Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 09:12 PM EDT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

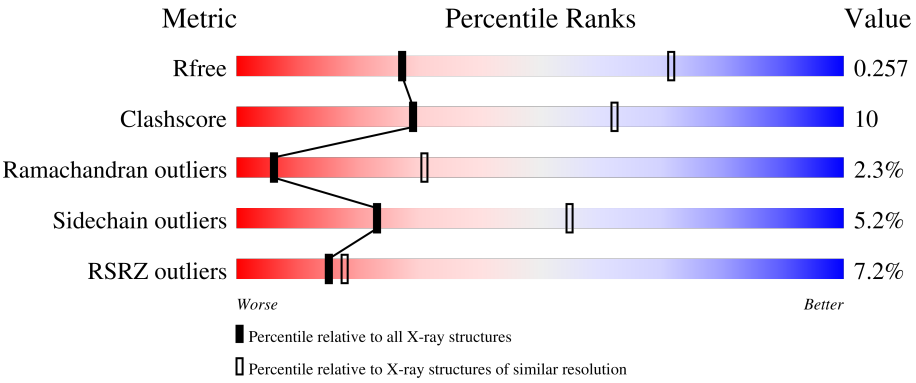
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	512	13% 73% 23%
1	B	512	7% 71% 23%
1	C	512	5% 67% 25% 5%
1	D	512	4% 71% 21% 5%
1	E	512	5% 70% 23%

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Mol	Chain	Length	Quality of chain
1	F	512	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	F	601	-	-	-	X
4	PO4	B	604	-	-	-	X
4	PO4	F	604	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24219 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3991	2511	701	763	1	15			
1	B	489	Total	C	N	O	P	S	0	0	0
			3861	2433	676	736	1	15			
1	C	488	Total	C	N	O	P	S	0	0	0
			3852	2427	674	735	1	15			
1	D	485	Total	C	N	O	P	S	0	0	0
			3828	2413	671	728	1	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3884	2447	679	742	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3987	2509	701	761	1	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	VAL	ALA	engineered mutation	UNP Q79PF4
A	520	HIS	-	expression tag	UNP Q79PF4
A	521	HIS	-	expression tag	UNP Q79PF4
A	522	HIS	-	expression tag	UNP Q79PF4
A	523	HIS	-	expression tag	UNP Q79PF4
A	524	HIS	-	expression tag	UNP Q79PF4
A	525	HIS	-	expression tag	UNP Q79PF4
B	422	VAL	ALA	engineered mutation	UNP Q79PF4
B	520	HIS	-	expression tag	UNP Q79PF4
B	521	HIS	-	expression tag	UNP Q79PF4
B	522	HIS	-	expression tag	UNP Q79PF4
B	523	HIS	-	expression tag	UNP Q79PF4
B	524	HIS	-	expression tag	UNP Q79PF4
B	525	HIS	-	expression tag	UNP Q79PF4
C	422	VAL	ALA	engineered mutation	UNP Q79PF4
C	520	HIS	-	expression tag	UNP Q79PF4
C	521	HIS	-	expression tag	UNP Q79PF4

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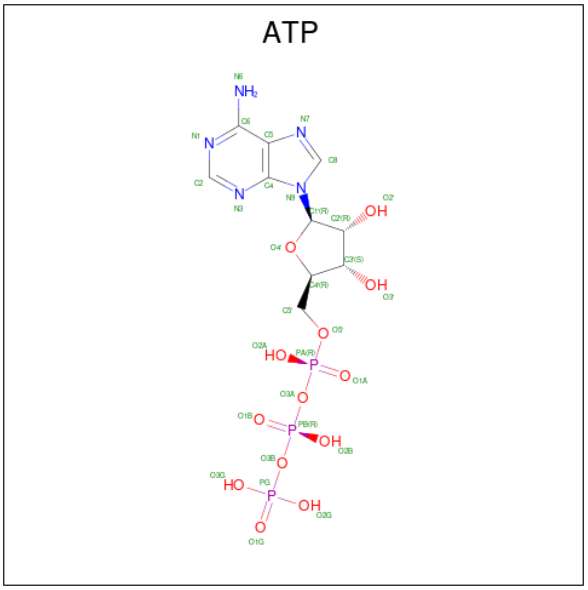
Chain	Residue	Modelled	Actual	Comment	Reference
C	522	HIS	-	expression tag	UNP Q79PF4
C	523	HIS	-	expression tag	UNP Q79PF4
C	524	HIS	-	expression tag	UNP Q79PF4
C	525	HIS	-	expression tag	UNP Q79PF4
D	422	VAL	ALA	engineered mutation	UNP Q79PF4
D	520	HIS	-	expression tag	UNP Q79PF4
D	521	HIS	-	expression tag	UNP Q79PF4
D	522	HIS	-	expression tag	UNP Q79PF4
D	523	HIS	-	expression tag	UNP Q79PF4
D	524	HIS	-	expression tag	UNP Q79PF4
D	525	HIS	-	expression tag	UNP Q79PF4
E	422	VAL	ALA	engineered mutation	UNP Q79PF4
E	520	HIS	-	expression tag	UNP Q79PF4
E	521	HIS	-	expression tag	UNP Q79PF4
E	522	HIS	-	expression tag	UNP Q79PF4
E	523	HIS	-	expression tag	UNP Q79PF4
E	524	HIS	-	expression tag	UNP Q79PF4
E	525	HIS	-	expression tag	UNP Q79PF4
F	422	VAL	ALA	engineered mutation	UNP Q79PF4
F	520	HIS	-	expression tag	UNP Q79PF4
F	521	HIS	-	expression tag	UNP Q79PF4
F	522	HIS	-	expression tag	UNP Q79PF4
F	523	HIS	-	expression tag	UNP Q79PF4
F	524	HIS	-	expression tag	UNP Q79PF4
F	525	HIS	-	expression tag	UNP Q79PF4

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

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

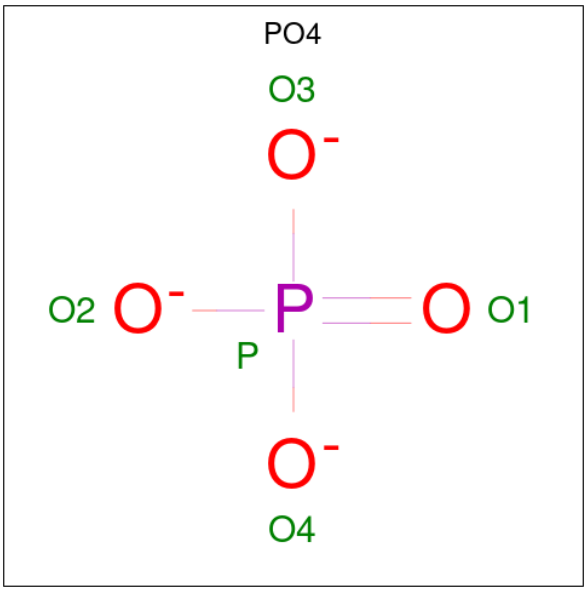
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

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



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	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

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

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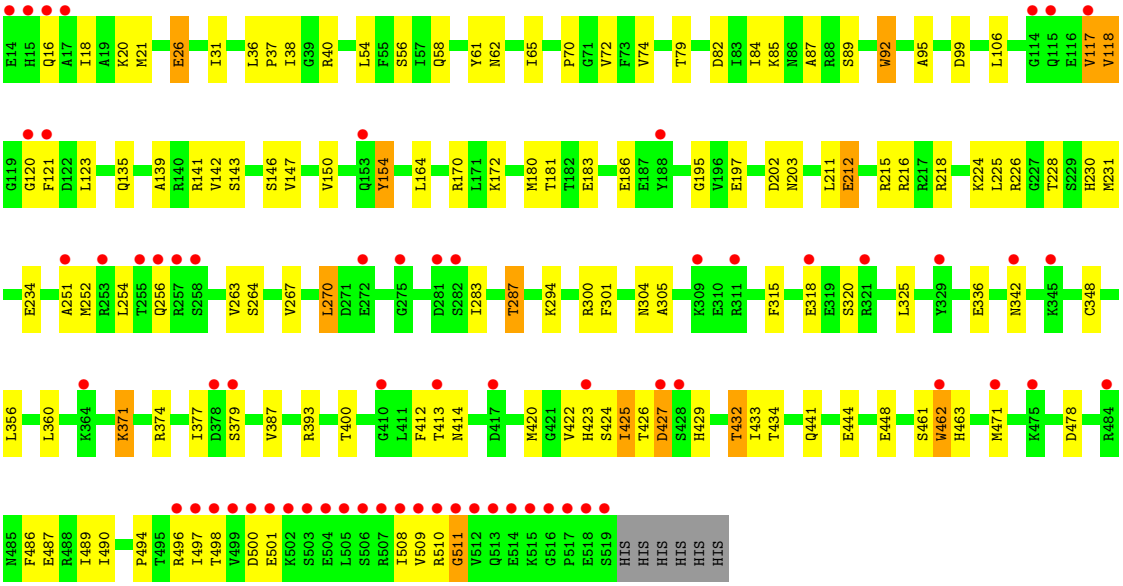
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	54	Total O 54 54	0	0
5	F	67	Total O 67 67	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

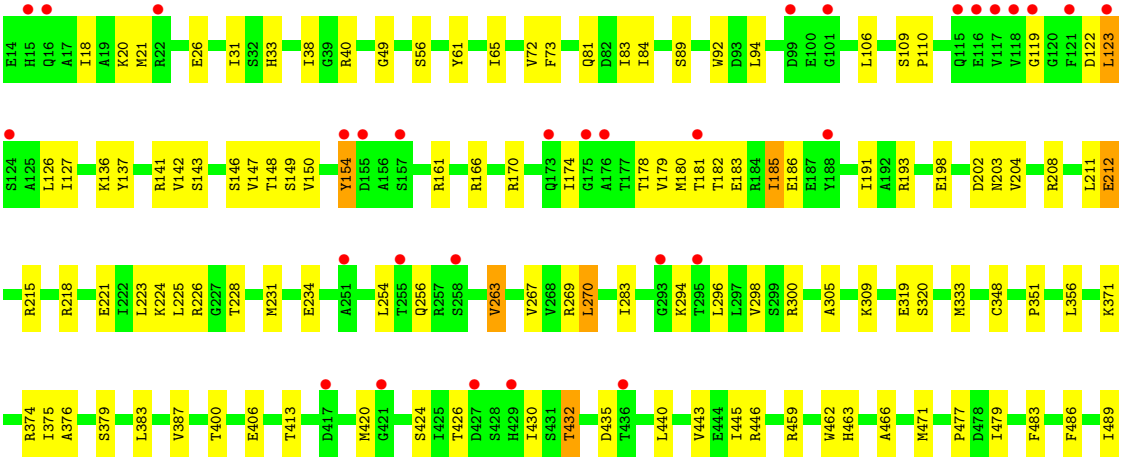
• Molecule 1: Circadian clock protein kinase KaiC

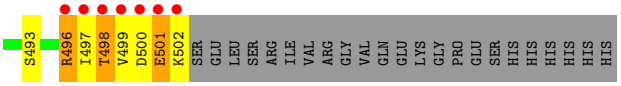
Chain A:



• Molecule 1: Circadian clock protein kinase KaiC

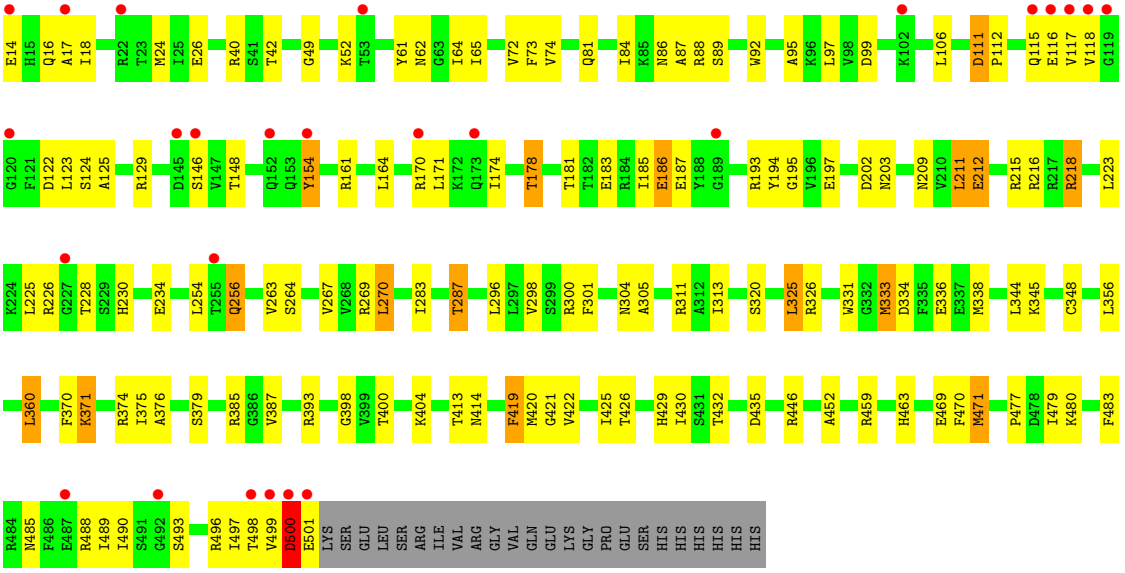
Chain B:





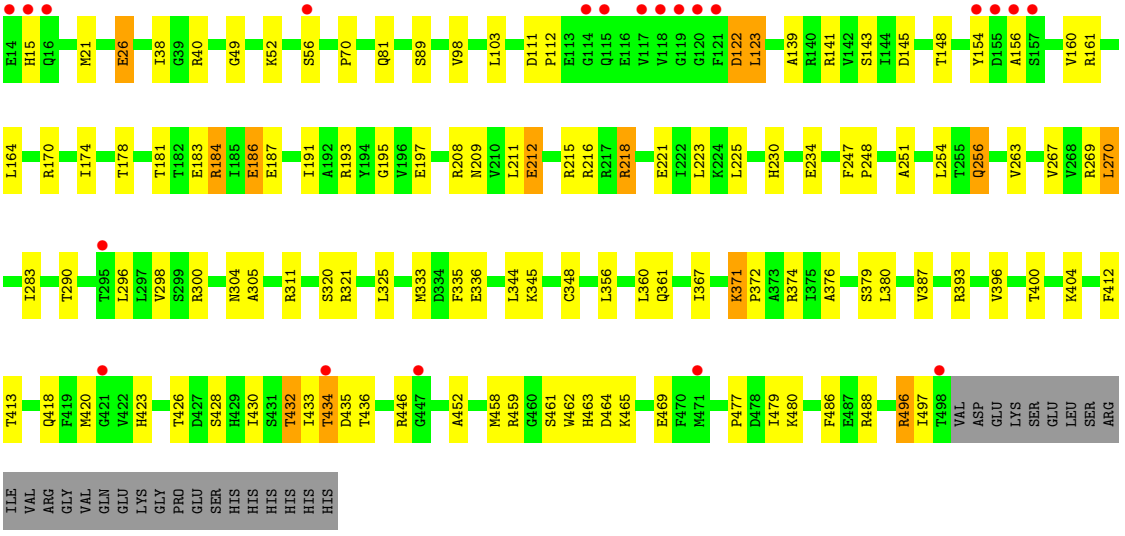
• Molecule 1: Circadian clock protein kinase KaiC

Chain C:



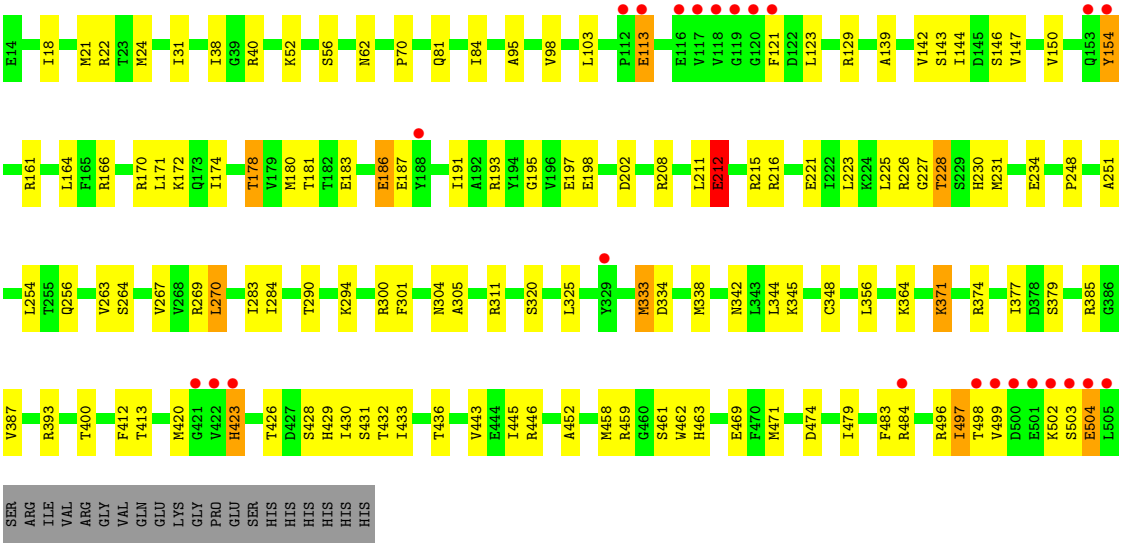
• Molecule 1: Circadian clock protein kinase KaiC

Chain D:

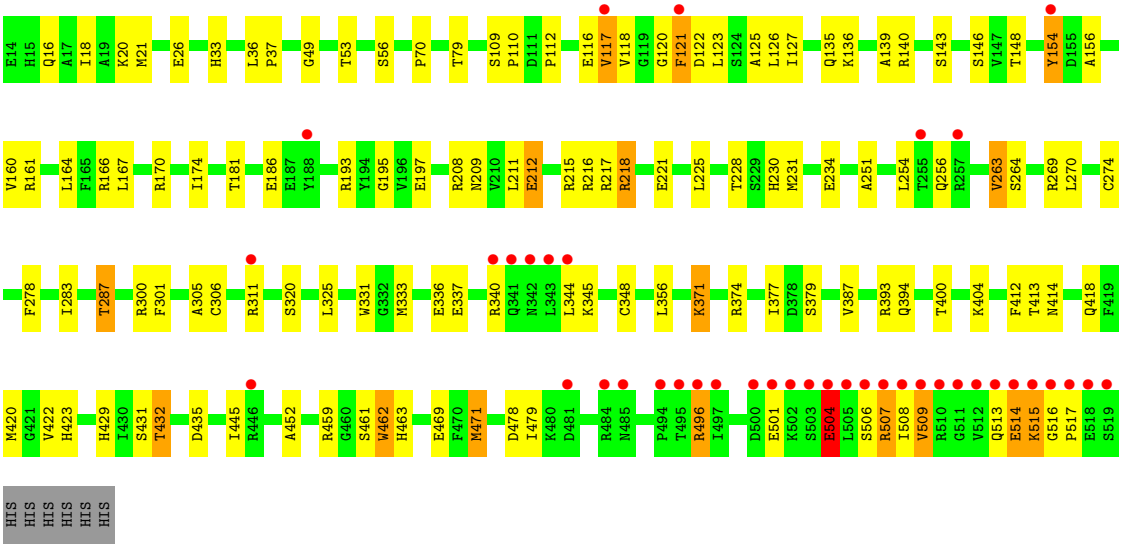


• Molecule 1: Circadian clock protein kinase KaiC

Chain E:



• Molecule 1: Circadian clock protein kinase KaiC



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.36Å 134.47Å 203.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.35 29.96 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.96-3.35) 95.0 (29.96-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.60 (at 3.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168), CNS	Depositor
R, R_{free}	0.217 , 0.261 0.217 , 0.257	Depositor DCC
R_{free} test set	2665 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	24219	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ATP, PO4, TPO, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/4045	0.41	2/5448 (0.0%)
1	B	0.25	0/3914	0.41	0/5273
1	C	0.22	0/3905	0.39	0/5262
1	D	0.22	0/3881	0.39	0/5229
1	E	0.23	0/3937	0.41	0/5304
1	F	0.22	0/4041	0.40	0/5443
All	All	0.23	0/23723	0.40	2/31959 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3991	0	3988	73	0
1	B	3861	0	3854	85	0
1	C	3852	0	3842	98	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (453) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:SER:HB3	1:E:504:GLU:HB2	1.29	1.12
1:B:499:VAL:C	1:B:501:GLU:HA	1.76	1.06
1:D:379:SER:H	1:D:413:THR:HB	1.41	0.83
1:F:379:SER:H	1:F:413:THR:HB	1.41	0.82
1:E:379:SER:H	1:E:413:THR:HB	1.43	0.82
1:C:485:ASN:HB2	1:C:497:ILE:CG1	2.12	0.80
1:C:485:ASN:HB2	1:C:497:ILE:HG12	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:SER:H	1:B:413:THR:HB	1.48	0.78
1:C:379:SER:H	1:C:413:THR:HB	1.48	0.77
1:B:496:ARG:CB	1:B:496:ARG:HH11	1.99	0.76
1:C:146:SER:H	1:C:181:THR:HB	1.50	0.76
1:D:283:ILE:HG13	1:D:400:THR:HG23	1.68	0.74
1:B:499:VAL:O	1:B:501:GLU:HA	1.86	0.74
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.22	0.73
1:C:283:ILE:HG13	1:C:400:THR:HG23	1.70	0.72
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.22	0.72
1:B:148:THR:HG21	1:B:193:ARG:HD2	1.71	0.72
1:F:49:GLY:O	1:F:218:ARG:NH2	2.22	0.72
1:C:269:ARG:HG2	1:C:479:ILE:HB	1.70	0.71
1:C:164:LEU:HD11	1:C:197:GLU:HG3	1.71	0.71
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.73	0.70
1:E:283:ILE:HG13	1:E:400:THR:HG23	1.73	0.68
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.27	0.68
1:B:497:ILE:HD12	1:B:498:THR:N	2.09	0.67
1:C:148:THR:HG21	1:C:193:ARG:HD2	1.76	0.67
1:F:283:ILE:HG13	1:F:400:THR:HG23	1.75	0.67
1:F:148:THR:HG21	1:F:193:ARG:HD2	1.76	0.66
1:C:215:ARG:NH2	1:D:234:GLU:O	2.28	0.66
1:C:49:GLY:O	1:C:218:ARG:NH2	2.28	0.66
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.76	0.66
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.77	0.66
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.77	0.66
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.78	0.66
1:D:356:LEU:HD22	1:D:387:VAL:HG11	1.76	0.66
1:D:305:ALA:HB2	1:D:374:ARG:HD2	1.77	0.65
1:F:218:ARG:NH1	4:F:604:PO4:O2	2.29	0.65
1:A:379:SER:H	1:A:413:THR:HB	1.61	0.64
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.61	0.64
1:B:500:ASP:N	1:B:501:GLU:HA	2.12	0.64
1:B:49:GLY:O	1:B:218:ARG:NH2	2.31	0.64
1:B:193:ARG:NH2	1:C:195:GLY:O	2.22	0.63
1:C:485:ASN:O	1:C:497:ILE:HG12	1.97	0.63
1:C:435:ASP:OD1	1:C:459:ARG:NH1	2.31	0.63
1:D:49:GLY:O	1:D:218:ARG:NH2	2.30	0.63
1:D:311:ARG:HD2	1:D:371:LYS:HE3	1.81	0.63
1:C:393:ARG:HH21	1:C:429:HIS:HB2	1.63	0.63
1:D:184:ARG:NH1	1:D:187:GLU:O	2.32	0.63
1:E:503:SER:HB3	1:E:504:GLU:CB	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:SER:O	1:F:374:ARG:NH2	2.32	0.61
1:B:146:SER:H	1:B:181:THR:HB	1.65	0.61
1:C:202:ASP:HA	1:C:226:ARG:HD2	1.82	0.61
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.82	0.61
1:B:499:VAL:O	1:B:499:VAL:HG23	2.01	0.61
1:C:497:ILE:HG22	1:C:498:THR:HG23	1.82	0.61
1:F:513:GLN:HG3	1:F:514:GLU:H	1.65	0.61
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.84	0.60
1:E:193:ARG:NH2	1:F:195:GLY:O	2.24	0.60
1:C:485:ASN:HB2	1:C:497:ILE:HG13	1.83	0.60
1:D:256:GLN:HG3	1:D:404:LYS:HD3	1.83	0.60
1:B:320:SER:HA	1:C:254:LEU:HG	1.83	0.60
1:E:22:ARG:NH1	5:E:740:HOH:O	2.35	0.60
1:A:393:ARG:HH21	1:A:429:HIS:HB2	1.66	0.59
1:D:269:ARG:HG2	1:D:479:ILE:HB	1.84	0.59
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.85	0.59
1:A:141:ARG:NH1	5:A:938:HOH:O	2.36	0.59
1:B:202:ASP:HA	1:B:226:ARG:HD2	1.85	0.59
1:C:499:VAL:HG13	1:C:499:VAL:O	2.03	0.59
1:C:40:ARG:NH1	1:C:226:ARG:O	2.34	0.59
1:D:21:MET:HB2	1:D:38:ILE:HG12	1.85	0.59
1:D:290:THR:HG21	1:E:431:SER:HB2	1.85	0.59
1:E:426:THR:HG21	1:E:430:ILE:HG12	1.85	0.59
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.84	0.59
1:A:371:LYS:NZ	5:A:968:HOH:O	2.36	0.58
1:B:496:ARG:HH11	1:B:496:ARG:HB3	1.68	0.58
1:C:72:VAL:N	5:C:715:HOH:O	2.34	0.58
1:B:499:VAL:O	1:B:501:GLU:HB3	2.04	0.58
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.83	0.58
1:E:40:ARG:HG2	1:E:172:LYS:HE3	1.84	0.58
1:A:31:ILE:HG23	1:A:231:MET:HB2	1.84	0.58
1:F:209:ASN:O	1:F:216:ARG:NH1	2.35	0.58
1:C:452:ALA:HA	1:C:469:GLU:HA	1.85	0.58
1:E:164:LEU:HD11	1:E:197:GLU:HG3	1.86	0.58
1:E:320:SER:HA	1:F:254:LEU:HG	1.85	0.58
1:D:164:LEU:HD11	1:D:197:GLU:HG3	1.85	0.57
1:A:195:GLY:O	1:F:193:ARG:NH2	2.26	0.57
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.69	0.57
1:F:404:LYS:NZ	5:F:742:HOH:O	2.38	0.57
1:F:452:ALA:HA	1:F:469:GLU:HA	1.86	0.57
1:A:164:LEU:HD11	1:A:197:GLU:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLU:HG3	1:C:193:ARG:HE	1.69	0.57
1:C:42:THR:HA	1:C:203:ASN:HB2	1.86	0.57
1:E:385:ARG:NH2	5:E:723:HOH:O	2.37	0.57
1:C:305:ALA:HB2	1:C:374:ARG:HD2	1.87	0.57
1:D:215:ARG:NH2	1:E:234:GLU:O	2.38	0.57
1:A:254:LEU:HG	1:F:320:SER:HA	1.88	0.56
1:A:294:LYS:N	3:A:802:ATP:O2B	2.38	0.56
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.69	0.56
1:B:89:SER:OG	3:B:603:ATP:N6	2.33	0.56
1:D:148:THR:HG21	1:D:193:ARG:HD2	1.87	0.56
1:E:304:ASN:OD1	1:E:374:ARG:NH2	2.39	0.56
1:A:318:GLU:OE2	1:B:432:TPO:O1P	2.24	0.56
1:E:364:LYS:NZ	5:E:711:HOH:O	2.38	0.56
1:C:287:THR:HG23	1:C:414:ASN:HB3	1.88	0.56
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.87	0.56
1:B:183:GLU:OE2	1:C:161:ARG:NH1	2.25	0.55
1:D:70:PRO:HB2	1:D:139:ALA:HA	1.88	0.55
1:C:498:THR:O	1:C:499:VAL:HG12	2.06	0.55
1:D:283:ILE:H	1:D:435:ASP:HB2	1.72	0.55
1:A:487:GLU:HG3	1:A:497:ILE:HG12	1.88	0.55
1:B:446:ARG:HH21	1:B:496:ARG:NH2	2.03	0.55
1:E:301:PHE:O	1:E:374:ARG:NH1	2.39	0.55
1:A:135:GLN:NE2	5:A:943:HOH:O	2.40	0.54
1:D:304:ASN:HB3	1:D:374:ARG:HH12	1.72	0.54
1:E:294:LYS:N	3:E:602:ATP:O2B	2.41	0.54
1:E:146:SER:H	1:E:181:THR:HB	1.71	0.54
1:B:497:ILE:O	1:B:498:THR:OG1	2.21	0.54
1:D:325:LEU:HD22	1:D:336:GLU:HG2	1.89	0.54
1:A:56:SER:HB2	1:A:143:SER:HB3	1.89	0.54
1:A:325:LEU:HD22	1:A:336:GLU:HG2	1.90	0.54
1:B:123:LEU:HD12	1:B:166:ARG:HD2	1.89	0.54
1:B:225:LEU:N	5:B:729:HOH:O	2.24	0.54
1:F:127:ILE:HD11	1:F:167:LEU:HA	1.90	0.54
1:C:14:GLU:HG3	1:C:16:GLN:H	1.74	0.53
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.74	0.53
1:C:89:SER:OG	3:C:603:ATP:N6	2.29	0.53
1:C:404:LYS:NZ	5:C:777:HOH:O	2.40	0.53
1:F:122:ASP:O	1:F:126:LEU:N	2.37	0.53
1:B:21:MET:HB2	1:B:38:ILE:HG12	1.90	0.53
1:D:193:ARG:NH2	1:E:195:GLY:O	2.24	0.53
1:E:300:ARG:HA	1:E:333:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:HA	1:A:226:ARG:HD2	1.90	0.53
1:A:509:VAL:O	1:A:511:GLY:N	2.42	0.53
1:C:97:LEU:HB3	5:C:735:HOH:O	2.07	0.53
1:C:313:ILE:HD11	1:C:370:PHE:HB3	1.90	0.53
1:D:183:GLU:OE2	1:E:161:ARG:NH1	2.34	0.53
1:A:224:LYS:NZ	3:A:804:ATP:O3G	2.33	0.53
1:E:215:ARG:NH2	1:F:234:GLU:O	2.41	0.53
1:C:421:GLY:HA2	1:C:490:ILE:O	2.09	0.53
1:D:209:ASN:O	1:D:216:ARG:NH1	2.39	0.53
1:A:320:SER:HA	1:B:254:LEU:HG	1.91	0.53
1:C:87:ALA:HB1	1:C:92:TRP:CD1	2.44	0.53
1:C:171:LEU:HD13	1:C:178:THR:HG21	1.90	0.53
1:F:117:VAL:HA	1:F:154:TYR:HE2	1.74	0.53
1:F:301:PHE:O	1:F:374:ARG:NH1	2.39	0.52
1:B:84:ILE:HG23	1:B:94:LEU:HB2	1.90	0.52
1:C:183:GLU:OE2	1:D:161:ARG:NH1	2.33	0.52
1:F:393:ARG:HH21	1:F:429:HIS:HB2	1.73	0.52
1:B:185:ILE:HD11	1:B:193:ARG:HG2	1.90	0.52
1:C:300:ARG:HA	1:C:333:MET:HE1	1.91	0.52
1:A:215:ARG:NH2	1:B:234:GLU:O	2.43	0.52
1:A:301:PHE:O	1:A:374:ARG:NH1	2.41	0.52
1:D:225:LEU:HD12	1:D:230:HIS:HB3	1.91	0.52
1:C:209:ASN:O	1:C:216:ARG:NH1	2.42	0.52
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.75	0.52
1:B:89:SER:HG	3:B:603:ATP:HN61	1.52	0.52
1:B:191:ILE:HB	1:B:198:GLU:HG2	1.90	0.52
1:F:435:ASP:OD1	1:F:459:ARG:NH1	2.42	0.52
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.92	0.52
1:A:432:TPO:O2P	1:F:379:SER:OG	2.23	0.52
1:B:319:GLU:OE2	5:B:720:HOH:O	2.19	0.52
1:B:300:ARG:HA	1:B:333:MET:HE1	1.92	0.51
1:E:344:LEU:HD22	1:E:345:LYS:H	1.75	0.51
1:A:72:VAL:HB	1:A:142:VAL:HG22	1.91	0.51
1:B:443:VAL:HG12	1:B:445:ILE:HG12	1.92	0.51
1:D:208:ARG:NH2	1:D:221:GLU:OE2	2.33	0.51
1:A:58:GLN:O	1:A:62:ASN:ND2	2.42	0.51
1:D:434:THR:OG1	1:D:435:ASP:HA	2.09	0.51
1:F:287:THR:HG23	1:F:414:ASN:HB3	1.92	0.51
1:C:469:GLU:HG3	1:C:480:LYS:HE3	1.92	0.51
1:E:40:ARG:NH1	1:E:226:ARG:O	2.44	0.51
1:E:344:LEU:HD22	1:E:345:LYS:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:CYS:HG	1:F:278:PHE:HE1	1.59	0.51
1:A:118:VAL:HG12	1:A:121:PHE:HE1	1.74	0.51
1:B:499:VAL:O	1:B:501:GLU:CB	2.59	0.51
1:C:267:VAL:HB	1:C:270:LEU:HB2	1.93	0.51
1:D:320:SER:HA	1:E:254:LEU:HG	1.93	0.51
1:D:56:SER:HB2	1:D:143:SER:HB3	1.93	0.51
1:A:146:SER:H	1:A:181:THR:HB	1.76	0.50
1:C:52:LYS:N	3:C:603:ATP:O2B	2.44	0.50
1:D:298:VAL:HG13	1:D:376:ALA:HB1	1.92	0.50
1:B:309:LYS:NZ	5:B:727:HOH:O	2.42	0.50
1:B:493:SER:HB3	1:C:488:ARG:HG2	1.91	0.50
1:C:74:VAL:HG22	1:C:106:LEU:HD23	1.94	0.50
1:B:497:ILE:HD12	1:B:497:ILE:C	2.32	0.50
1:C:186:GLU:OE2	1:C:187:GLU:N	2.45	0.50
1:E:284:ILE:N	5:E:730:HOH:O	2.44	0.50
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.93	0.50
1:C:24:MET:HB2	1:C:62:ASN:HB3	1.94	0.50
1:A:304:ASN:OD1	1:A:374:ARG:NH2	2.45	0.50
1:B:193:ARG:NH1	5:B:701:HOH:O	2.43	0.50
1:A:218:ARG:NH2	5:A:915:HOH:O	2.45	0.49
1:A:85:LYS:HE3	1:B:18:ILE:HD13	1.93	0.49
1:A:489:ILE:HA	1:A:494:PRO:HG3	1.93	0.49
1:B:499:VAL:O	1:B:501:GLU:CA	2.58	0.49
1:E:503:SER:CB	1:E:504:GLU:HB2	2.21	0.49
1:F:311:ARG:HD2	1:F:371:LYS:HE3	1.93	0.49
1:D:248:PRO:HB2	1:D:251:ALA:HB3	1.94	0.49
1:A:89:SER:OG	3:A:803:ATP:N6	2.44	0.49
1:C:356:LEU:HD22	1:C:387:VAL:HG11	1.94	0.49
1:D:184:ARG:HH21	1:D:191:ILE:HA	1.77	0.49
1:E:216:ARG:NE	1:F:221:GLU:OE1	2.38	0.49
1:B:31:ILE:HG23	1:B:231:MET:HB2	1.95	0.49
1:B:435:ASP:OD1	1:B:459:ARG:NH1	2.45	0.49
1:F:514:GLU:OE1	1:F:515:LYS:N	2.45	0.49
1:E:311:ARG:HD2	1:E:371:LYS:HE3	1.93	0.49
1:C:360:LEU:HD11	1:C:398:GLY:HA3	1.95	0.48
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.95	0.48
1:F:356:LEU:HD22	1:F:387:VAL:HG11	1.95	0.48
1:F:504:GLU:HA	1:F:507:ARG:HE	1.78	0.48
1:C:211:LEU:HA	1:C:216:ARG:HD3	1.96	0.48
1:F:117:VAL:HA	1:F:154:TYR:CE2	2.49	0.48
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.94	0.48
1:E:186:GLU:OE2	1:E:187:GLU:N	2.46	0.48
1:B:127:ILE:HD13	1:B:170:ARG:HG3	1.94	0.48
1:C:320:SER:HB3	1:D:256:GLN:HG2	1.96	0.48
1:B:294:LYS:HG3	1:B:440:LEU:HD12	1.95	0.48
3:C:602:ATP:O1G	1:D:459:ARG:NH1	2.46	0.48
1:F:20:LYS:HE3	1:F:228:THR:HG21	1.94	0.48
1:D:300:ARG:HA	1:D:333:MET:HE1	1.95	0.48
1:F:166:ARG:NH2	5:F:743:HOH:O	2.46	0.48
1:A:432:TPO:HG22	1:A:433:ILE:HG13	1.96	0.48
1:C:304:ASN:HB3	1:C:374:ARG:HH12	1.79	0.48
1:C:469:GLU:HB3	1:C:483:PHE:CZ	2.48	0.48
1:E:183:GLU:OE2	1:F:161:ARG:NH1	2.28	0.48
1:E:290:THR:HG21	1:F:431:SER:HB2	1.95	0.48
1:F:53:THR:OG1	5:F:715:HOH:O	2.20	0.48
1:B:497:ILE:HD12	1:B:498:THR:C	2.34	0.47
1:C:320:SER:HA	1:D:254:LEU:HG	1.94	0.47
1:F:225:LEU:HD12	1:F:230:HIS:HB3	1.96	0.47
1:C:426:THR:HG21	1:C:430:ILE:HG12	1.95	0.47
1:C:497:ILE:O	1:C:498:THR:HG22	2.14	0.47
1:A:471:MET:HG3	1:A:478:ASP:HB3	1.96	0.47
1:B:426:THR:HG21	1:B:430:ILE:HG12	1.96	0.47
1:C:326:ARG:NH2	5:D:753:HOH:O	2.46	0.47
1:D:426:THR:HG22	1:D:428:SER:H	1.78	0.47
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.95	0.47
1:F:70:PRO:HB2	1:F:139:ALA:HA	1.96	0.47
1:F:164:LEU:HD11	1:F:197:GLU:HG3	1.96	0.47
1:B:56:SER:HB2	1:B:143:SER:HB3	1.96	0.47
1:E:225:LEU:HD12	1:E:230:HIS:HB3	1.96	0.47
1:B:84:ILE:HA	1:B:94:LEU:HD12	1.97	0.47
1:E:461:SER:OG	1:E:462:TRP:N	2.48	0.47
1:A:82:ASP:HA	1:A:85:LYS:HB3	1.96	0.47
1:A:264:SER:O	1:A:374:ARG:NH2	2.48	0.47
1:A:300:ARG:NE	5:A:949:HOH:O	2.44	0.47
1:D:436:THR:HG23	1:D:458:MET:HG2	1.96	0.47
1:B:263:VAL:HB	1:B:374:ARG:HH21	1.80	0.46
1:C:264:SER:O	1:C:374:ARG:NH2	2.48	0.46
1:E:377:ILE:HD12	1:E:412:PHE:HE1	1.80	0.46
1:D:186:GLU:OE2	1:D:187:GLU:N	2.47	0.46
1:D:396:VAL:HG11	1:D:430:ILE:HG23	1.97	0.46
1:C:84:ILE:HG21	1:C:95:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.97	0.46
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.96	0.46
1:A:117:VAL:HA	1:A:154:TYR:OH	2.16	0.46
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.97	0.46
1:E:31:ILE:HG23	1:E:231:MET:HB2	1.95	0.46
1:B:204:VAL:HG23	1:B:224:LYS:HE2	1.97	0.46
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.97	0.46
1:F:217:ARG:NH2	1:F:394:GLN:OE1	2.48	0.46
1:C:344:LEU:HD22	1:C:345:LYS:N	2.31	0.46
1:E:393:ARG:HH21	1:E:429:HIS:HB2	1.79	0.46
1:C:393:ARG:NH2	1:C:429:HIS:HB2	2.29	0.46
1:E:144:ILE:N	5:E:743:HOH:O	2.30	0.46
1:E:443:VAL:HG12	1:E:445:ILE:HG12	1.97	0.46
1:B:40:ARG:NH1	1:B:226:ARG:O	2.48	0.46
1:C:225:LEU:HD12	1:C:230:HIS:HB3	1.98	0.46
1:D:418:GLN:HB2	1:E:423:HIS:O	2.16	0.46
1:E:426:THR:HG22	1:E:428:SER:H	1.81	0.46
1:A:234:GLU:O	1:F:215:ARG:NH2	2.49	0.46
1:C:301:PHE:O	1:C:374:ARG:NH1	2.42	0.46
1:D:170:ARG:O	1:D:174:ILE:HG12	2.15	0.46
1:E:212:GLU:O	1:E:212:GLU:HG2	2.16	0.46
1:E:264:SER:O	1:E:374:ARG:NH2	2.49	0.46
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.97	0.45
1:C:64:ILE:HG21	5:C:735:HOH:O	2.16	0.45
1:C:148:THR:HG23	1:C:194:TYR:HE2	1.81	0.45
1:D:267:VAL:HG12	1:D:270:LEU:H	1.80	0.45
1:E:56:SER:HB2	1:E:143:SER:HB3	1.97	0.45
1:D:296:LEU:HD11	1:D:477:PRO:HD3	1.97	0.45
1:F:16:GLN:NE2	1:F:33:HIS:HB3	2.31	0.45
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.97	0.45
1:D:267:VAL:HB	1:D:270:LEU:HB2	1.99	0.45
1:F:121:PHE:HD1	1:F:121:PHE:HA	1.67	0.45
1:F:461:SER:OG	1:F:462:TRP:N	2.50	0.45
1:C:64:ILE:HD13	5:C:735:HOH:O	2.15	0.45
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.99	0.45
1:C:18:ILE:HB	1:C:228:THR:HG23	1.99	0.45
1:A:427:ASP:OD1	1:A:427:ASP:N	2.39	0.45
1:C:193:ARG:NH2	1:D:195:GLY:O	2.23	0.45
1:C:488:ARG:HH22	1:D:488:ARG:HH21	1.64	0.45
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.97	0.45
1:E:142:VAL:HB	1:E:178:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:HB	1:A:228:THR:HG23	1.98	0.45
1:A:54:LEU:N	3:A:803:ATP:O2A	2.45	0.45
1:A:422:VAL:O	1:A:424:SER:N	2.50	0.45
1:C:311:ARG:HD2	1:C:371:LYS:HE3	1.98	0.45
3:A:803:ATP:O3'	5:A:915:HOH:O	2.20	0.45
1:B:170:ARG:O	1:B:174:ILE:HG12	2.16	0.45
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.99	0.45
1:A:422:VAL:C	1:A:424:SER:H	2.20	0.45
1:C:483:PHE:HB2	1:C:489:ILE:HD13	1.98	0.45
1:D:325:LEU:HD23	1:D:335:PHE:HB2	1.99	0.45
1:F:445:ILE:HA	1:F:496:ARG:HH12	1.82	0.45
1:F:515:LYS:HA	1:F:516:GLY:HA3	1.88	0.45
1:C:419:PHE:H	1:C:419:PHE:HD1	1.64	0.45
1:A:216:ARG:NE	1:B:221:GLU:OE1	2.38	0.44
1:B:73:PHE:O	1:B:106:LEU:N	2.49	0.44
1:D:283:ILE:O	1:D:435:ASP:N	2.31	0.44
1:E:433:ILE:O	5:E:703:HOH:O	2.21	0.44
1:C:500:ASP:HB3	1:C:501:GLU:H	1.67	0.44
1:F:325:LEU:HD22	1:F:336:GLU:HG2	1.99	0.44
1:A:315:PHE:HB2	1:A:377:ILE:HA	1.98	0.44
1:D:486:PHE:HE2	1:D:496:ARG:HH11	1.65	0.44
1:A:461:SER:OG	1:A:462:TRP:N	2.50	0.44
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.57	0.44
1:F:331:TRP:NE1	3:F:602:ATP:N7	2.65	0.44
1:F:513:GLN:HG3	1:F:514:GLU:N	2.33	0.44
1:C:73:PHE:O	1:C:106:LEU:N	2.45	0.44
1:E:267:VAL:HB	1:E:270:LEU:HB2	1.99	0.44
1:C:325:LEU:HD21	1:C:336:GLU:HG2	2.00	0.44
1:D:393:ARG:NH2	1:D:432:TPO:O3P	2.50	0.44
1:A:486:PHE:HE2	1:A:496:ARG:HG2	1.83	0.44
1:C:256:GLN:H	1:C:256:GLN:HG2	1.65	0.44
1:D:170:ARG:HH12	1:D:174:ILE:HD11	1.83	0.43
1:D:380:LEU:HD21	1:D:412:PHE:HD2	1.83	0.43
1:E:269:ARG:HB3	1:E:479:ILE:HD12	1.98	0.43
1:E:446:ARG:HH21	1:E:496:ARG:HH22	1.66	0.43
1:B:21:MET:HE1	1:B:141:ARG:HG2	2.00	0.43
1:C:497:ILE:C	1:C:498:THR:CG2	2.86	0.43
1:D:434:THR:HG1	1:D:435:ASP:HA	1.82	0.43
1:F:344:LEU:HD22	1:F:345:LYS:H	1.84	0.43
1:F:344:LEU:HD22	1:F:345:LYS:N	2.33	0.43
1:C:298:VAL:HG13	1:C:376:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ARG:O	1:E:174:ILE:HG12	2.18	0.43
1:F:146:SER:H	1:F:181:THR:HB	1.82	0.43
1:F:418:GLN:HG3	1:F:422:VAL:HB	2.00	0.43
1:B:136:LYS:HE3	1:B:137:TYR:CE2	2.53	0.43
1:C:170:ARG:O	1:C:174:ILE:HG12	2.18	0.43
1:E:178:THR:HG22	5:E:743:HOH:O	2.19	0.43
1:A:84:ILE:HG21	1:A:95:ALA:HB2	2.01	0.43
1:A:170:ARG:HG2	1:F:112:PRO:HB3	1.99	0.43
1:D:426:THR:HG21	1:D:430:ILE:HG12	2.00	0.43
1:E:183:GLU:HG3	1:E:193:ARG:HE	1.83	0.43
1:F:21:MET:N	1:F:36:LEU:O	2.42	0.43
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.43	0.43
1:F:122:ASP:HA	1:F:125:ALA:HB3	2.01	0.43
1:F:504:GLU:O	1:F:506:SER:N	2.51	0.43
1:C:471:MET:HG2	1:C:480:LYS:HD3	2.00	0.43
1:B:146:SER:O	1:B:149:SER:OG	2.36	0.43
1:F:170:ARG:O	1:F:174:ILE:HG12	2.18	0.43
1:A:444:GLU:O	5:A:932:HOH:O	2.21	0.43
1:C:88:ARG:CZ	1:D:15:HIS:HA	2.49	0.43
1:E:356:LEU:HD13	1:E:387:VAL:HG21	2.01	0.42
1:A:203:ASN:ND2	5:A:946:HOH:O	2.51	0.42
1:A:441:GLN:HE22	1:A:490:ILE:HA	1.83	0.42
1:C:385:ARG:HG2	1:D:393:ARG:CZ	2.48	0.42
1:C:488:ARG:NH2	1:D:488:ARG:HH21	2.16	0.42
1:D:344:LEU:HD22	1:D:345:LYS:H	1.84	0.42
1:F:515:LYS:HA	1:F:515:LYS:HD2	1.90	0.42
1:E:123:LEU:HD22	1:E:166:ARG:HD2	2.01	0.42
1:E:385:ARG:NE	1:F:432:TPO:O2P	2.52	0.42
1:C:122:ASP:O	1:C:124:SER:N	2.50	0.42
1:E:147:VAL:O	1:E:150:VAL:HG12	2.20	0.42
1:A:87:ALA:HB1	1:A:92:TRP:CD1	2.55	0.42
1:A:267:VAL:HB	1:A:270:LEU:HB2	2.00	0.42
1:B:215:ARG:NH2	1:C:234:GLU:O	2.52	0.42
1:C:344:LEU:HD22	1:C:345:LYS:H	1.85	0.42
1:C:493:SER:HB3	1:D:488:ARG:HG2	2.02	0.42
1:B:21:MET:SD	1:B:141:ARG:NE	2.91	0.42
1:B:179:VAL:HG11	5:B:726:HOH:O	2.19	0.42
1:D:461:SER:OG	1:D:462:TRP:N	2.53	0.42
1:D:469:GLU:HG3	1:D:480:LYS:HE3	2.02	0.42
1:E:502:LYS:O	1:E:503:SER:HB2	2.20	0.42
1:C:296:LEU:HD11	1:C:477:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ILE:HG23	1:D:372:PRO:HD2	2.01	0.42
1:D:396:VAL:HG12	1:D:433:ILE:HG21	2.02	0.42
1:E:21:MET:HB2	1:E:38:ILE:HG12	2.02	0.42
1:F:231:MET:SD	1:F:251:ALA:HB2	2.60	0.42
1:D:446:ARG:HB3	1:E:484:ARG:HG3	2.01	0.42
1:A:448:GLU:HA	1:B:466:ALA:HA	2.02	0.42
1:B:296:LEU:HD11	1:B:477:PRO:HD3	2.02	0.42
1:B:483:PHE:HB2	1:B:489:ILE:HD13	2.01	0.42
1:C:287:THR:HG21	1:C:425:ILE:O	2.19	0.42
1:E:231:MET:SD	1:E:251:ALA:HB2	2.59	0.42
1:A:74:VAL:HG22	1:A:106:LEU:HD23	2.01	0.41
1:D:111:ASP:HA	1:D:112:PRO:HD3	1.91	0.41
1:B:73:PHE:HE2	1:B:83:ILE:HD13	1.85	0.41
1:D:98:VAL:HA	1:D:103:LEU:O	2.20	0.41
1:E:459:ARG:NH1	5:E:752:HOH:O	2.52	0.41
1:E:469:GLU:HB3	1:E:483:PHE:CZ	2.54	0.41
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.84	0.41
1:B:61:TYR:CZ	1:B:65:ILE:HG13	2.55	0.41
1:B:72:VAL:HB	1:B:142:VAL:HG22	2.02	0.41
1:C:86:ASN:OD1	1:D:40:ARG:NH2	2.40	0.41
1:C:296:LEU:HD13	1:C:331:TRP:CD2	2.56	0.41
1:C:446:ARG:HG2	1:C:496:ARG:NH2	2.35	0.41
1:D:52:LYS:HE3	1:D:52:LYS:HB2	1.89	0.41
1:E:371:LYS:HD2	1:E:371:LYS:O	2.20	0.41
1:B:351:PRO:HB3	1:B:383:LEU:HD23	2.03	0.41
1:D:304:ASN:HB3	1:D:374:ARG:NH1	2.34	0.41
1:E:171:LEU:HD13	1:E:178:THR:HG21	2.01	0.41
1:A:40:ARG:HG2	1:A:172:LYS:HE3	2.03	0.41
1:D:145:ASP:HA	1:D:181:THR:HB	2.01	0.41
1:A:21:MET:HB2	1:A:38:ILE:HG12	2.03	0.41
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.95	0.41
1:B:180:MET:HB3	1:B:180:MET:HE2	1.84	0.41
1:D:464:ASP:OD1	1:D:465:LYS:N	2.53	0.41
1:A:61:TYR:O	1:A:65:ILE:HG12	2.21	0.41
1:A:377:ILE:HD12	1:A:412:PHE:HE1	1.86	0.41
1:B:356:LEU:HD13	1:B:387:VAL:HG21	2.02	0.41
1:C:61:TYR:CZ	1:C:65:ILE:HG13	2.56	0.41
1:D:497:ILE:H	1:D:497:ILE:HG13	1.65	0.41
1:B:147:VAL:O	1:B:150:VAL:HG12	2.21	0.41
1:B:294:LYS:HB2	1:B:294:LYS:HE2	1.87	0.41
1:B:486:PHE:CE1	1:B:496:ARG:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:LYS:HE3	1:E:52:LYS:HB2	1.89	0.41
1:A:20:LYS:HE3	1:A:228:THR:HG21	2.02	0.41
1:B:109:SER:HA	1:B:110:PRO:HD3	1.92	0.41
1:B:122:ASP:O	1:B:126:LEU:N	2.38	0.41
1:B:183:GLU:HG3	1:B:193:ARG:HE	1.84	0.41
1:C:87:ALA:HB1	1:C:92:TRP:HD1	1.84	0.41
1:C:116:GLU:C	1:C:118:VAL:H	2.25	0.41
1:D:122:ASP:HB3	1:D:123:LEU:H	1.56	0.41
1:D:247:PHE:HZ	1:D:361:GLN:HB2	1.86	0.41
1:D:452:ALA:HA	1:D:469:GLU:HA	2.03	0.41
1:E:98:VAL:HA	1:E:103:LEU:O	2.21	0.41
1:E:180:MET:HB3	1:E:180:MET:HE2	1.96	0.41
1:F:56:SER:HB2	1:F:143:SER:HB3	2.03	0.41
1:F:109:SER:HA	1:F:110:PRO:HD3	1.90	0.41
1:A:283:ILE:HD12	1:A:412:PHE:HE2	1.86	0.41
1:D:156:ALA:O	1:D:160:VAL:HG23	2.21	0.41
1:E:24:MET:HB2	1:E:62:ASN:HD22	1.86	0.41
1:E:334:ASP:O	1:E:338:MET:HG2	2.20	0.41
1:E:446:ARG:NH2	1:E:496:ARG:HH22	2.18	0.41
1:F:156:ALA:O	1:F:160:VAL:HG23	2.21	0.41
1:A:147:VAL:O	1:A:150:VAL:HG12	2.22	0.40
1:D:433:ILE:O	1:D:434:THR:HG22	2.21	0.40
1:C:52:LYS:HB2	1:C:52:LYS:HE3	1.82	0.40
1:C:334:ASP:O	1:C:338:MET:HG2	2.21	0.40
1:D:89:SER:HB2	1:E:227:GLY:O	2.21	0.40
1:E:129:ARG:NH1	5:E:746:HOH:O	2.33	0.40
1:E:436:THR:HG23	1:E:458:MET:HG2	2.02	0.40
1:F:337:GLU:HA	1:F:340:ARG:HD2	2.02	0.40
1:C:111:ASP:HA	1:C:112:PRO:HD3	1.85	0.40
1:D:21:MET:HE1	1:D:141:ARG:HG2	2.03	0.40
1:F:18:ILE:HG21	1:F:37:PRO:HB3	2.02	0.40
3:A:802:ATP:C2	1:B:462:TRP:HA	2.56	0.40
1:B:298:VAL:HG13	1:B:376:ALA:HB1	2.03	0.40
1:C:125:ALA:O	1:C:129:ARG:HG3	2.22	0.40
1:E:452:ALA:HA	1:E:469:GLU:HA	2.03	0.40
1:F:136:LYS:NZ	5:F:745:HOH:O	2.37	0.40

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	503/512 (98%)	448 (89%)	39 (8%)	16 (3%)	4	24
1	B	486/512 (95%)	449 (92%)	28 (6%)	9 (2%)	8	34
1	C	485/512 (95%)	442 (91%)	31 (6%)	12 (2%)	5	29
1	D	482/512 (94%)	448 (93%)	27 (6%)	7 (2%)	10	39
1	E	489/512 (96%)	442 (90%)	37 (8%)	10 (2%)	7	33
1	F	503/512 (98%)	452 (90%)	37 (7%)	14 (3%)	5	26
All	All	2948/3072 (96%)	2681 (91%)	199 (7%)	68 (2%)	6	31

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ILE
1	C	17	ALA
1	C	117	VAL
1	E	463	HIS
1	F	154	TYR
1	F	517	PRO
1	A	154	TYR
1	A	211	LEU
1	A	463	HIS
1	A	498	THR
1	A	510	ARG
1	B	154	TYR
1	C	211	LEU
1	C	463	HIS
1	D	211	LEU
1	D	463	HIS
1	E	154	TYR
1	E	211	LEU
1	E	504	GLU
1	F	211	LEU

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Mol	Chain	Res	Type
1	F	463	HIS
1	A	212	GLU
1	A	348	CYS
1	A	423	HIS
1	A	500	ASP
1	B	211	LEU
1	B	212	GLU
1	B	348	CYS
1	B	420	MET
1	B	463	HIS
1	B	498	THR
1	C	115	GLN
1	C	154	TYR
1	C	212	GLU
1	C	420	MET
1	D	26	GLU
1	D	154	TYR
1	D	348	CYS
1	D	420	MET
1	E	113	GLU
1	E	212	GLU
1	E	348	CYS
1	E	420	MET
1	E	498	THR
1	F	212	GLU
1	F	348	CYS
1	F	504	GLU
1	F	507	ARG
1	A	420	MET
1	B	424	SER
1	C	348	CYS
1	D	212	GLU
1	F	118	VAL
1	F	420	MET
1	F	509	VAL
1	A	26	GLU
1	A	117	VAL
1	A	511	GLY
1	B	119	GLY
1	C	123	LEU
1	F	508	ILE
1	A	501	GLU

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Mol	Chain	Res	Type
1	C	422	VAL
1	C	500	ASP
1	F	117	VAL
1	E	497	ILE
1	A	120	GLY
1	F	120	GLY

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	432/438 (99%)	411 (95%)	21 (5%)	25	57
1	B	417/438 (95%)	395 (95%)	22 (5%)	22	54
1	C	416/438 (95%)	392 (94%)	24 (6%)	20	52
1	D	413/438 (94%)	394 (95%)	19 (5%)	27	59
1	E	420/438 (96%)	400 (95%)	20 (5%)	25	57
1	F	431/438 (98%)	405 (94%)	26 (6%)	19	50
All	All	2529/2628 (96%)	2397 (95%)	132 (5%)	23	55

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	26	GLU
1	A	79	THR
1	A	92	TRP
1	A	99	ASP
1	A	118	VAL
1	A	123	LEU
1	A	186	GLU
1	A	212	GLU
1	A	256	GLN
1	A	270	LEU
1	A	287	THR

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Mol	Chain	Res	Type
1	A	342	ASN
1	A	360	LEU
1	A	371	LYS
1	A	425	ILE
1	A	426	THR
1	A	427	ASP
1	A	434	THR
1	A	462	TRP
1	A	508	ILE
1	B	26	GLU
1	B	33	HIS
1	B	81	GLN
1	B	92	TRP
1	B	123	LEU
1	B	154	TYR
1	B	178	THR
1	B	182	THR
1	B	185	ILE
1	B	186	GLU
1	B	212	GLU
1	B	223	LEU
1	B	256	GLN
1	B	263	VAL
1	B	270	LEU
1	B	371	LYS
1	B	375	ILE
1	B	406	GLU
1	B	471	MET
1	B	496	ARG
1	B	501	GLU
1	B	502	LYS
1	C	26	GLU
1	C	81	GLN
1	C	99	ASP
1	C	111	ASP
1	C	154	TYR
1	C	178	THR
1	C	185	ILE
1	C	186	GLU
1	C	212	GLU
1	C	218	ARG
1	C	223	LEU

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Mol	Chain	Res	Type
1	C	256	GLN
1	C	263	VAL
1	C	270	LEU
1	C	287	THR
1	C	325	LEU
1	C	333	MET
1	C	360	LEU
1	C	371	LYS
1	C	375	ILE
1	C	419	PHE
1	C	470	PHE
1	C	471	MET
1	C	500	ASP
1	D	26	GLU
1	D	81	GLN
1	D	122	ASP
1	D	123	LEU
1	D	178	THR
1	D	184	ARG
1	D	186	GLU
1	D	212	GLU
1	D	218	ARG
1	D	223	LEU
1	D	256	GLN
1	D	263	VAL
1	D	270	LEU
1	D	321	ARG
1	D	360	LEU
1	D	371	LYS
1	D	423	HIS
1	D	434	THR
1	D	496	ARG
1	E	81	GLN
1	E	113	GLU
1	E	121	PHE
1	E	154	TYR
1	E	178	THR
1	E	186	GLU
1	E	212	GLU
1	E	223	LEU
1	E	228	THR
1	E	256	GLN

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Mol	Chain	Res	Type
1	E	270	LEU
1	E	325	LEU
1	E	333	MET
1	E	342	ASN
1	E	371	LYS
1	E	423	HIS
1	E	471	MET
1	E	474	ASP
1	E	497	ILE
1	E	499	VAL
1	F	26	GLU
1	F	79	THR
1	F	116	GLU
1	F	121	PHE
1	F	123	LEU
1	F	135	GLN
1	F	140	ARG
1	F	186	GLU
1	F	212	GLU
1	F	218	ARG
1	F	256	GLN
1	F	263	VAL
1	F	270	LEU
1	F	287	THR
1	F	300	ARG
1	F	333	MET
1	F	371	LYS
1	F	423	HIS
1	F	462	TRP
1	F	471	MET
1	F	496	ARG
1	F	501	GLU
1	F	504	GLU
1	F	509	VAL
1	F	514	GLU
1	F	515	LYS

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	E	432	1	8,10,11	1.07	0	10,14,16	1.88	2 (20%)
1	TPO	B	432	1	8,10,11	1.59	1 (12%)	10,14,16	1.81	2 (20%)
1	TPO	A	432	1	8,10,11	1.58	1 (12%)	10,14,16	1.91	2 (20%)
1	TPO	F	432	1	8,10,11	1.07	0	10,14,16	1.91	2 (20%)
1	TPO	D	432	1	8,10,11	1.10	0	10,14,16	2.00	2 (20%)
1	TPO	C	432	1	8,10,11	1.57	1 (12%)	10,14,16	1.94	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
1	TPO	E	432	1	-	0/9/11/13	-
1	TPO	B	432	1	-	3/9/11/13	-
1	TPO	A	432	1	-	2/9/11/13	-
1	TPO	F	432	1	-	2/9/11/13	-
1	TPO	D	432	1	-	4/9/11/13	-
1	TPO	C	432	1	-	3/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	432	TPO	P-O1P	3.38	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	TPO	P-O1P	3.36	1.61	1.50
1	C	432	TPO	P-O1P	3.33	1.61	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	432	TPO	P-OG1-CB	-5.37	106.98	123.21
1	D	432	TPO	P-OG1-CB	-5.32	107.15	123.21
1	F	432	TPO	P-OG1-CB	-5.25	107.36	123.21
1	A	432	TPO	P-OG1-CB	-5.22	107.45	123.21
1	E	432	TPO	P-OG1-CB	-5.12	107.73	123.21
1	B	432	TPO	P-OG1-CB	-4.93	108.31	123.21
1	D	432	TPO	CG2-CB-CA	-2.66	107.91	113.16
1	A	432	TPO	CG2-CB-CA	-2.24	108.75	113.16
1	E	432	TPO	CG2-CB-CA	-2.17	108.89	113.16
1	F	432	TPO	CG2-CB-CA	-2.12	108.97	113.16
1	B	432	TPO	CG2-CB-CA	-2.07	109.08	113.16
1	C	432	TPO	CG2-CB-CA	-2.06	109.09	113.16

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	432	TPO	N-CA-CB-OG1
1	A	432	TPO	O-C-CA-CB
1	B	432	TPO	N-CA-CB-CG2
1	B	432	TPO	N-CA-CB-OG1
1	D	432	TPO	N-CA-CB-CG2
1	D	432	TPO	N-CA-CB-OG1
1	D	432	TPO	C-CA-CB-CG2
1	C	432	TPO	CB-OG1-P-O3P
1	C	432	TPO	N-CA-CB-CG2
1	B	432	TPO	CB-OG1-P-O1P
1	F	432	TPO	CB-OG1-P-O1P
1	C	432	TPO	CB-OG1-P-O2P
1	F	432	TPO	CB-OG1-P-O2P
1	D	432	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 7 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	E	603	-	26,33,33	0.94	1 (3%)	31,52,52	1.53	5 (16%)
3	ATP	A	803	-	26,33,33	0.95	1 (3%)	31,52,52	1.48	5 (16%)
4	PO4	B	604	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	C	604	-	4,4,4	0.94	0	6,6,6	0.44	0
3	ATP	F	602	2	26,33,33	0.94	1 (3%)	31,52,52	1.53	5 (16%)
3	ATP	D	603	-	26,33,33	0.96	1 (3%)	31,52,52	1.51	5 (16%)
3	ATP	A	804	-	26,33,33	0.95	1 (3%)	31,52,52	1.51	5 (16%)
4	PO4	E	605	-	4,4,4	0.93	0	6,6,6	0.43	0
4	PO4	F	603	-	4,4,4	0.93	0	6,6,6	0.41	0
4	PO4	B	605	-	4,4,4	0.94	0	6,6,6	0.43	0
3	ATP	C	602	2	26,33,33	0.96	1 (3%)	31,52,52	1.53	5 (16%)
3	ATP	E	602	2	26,33,33	0.95	1 (3%)	31,52,52	1.48	5 (16%)
3	ATP	A	802	2	26,33,33	0.94	1 (3%)	31,52,52	1.40	4 (12%)
3	ATP	D	602	2	26,33,33	0.94	1 (3%)	31,52,52	1.49	5 (16%)
3	ATP	C	603	-	26,33,33	0.94	1 (3%)	31,52,52	1.45	5 (16%)
4	PO4	E	604	-	4,4,4	0.93	0	6,6,6	0.45	0
3	ATP	B	603	-	26,33,33	0.95	1 (3%)	31,52,52	1.56	6 (19%)
4	PO4	D	604	-	4,4,4	0.93	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ATP	B	602	2	26,33,33	0.94	1 (3%)	31,52,52	1.35	4 (12%)
4	PO4	F	604	-	4,4,4	0.93	0	6,6,6	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	804	-	-	5/18/38/38	0/3/3/3
3	ATP	E	603	-	-	3/18/38/38	0/3/3/3
3	ATP	A	803	-	-	3/18/38/38	0/3/3/3
3	ATP	B	602	2	-	7/18/38/38	0/3/3/3
3	ATP	A	802	2	-	3/18/38/38	0/3/3/3
3	ATP	C	602	2	-	3/18/38/38	0/3/3/3
3	ATP	C	603	-	-	5/18/38/38	0/3/3/3
3	ATP	D	602	2	-	8/18/38/38	0/3/3/3
3	ATP	B	603	-	-	3/18/38/38	0/3/3/3
3	ATP	F	602	2	-	5/18/38/38	0/3/3/3
3	ATP	D	603	-	-	4/18/38/38	0/3/3/3
3	ATP	E	602	2	-	1/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	ATP	C5-C4	2.57	1.47	1.40
3	D	603	ATP	C5-C4	2.56	1.47	1.40
3	C	602	ATP	C5-C4	2.55	1.47	1.40
3	D	602	ATP	C5-C4	2.54	1.47	1.40
3	A	803	ATP	C5-C4	2.54	1.47	1.40
3	A	802	ATP	C5-C4	2.53	1.47	1.40
3	C	603	ATP	C5-C4	2.52	1.47	1.40
3	A	804	ATP	C5-C4	2.52	1.47	1.40
3	B	602	ATP	C5-C4	2.52	1.47	1.40
3	E	602	ATP	C5-C4	2.51	1.47	1.40
3	B	603	ATP	C5-C4	2.49	1.47	1.40
3	E	603	ATP	C5-C4	2.49	1.47	1.40

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	ATP	PB-O3B-PG	-3.74	119.99	132.83
3	F	602	ATP	C3'-C2'-C1'	3.50	106.24	100.98
3	D	602	ATP	C3'-C2'-C1'	3.48	106.22	100.98
3	B	603	ATP	PB-O3B-PG	-3.48	120.90	132.83
3	B	602	ATP	C3'-C2'-C1'	3.46	106.18	100.98
3	A	802	ATP	C3'-C2'-C1'	3.46	106.18	100.98
3	E	602	ATP	C3'-C2'-C1'	3.44	106.16	100.98
3	C	602	ATP	PB-O3B-PG	-3.42	121.08	132.83
3	E	603	ATP	PB-O3B-PG	-3.42	121.09	132.83
3	C	602	ATP	C3'-C2'-C1'	3.32	105.97	100.98
3	A	804	ATP	PB-O3B-PG	-3.31	121.46	132.83
3	D	602	ATP	PB-O3B-PG	-3.29	121.54	132.83
3	A	803	ATP	C3'-C2'-C1'	3.28	105.92	100.98
3	E	602	ATP	PB-O3B-PG	-3.28	121.57	132.83
3	B	603	ATP	PA-O3A-PB	-3.24	121.72	132.83
3	E	603	ATP	C3'-C2'-C1'	3.19	105.79	100.98
3	D	603	ATP	C3'-C2'-C1'	3.19	105.78	100.98
3	B	603	ATP	N3-C2-N1	-3.19	123.70	128.68
3	C	603	ATP	PB-O3B-PG	-3.16	121.97	132.83
3	E	602	ATP	N3-C2-N1	-3.16	123.74	128.68
3	E	603	ATP	PA-O3A-PB	-3.16	121.98	132.83
3	B	603	ATP	C3'-C2'-C1'	3.16	105.73	100.98
3	A	803	ATP	N3-C2-N1	-3.15	123.76	128.68
3	C	603	ATP	N3-C2-N1	-3.13	123.79	128.68
3	B	602	ATP	N3-C2-N1	-3.13	123.79	128.68
3	E	603	ATP	N3-C2-N1	-3.12	123.80	128.68
3	A	804	ATP	N3-C2-N1	-3.12	123.80	128.68
3	A	802	ATP	N3-C2-N1	-3.11	123.81	128.68
3	D	603	ATP	PA-O3A-PB	-3.11	122.17	132.83
3	C	603	ATP	C3'-C2'-C1'	3.10	105.65	100.98
3	D	602	ATP	N3-C2-N1	-3.10	123.84	128.68
3	D	603	ATP	PB-O3B-PG	-3.10	122.20	132.83
3	D	603	ATP	N3-C2-N1	-3.08	123.87	128.68
3	F	602	ATP	N3-C2-N1	-3.07	123.87	128.68
3	C	602	ATP	N3-C2-N1	-3.06	123.90	128.68
3	A	804	ATP	PA-O3A-PB	-3.04	122.39	132.83
3	A	804	ATP	C3'-C2'-C1'	3.01	105.51	100.98
3	D	603	ATP	C4-C5-N7	-2.98	106.29	109.40
3	A	803	ATP	PB-O3B-PG	-2.98	122.60	132.83
3	C	603	ATP	C4-C5-N7	-2.96	106.31	109.40
3	A	804	ATP	C4-C5-N7	-2.96	106.32	109.40
3	C	602	ATP	PA-O3A-PB	-2.96	122.67	132.83
3	E	603	ATP	C4-C5-N7	-2.87	106.40	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	603	ATP	C4-C5-N7	-2.87	106.41	109.40
3	C	602	ATP	C4-C5-N7	-2.87	106.41	109.40
3	A	803	ATP	PA-O3A-PB	-2.84	123.08	132.83
3	F	602	ATP	C4-C5-N7	-2.78	106.50	109.40
3	A	803	ATP	C4-C5-N7	-2.77	106.52	109.40
3	E	602	ATP	C4-C5-N7	-2.76	106.52	109.40
3	D	602	ATP	C4-C5-N7	-2.76	106.52	109.40
3	B	602	ATP	C4-C5-N7	-2.74	106.54	109.40
3	A	802	ATP	C4-C5-N7	-2.73	106.55	109.40
3	A	802	ATP	PB-O3B-PG	-2.60	123.91	132.83
3	F	602	ATP	PA-O3A-PB	-2.54	124.12	132.83
3	D	602	ATP	PA-O3A-PB	-2.47	124.34	132.83
3	E	602	ATP	PA-O3A-PB	-2.31	124.89	132.83
3	B	602	ATP	PB-O3B-PG	-2.18	125.34	132.83
3	C	603	ATP	PA-O3A-PB	-2.05	125.78	132.83
3	B	603	ATP	O3G-PG-O2G	2.01	115.31	107.64

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	ATP	C5'-O5'-PA-O1A
3	A	803	ATP	C5'-O5'-PA-O2A
3	A	804	ATP	C5'-O5'-PA-O1A
3	A	804	ATP	C5'-O5'-PA-O2A
3	B	602	ATP	PB-O3A-PA-O5'
3	B	602	ATP	C5'-O5'-PA-O1A
3	B	603	ATP	C5'-O5'-PA-O1A
3	B	603	ATP	C5'-O5'-PA-O2A
3	C	602	ATP	C5'-O5'-PA-O1A
3	C	602	ATP	C5'-O5'-PA-O2A
3	C	603	ATP	C5'-O5'-PA-O2A
3	D	602	ATP	PB-O3A-PA-O5'
3	D	602	ATP	C5'-O5'-PA-O1A
3	D	602	ATP	C5'-O5'-PA-O2A
3	D	603	ATP	C5'-O5'-PA-O1A
3	D	603	ATP	C5'-O5'-PA-O2A
3	E	603	ATP	C5'-O5'-PA-O2A
3	F	602	ATP	C5'-O5'-PA-O1A
3	F	602	ATP	C5'-O5'-PA-O2A
3	A	802	ATP	PB-O3A-PA-O5'
3	C	603	ATP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
3	E	602	ATP	PB-O3A-PA-O5'
3	F	602	ATP	PB-O3A-PA-O5'
3	B	602	ATP	PB-O3B-PG-O3G
3	D	603	ATP	PB-O3B-PG-O2G
3	B	602	ATP	C5'-O5'-PA-O3A
3	B	603	ATP	C5'-O5'-PA-O3A
3	C	603	ATP	C5'-O5'-PA-O3A
3	D	603	ATP	C5'-O5'-PA-O3A
3	E	603	ATP	C5'-O5'-PA-O3A
3	A	802	ATP	PB-O3A-PA-O1A
3	D	602	ATP	PA-O3A-PB-O2B
3	B	602	ATP	C5'-O5'-PA-O2A
3	C	603	ATP	C5'-O5'-PA-O1A
3	E	603	ATP	C5'-O5'-PA-O1A
3	A	804	ATP	PA-O3A-PB-O1B
3	A	804	ATP	PA-O3A-PB-O2B
3	D	602	ATP	PA-O3A-PB-O1B
3	D	602	ATP	PB-O3B-PG-O1G
3	C	603	ATP	PB-O3B-PG-O2G
3	D	602	ATP	PB-O3B-PG-O2G
3	F	602	ATP	PB-O3B-PG-O2G
3	A	802	ATP	C5'-O5'-PA-O3A
3	A	803	ATP	C5'-O5'-PA-O3A
3	A	804	ATP	C5'-O5'-PA-O3A
3	C	602	ATP	C5'-O5'-PA-O3A
3	D	602	ATP	C5'-O5'-PA-O3A
3	F	602	ATP	C5'-O5'-PA-O3A
3	B	602	ATP	PB-O3A-PA-O1A
3	B	602	ATP	PB-O3A-PA-O2A

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	ATP	3	0
3	F	602	ATP	1	0
3	A	804	ATP	1	0
3	C	602	ATP	1	0
3	E	602	ATP	1	0
3	A	802	ATP	2	0
3	C	603	ATP	2	0
3	B	603	ATP	2	0

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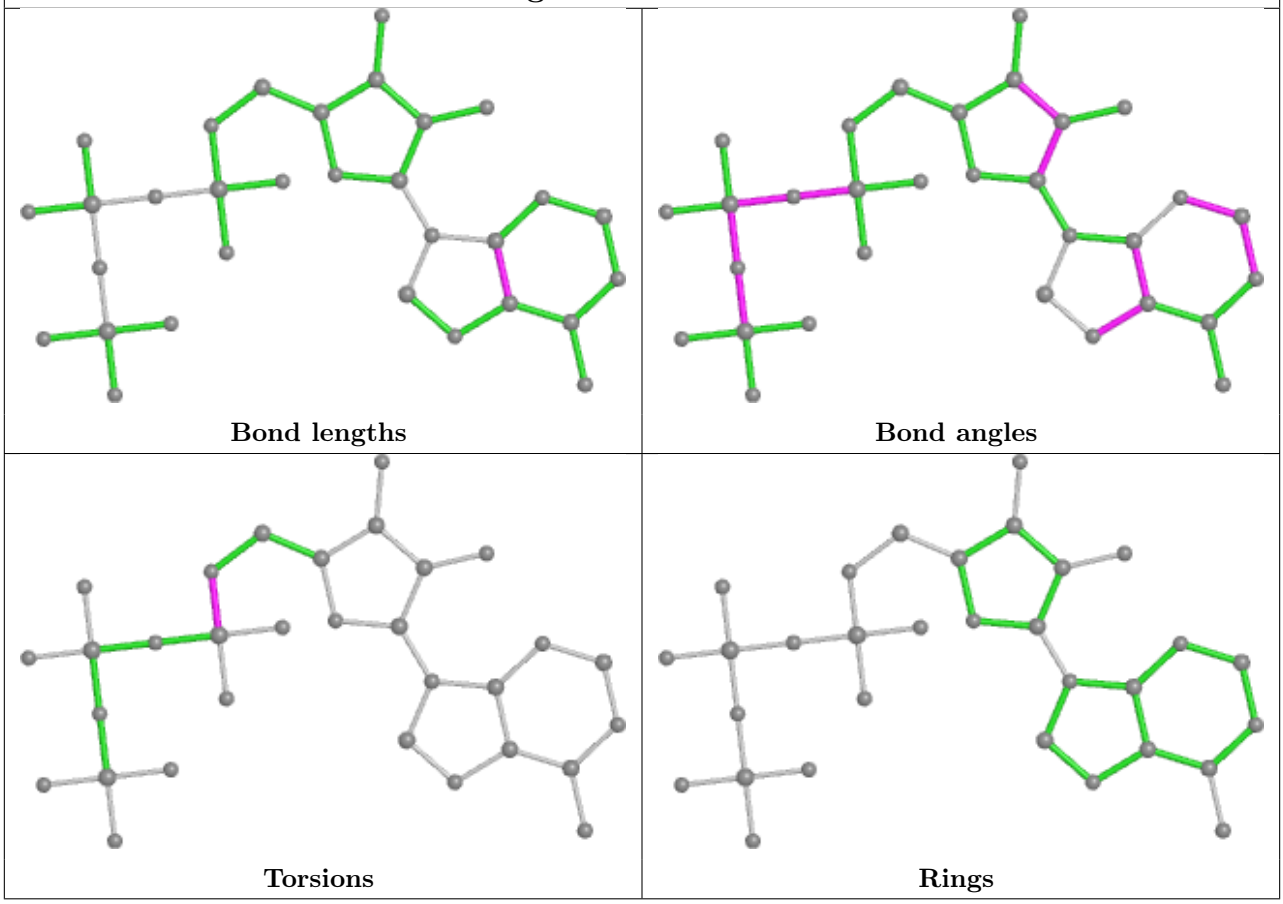
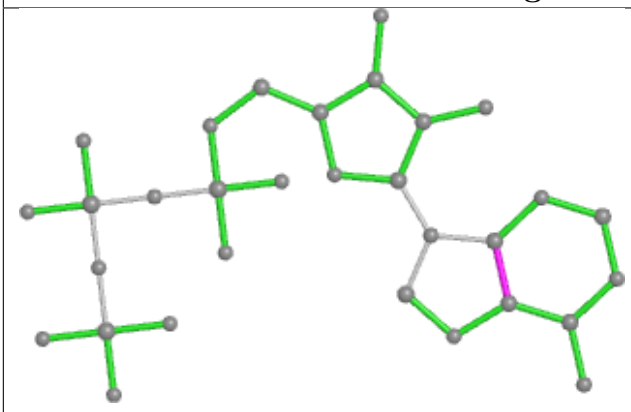
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	604	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

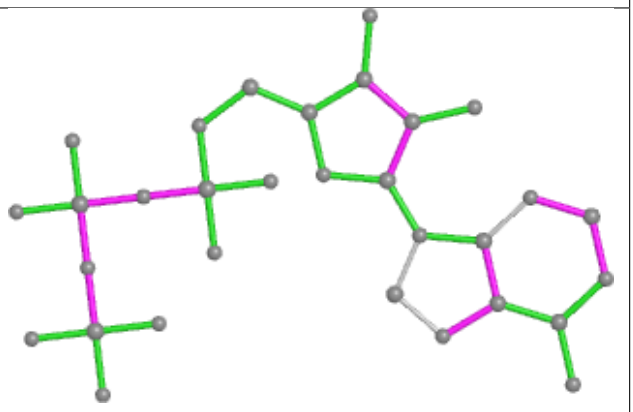
Ligand ATP E 603



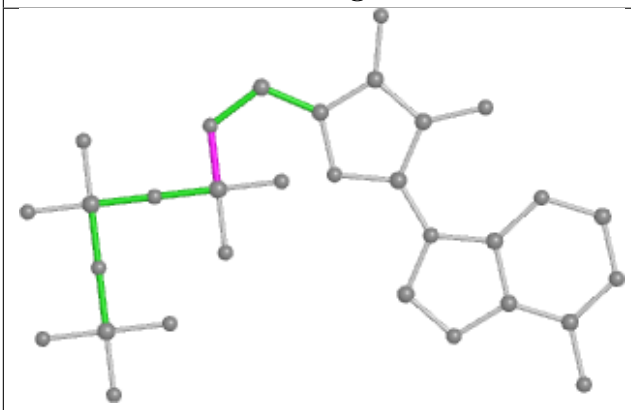
Ligand ATP A 803



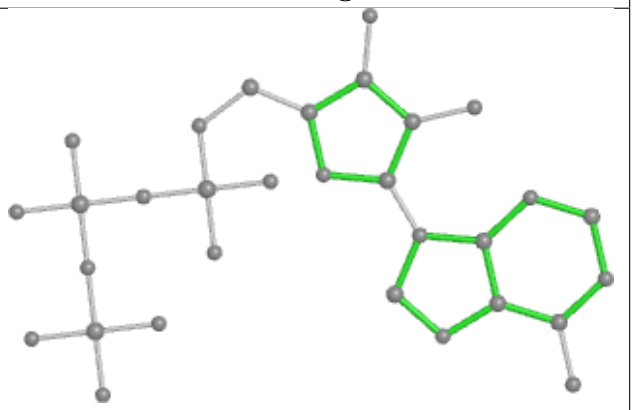
Bond lengths



Bond angles

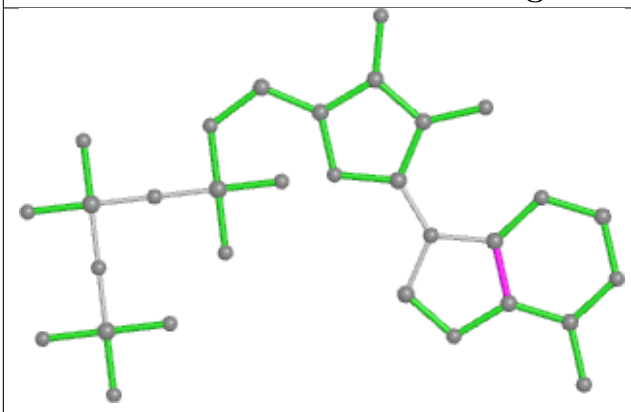


Torsions

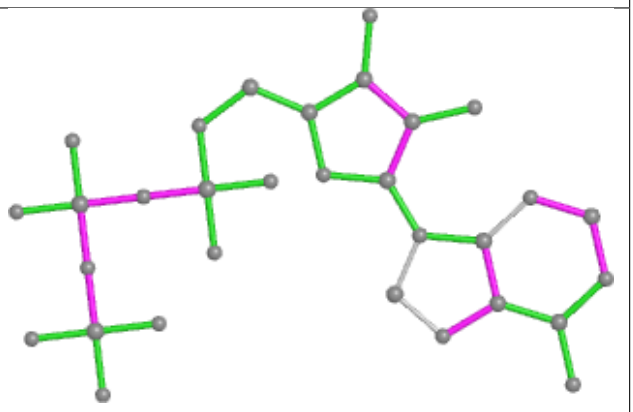


Rings

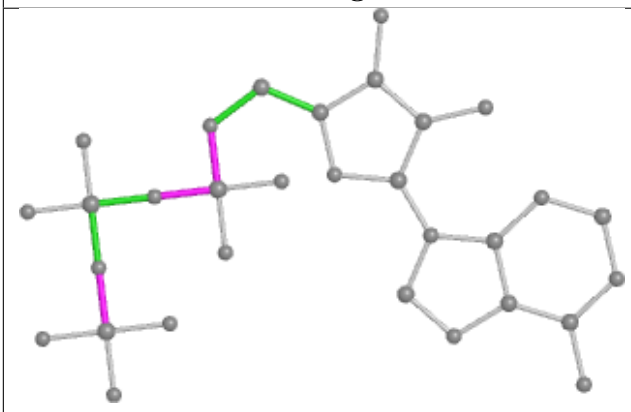
Ligand ATP F 602



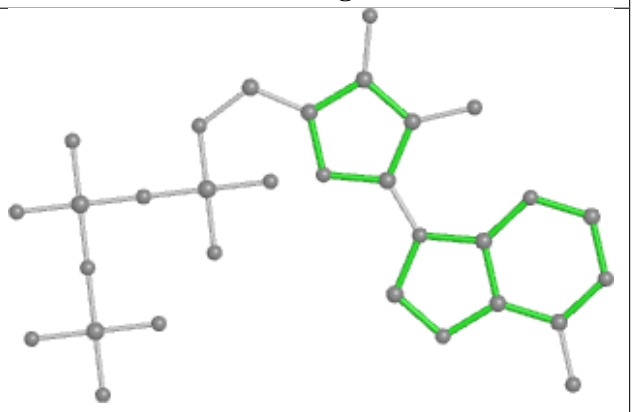
Bond lengths



Bond angles

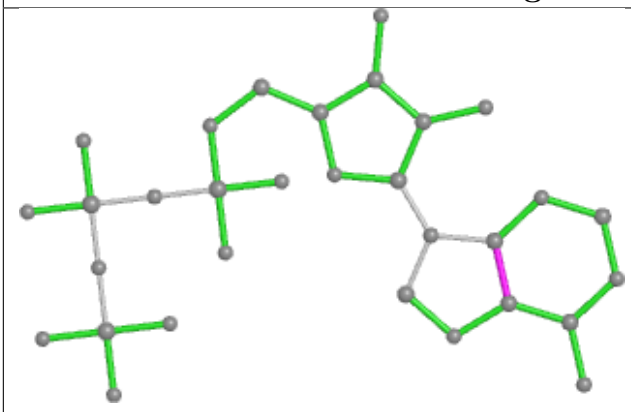


Torsions

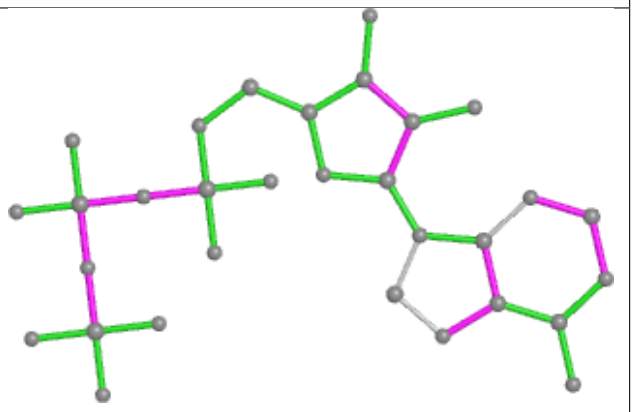


Rings

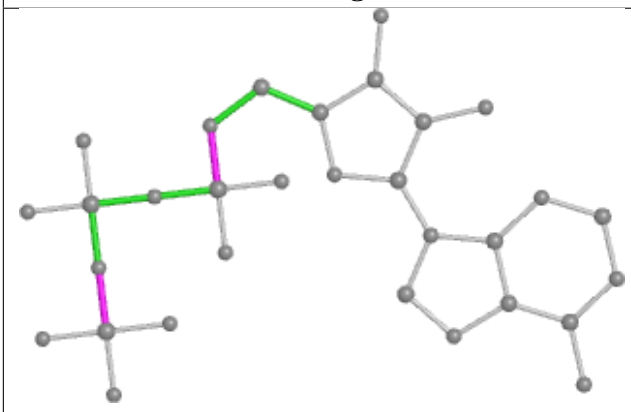
Ligand ATP D 603



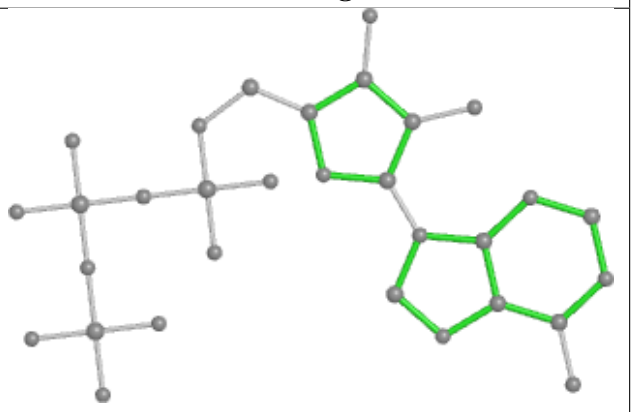
Bond lengths



Bond angles

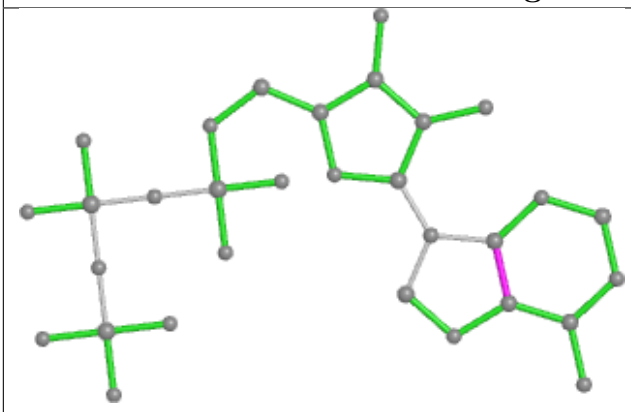


Torsions

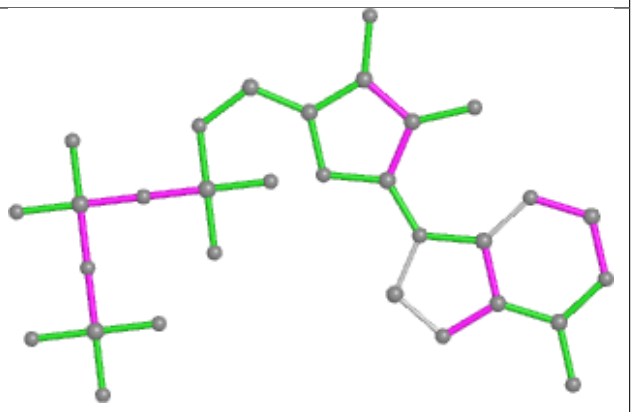


Rings

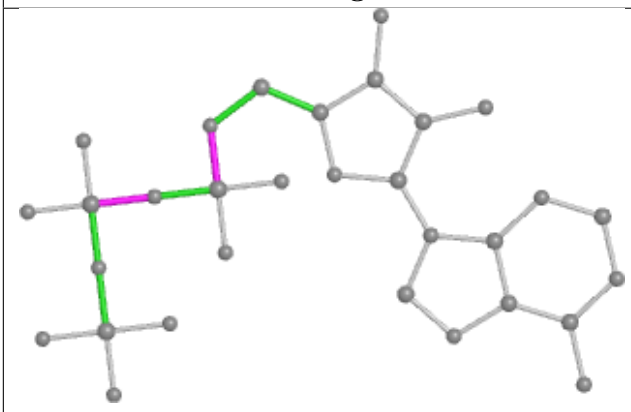
Ligand ATP A 804



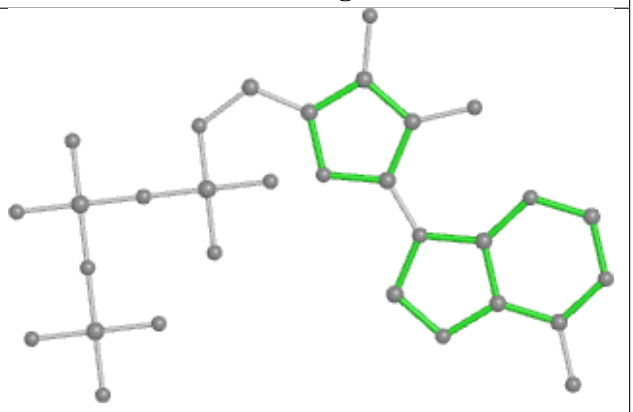
Bond lengths



Bond angles

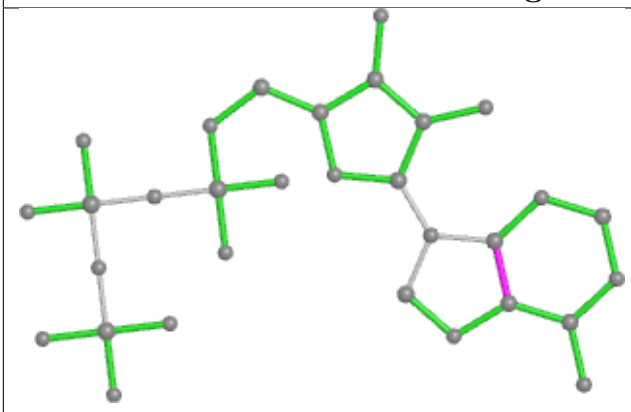


Torsions

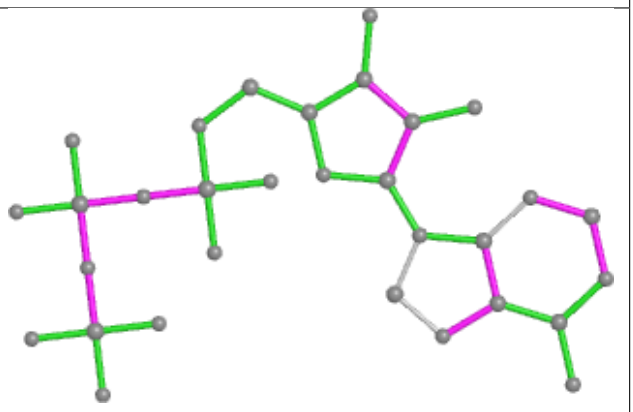


Rings

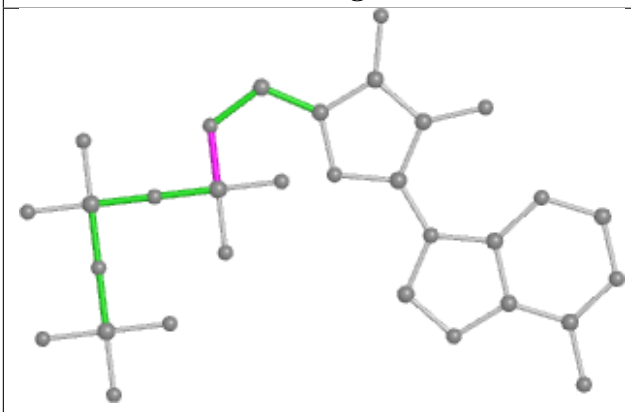
Ligand ATP C 602



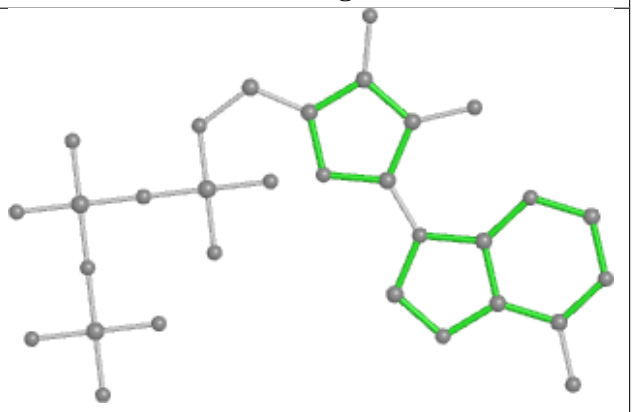
Bond lengths



Bond angles

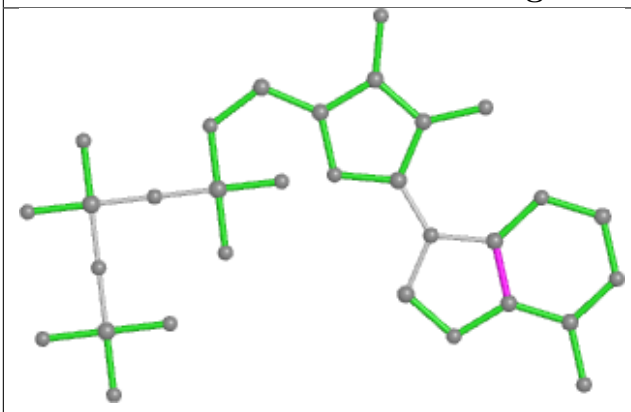


Torsions

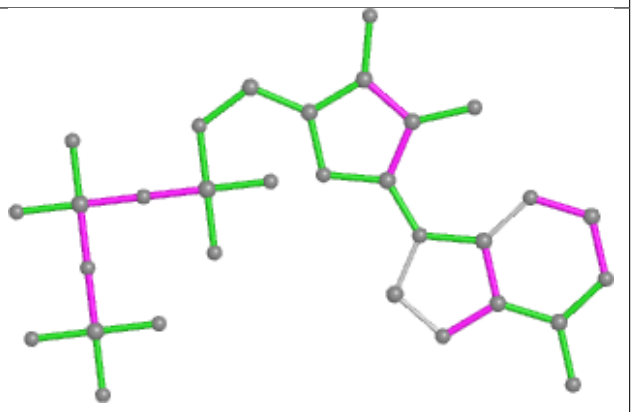


Rings

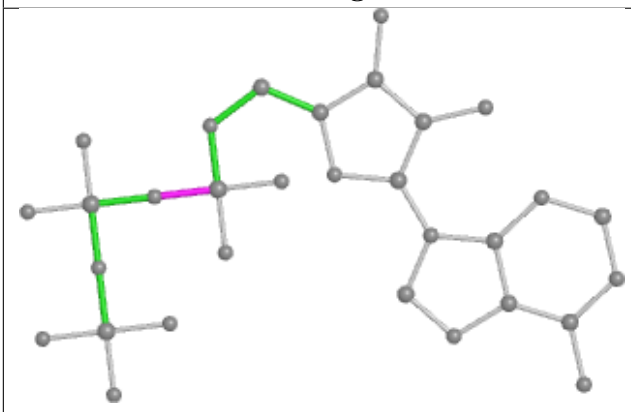
Ligand ATP E 602



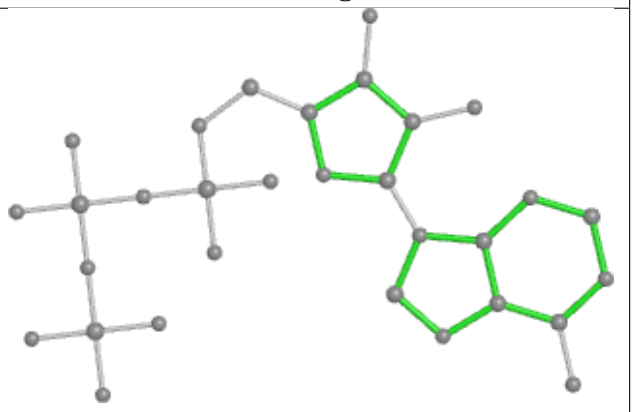
Bond lengths



Bond angles

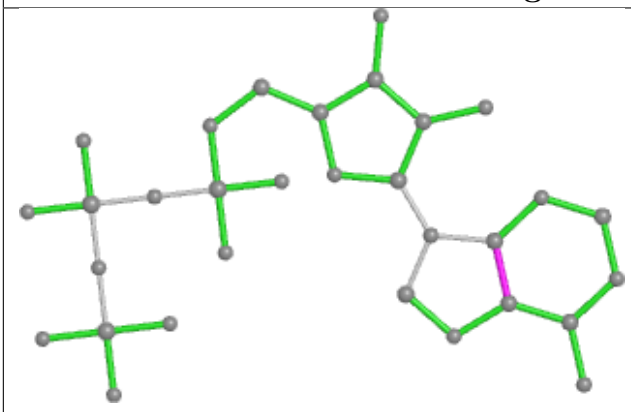


Torsions

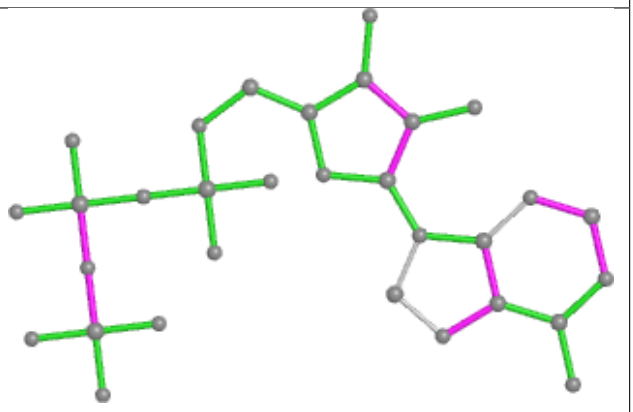


Rings

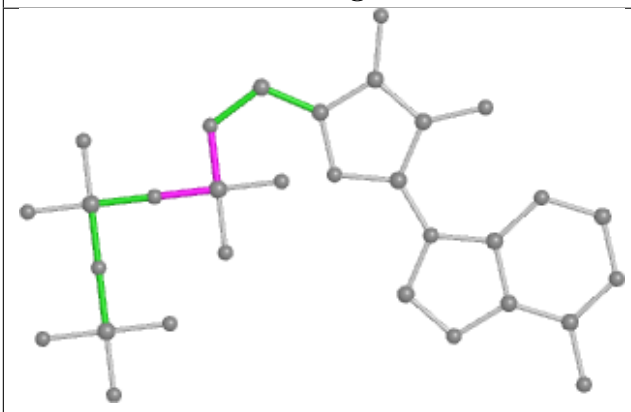
Ligand ATP A 802



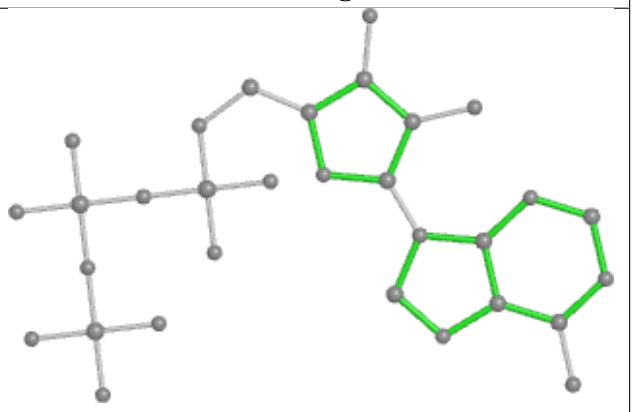
Bond lengths



Bond angles

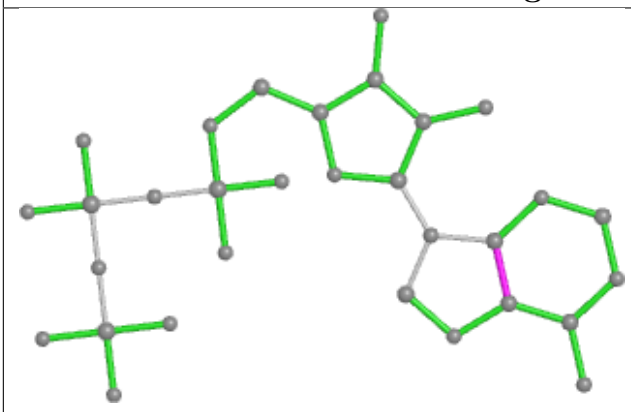


Torsions

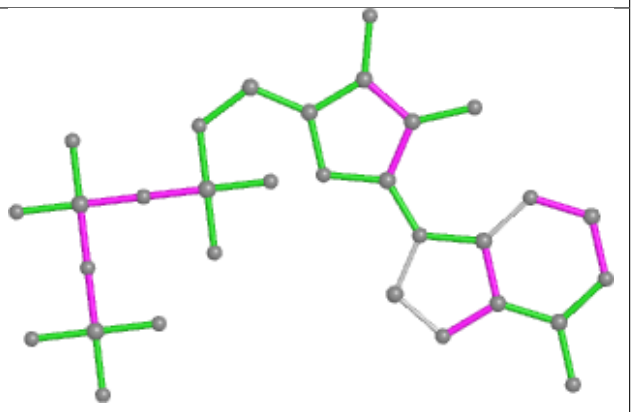


Rings

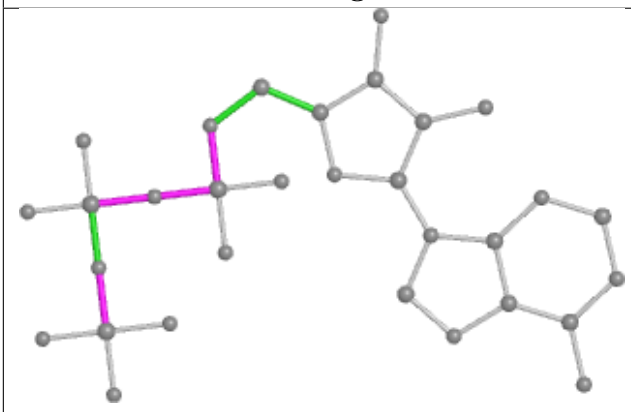
Ligand ATP D 602



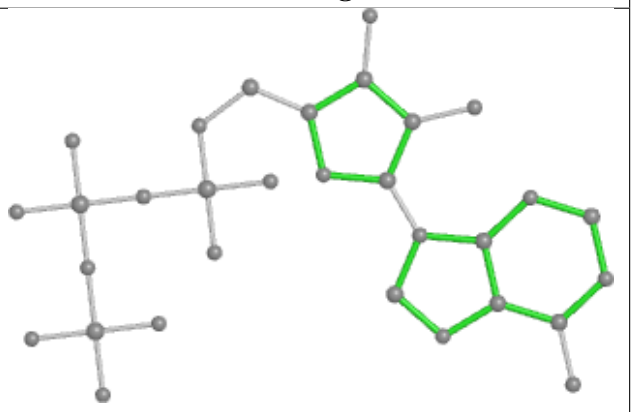
Bond lengths



Bond angles

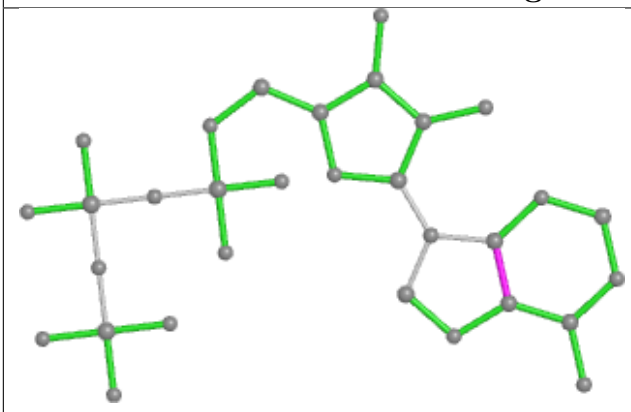


Torsions

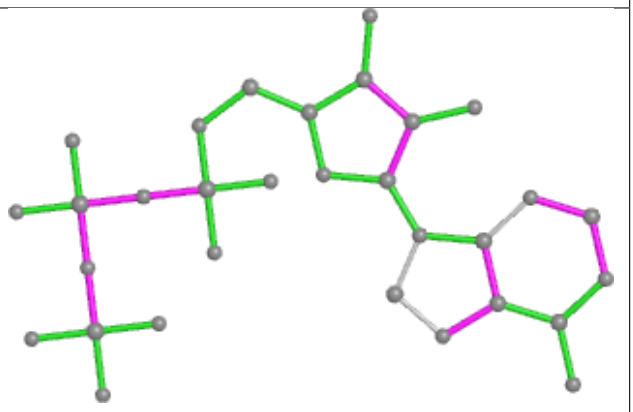


Rings

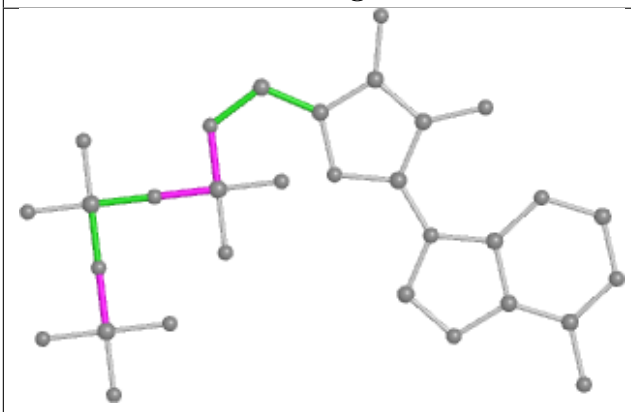
Ligand ATP C 603



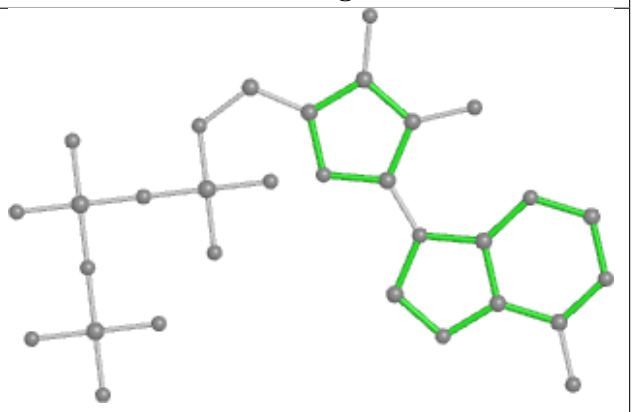
Bond lengths



Bond angles

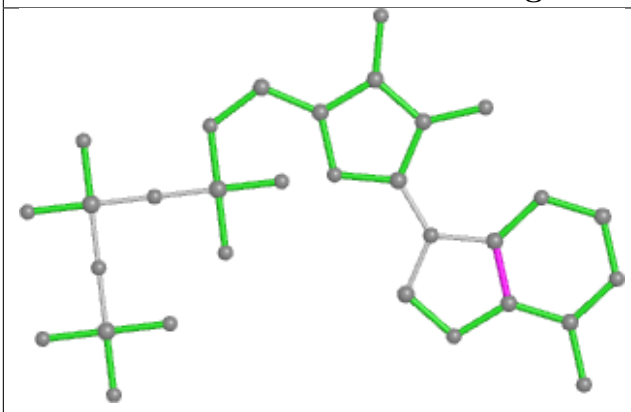


Torsions

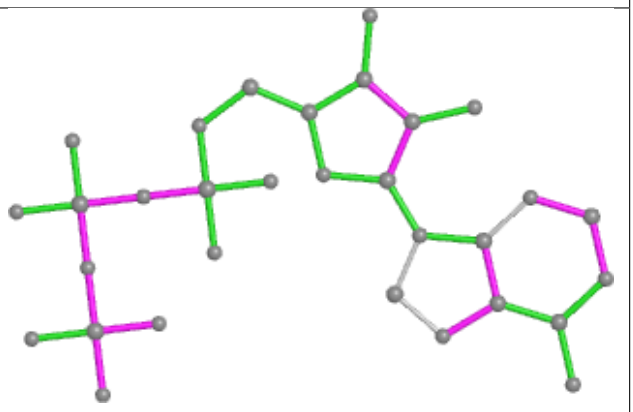


Rings

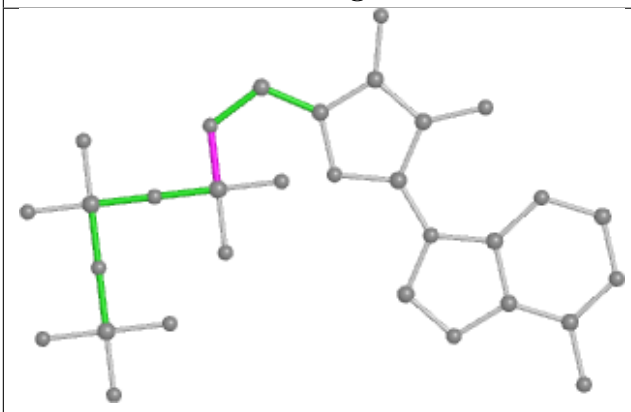
Ligand ATP B 603



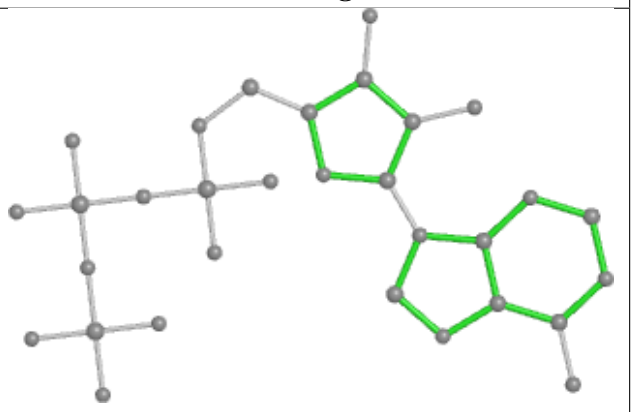
Bond lengths



Bond angles

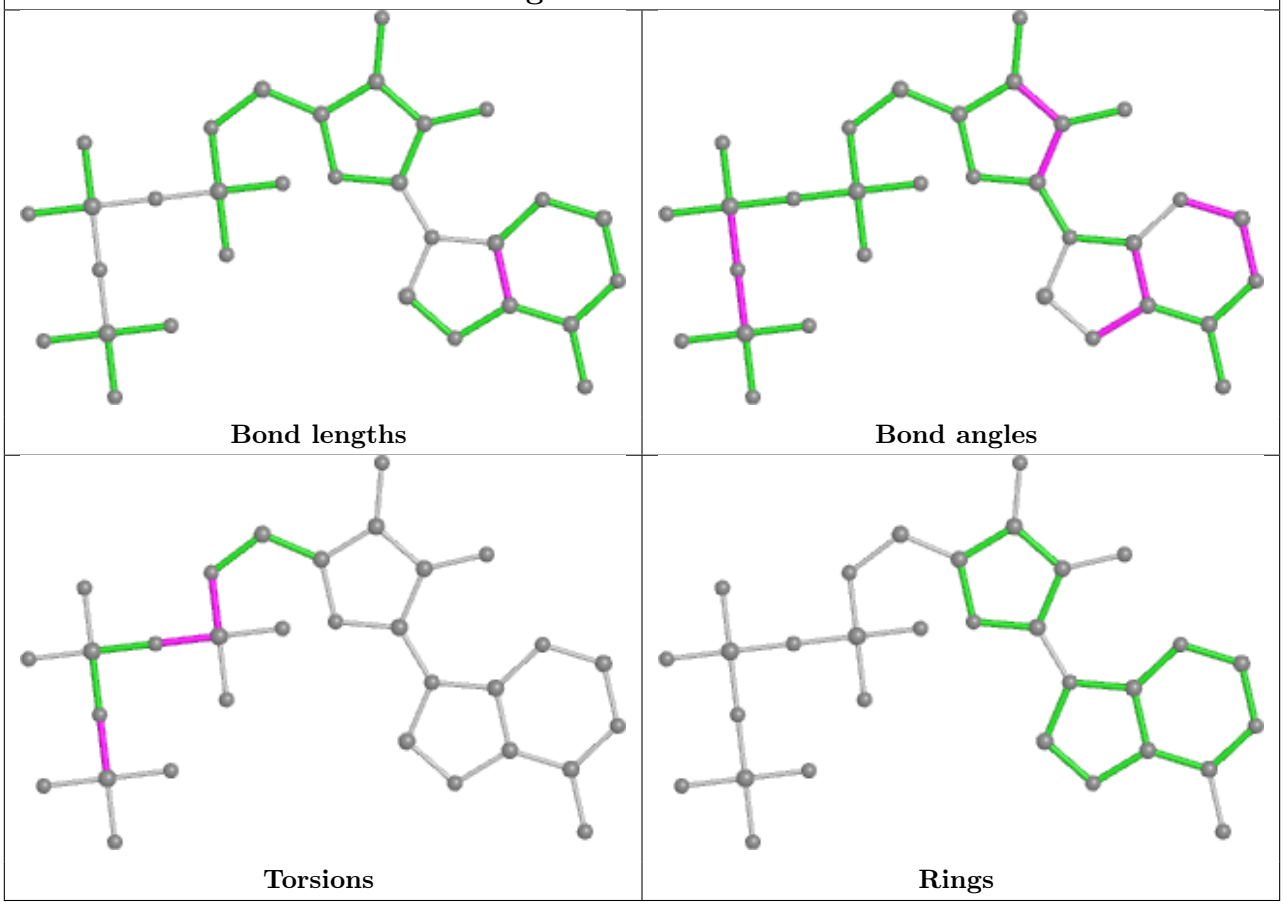


Torsions



Rings

Ligand ATP B 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	505/512 (98%)	0.58	65 (12%) 3 4	27, 84, 140, 180	0
1	B	488/512 (95%)	0.46	38 (7%) 13 15	38, 84, 134, 171	0
1	C	487/512 (95%)	0.17	26 (5%) 26 28	29, 67, 120, 176	0
1	D	484/512 (94%)	0.07	21 (4%) 35 38	13, 50, 114, 144	0
1	E	491/512 (95%)	0.12	24 (4%) 29 31	8, 54, 120, 167	0
1	F	505/512 (98%)	0.28	40 (7%) 12 14	8, 66, 136, 181	0
All	All	2960/3072 (96%)	0.28	214 (7%) 15 18	8, 69, 130, 181	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	GLY	8.5
1	A	507	ARG	8.0
1	A	516	GLY	7.7
1	A	519	SER	7.4
1	B	117	VAL	7.4
1	F	516	GLY	7.4
1	F	501	GLU	7.3
1	A	498	THR	7.0
1	E	500	ASP	7.0
1	A	257	ARG	7.0
1	B	118	VAL	6.9
1	B	500	ASP	6.7
1	B	121	PHE	6.7
1	F	509	VAL	6.6
1	A	500	ASP	6.5
1	C	500	ASP	6.2
1	F	500	ASP	6.1
1	B	498	THR	6.1
1	F	518	GLU	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	511	GLY	6.0
1	B	15	HIS	5.9
1	F	506	SER	5.9
1	D	117	VAL	5.8
1	F	519	SER	5.6
1	F	517	PRO	5.6
1	E	421	GLY	5.5
1	A	514	GLU	5.5
1	A	503	SER	5.5
1	D	119	GLY	5.4
1	A	504	GLU	5.3
1	A	513	GLN	5.3
1	C	117	VAL	5.2
1	A	515	LYS	5.2
1	A	506	SER	5.2
1	A	502	LYS	5.2
1	A	496	ARG	5.1
1	D	157	SER	5.0
1	C	501	GLU	4.9
1	E	505	LEU	4.9
1	F	341	GLN	4.8
1	A	255	THR	4.8
1	F	503	SER	4.7
1	F	508	ILE	4.6
1	E	503	SER	4.6
1	F	507	ARG	4.6
1	F	497	ILE	4.6
1	E	154	TYR	4.5
1	B	119	GLY	4.5
1	F	485	ASN	4.5
1	C	119	GLY	4.5
1	A	501	GLU	4.4
1	D	15	HIS	4.4
1	E	504	GLU	4.4
1	E	121	PHE	4.3
1	A	120	GLY	4.3
1	A	508	ILE	4.2
1	F	495	THR	4.2
1	E	501	GLU	4.2
1	A	518	GLU	4.2
1	E	120	GLY	4.1
1	A	253	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	501	GLU	4.1
1	D	121	PHE	4.0
1	C	499	VAL	4.0
1	D	471	MET	4.0
1	A	417	ASP	4.0
1	C	498	THR	4.0
1	A	475	LYS	4.0
1	A	256	GLN	4.0
1	F	504	GLU	4.0
1	F	515	LYS	4.0
1	F	513	GLN	3.9
1	B	496	ARG	3.8
1	F	311	ARG	3.8
1	B	16	GLN	3.8
1	A	499	VAL	3.8
1	A	121	PHE	3.7
1	F	496	ARG	3.7
1	D	118	VAL	3.7
1	A	517	PRO	3.6
1	B	115	GLN	3.6
1	E	499	VAL	3.6
1	F	512	VAL	3.6
1	A	342	ASN	3.5
1	A	16	GLN	3.5
1	F	514	GLU	3.5
1	B	188	TYR	3.5
1	F	505	LEU	3.5
1	B	497	ILE	3.4
1	A	15	HIS	3.4
1	F	342	ASN	3.4
1	B	157	SER	3.3
1	E	498	THR	3.3
1	F	154	TYR	3.3
1	D	16	GLN	3.3
1	E	117	VAL	3.2
1	E	423	HIS	3.2
1	A	510	ARG	3.2
1	C	118	VAL	3.2
1	B	116	GLU	3.2
1	A	509	VAL	3.1
1	C	154	TYR	3.1
1	B	258	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	329	TYR	3.1
1	A	427	ASP	3.1
1	F	510	ARG	3.1
1	C	152	GLN	3.1
1	C	145	ASP	3.1
1	B	421	GLY	3.1
1	D	447	GLY	3.1
1	A	512	VAL	3.1
1	B	173	GLN	3.0
1	B	502	LYS	3.0
1	A	14	GLU	3.0
1	E	116	GLU	3.0
1	F	511	GLY	3.0
1	F	343	LEU	3.0
1	F	255	THR	3.0
1	C	53	THR	3.0
1	E	329	TYR	3.0
1	B	124	SER	2.9
1	E	484	ARG	2.9
1	C	116	GLU	2.9
1	E	113	GLU	2.9
1	A	114	GLY	2.9
1	F	117	VAL	2.9
1	A	258	SER	2.9
1	A	275	GLY	2.9
1	B	436	THR	2.8
1	C	120	GLY	2.8
1	E	502	LYS	2.8
1	F	340	ARG	2.8
1	D	14	GLU	2.8
1	D	156	ALA	2.8
1	C	22	ARG	2.8
1	F	502	LYS	2.8
1	C	492	GLY	2.8
1	E	112	PRO	2.8
1	C	17	ALA	2.7
1	B	251	ALA	2.7
1	D	154	TYR	2.7
1	A	484	ARG	2.7
1	E	118	VAL	2.7
1	A	505	LEU	2.7
1	F	494	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	413	THR	2.7
1	A	17	ALA	2.7
1	A	115	GLN	2.7
1	B	101	GLY	2.7
1	A	311	ARG	2.6
1	A	379	SER	2.6
1	F	121	PHE	2.6
1	B	429	HIS	2.6
1	B	181	THR	2.6
1	A	423	HIS	2.6
1	F	481	ASP	2.6
1	A	309	LYS	2.6
1	A	321	ARG	2.5
1	E	119	GLY	2.5
1	C	170	ARG	2.5
1	E	188	TYR	2.5
1	F	344	LEU	2.5
1	B	255	THR	2.5
1	C	14	GLU	2.5
1	D	421	GLY	2.5
1	B	293	GLY	2.5
1	A	428	SER	2.4
1	B	123	LEU	2.4
1	A	462	TRP	2.4
1	C	227	GLY	2.4
1	D	434	THR	2.4
1	A	378	ASP	2.4
1	B	99	ASP	2.4
1	A	410	GLY	2.4
1	B	176	ALA	2.4
1	A	471	MET	2.4
1	B	154	TYR	2.3
1	F	188	TYR	2.3
1	A	364	LYS	2.3
1	B	155	ASP	2.3
1	B	499	VAL	2.3
1	A	318	GLU	2.3
1	B	22	ARG	2.3
1	C	173	GLN	2.3
1	A	281	ASP	2.2
1	F	446	ARG	2.2
1	C	146	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	282	SER	2.2
1	D	115	GLN	2.2
1	E	153	GLN	2.2
1	C	102	LYS	2.2
1	A	497	ILE	2.2
1	B	417	ASP	2.2
1	D	295	THR	2.2
1	A	153	GLN	2.2
1	C	115	GLN	2.2
1	A	117	VAL	2.1
1	F	484	ARG	2.1
1	C	487	GLU	2.1
1	C	189	GLY	2.1
1	A	272	GLU	2.1
1	C	255	THR	2.1
1	A	345	LYS	2.1
1	B	295	THR	2.1
1	D	498	THR	2.1
1	A	251	ALA	2.1
1	D	155	ASP	2.1
1	B	427	ASP	2.1
1	E	422	VAL	2.0
1	B	175	GLY	2.0
1	D	114	GLY	2.0
1	F	257	ARG	2.0
1	A	188	TYR	2.0
1	D	56	SER	2.0

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. 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	B-factors(Å^2)	Q<0.9
1	TPO	A	432	11/12	0.78	0.26	83,90,112,116	0
1	TPO	F	432	11/12	0.83	0.26	46,73,98,100	0
1	TPO	D	432	11/12	0.86	0.30	38,55,98,100	0
1	TPO	B	432	11/12	0.92	0.30	68,87,103,106	0
1	TPO	E	432	11/12	0.93	0.22	33,45,78,90	0
1	TPO	C	432	11/12	0.93	0.20	45,57,76,83	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

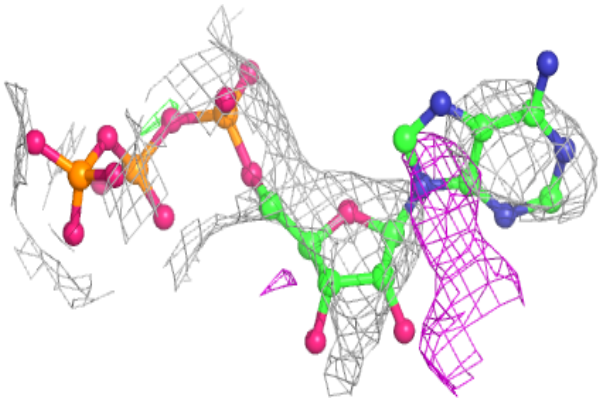
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

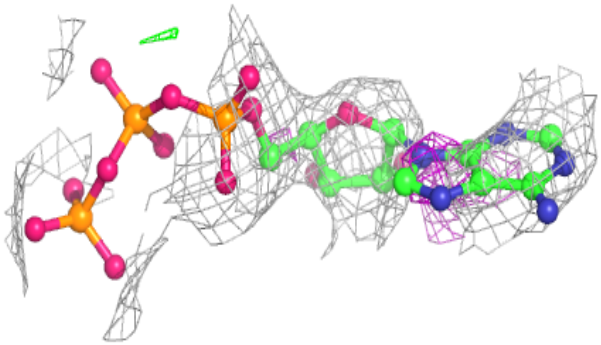
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PO4	B	604	5/5	0.56	0.51	126,129,146,151	0
2	MG	F	601	1/1	0.61	0.56	85,85,85,85	0
2	MG	C	601	1/1	0.71	0.27	43,43,43,43	0
4	PO4	F	604	5/5	0.71	0.43	77,78,106,143	0
2	MG	B	601	1/1	0.78	0.30	63,63,63,63	0
3	ATP	F	602	31/31	0.78	0.35	66,101,113,120	0
4	PO4	D	604	5/5	0.82	0.75	71,83,87,111	0
3	ATP	A	803	31/31	0.82	0.29	34,64,97,99	0
4	PO4	E	605	5/5	0.83	0.66	55,64,81,115	0
4	PO4	F	603	5/5	0.84	0.45	62,66,103,119	0
3	ATP	A	802	31/31	0.85	0.29	58,82,97,100	0
3	ATP	B	603	31/31	0.86	0.28	55,80,104,117	0
3	ATP	E	602	31/31	0.86	0.26	38,79,94,95	0
4	PO4	E	604	5/5	0.87	0.20	112,123,141,148	0
4	PO4	B	605	5/5	0.87	0.73	81,94,105,120	0
3	ATP	D	602	31/31	0.89	0.27	32,54,66,77	0
3	ATP	C	603	31/31	0.90	0.28	22,50,78,105	0
3	ATP	B	602	31/31	0.90	0.23	52,66,86,93	0
3	ATP	D	603	31/31	0.90	0.28	3,17,54,88	0
2	MG	E	601	1/1	0.90	0.25	59,59,59,59	0
4	PO4	C	604	5/5	0.91	0.31	43,74,89,107	0
3	ATP	C	602	31/31	0.91	0.24	23,46,74,82	0
3	ATP	E	603	31/31	0.92	0.23	7,18,53,72	0
3	ATP	A	804	31/31	0.92	0.24	8,37,63,78	0
2	MG	A	801	1/1	0.93	0.33	82,82,82,82	0
2	MG	D	601	1/1	0.95	0.26	55,55,55,55	0
2	MG	B	606	1/1	0.96	0.29	69,69,69,69	0

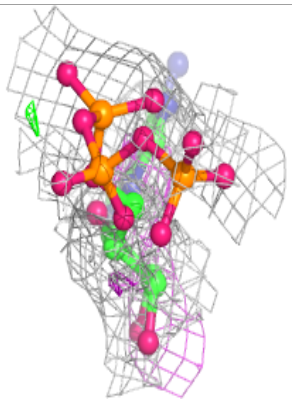
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP F 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

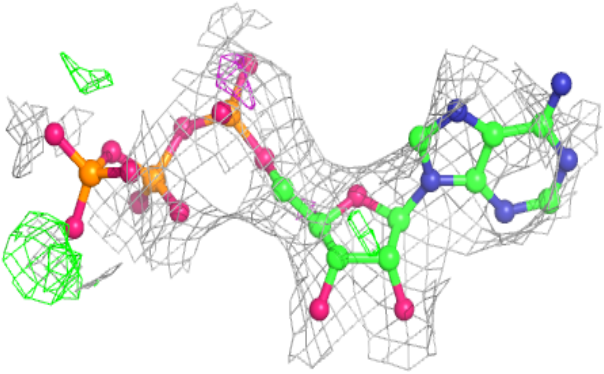


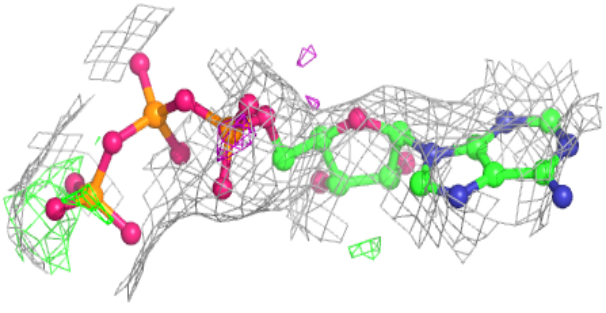


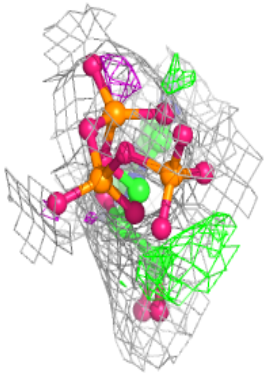


Electron density around ATP A 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

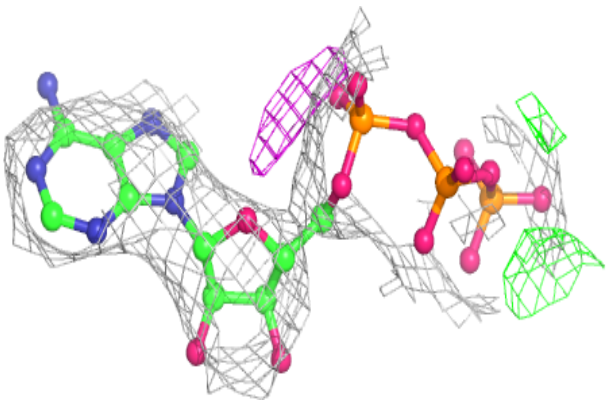


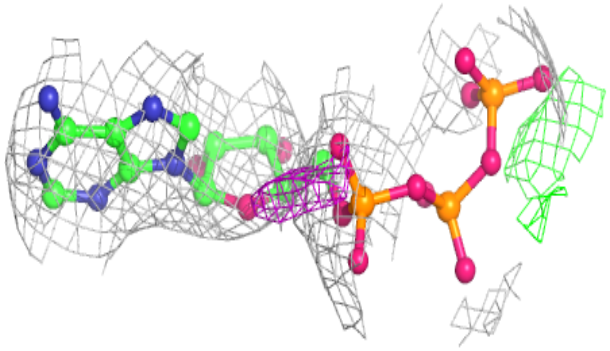


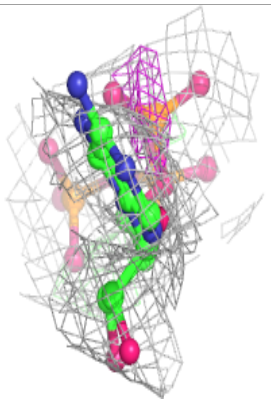


Electron density around ATP A 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

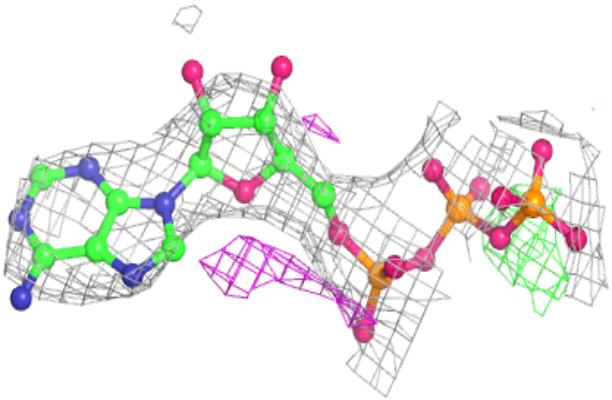


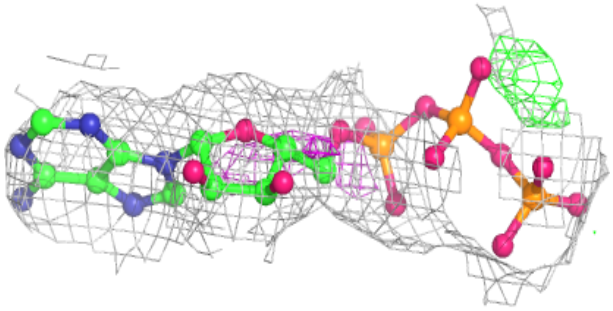


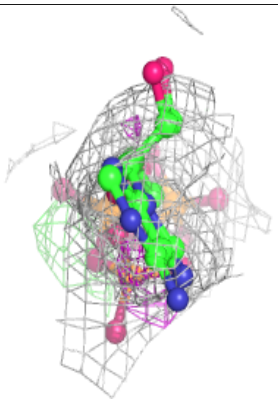


Electron density around ATP B 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

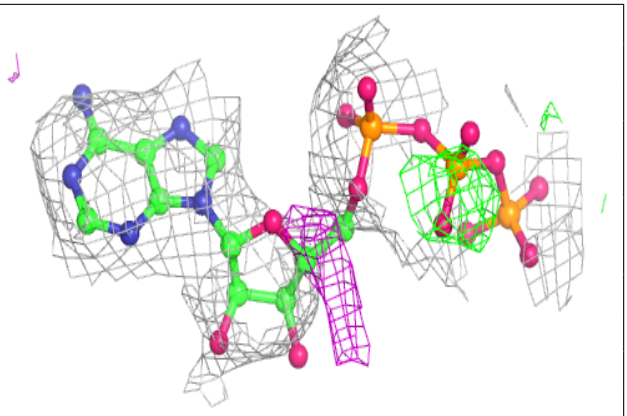


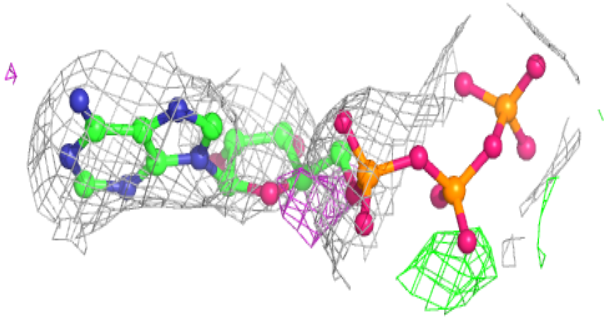


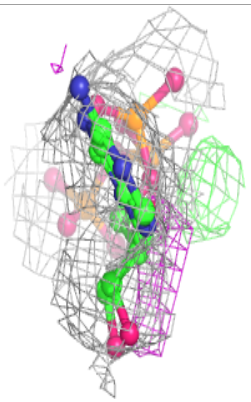


Electron density around ATP E 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

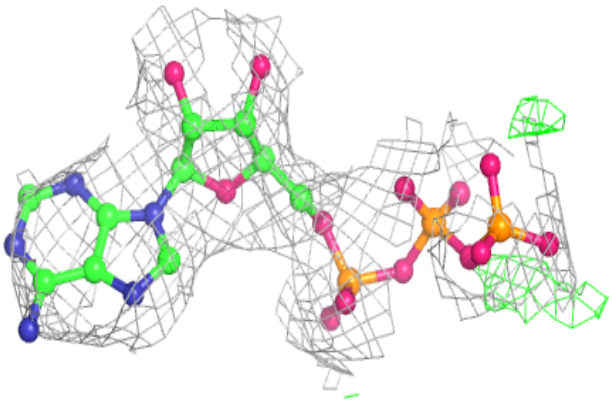


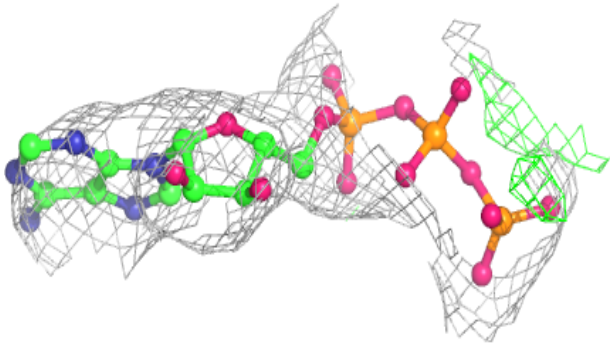


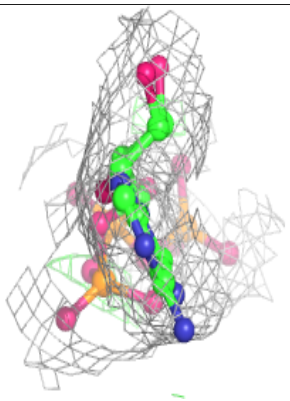


Electron density around ATP D 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

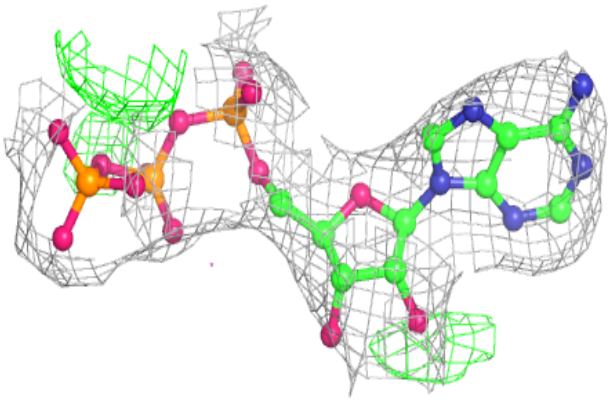


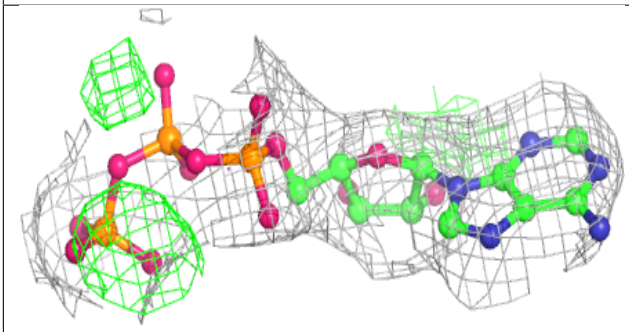


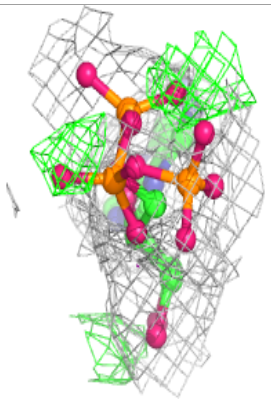


Electron density around ATP C 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

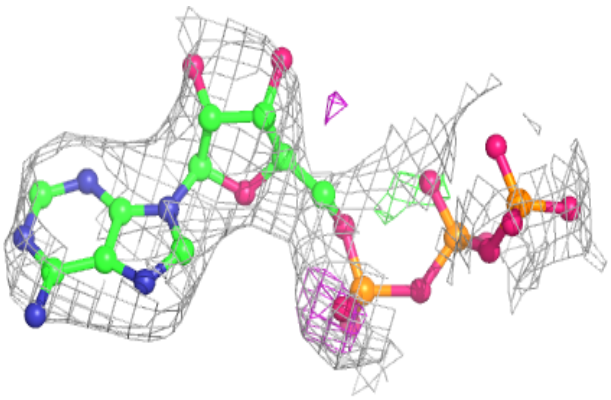


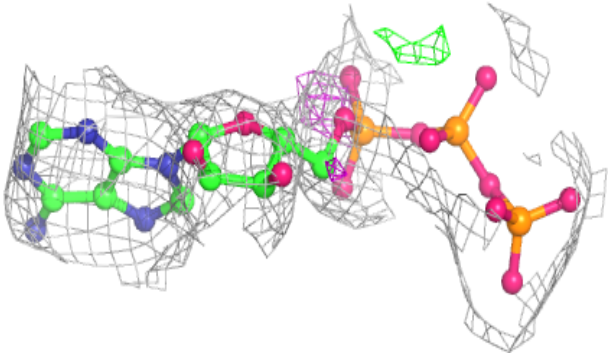


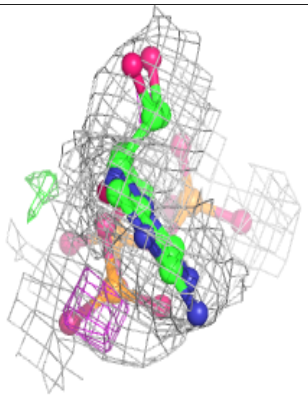


Electron density around ATP B 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

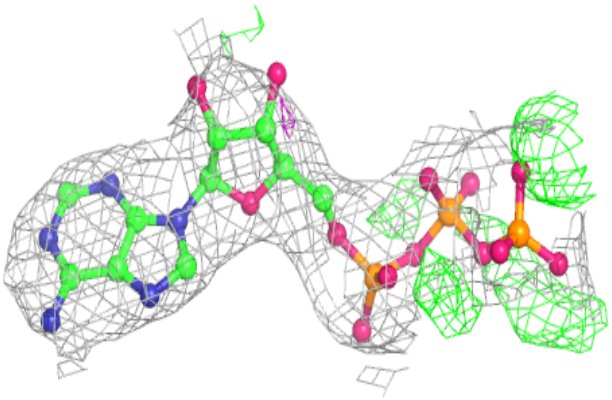


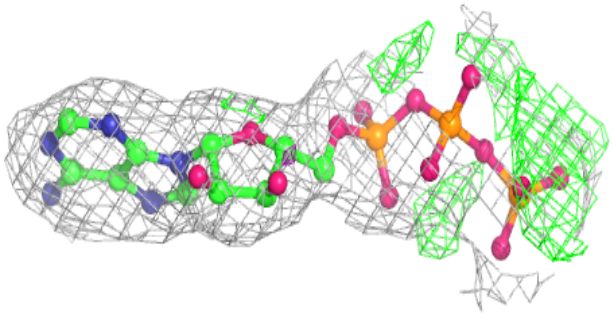


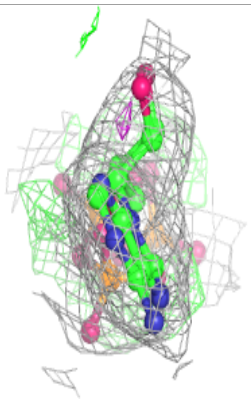


Electron density around ATP D 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

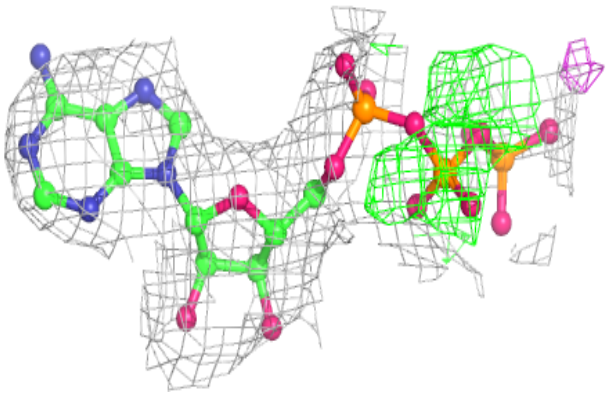


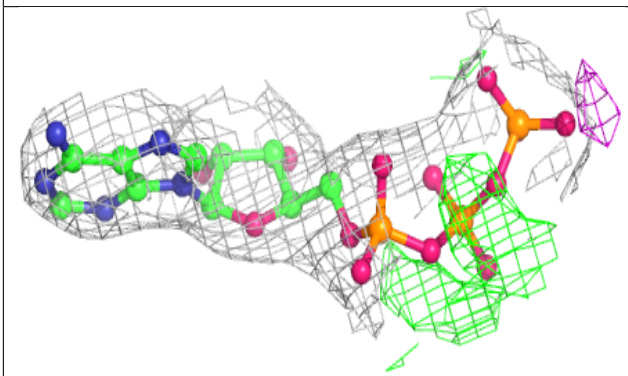


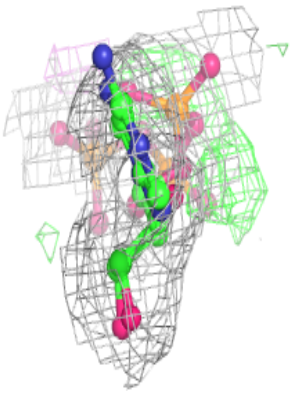


Electron density around ATP C 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

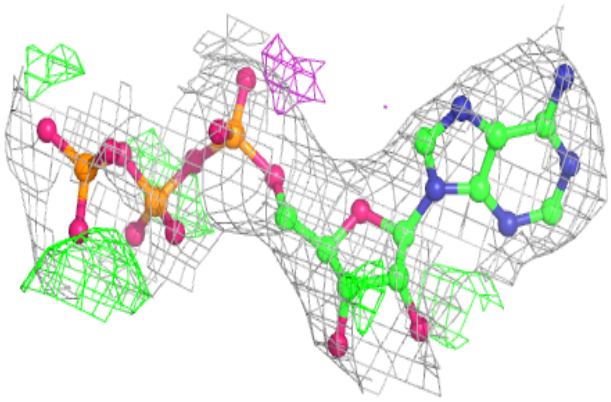


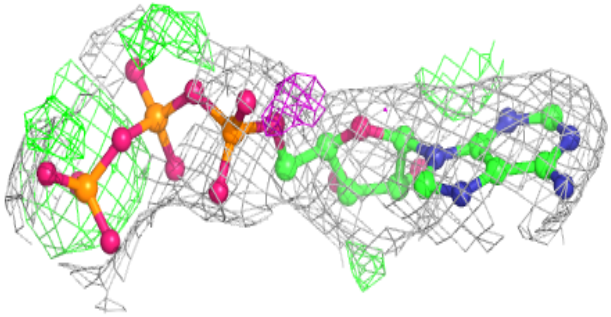


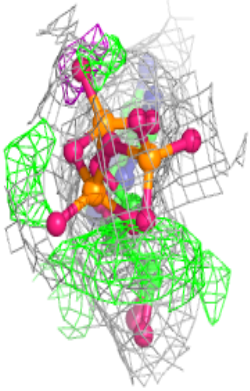


Electron density around ATP E 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

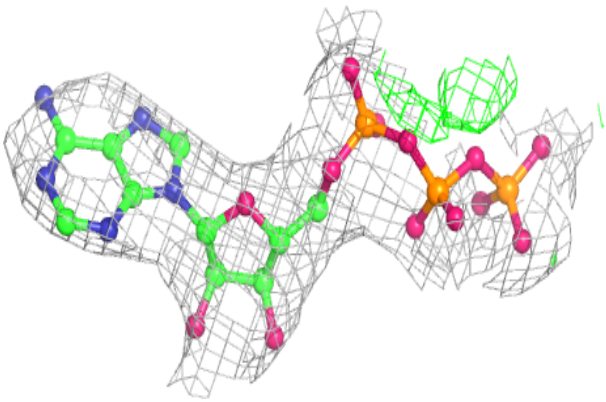


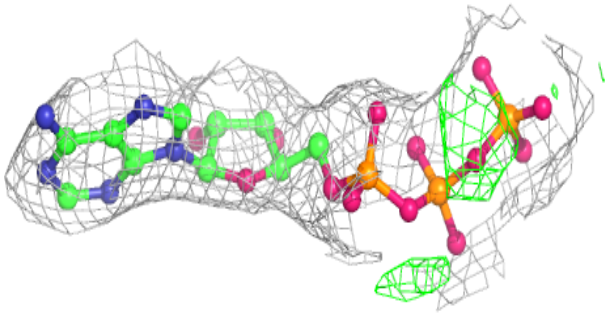


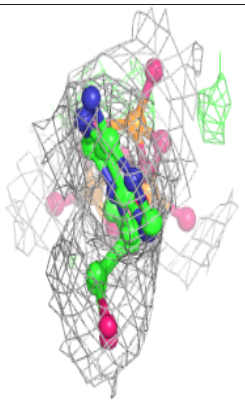


Electron density around ATP A 804:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.