4	MG	D	701	1/1	0.34	5.26	59,59,59,59	0
4	MG	C	702	1/1	0.44	4.85	65,65,65,65	0
4	MG	D	702	1/1	0.24	4.68	49,49,49,49	0
4	MG	F	702	1/1	0.24	4.41	68,68,68,68	0
4	MG	D	801	1/1	0.34	2.94	44,44,44,44	0
4	MG	A	526	1/1	0.47	2.32	58,58,58,58	0
4	MG	A	701	1/1	0.28	2.00	63,63,63,63	0
4	MG	C	701	1/1	0.23	1.28	70,70,70,70	0
4	MG	B	702	1/1	0.27	1.15	79,79,79,79	0
4	MG	A	802	1/1	0.32	1.12	82,82,82,82	0
4	MG	F	701	1/1	0.16	0.67	45,45,45,45	0
3	ATP	C	903	31/31	0.18	0.39	42,52,85,85	0
3	ATP	D	903	31/31	0.15	0.37	26,35,60,62	0
3	ATP	B	901	31/31	0.19	0.05	67,70,85,87	0
3	ATP	D	901	31/31	0.17	-0.12	50,54,60,62	0
4	MG	E	802	1/1	0.19	-0.23	46,46,46,46	0
4	MG	B	701	1/1	0.18	-0.23	58,58,58,58	0
3	ATP	C	901	31/31	0.15	-0.32	36,47,56,56	0
3	ATP	A	903	31/31	0.18	-0.33	61,66,76,77	0
3	ATP	E	903	31/31	0.14	-0.46	22,28,60,62	0
3	ATP	F	903	31/31	0.14	-0.51	44,48,62,62	0
3	ATP	F	901	31/31	0.17	-0.55	74,83,88,89	0
4	MG	C	802	1/1	0.14	-0.60	41,41,41,41	0
4	MG	E	801	1/1	0.19	-0.61	38,38,38,38	0
3	ATP	A	901	31/31	0.19	-0.65	84,86,89,90	0
3	ATP	E	901	31/31	0.16	-0.71	65,72,81,81	0
4	MG	F	802	1/1	0.24	-0.79	53,53,53,53	0
3	ATP	B	903	31/31	0.18	-0.84	77,81,94,95	0
4	MG	B	802	1/1	0.17	-0.86	64,64,64,64	0
4	MG	B	801	1/1	0.12	-2.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	D	802	1/1	0.12	-2.28	17,17,17,17	0
4	MG	C	801	1/1	0.09	-2.68	25,25,25,25	0
4	MG	A	801	1/1	0.17	-3.15	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.