wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 12:20 AM JST

PDB ID	:	7DY2
Title	:	Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC
Authors	:	Furuike, Y.; Akiyama, S.
Deposited on	:	2021-01-20
Resolution	:	3.04 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

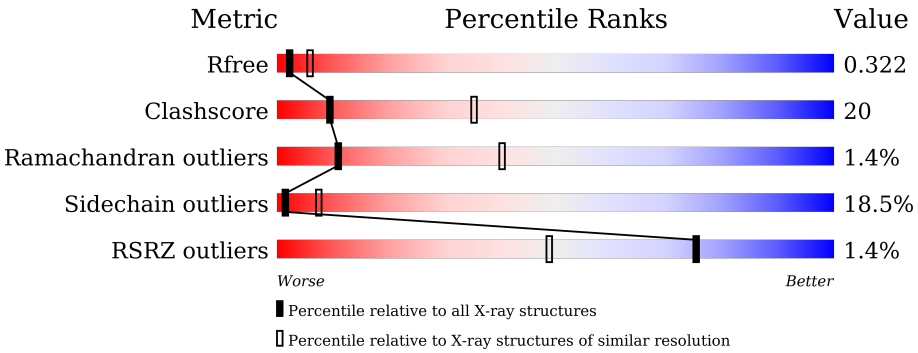
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 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	519	58% 25% 6% 11%
1	B	519	58% 27% • 11%
1	C	519	55% 27% 6% 11%
1	D	519	55% 28% 6% 12%
1	E	519	55% 29% 6% 11%
1	F	519	64% 23% • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	519	2% 65% 18% 6% 12%
1	I	519	58% 26% 6% 10%
1	J	519	% 56% 27% 6% 11%
1	K	519	2% 61% 25% 10%
1	L	519	2% 57% 26% 5% 12%
2	H	519	% 60% 25% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	K	431	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 39277 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.

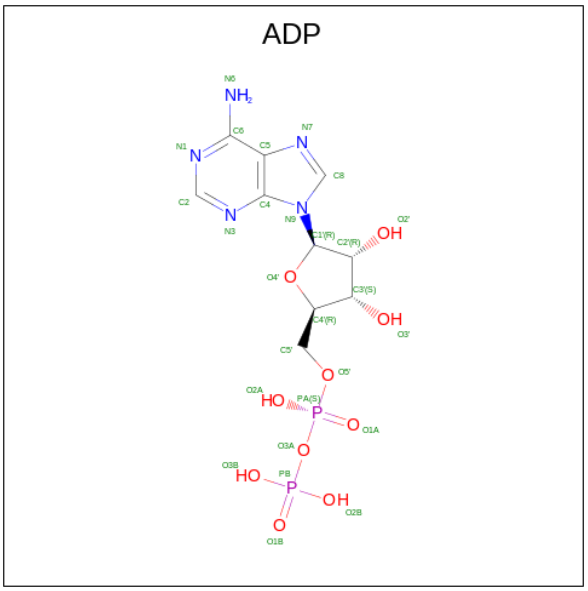
- Molecule 1 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	P	S	0	0	0
			3300	2058	575	653	1	13			
1	B	461	Total	C	N	O	P	S	0	0	0
			3204	1995	566	631	1	11			
1	E	464	Total	C	N	O	P	S	0	0	0
			3287	2046	580	647	1	13			
1	F	467	Total	C	N	O	P	S	0	0	0
			3245	2013	575	644	1	12			
1	C	462	Total	C	N	O	P	S	0	0	0
			3236	2016	563	644	1	12			
1	D	458	Total	C	N	O	P	S	0	0	0
			3173	1958	567	634	1	13			
1	G	459	Total	C	N	O	P	S	0	0	0
			3000	1835	546	607	1	11			
1	K	465	Total	C	N	O	P	S	0	0	0
			3132	1933	563	623	1	12			
1	L	457	Total	C	N	O	P	S	0	0	0
			3082	1905	548	617	1	11			
1	I	467	Total	C	N	O	P	S	0	0	0
			3349	2087	585	662	1	14			
1	J	464	Total	C	N	O	P	S	0	0	0
			3342	2098	581	648	1	14			

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

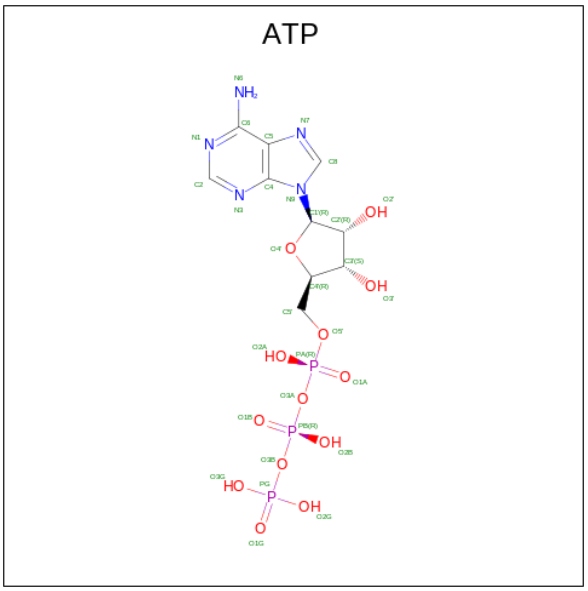
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	460	Total	C	N	O	S	0	0	0
			3197	1998	553	634	12			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	E	2	Total Mg 2 2	0	0
5	F	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0
5	K	1	Total Mg 1 1	0	0
5	L	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0

- Molecule 6 is water.

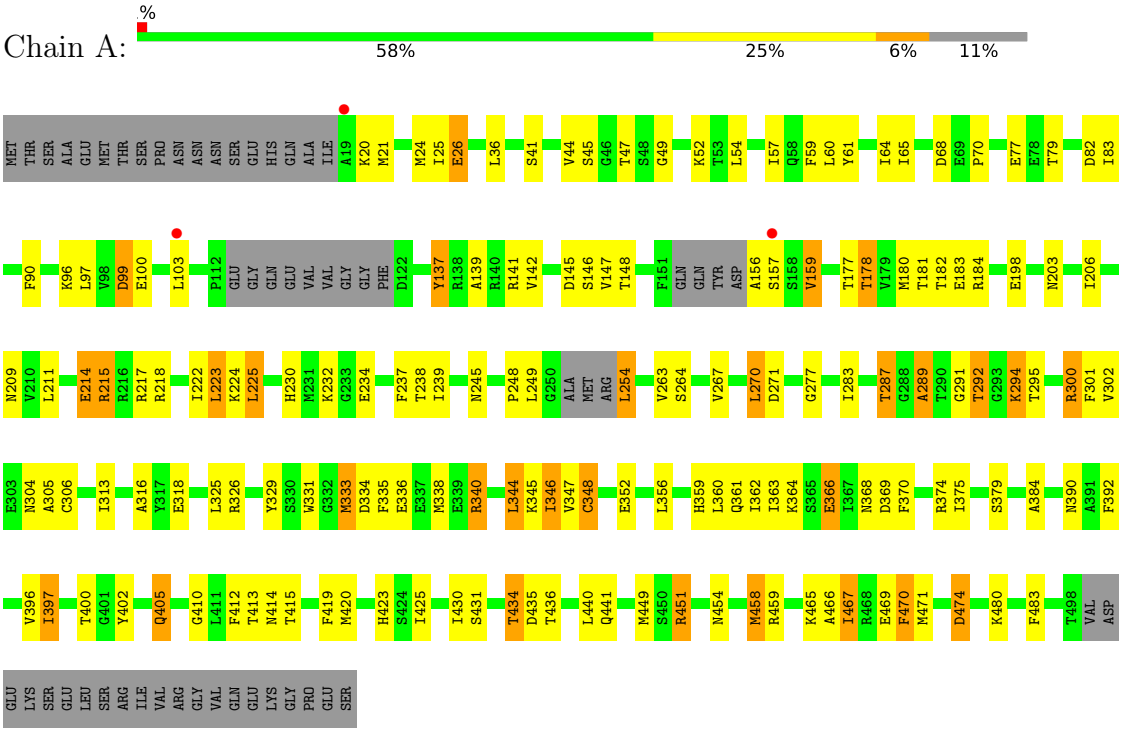
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	B	1	Total O 1 1	0	0
6	E	1	Total O 1 1	0	0
6	F	2	Total O 2 2	0	0
6	D	1	Total O 1 1	0	0
6	G	2	Total O 2 2	0	0
6	H	4	Total O 4 4	0	0
6	K	1	Total O 1 1	0	0
6	I	2	Total O 2 2	0	0

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.

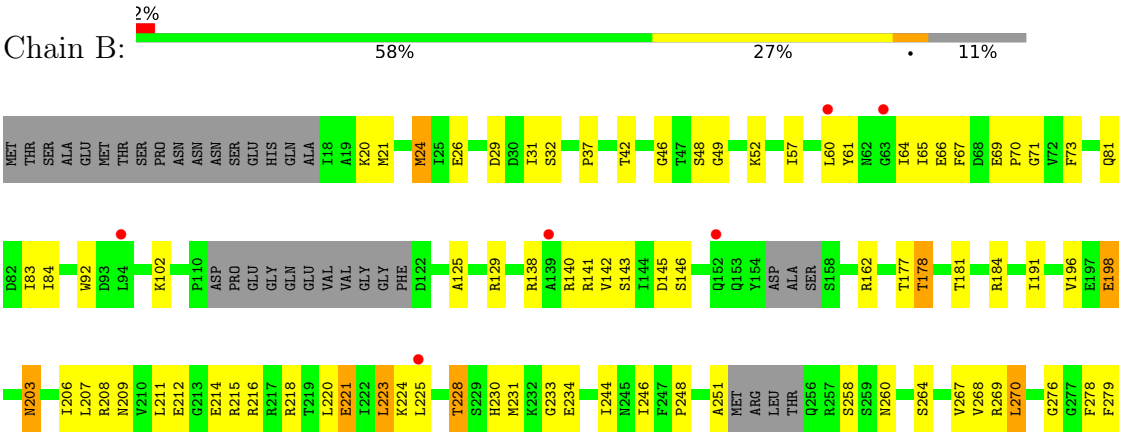
• Molecule 1: Circadian clock protein kinase KaiC

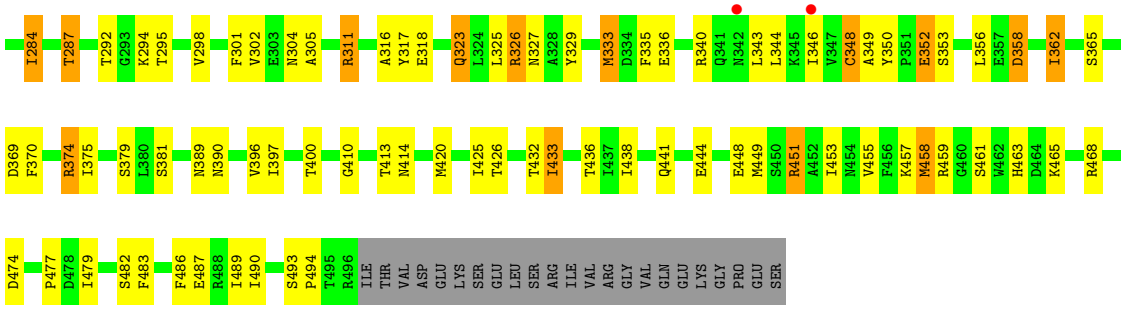
Chain A:



• Molecule 1: Circadian clock protein kinase KaiC

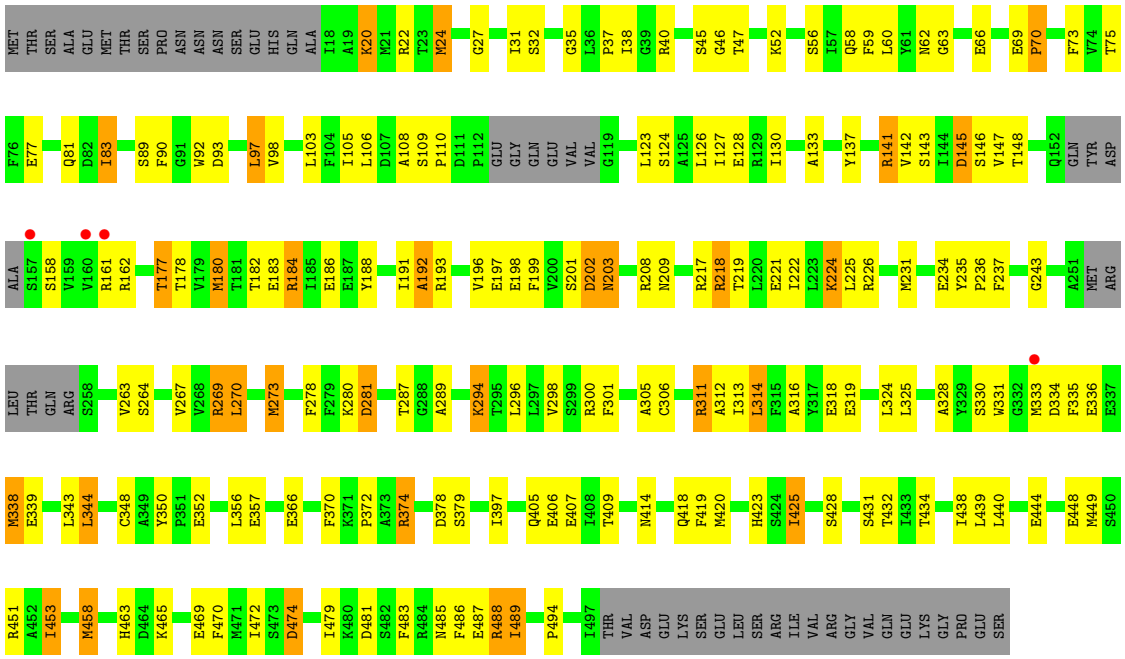
Chain B:





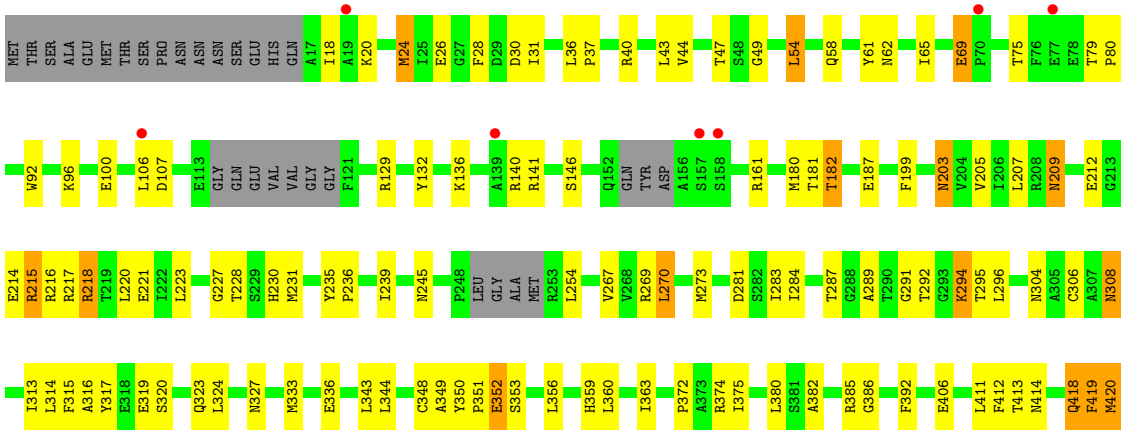
• Molecule 1: Circadian clock protein kinase KaiC

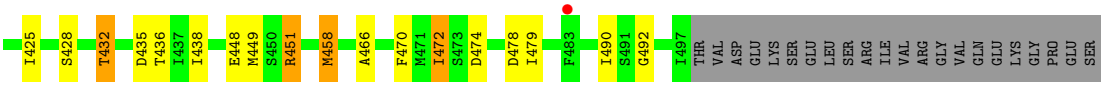
Chain E:



• Molecule 1: Circadian clock protein kinase KaiC

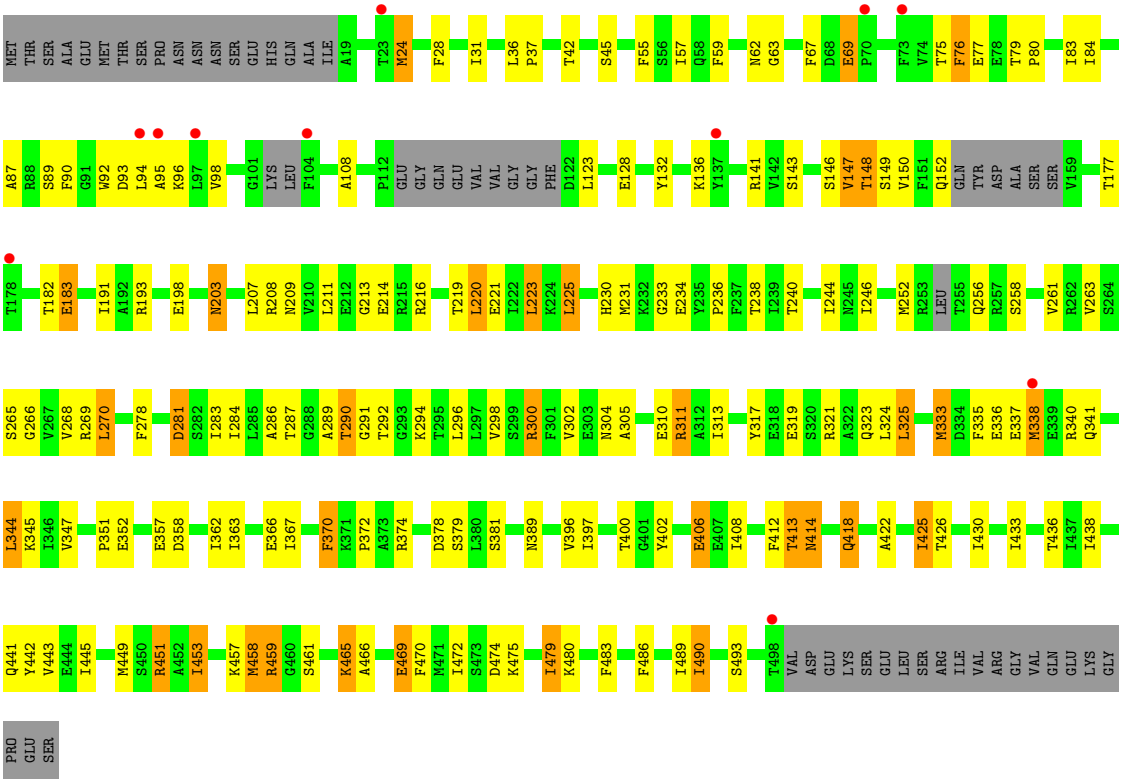
Chain F:





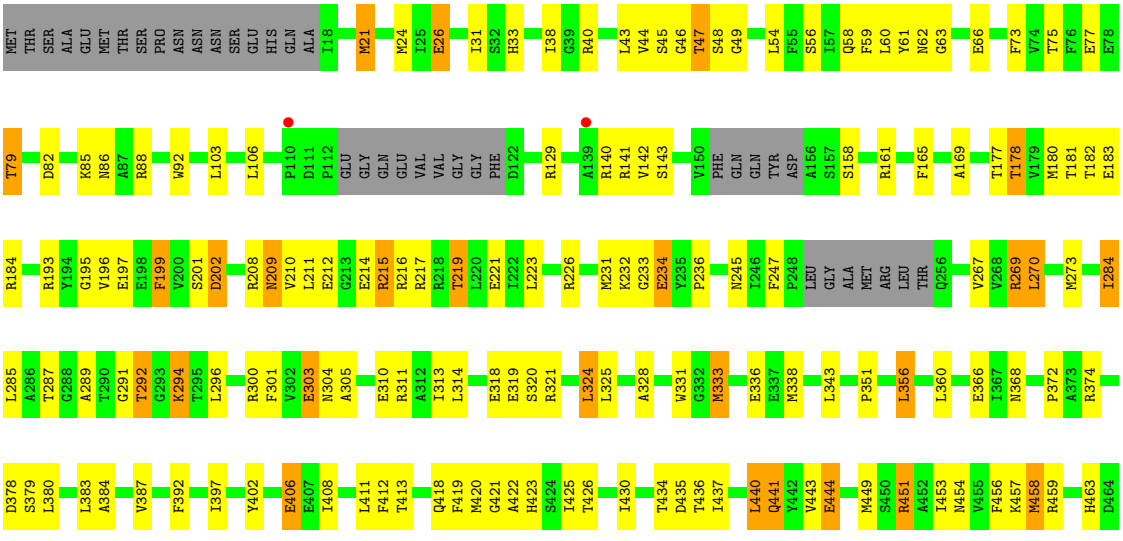
• Molecule 1: Circadian clock protein kinase KaiC

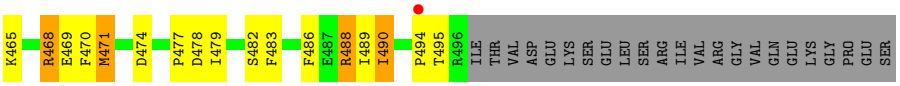
Chain C:



• Molecule 1: Circadian clock protein kinase KaiC

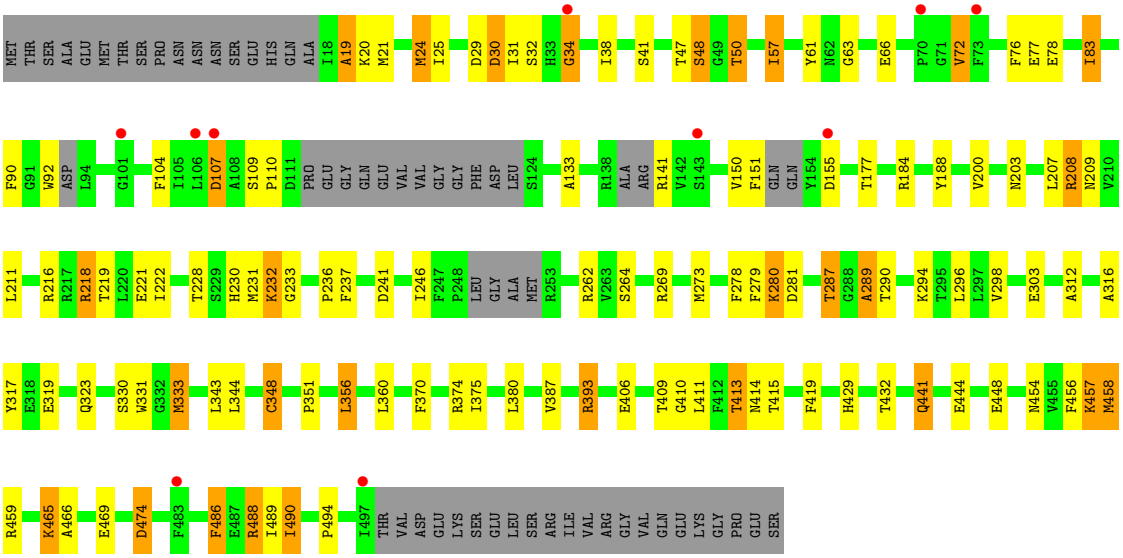
Chain D:





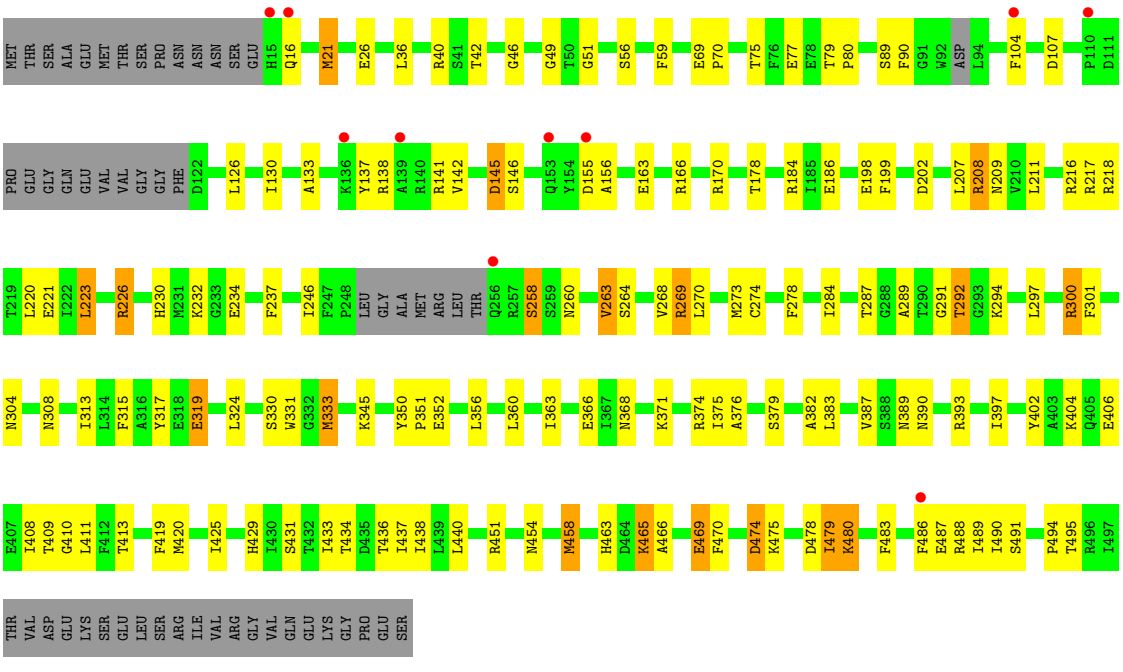
• Molecule 1: Circadian clock protein kinase KaiC

Chain G:



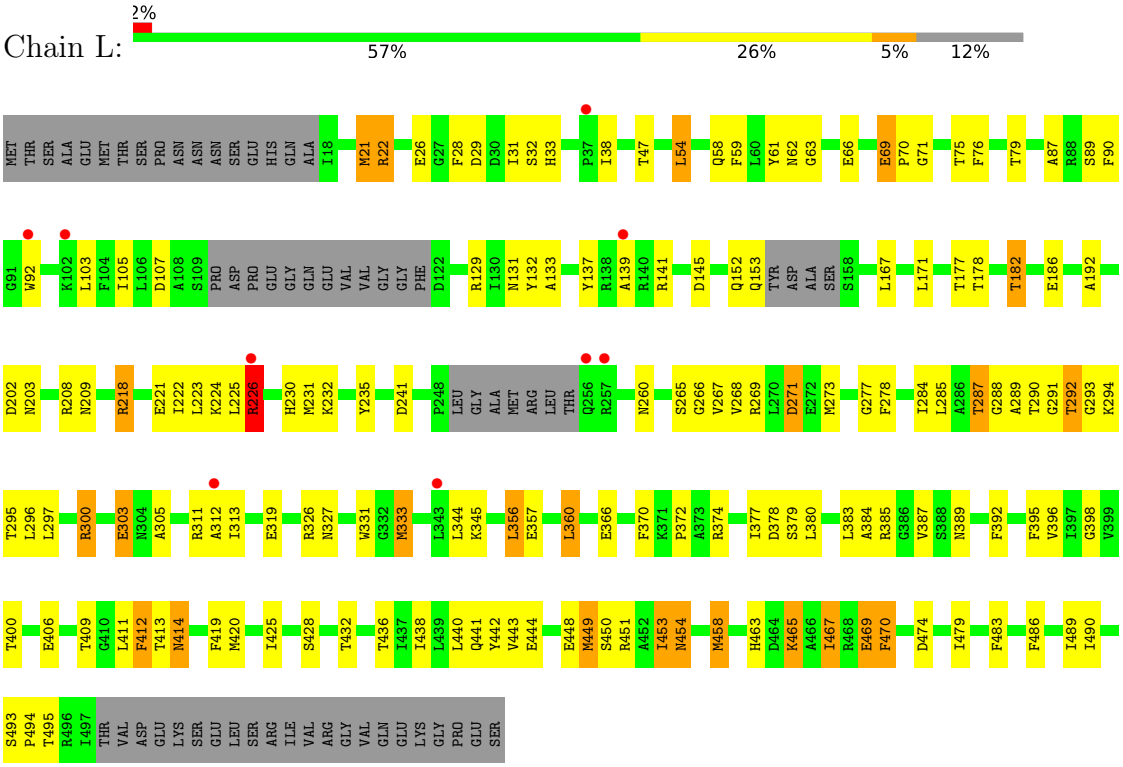
• Molecule 1: Circadian clock protein kinase KaiC

Chain K:



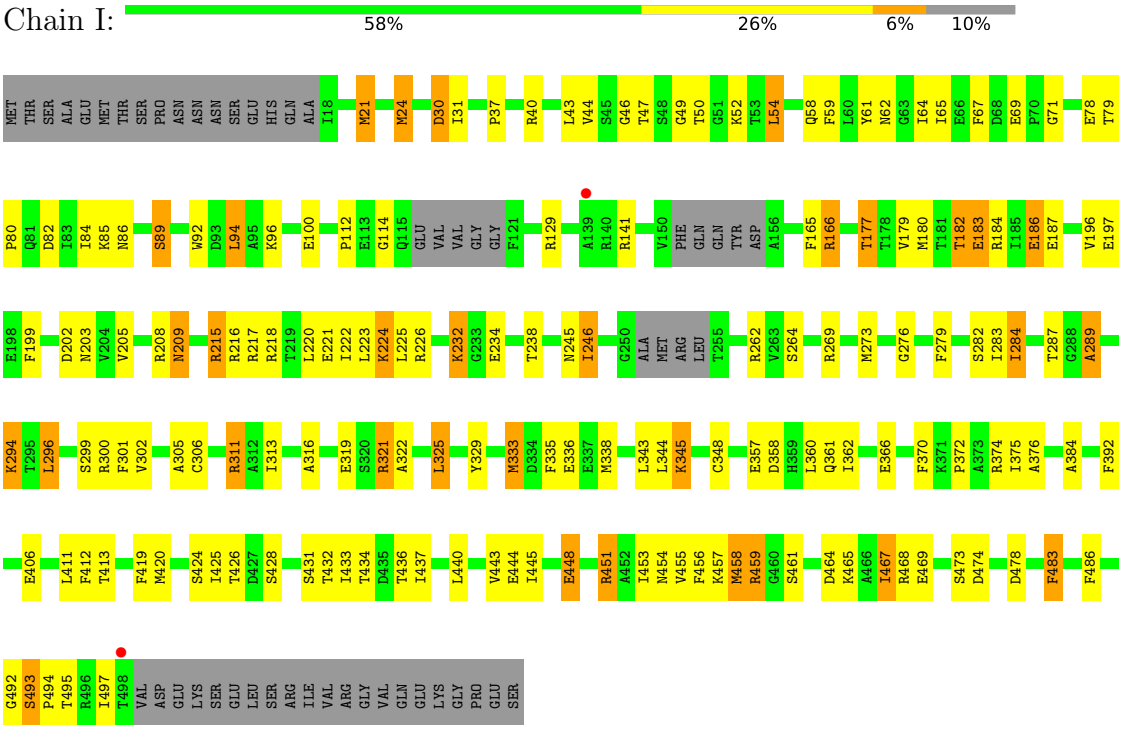
• Molecule 1: Circadian clock protein kinase KaiC

Chain L:



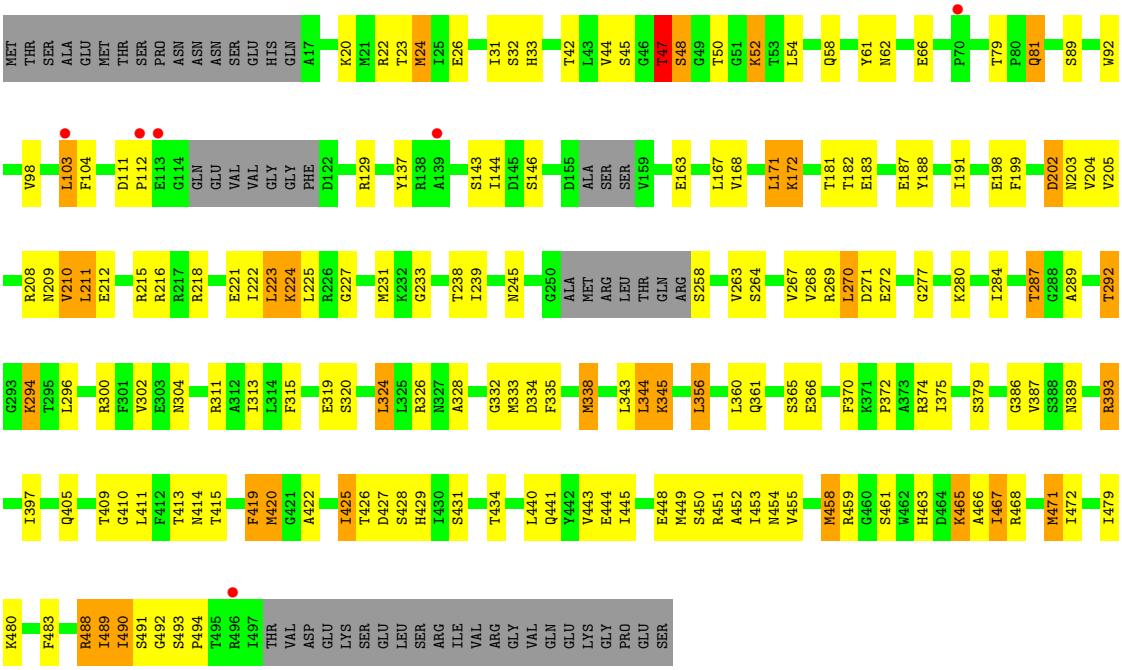
• Molecule 1: Circadian clock protein kinase KaiC

Chain I:



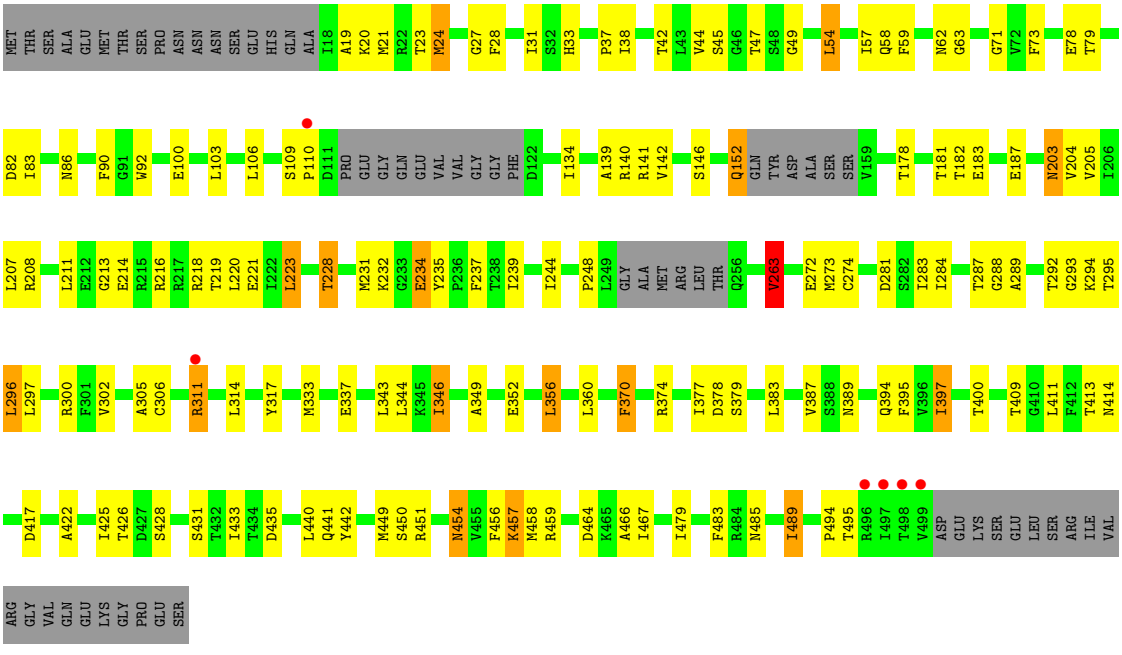
• Molecule 1: Circadian clock protein kinase KaiC

Chain J:



• Molecule 2: Circadian clock protein kinase KaiC

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.80Å 206.60Å 168.38Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	49.24 – 3.04 49.19 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.24-3.04) 99.0 (49.19-3.04)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.263 , 0.326 0.261 , 0.322	Depositor DCC
R_{free} test set	6048 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	71.4	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	39277	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: SEP, ADP, MG, ATP

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	0.68	0/3342	0.75	0/4539
1	B	0.70	0/3244	0.75	0/4413
1	C	0.69	0/3275	0.76	0/4450
1	D	0.69	0/3213	0.76	0/4366
1	E	0.69	0/3330	0.76	0/4516
1	F	0.70	0/3286	0.75	0/4465
1	G	0.72	0/3032	0.77	0/4131
1	I	0.68	0/3394	0.75	0/4600
1	J	0.68	0/3388	0.75	0/4597
1	K	0.71	0/3171	0.76	0/4311
1	L	0.71	0/3119	0.76	0/4249
2	H	0.70	0/3251	0.75	0/4424
All	All	0.70	0/39045	0.76	0/53061

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	155	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3300	0	2905	136	0
1	B	3204	0	2737	127	0
1	C	3236	0	2796	130	0
1	D	3173	0	2656	123	0
1	E	3287	0	2870	158	0
1	F	3245	0	2754	113	0
1	G	3000	0	2290	89	0
1	I	3349	0	2937	135	0
1	J	3342	0	2998	153	0
1	K	3132	0	2519	112	0
1	L	3082	0	2480	136	0
2	H	3197	0	2704	126	0
3	A	27	0	12	2	0
3	C	27	0	12	2	0
3	D	54	0	24	2	0
3	F	27	0	12	3	0
3	G	27	0	12	0	0
3	H	27	0	12	2	0
3	I	54	0	24	3	0
3	K	27	0	12	3	0
3	L	27	0	12	3	0
4	A	31	0	12	3	0
4	B	62	0	24	2	0
4	C	31	0	12	2	0
4	E	62	0	24	3	0
4	F	31	0	12	2	0
4	G	31	0	12	1	0
4	H	31	0	12	2	0
4	J	62	0	24	6	0
4	K	31	0	12	0	0
4	L	31	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	4	0	0	0	0
6	I	2	0	0	0	0
6	K	1	0	0	0	0
All	All	39277	0	32934	1413	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 20.

The worst 5 of 1413 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:K:207:LEU:HD21	1:K:220:LEU:HD12	1.30	1.10
1:C:311:ARG:HD3	1:C:370:PHE:CE2	1.90	1.07
1:L:384:ALA:HB2	1:L:392:PHE:CE1	1.92	1.04
1:F:352:GLU:OE2	1:F:385:ARG:NH2	1.91	1.03
1:J:52:LYS:HB3	1:J:181:THR:HG23	1.38	1.03

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	455/519 (88%)	409 (90%)	42 (9%)	4 (1%)	17 52
1	B	452/519 (87%)	401 (89%)	46 (10%)	5 (1%)	14 47
1	C	451/519 (87%)	399 (88%)	41 (9%)	11 (2%)	6 26
1	D	449/519 (86%)	392 (87%)	50 (11%)	7 (2%)	9 37
1	E	455/519 (88%)	411 (90%)	40 (9%)	4 (1%)	17 52
1	F	458/519 (88%)	404 (88%)	51 (11%)	3 (1%)	22 57
1	G	446/519 (86%)	372 (83%)	60 (14%)	14 (3%)	4 20
1	I	458/519 (88%)	410 (90%)	41 (9%)	7 (2%)	10 39
1	J	455/519 (88%)	410 (90%)	41 (9%)	4 (1%)	17 52
1	K	456/519 (88%)	413 (91%)	40 (9%)	3 (1%)	22 57
1	L	448/519 (86%)	393 (88%)	45 (10%)	10 (2%)	6 28
2	H	452/519 (87%)	411 (91%)	35 (8%)	6 (1%)	12 42
All	All	5435/6228 (87%)	4825 (89%)	532 (10%)	78 (1%)	11 40

5 of 78 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ALA
1	F	26	GLU
1	C	422	ALA
1	D	421	GLY
1	G	200	VAL

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	297/443 (67%)	243 (82%)	54 (18%)	1 8
1	B	272/443 (61%)	226 (83%)	46 (17%)	2 9
1	C	282/443 (64%)	220 (78%)	62 (22%)	1 4
1	D	266/443 (60%)	207 (78%)	59 (22%)	1 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	290/443 (66%)	231 (80%)	59 (20%)	1 5
1	F	275/443 (62%)	234 (85%)	41 (15%)	3 13
1	G	213/443 (48%)	174 (82%)	39 (18%)	1 8
1	I	301/443 (68%)	242 (80%)	59 (20%)	1 6
1	J	307/443 (69%)	253 (82%)	54 (18%)	2 8
1	K	240/443 (54%)	199 (83%)	41 (17%)	2 9
1	L	239/443 (54%)	190 (80%)	49 (20%)	1 5
2	H	273/444 (62%)	233 (85%)	40 (15%)	3 13
All	All	3255/5317 (61%)	2652 (82%)	603 (18%)	1 7

5 of 603 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	300	ARG
1	J	238	THR
1	L	414	ASN
1	L	296	LEU
1	I	311	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	203	ASN
1	J	389	ASN
1	L	323	GLN
1	I	414	ASN
1	F	209	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)

11 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	K	431	1	8,9,10	0.61	0	8,12,14	0.64	0
1	SEP	I	431	1	8,9,10	0.59	0	8,12,14	0.61	0
1	SEP	J	431	1	8,9,10	0.55	0	8,12,14	0.75	0
1	SEP	F	431	1	8,9,10	0.58	0	8,12,14	0.63	0
1	SEP	A	431	1	8,9,10	0.60	0	8,12,14	0.68	0
1	SEP	D	431	1	8,9,10	0.58	0	8,12,14	0.75	0
1	SEP	E	431	1	8,9,10	0.62	0	8,12,14	0.68	0
1	SEP	B	431	1	8,9,10	0.57	0	8,12,14	0.58	0
1	SEP	L	431	1	8,9,10	0.61	0	8,12,14	0.71	0
1	SEP	G	431	1	8,9,10	0.70	0	8,12,14	0.77	0
1	SEP	C	431	1	8,9,10	0.59	0	8,12,14	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	K	431	1	-	1/5/8/10	-
1	SEP	I	431	1	-	4/5/8/10	-
1	SEP	J	431	1	-	2/5/8/10	-
1	SEP	F	431	1	-	1/5/8/10	-
1	SEP	A	431	1	-	1/5/8/10	-
1	SEP	D	431	1	-	1/5/8/10	-
1	SEP	E	431	1	-	2/5/8/10	-
1	SEP	B	431	1	-	1/5/8/10	-
1	SEP	L	431	1	-	1/5/8/10	-
1	SEP	G	431	1	-	2/5/8/10	-
1	SEP	C	431	1	-	3/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	431	SEP	N-CA-CB-OG
1	B	431	SEP	N-CA-CB-OG
1	F	431	SEP	N-CA-CB-OG
1	C	431	SEP	N-CA-CB-OG
1	D	431	SEP	N-CA-CB-OG

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	K	431	SEP	4	0
1	I	431	SEP	1	0
1	J	431	SEP	2	0
1	A	431	SEP	1	0
1	E	431	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	E	602	5	26,33,33	0.65	0	31,52,52	0.85	2 (6%)
4	ATP	A	602	5	26,33,33	0.65	0	31,52,52	0.84	1 (3%)
4	ATP	K	602	5	26,33,33	0.65	0	31,52,52	0.76	1 (3%)
3	ADP	A	601	-	24,29,29	0.66	0	29,45,45	0.74	1 (3%)
4	ATP	C	602	5	26,33,33	0.65	0	31,52,52	0.74	1 (3%)
4	ATP	B	701	5	26,33,33	0.66	0	31,52,52	1.00	2 (6%)
4	ATP	J	701	5	26,33,33	0.66	0	31,52,52	0.75	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ATP	J	702	-	26,33,33	0.66	0	31,52,52	0.74	1 (3%)
3	ADP	G	601	-	24,29,29	0.63	0	29,45,45	0.80	1 (3%)
4	ATP	F	602	5	26,33,33	0.66	0	31,52,52	0.77	1 (3%)
4	ATP	B	702	-	26,33,33	0.65	0	31,52,52	0.81	1 (3%)
3	ADP	I	602	-	24,29,29	0.62	0	29,45,45	0.83	1 (3%)
4	ATP	H	602	5	26,33,33	0.66	0	31,52,52	0.81	1 (3%)
3	ADP	K	601	-	24,29,29	0.66	0	29,45,45	0.81	2 (6%)
3	ADP	H	601	-	24,29,29	0.69	0	29,45,45	0.73	1 (3%)
3	ADP	D	601	-	24,29,29	0.66	0	29,45,45	0.77	1 (3%)
3	ADP	I	601	-	24,29,29	0.66	0	29,45,45	0.80	1 (3%)
3	ADP	D	602	-	24,29,29	0.66	0	29,45,45	0.72	1 (3%)
3	ADP	F	601	-	24,29,29	0.66	0	29,45,45	0.75	1 (3%)
4	ATP	L	602	-	26,33,33	0.67	0	31,52,52	0.84	2 (6%)
4	ATP	G	602	5	26,33,33	0.66	0	31,52,52	0.75	1 (3%)
3	ADP	C	601	-	24,29,29	0.66	0	29,45,45	0.69	1 (3%)
4	ATP	E	601	5	26,33,33	0.68	0	31,52,52	0.77	1 (3%)
3	ADP	L	601	-	24,29,29	0.66	0	29,45,45	0.70	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	E	602	5	-	4/18/38/38	0/3/3/3
4	ATP	A	602	5	-	1/18/38/38	0/3/3/3
4	ATP	K	602	5	-	1/18/38/38	0/3/3/3
3	ADP	A	601	-	-	5/12/32/32	0/3/3/3
4	ATP	C	602	5	-	4/18/38/38	0/3/3/3
4	ATP	B	701	5	-	3/18/38/38	0/3/3/3
4	ATP	J	701	5	-	7/18/38/38	0/3/3/3
4	ATP	J	702	-	-	5/18/38/38	0/3/3/3
3	ADP	G	601	-	-	4/12/32/32	0/3/3/3
4	ATP	F	602	5	-	6/18/38/38	0/3/3/3
4	ATP	B	702	-	-	5/18/38/38	0/3/3/3
3	ADP	I	602	-	-	2/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	H	602	5	-	5/18/38/38	0/3/3/3
3	ADP	K	601	-	-	5/12/32/32	0/3/3/3
3	ADP	H	601	-	-	3/12/32/32	0/3/3/3
3	ADP	D	601	-	-	8/12/32/32	0/3/3/3
3	ADP	I	601	-	-	6/12/32/32	0/3/3/3
3	ADP	D	602	-	-	2/12/32/32	0/3/3/3
3	ADP	F	601	-	-	6/12/32/32	0/3/3/3
4	ATP	L	602	-	-	0/18/38/38	0/3/3/3
4	ATP	G	602	5	-	6/18/38/38	0/3/3/3
3	ADP	C	601	-	-	3/12/32/32	0/3/3/3
4	ATP	E	601	5	-	6/18/38/38	0/3/3/3
3	ADP	L	601	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	701	ATP	C3'-C2'-C1'	2.87	105.30	100.98
4	G	602	ATP	C5-C6-N6	2.37	123.96	120.35
4	J	701	ATP	C5-C6-N6	2.36	123.94	120.35
4	E	602	ATP	C5-C6-N6	2.35	123.93	120.35
3	I	601	ADP	C5-C6-N6	2.32	123.87	120.35

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	C5'-O5'-PA-O1A
3	A	601	ADP	C5'-O5'-PA-O2A
3	F	601	ADP	C5'-O5'-PA-O1A
3	F	601	ADP	C5'-O5'-PA-O2A
3	C	601	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

21 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ATP	3	0

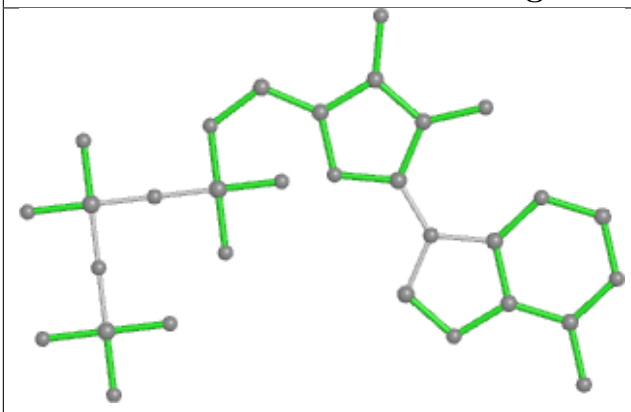
Continued on next page...

Continued from previous page...

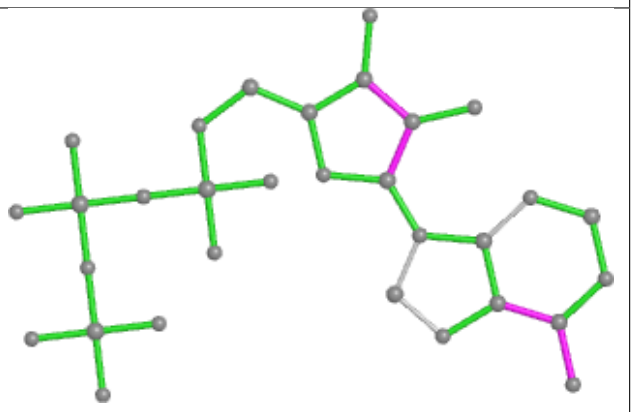
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ADP	2	0
4	C	602	ATP	2	0
4	B	701	ATP	1	0
4	J	701	ATP	1	0
4	J	702	ATP	5	0
4	F	602	ATP	2	0
4	B	702	ATP	1	0
3	I	602	ADP	2	0
4	H	602	ATP	2	0
3	K	601	ADP	3	0
3	H	601	ADP	2	0
3	D	601	ADP	1	0
3	I	601	ADP	1	0
3	D	602	ADP	1	0
3	F	601	ADP	3	0
4	L	602	ATP	4	0
4	G	602	ATP	1	0
3	C	601	ADP	2	0
4	E	601	ATP	3	0
3	L	601	ADP	3	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.

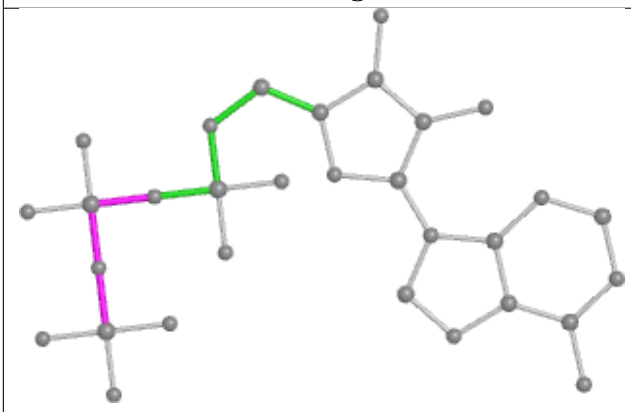
Ligand ATP E 602



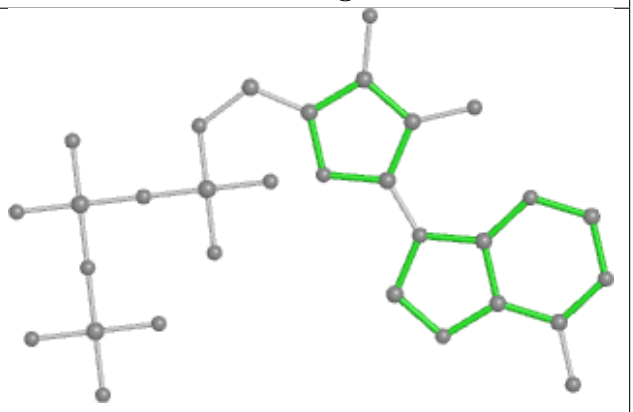
Bond lengths



Bond angles

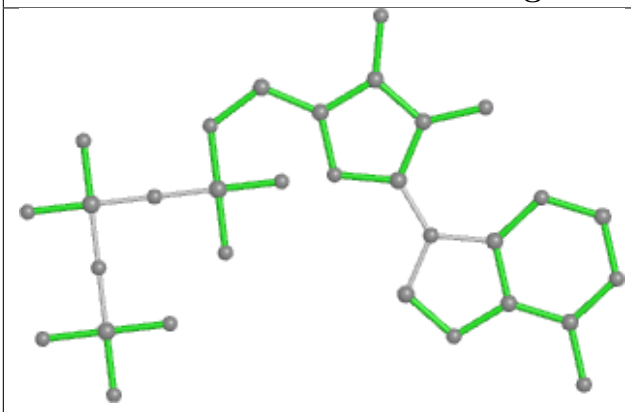


Torsions

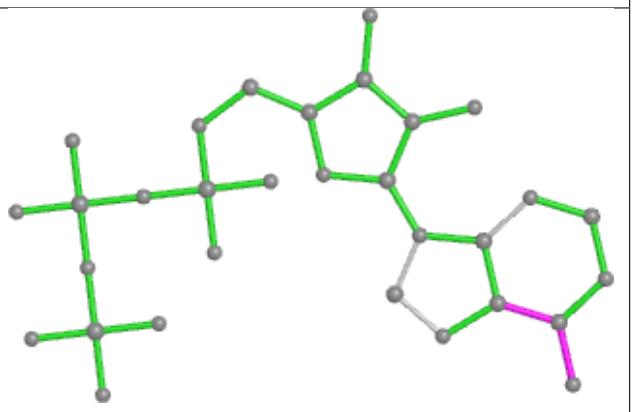


Rings

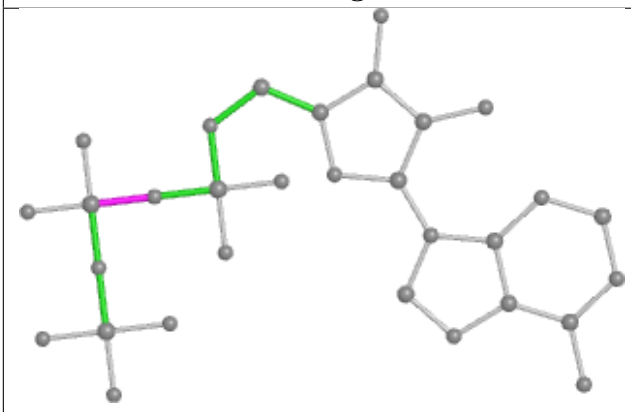
Ligand ATP A 602



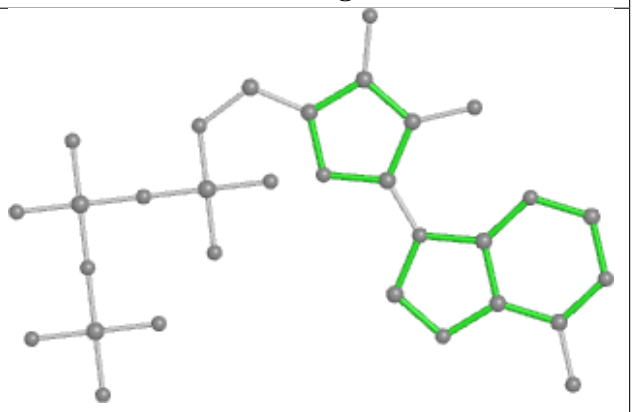
Bond lengths



Bond angles

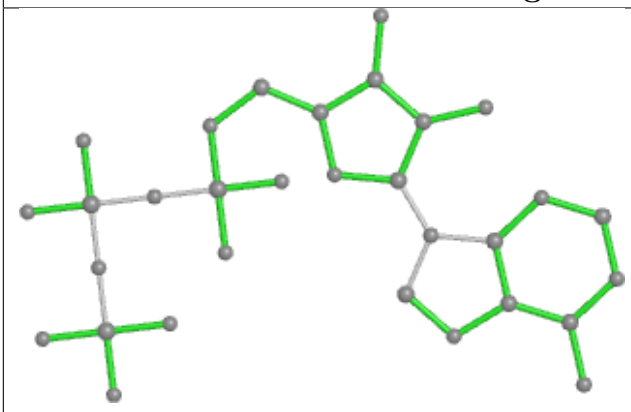


Torsions

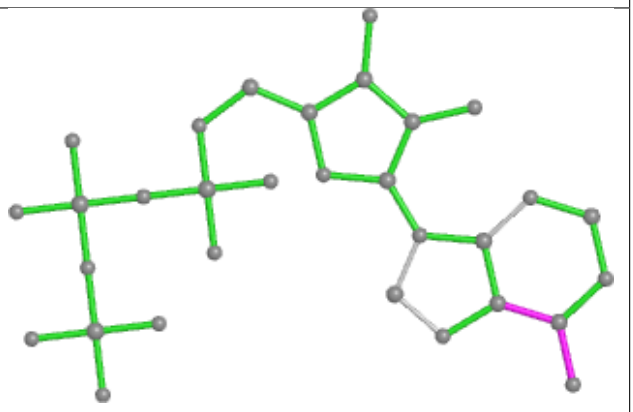


Rings

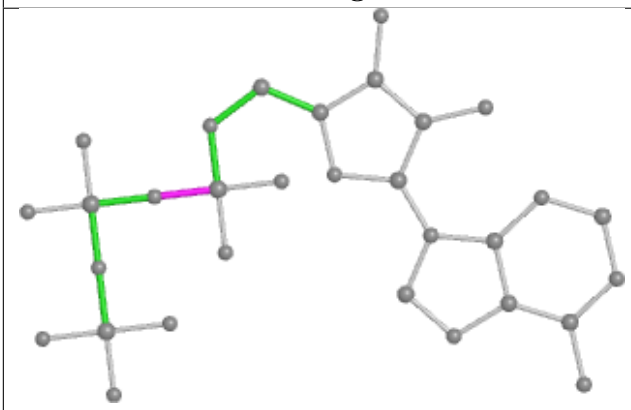
Ligand ATP K 602



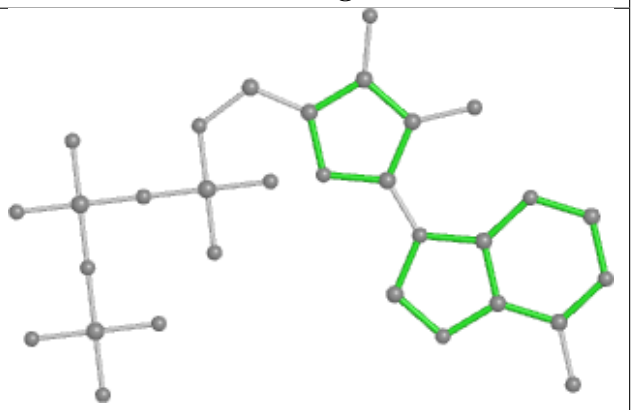
Bond lengths



Bond angles

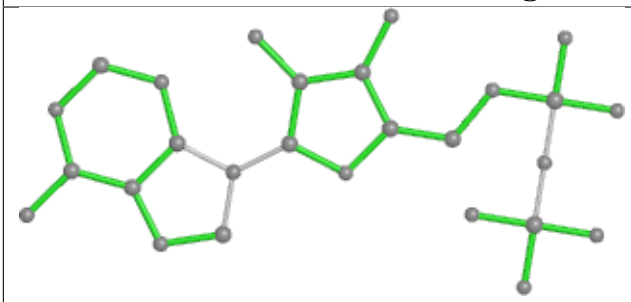


Torsions

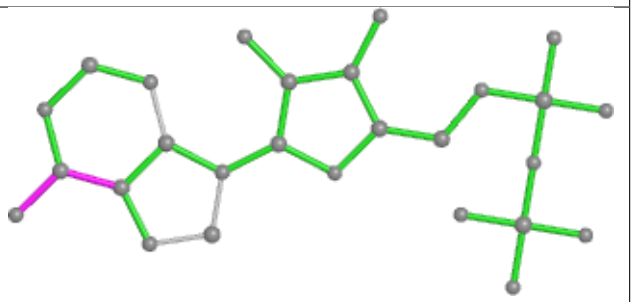


Rings

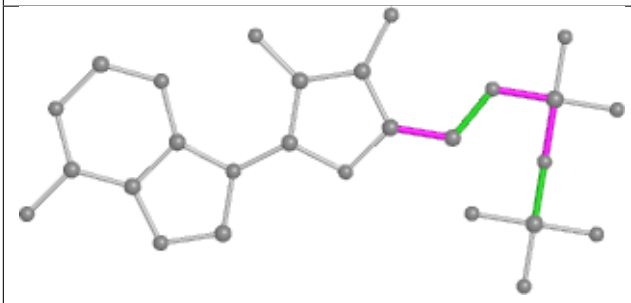
Ligand ADP A 601



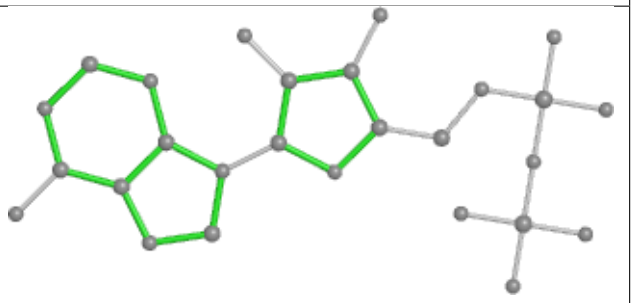
Bond lengths



Bond angles

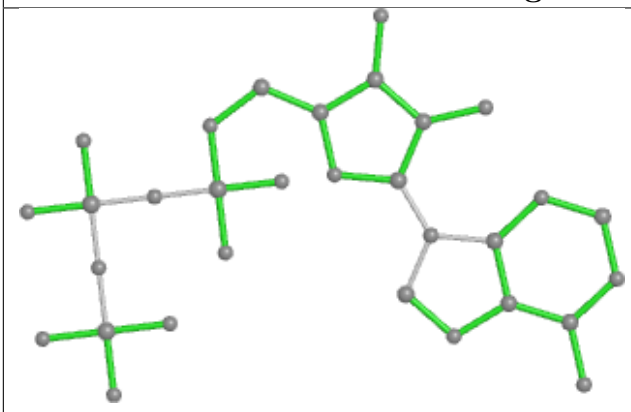


Torsions

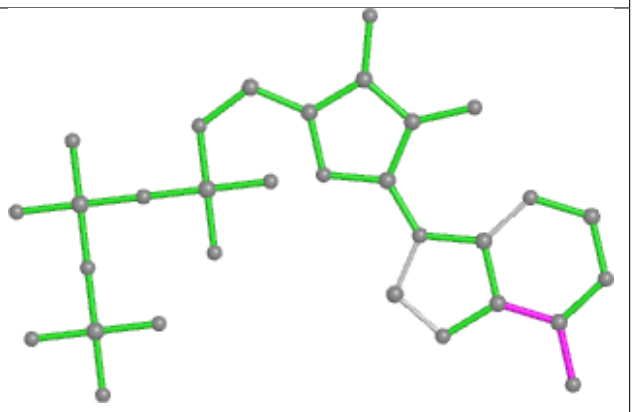


Rings

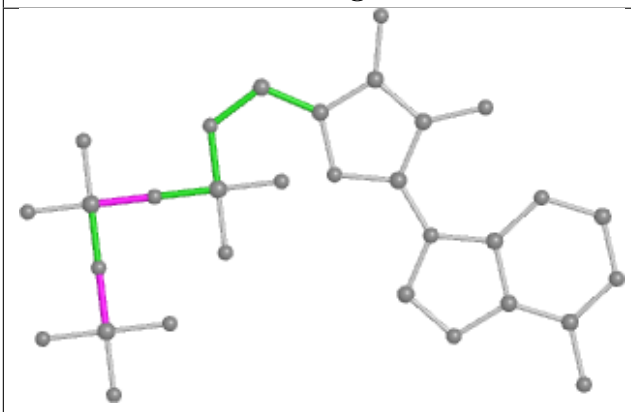
Ligand ATP C 602



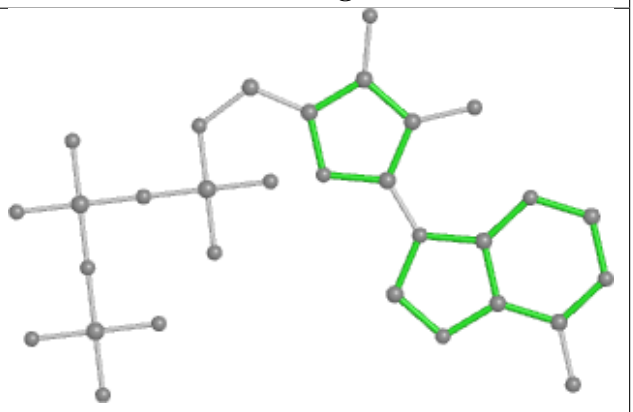
Bond lengths



Bond angles

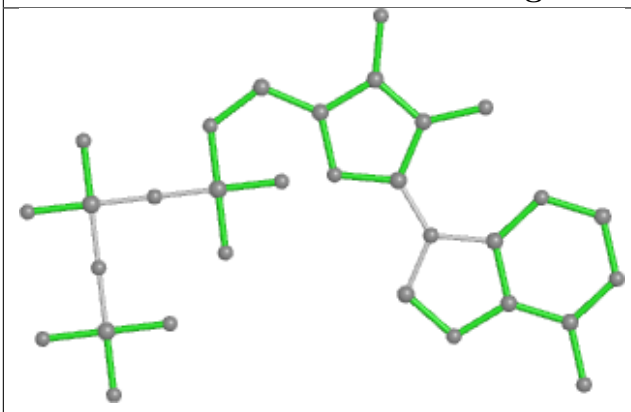


Torsions

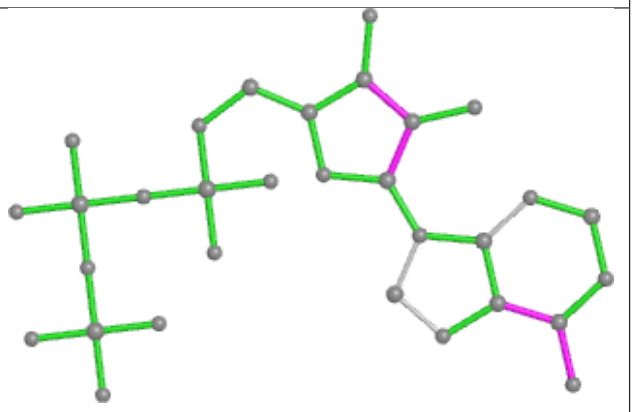


Rings

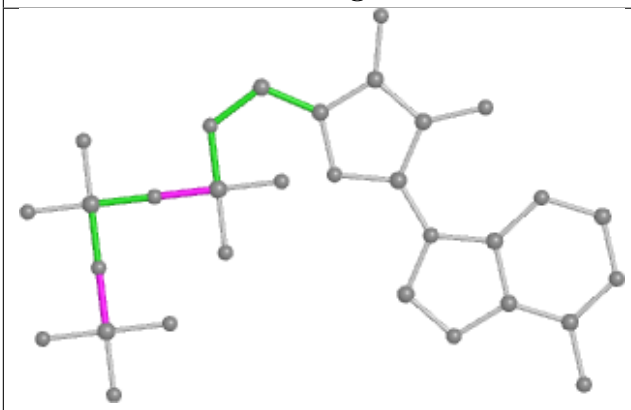
Ligand ATP B 701



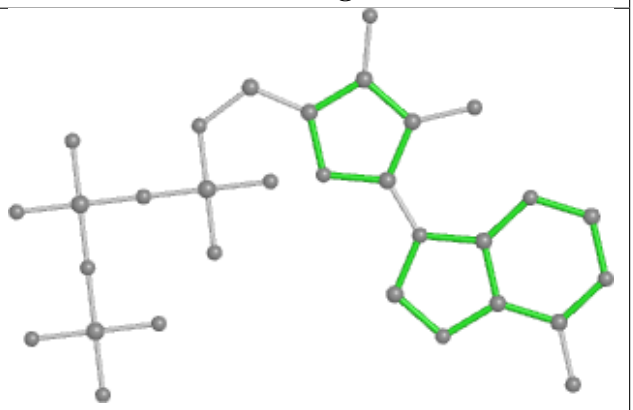
Bond lengths



Bond angles

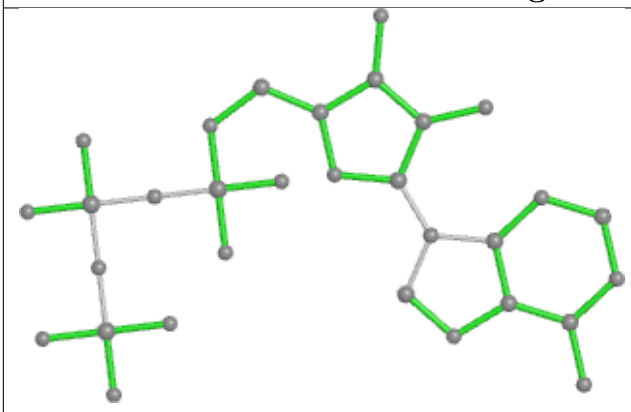


Torsions

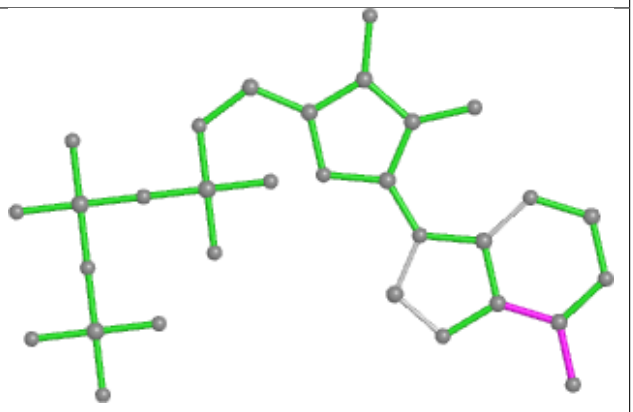


Rings

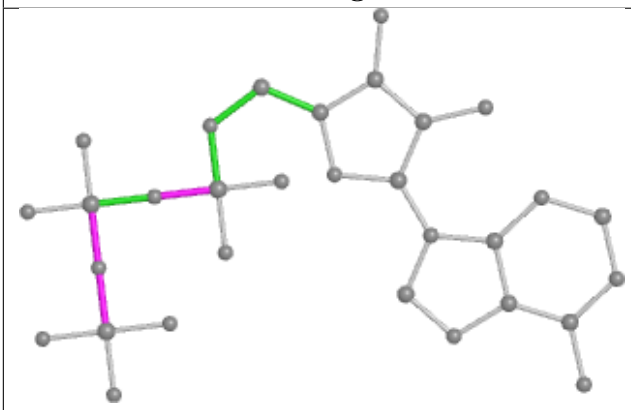
Ligand ATP J 701



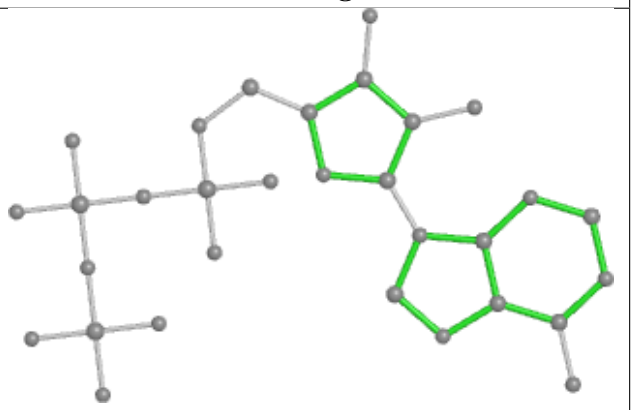
Bond lengths



Bond angles

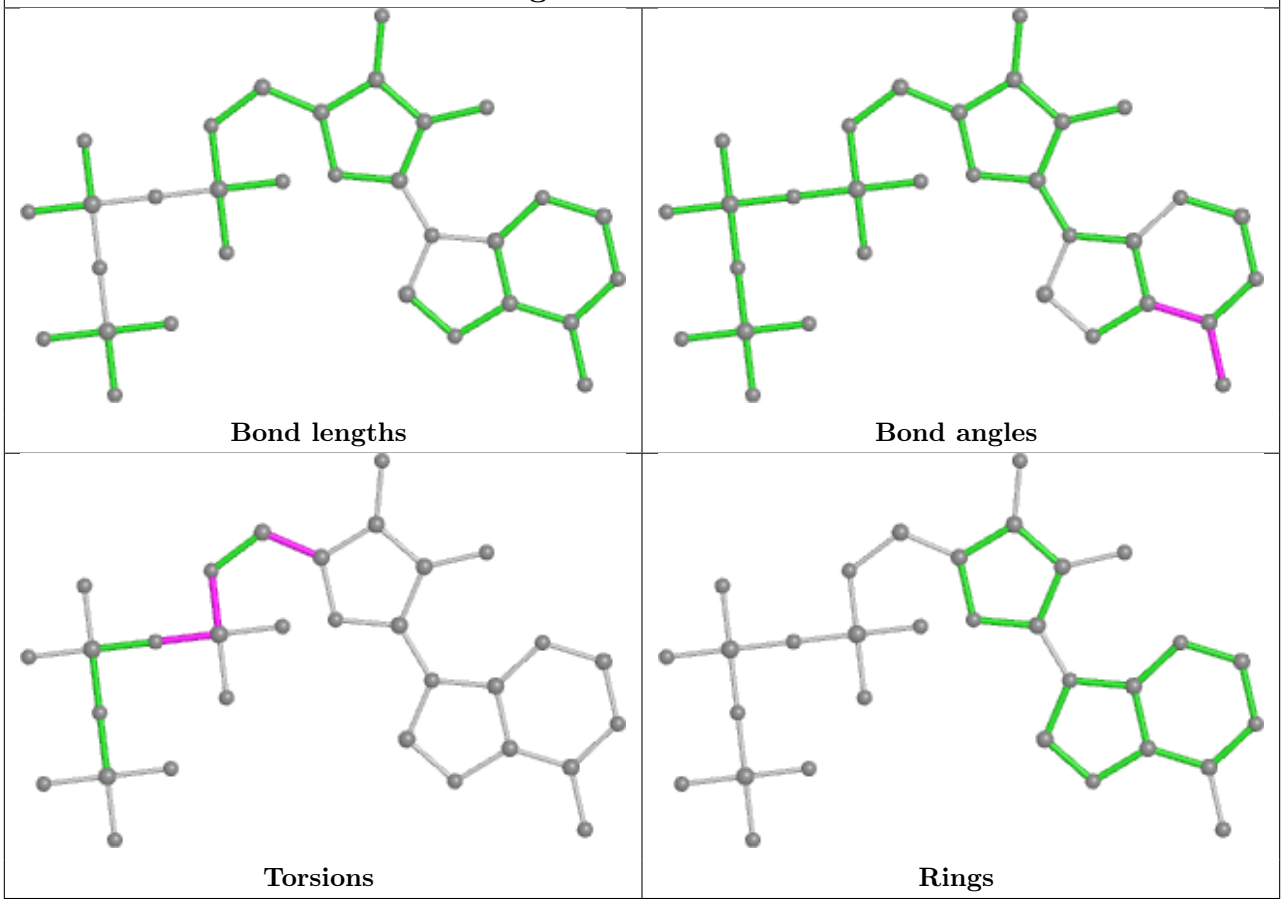


Torsions

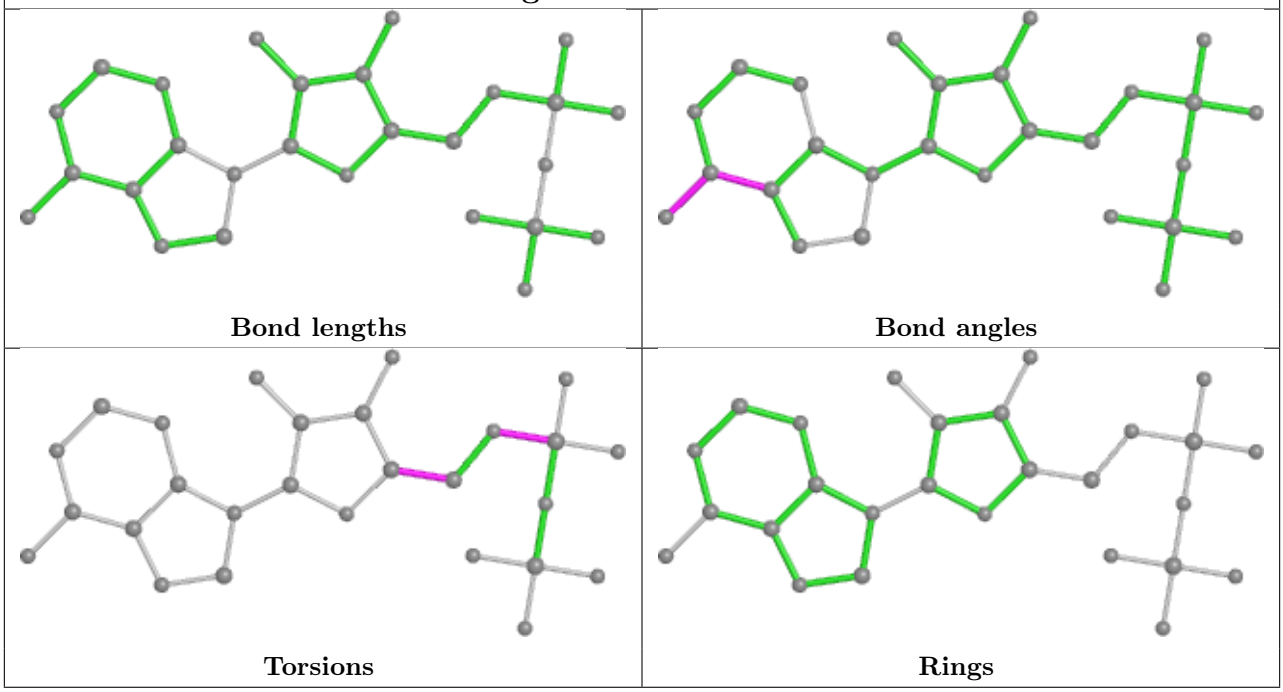


Rings

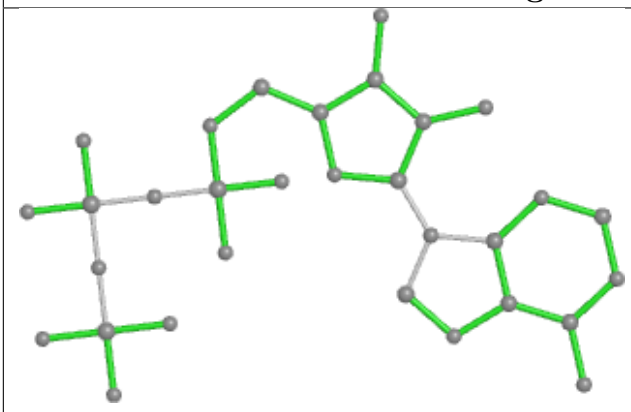
Ligand ATP J 702



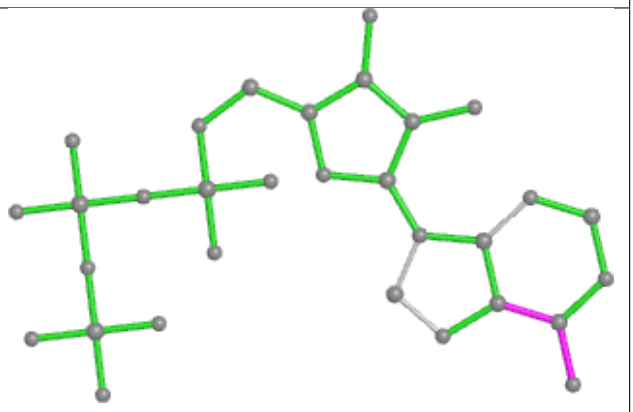
Ligand ADP G 601



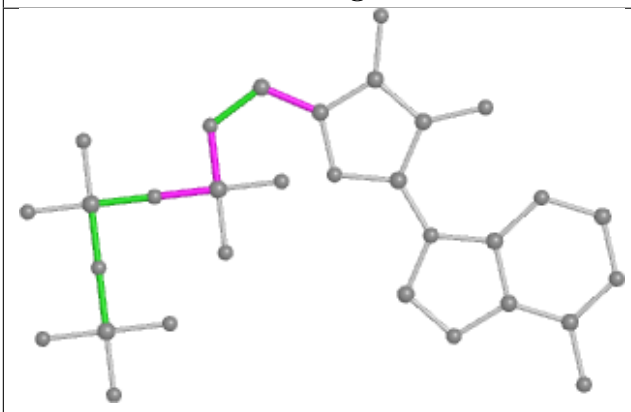
Ligand ATP F 602



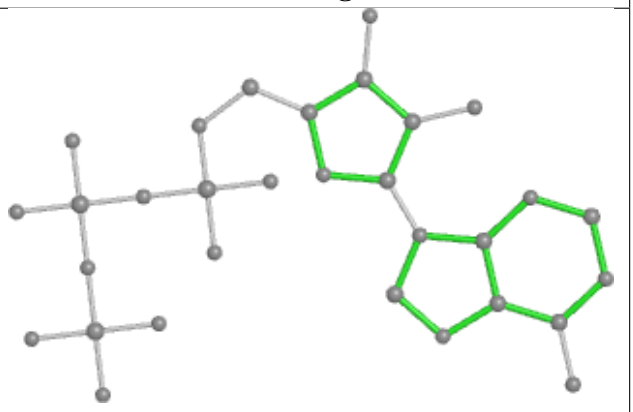
Bond lengths



Bond angles

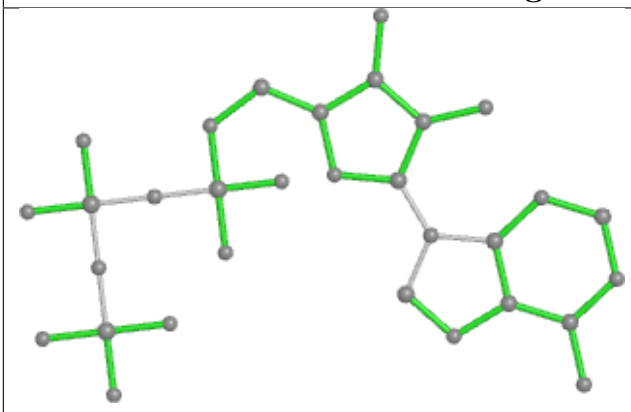


Torsions

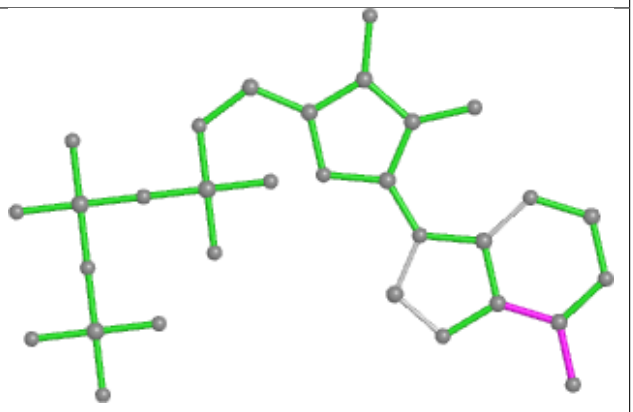


Rings

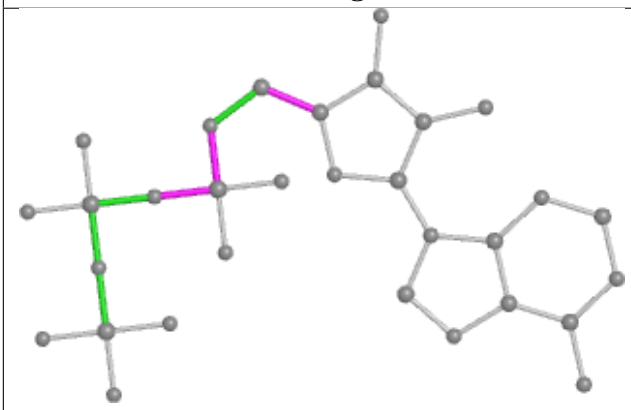
Ligand ATP B 702



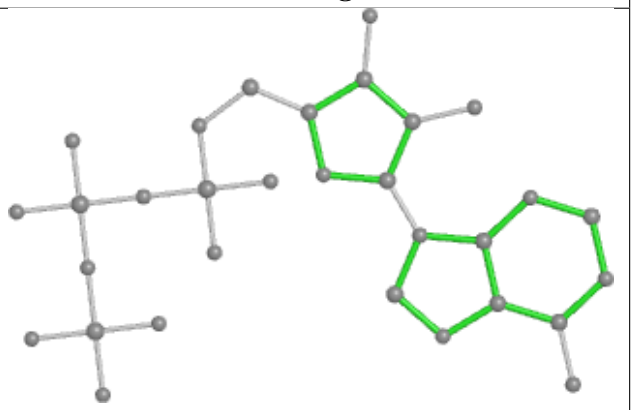
Bond lengths



Bond angles

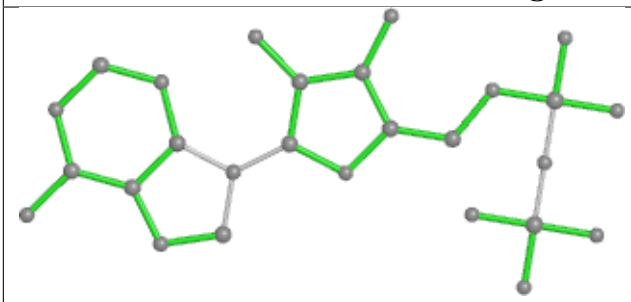


Torsions

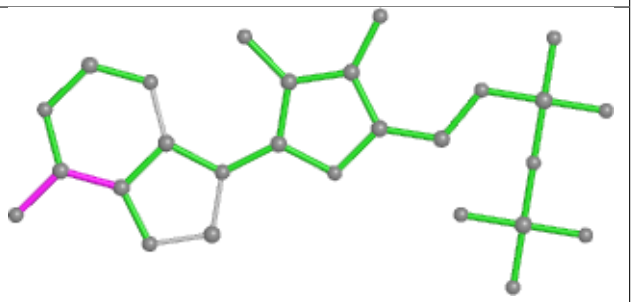


Rings

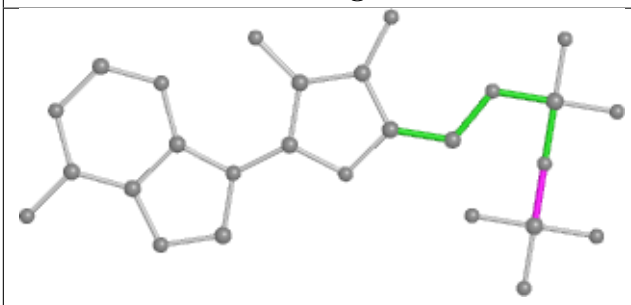
Ligand ADP I 602



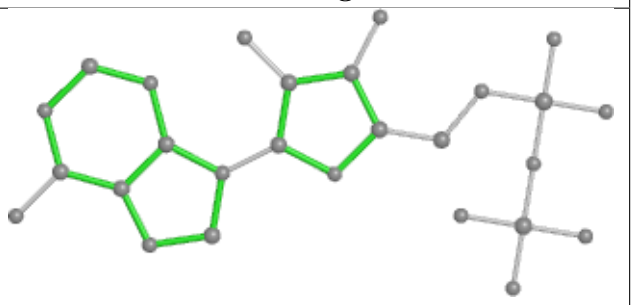
Bond lengths



Bond angles

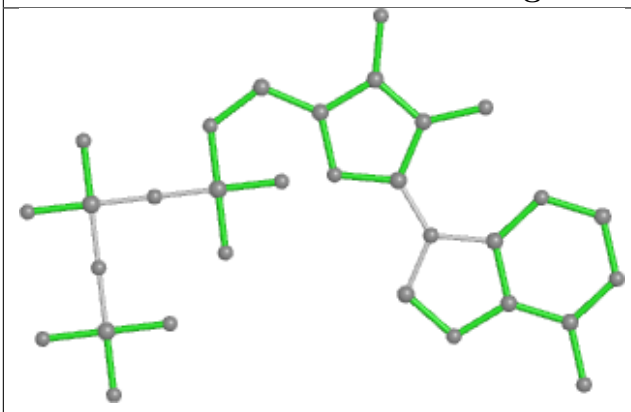


Torsions

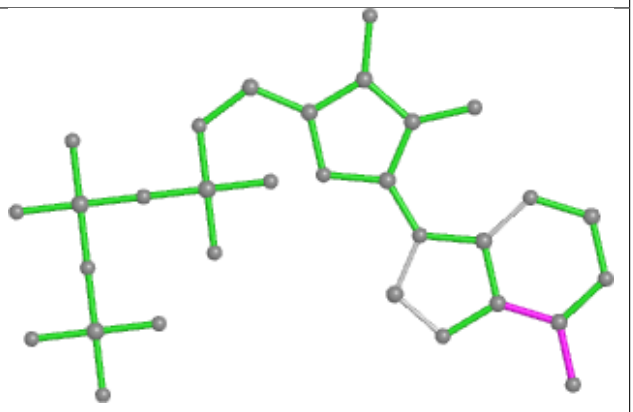


Rings

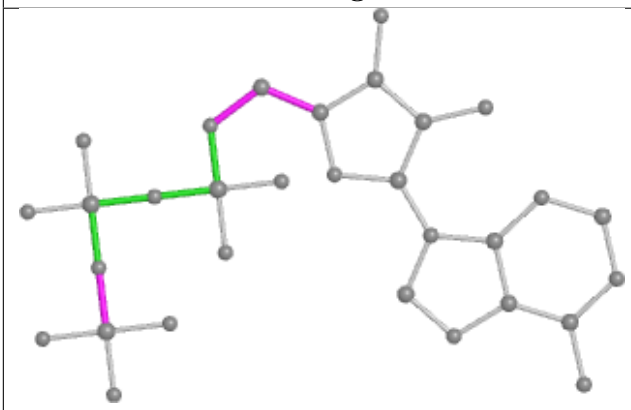
Ligand ATP H 602



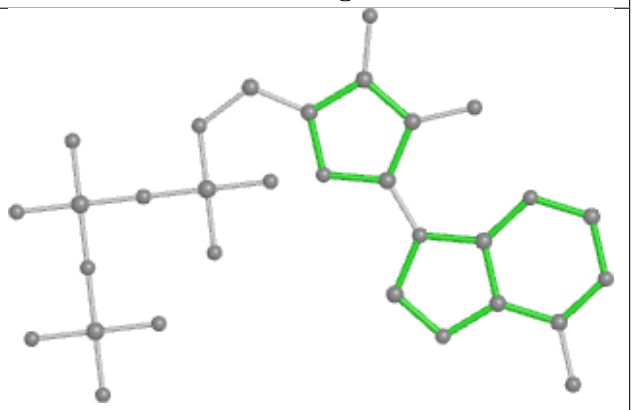
Bond lengths



Bond angles

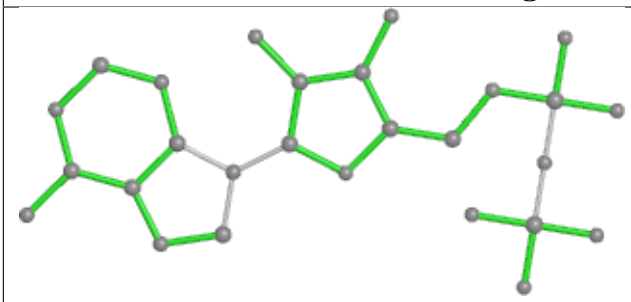


Torsions

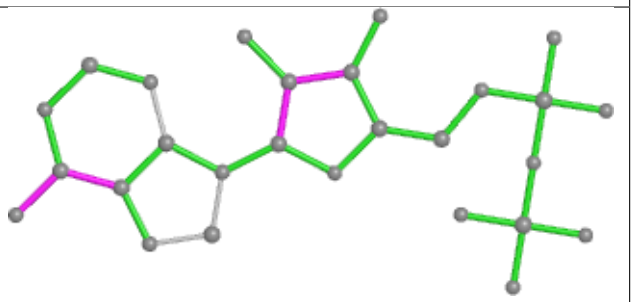


Rings

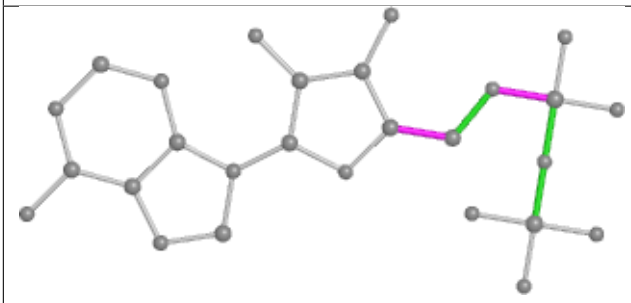
Ligand ADP K 601



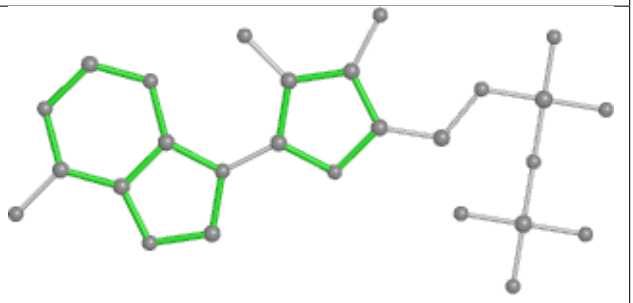
Bond lengths



Bond angles

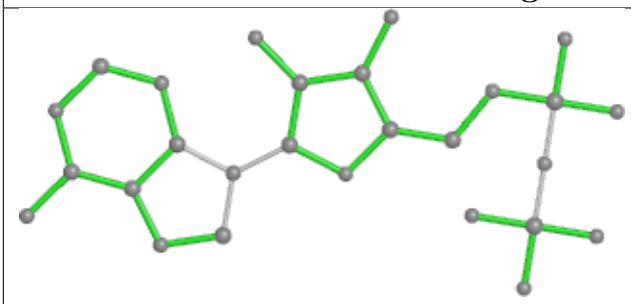


Torsions

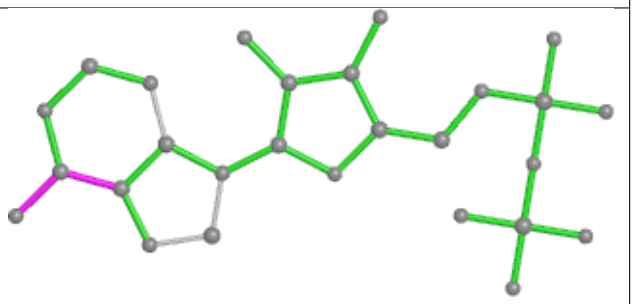


Rings

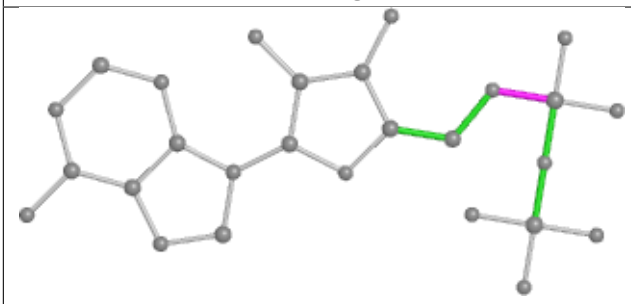
Ligand ADP H 601



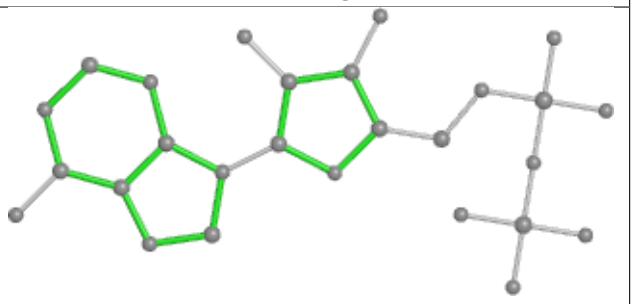
Bond lengths



Bond angles

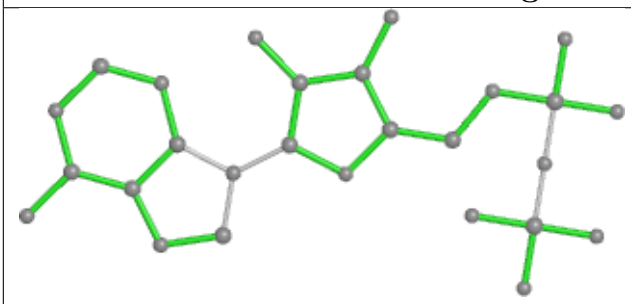


Torsions

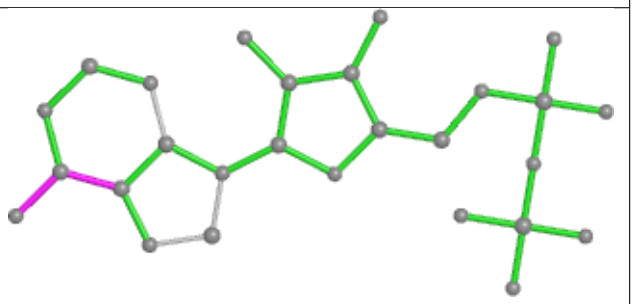


Rings

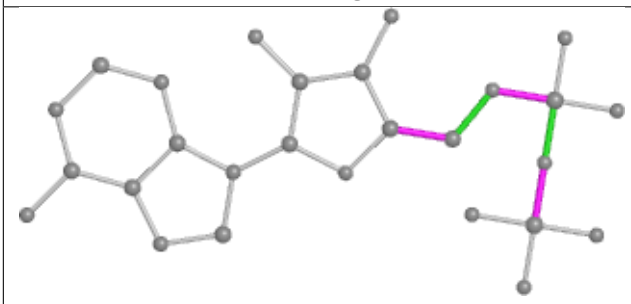
Ligand ADP D 601



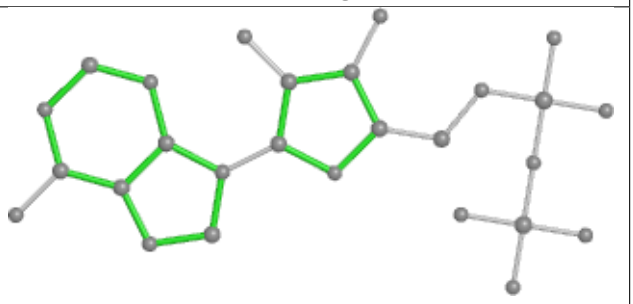
Bond lengths



Bond angles

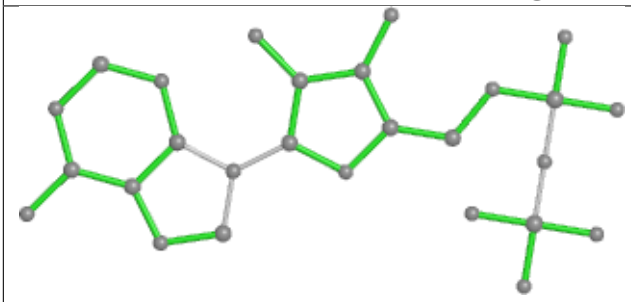


Torsions

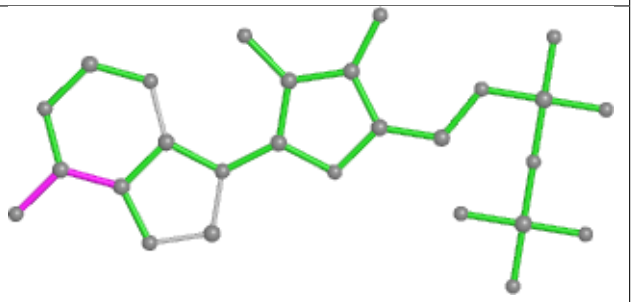


Rings

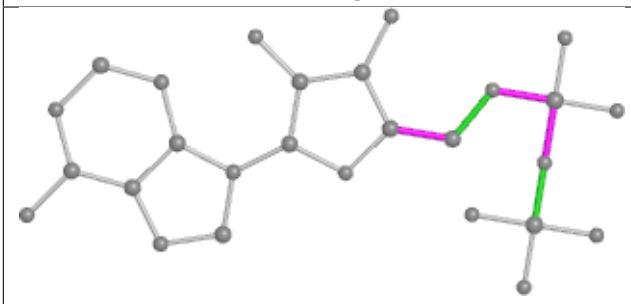
Ligand ADP I 601



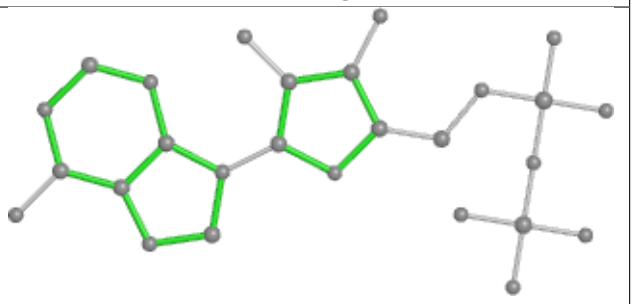
Bond lengths



Bond angles

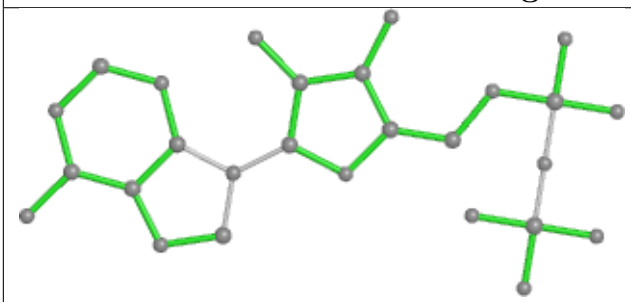


Torsions

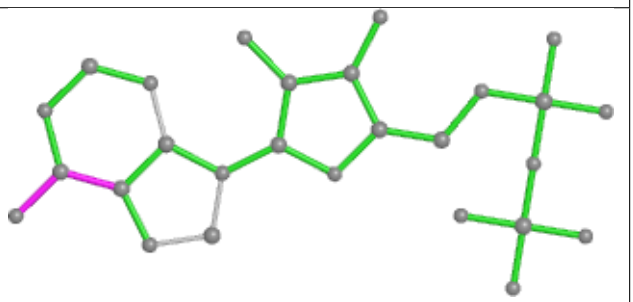


Rings

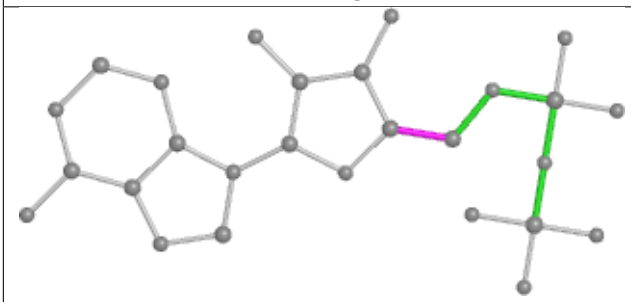
Ligand ADP D 602



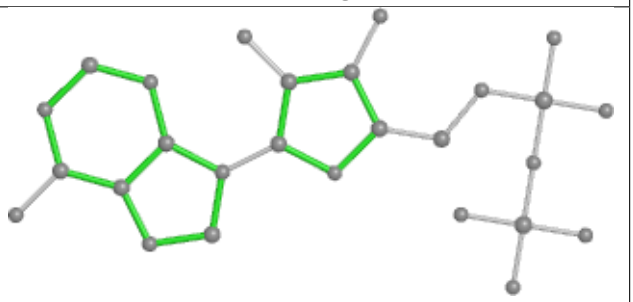
Bond lengths



Bond angles

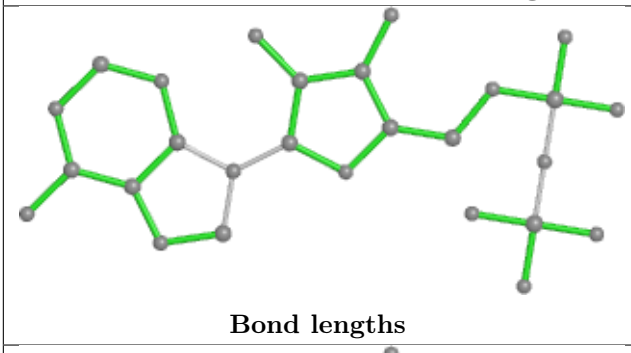


Torsions

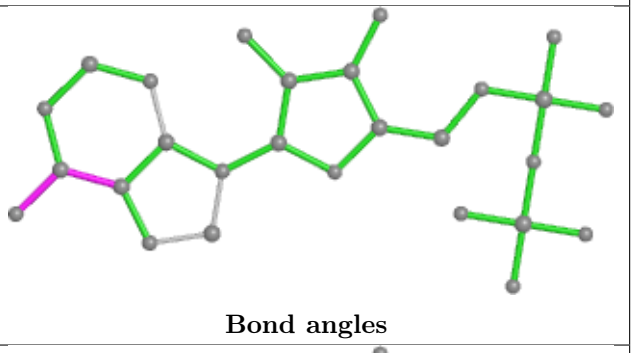


Rings

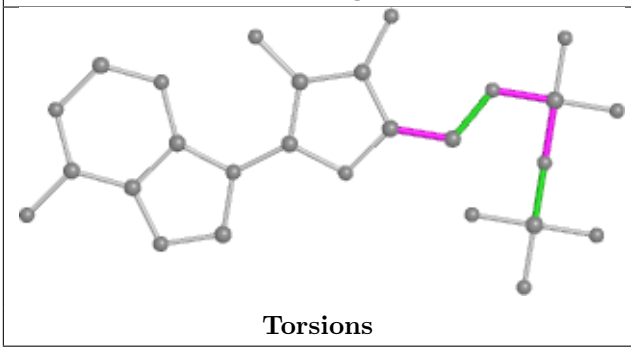
Ligand ADP F 601



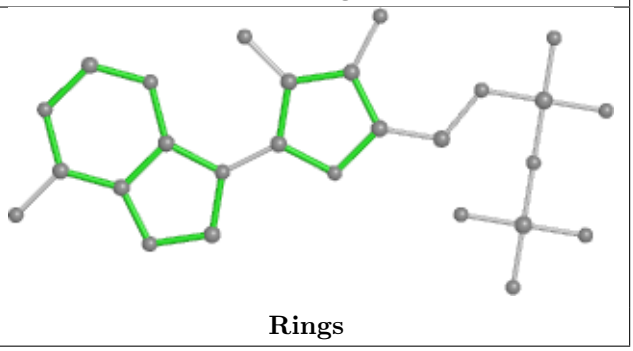
Bond lengths



Bond angles

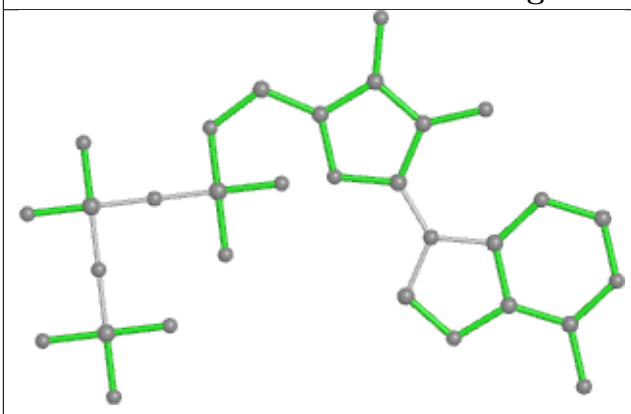


Torsions

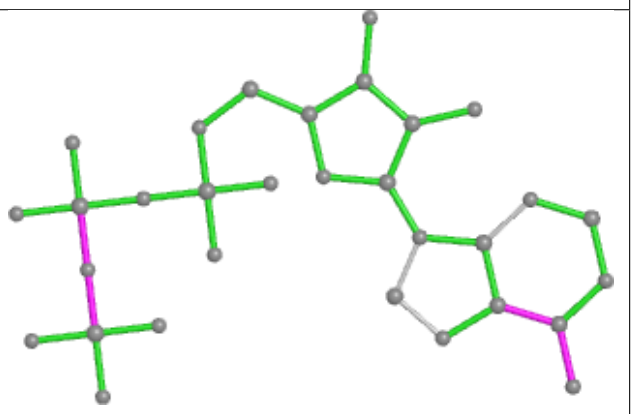


Rings

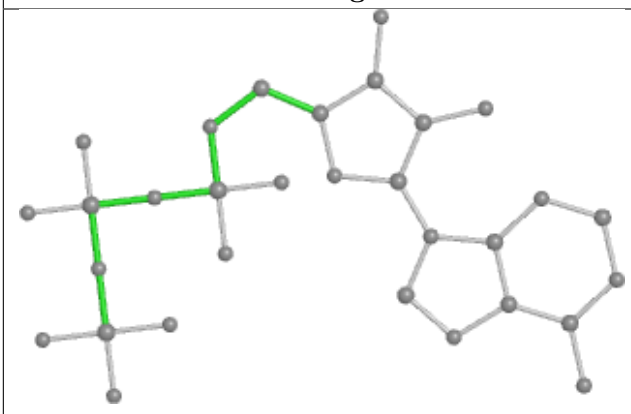
Ligand ATP L 602



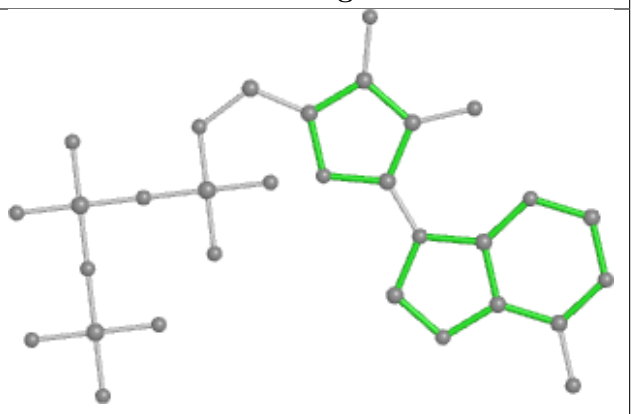
Bond lengths



Bond angles

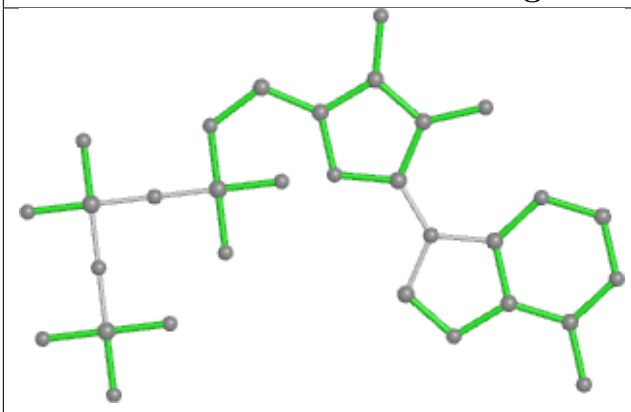


Torsions

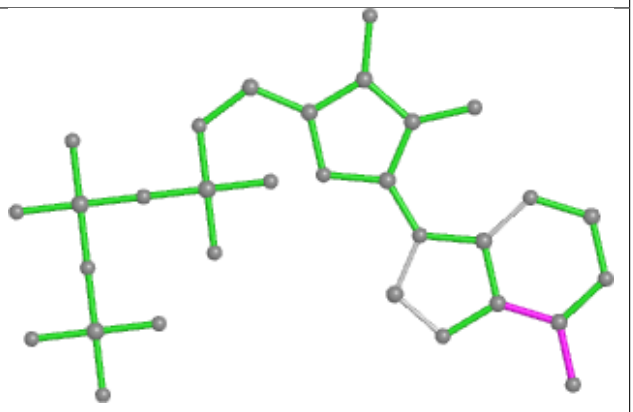


Rings

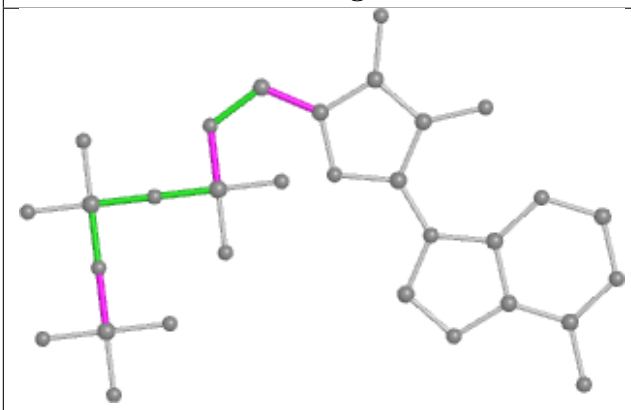
Ligand ATP G 602



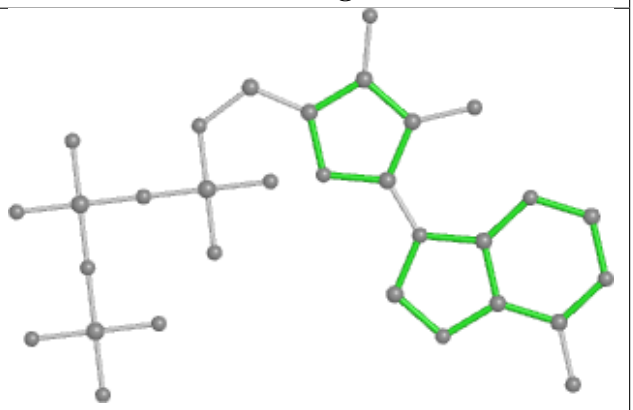
Bond lengths



Bond angles

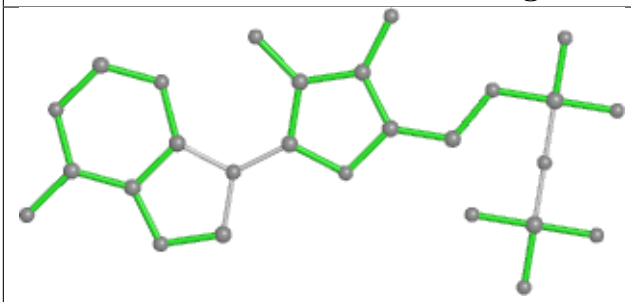


Torsions

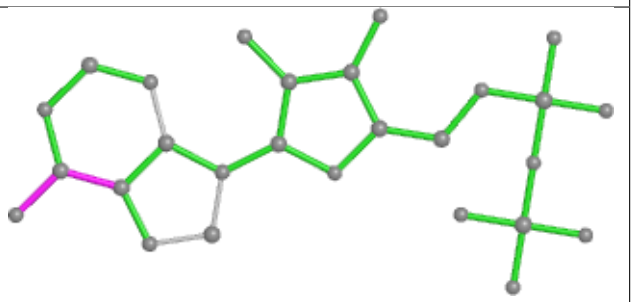


Rings

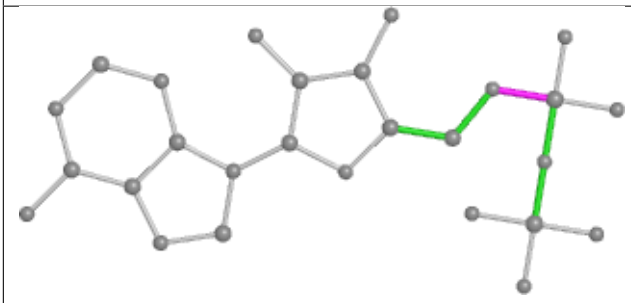
Ligand ADP C 601



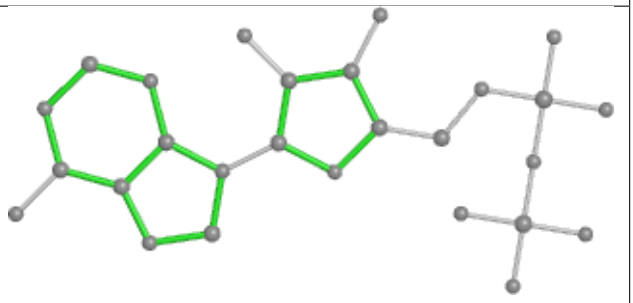
Bond lengths



Bond angles

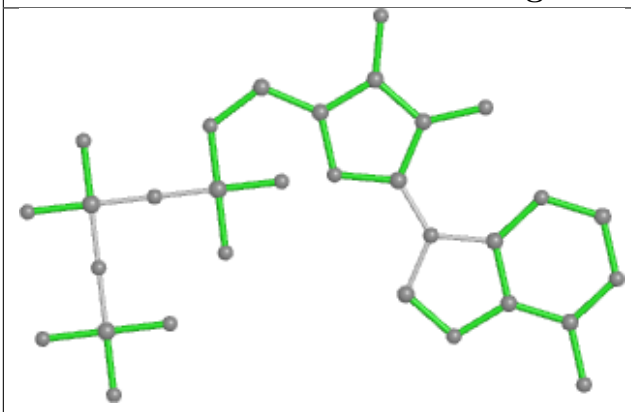


Torsions

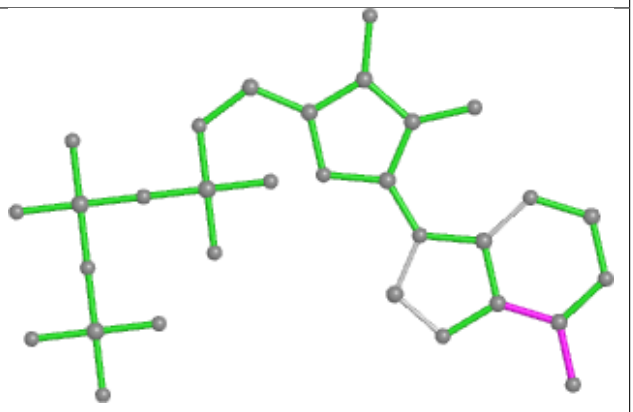


Rings

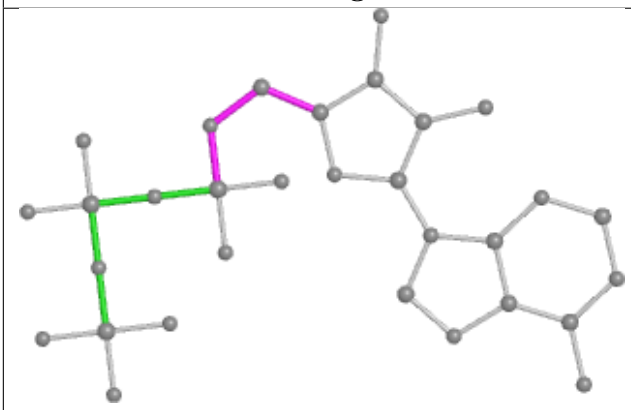
Ligand ATP E 601



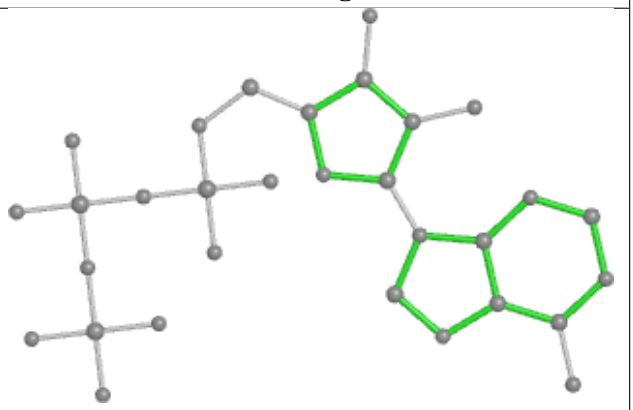
Bond lengths



Bond angles

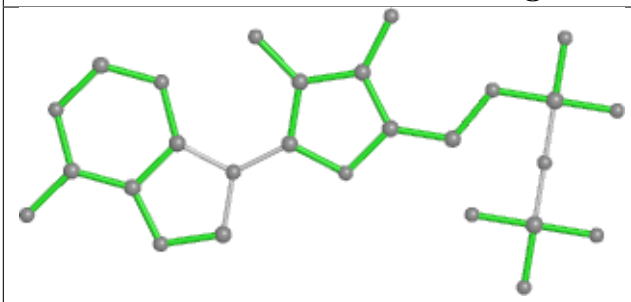


Torsions

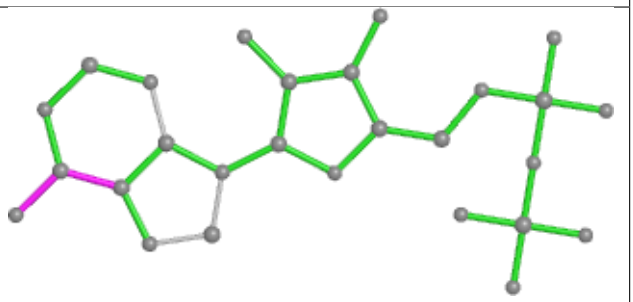


Rings

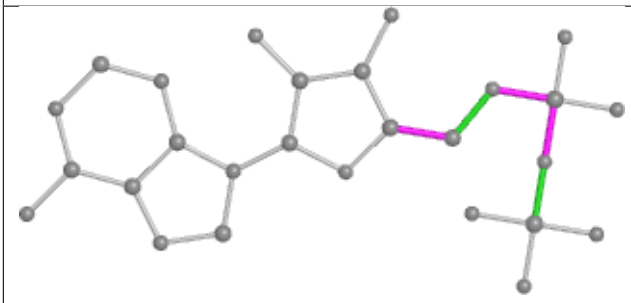
Ligand ADP L 601



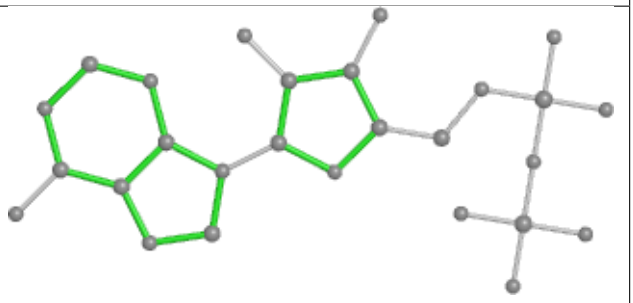
Bond lengths



Bond angles



Torsions



Rings

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	463/519 (89%)	-0.12	3 (0%)	89	72	48, 69, 111, 145	0
1	B	460/519 (88%)	-0.10	8 (1%)	70	42	51, 77, 107, 125	0
1	C	461/519 (88%)	-0.07	11 (2%)	59	30	46, 69, 113, 153	0
1	D	457/519 (88%)	-0.12	3 (0%)	87	69	45, 70, 104, 122	0
1	E	463/519 (89%)	-0.21	4 (0%)	84	62	44, 71, 95, 126	0
1	F	466/519 (89%)	-0.20	8 (1%)	70	42	46, 71, 100, 125	0
1	G	458/519 (88%)	-0.05	10 (2%)	62	33	56, 82, 129, 145	0
1	I	466/519 (89%)	-0.24	2 (0%)	92	79	44, 65, 94, 119	0
1	J	463/519 (89%)	-0.19	6 (1%)	77	51	44, 62, 92, 159	0
1	K	464/519 (89%)	-0.11	10 (2%)	62	33	56, 78, 124, 145	0
1	L	456/519 (87%)	-0.02	9 (1%)	65	36	62, 88, 119, 144	0
2	H	460/519 (88%)	-0.18	6 (1%)	77	51	48, 70, 99, 124	0
All	All	5537/6228 (88%)	-0.13	80 (1%)	75	49	44, 72, 111, 159	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	ALA	5.8
1	C	97	LEU	4.7
1	K	153	GLN	4.7
2	H	498	THR	4.6
1	J	113	GLU	4.2

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. 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	SEP	G	431	10/11	0.87	0.25	61,62,62,62	4
1	SEP	K	431	10/11	0.87	0.21	63,65,70,70	0
1	SEP	L	431	10/11	0.88	0.19	78,80,84,84	0
1	SEP	D	431	10/11	0.89	0.23	73,76,78,78	0
1	SEP	B	431	10/11	0.91	0.20	67,68,72,72	0
1	SEP	J	431	10/11	0.92	0.15	63,67,73,73	0
1	SEP	F	431	10/11	0.93	0.15	59,60,64,65	0
1	SEP	A	431	10/11	0.93	0.22	65,67,68,68	4
1	SEP	C	431	10/11	0.94	0.14	63,64,65,66	0
1	SEP	E	431	10/11	0.96	0.13	74,77,79,80	0
1	SEP	I	431	10/11	0.97	0.22	62,63,63,63	4

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
5	MG	E	603	1/1	0.84	0.18	59,59,59,59	0
5	MG	A	603	1/1	0.85	0.07	68,68,68,68	0
5	MG	B	703	1/1	0.87	0.28	60,60,60,60	0
3	ADP	L	601	27/27	0.89	0.19	82,86,87,89	0
3	ADP	C	601	27/27	0.91	0.22	74,79,83,84	0
3	ADP	D	601	27/27	0.91	0.17	68,73,74,75	0
3	ADP	K	601	27/27	0.92	0.18	83,87,89,90	0
5	MG	K	603	1/1	0.92	0.21	84,84,84,84	0
5	MG	L	603	1/1	0.92	0.20	73,73,73,73	0
4	ATP	G	602	31/31	0.93	0.17	74,76,80,80	0
5	MG	E	604	1/1	0.93	0.23	84,84,84,84	0
4	ATP	C	602	31/31	0.94	0.18	63,66,70,71	0
3	ADP	G	601	27/27	0.94	0.18	64,70,76,78	0
4	ATP	H	602	31/31	0.94	0.20	68,71,78,78	0
4	ATP	K	602	31/31	0.94	0.17	70,72,75,76	0

Continued on next page...

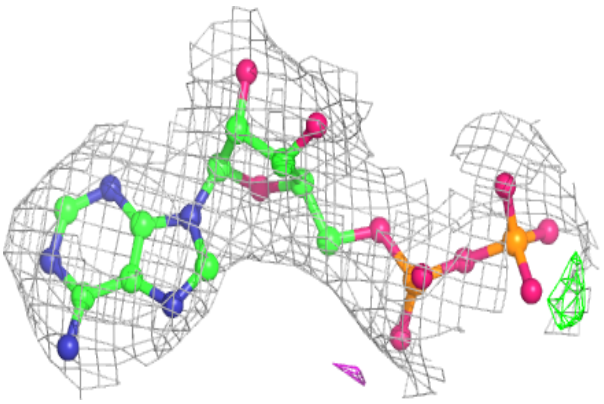
Continued from previous page...

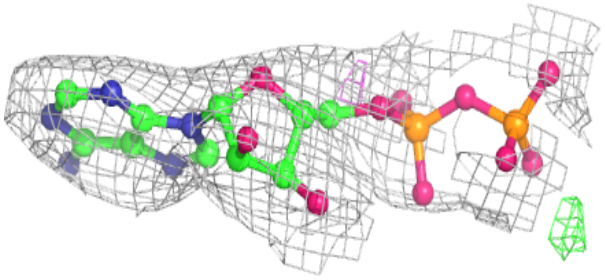
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ATP	J	702	31/31	0.94	0.16	70,72,82,83	0
3	ADP	H	601	27/27	0.94	0.18	49,50,52,52	0
3	ADP	A	601	27/27	0.94	0.20	67,70,72,73	0
3	ADP	F	601	27/27	0.94	0.15	60,61,62,63	0
4	ATP	A	602	31/31	0.94	0.18	59,63,67,68	0
4	ATP	B	702	31/31	0.94	0.14	75,77,81,83	0
4	ATP	E	601	31/31	0.94	0.15	78,79,93,94	0
5	MG	J	703	1/1	0.94	0.20	83,83,83,83	0
5	MG	D	603	1/1	0.95	0.15	49,49,49,49	0
4	ATP	L	602	31/31	0.95	0.17	74,76,84,84	0
3	ADP	I	602	27/27	0.95	0.17	37,42,46,47	0
3	ADP	D	602	27/27	0.95	0.18	53,59,63,64	0
4	ATP	J	701	31/31	0.96	0.15	65,68,72,73	0
5	MG	C	603	1/1	0.96	0.26	73,73,73,73	0
4	ATP	B	701	31/31	0.96	0.15	61,66,71,71	0
4	ATP	E	602	31/31	0.96	0.16	59,60,72,73	0
4	ATP	F	602	31/31	0.96	0.14	59,60,62,63	0
3	ADP	I	601	27/27	0.96	0.15	46,47,49,50	0
5	MG	H	603	1/1	0.97	0.11	48,48,48,48	0
5	MG	G	603	1/1	0.97	0.05	41,41,41,41	0
5	MG	F	603	1/1	0.99	0.27	76,76,76,76	0

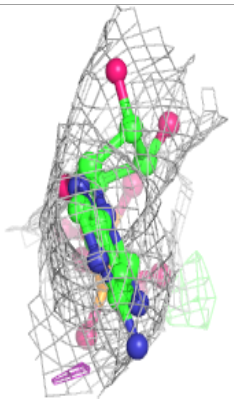
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP L 601:

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

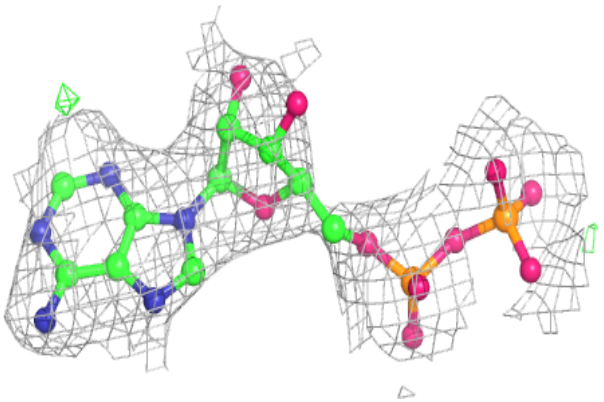


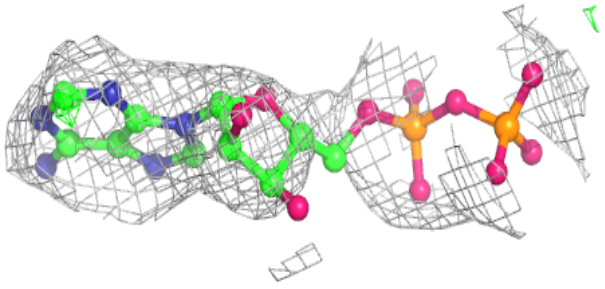


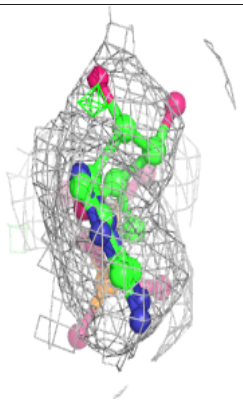


Electron density around ADP C 601:

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

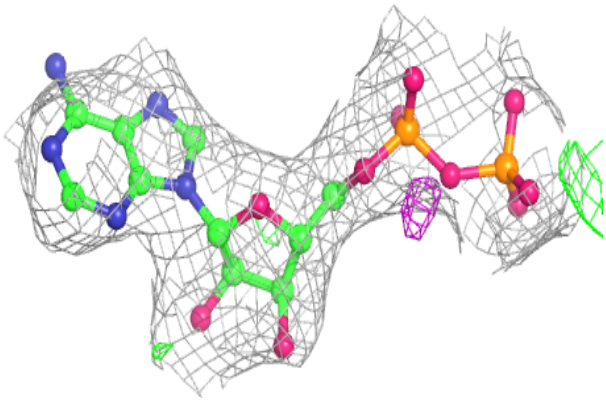


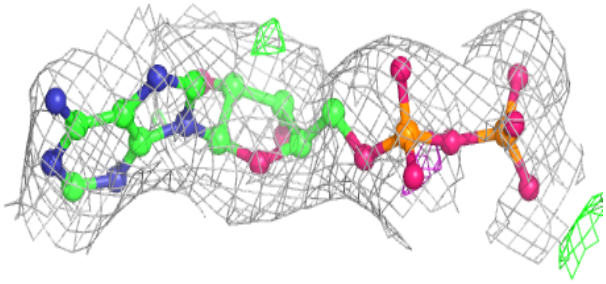


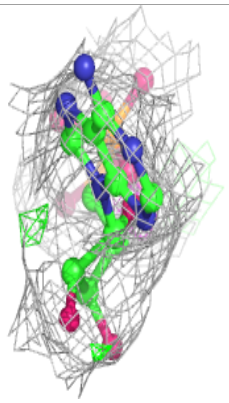


Electron density around ADP D 601:

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

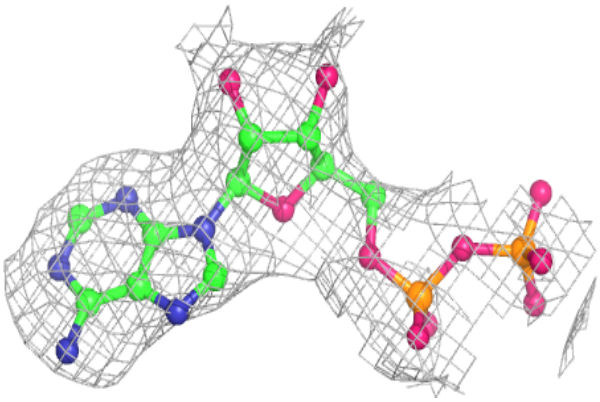


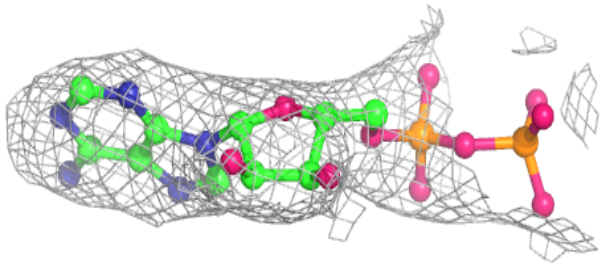


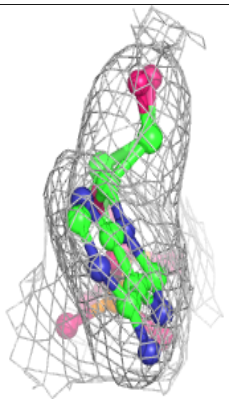


Electron density around ADP K 601:

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

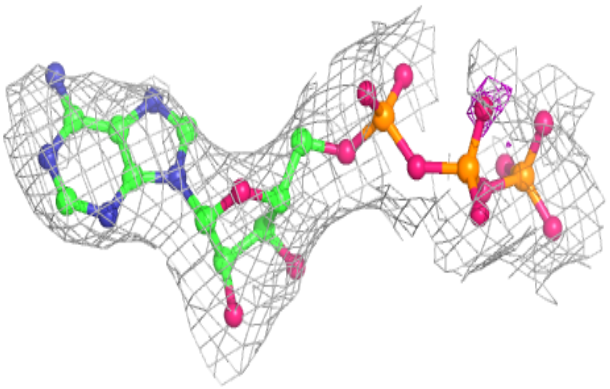


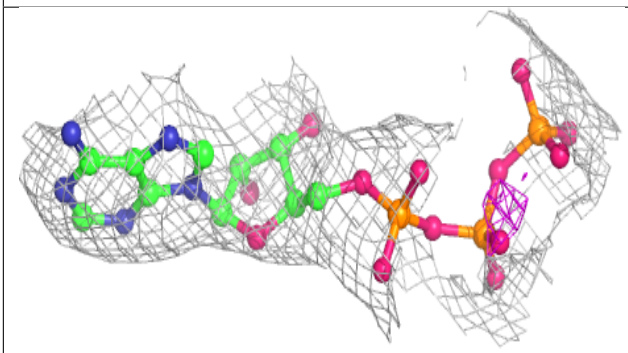


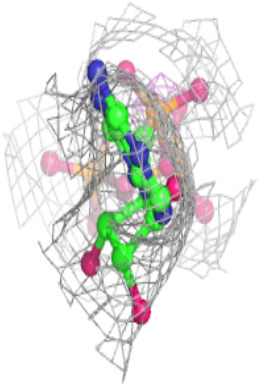


Electron density around ATP G 602:

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

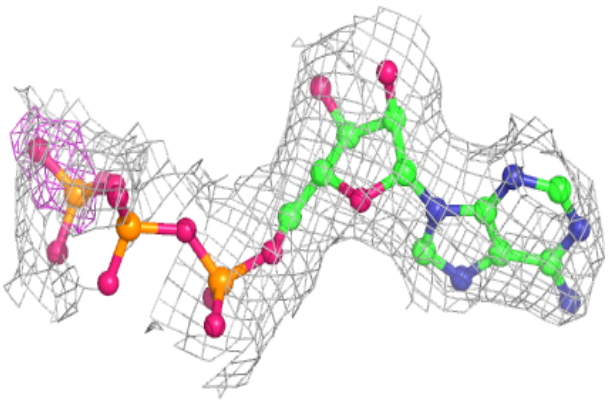


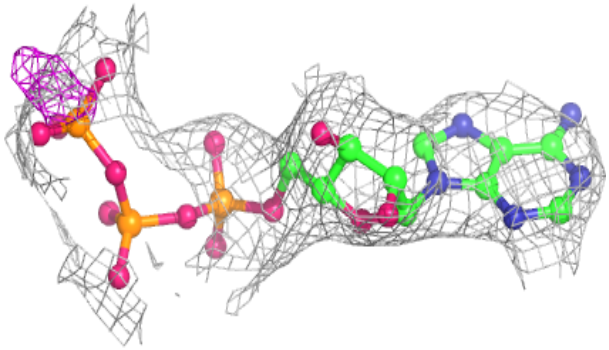


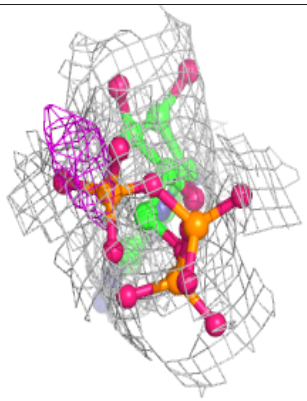


Electron density around ATP C 602:

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

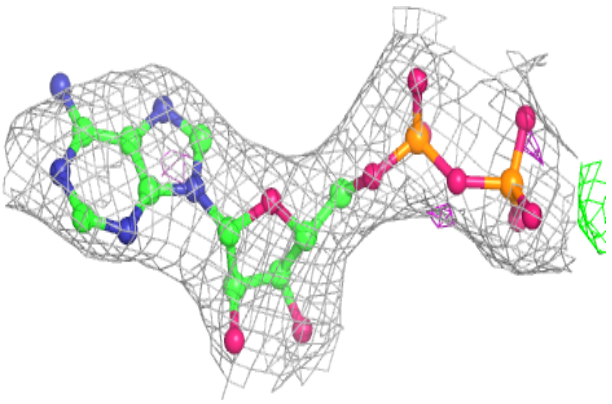


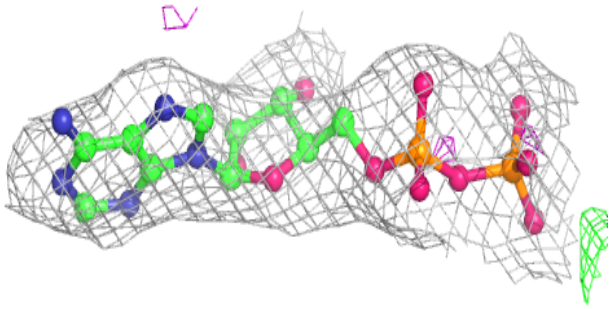


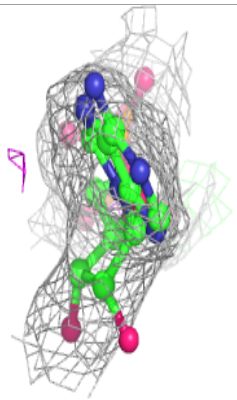


Electron density around ADP G 601:

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

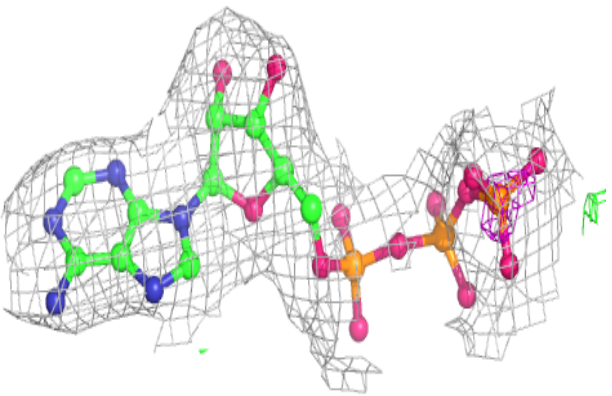


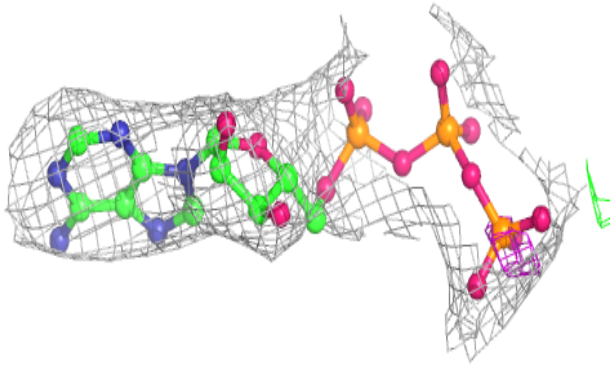


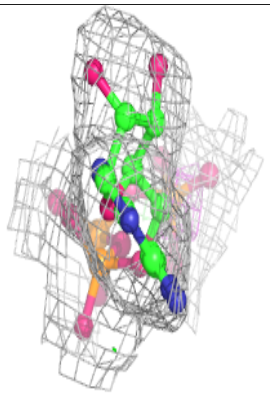


Electron density around ATP H 602:

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

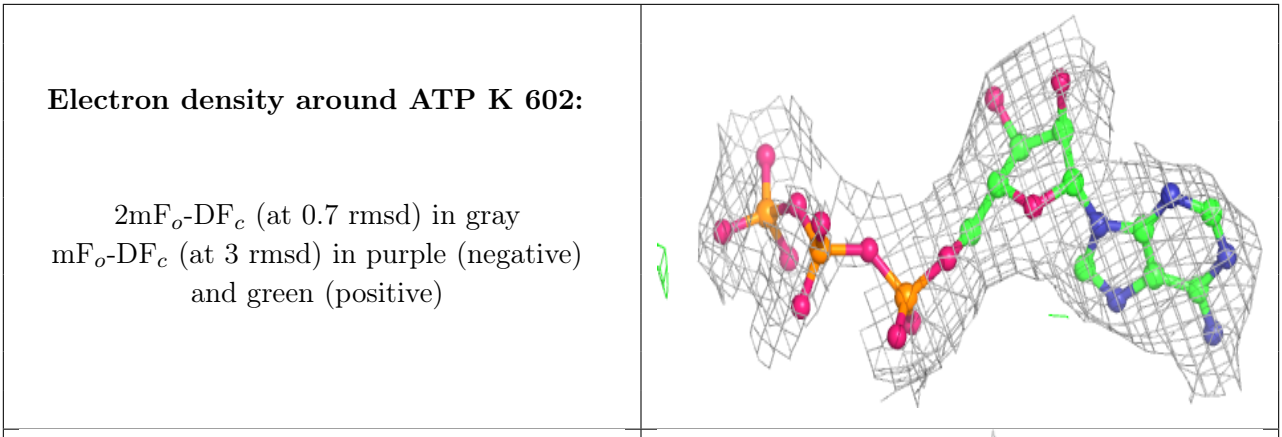






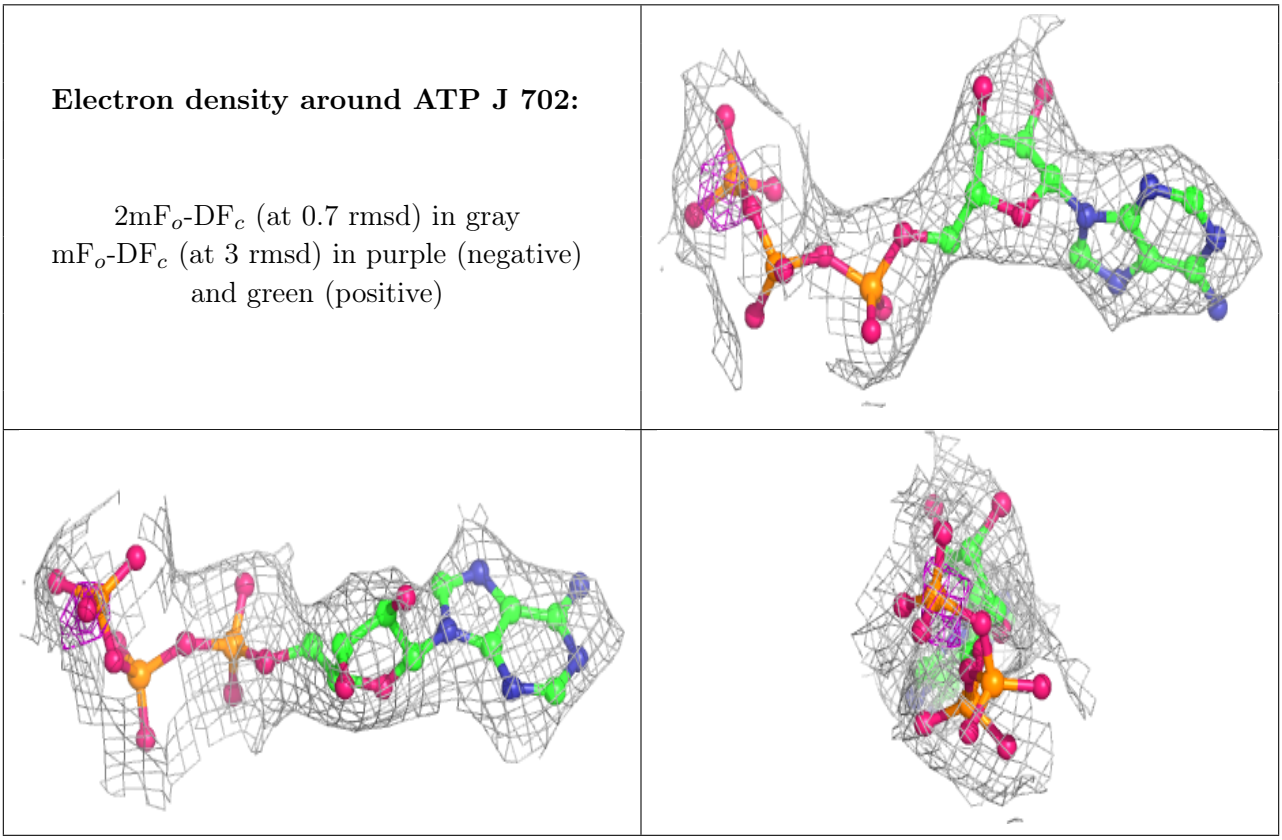
Electron density around ATP K 602:

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



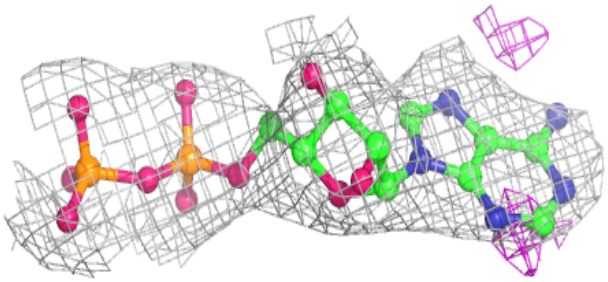
Electron density around ATP J 702:

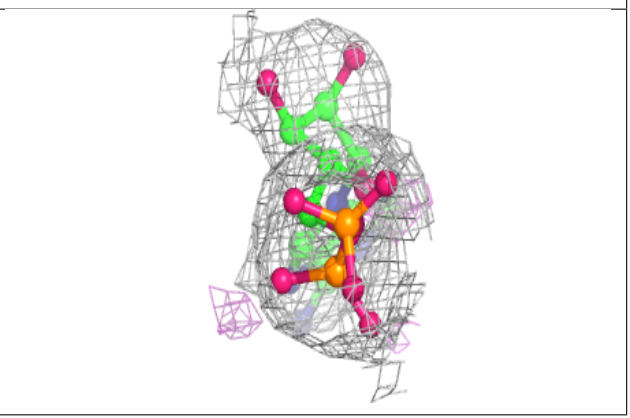
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADP H 601:

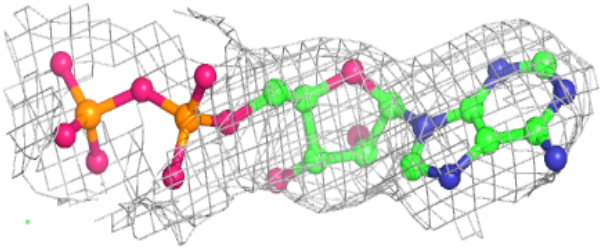
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

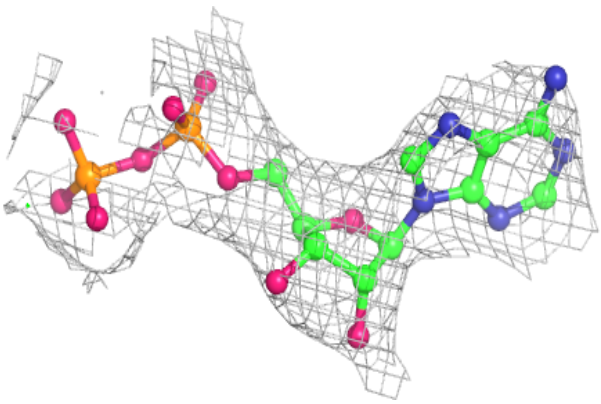




Electron density around ADP A 601:

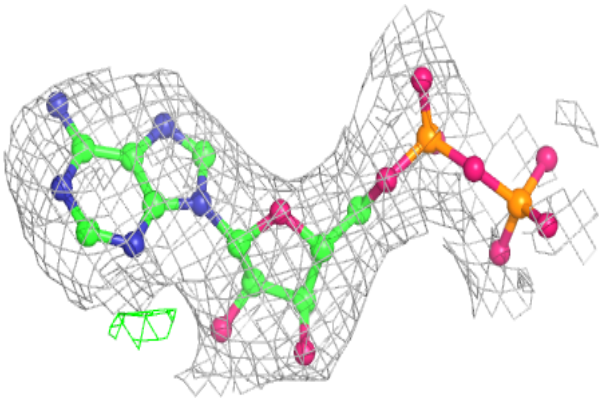
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

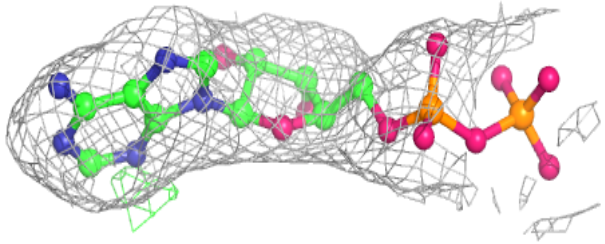


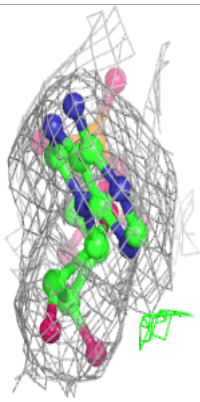


Electron density around ADP F 601:

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

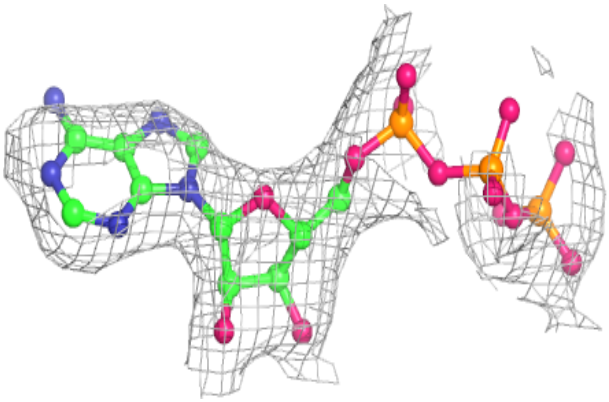


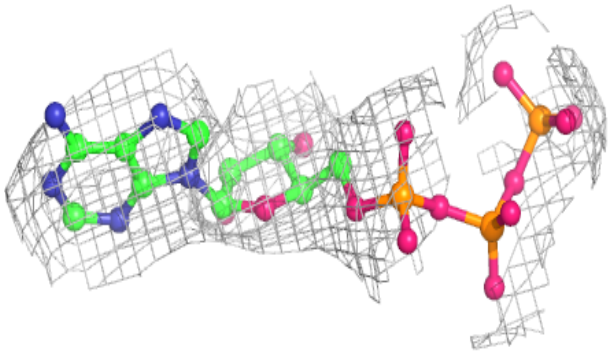


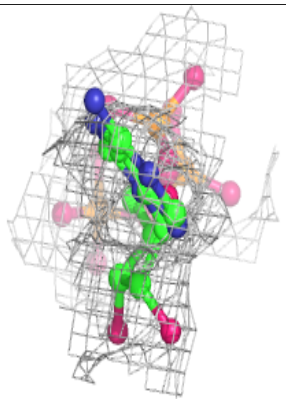


Electron density around ATP A 602:

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

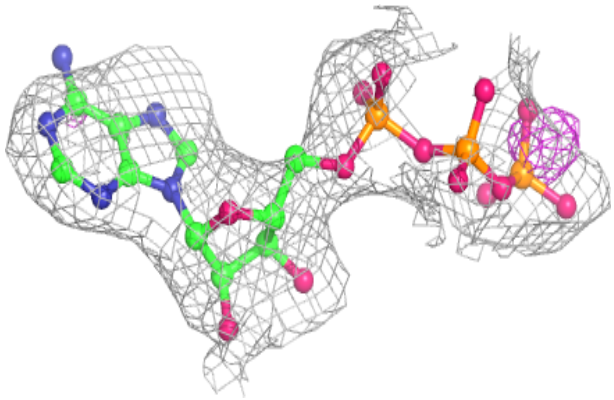


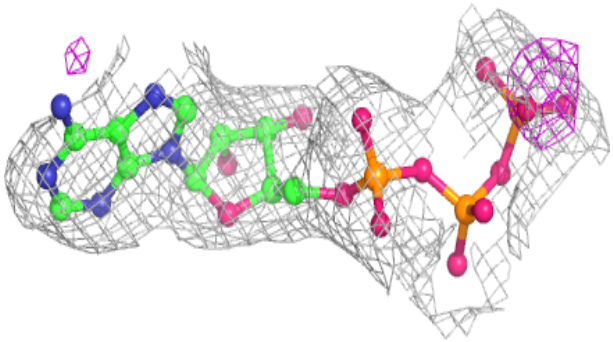


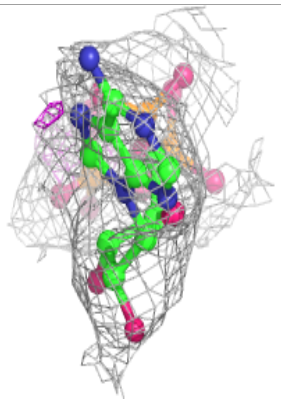


Electron density around ATP B 702:

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

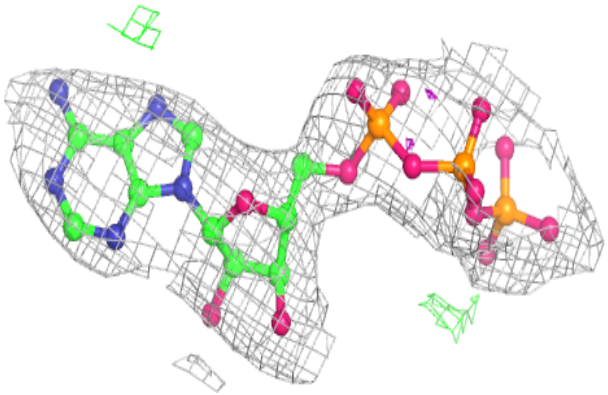


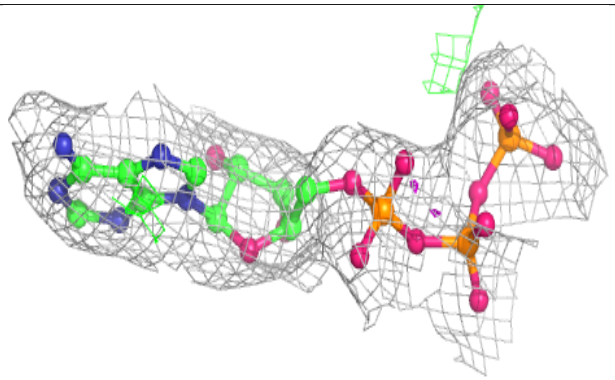


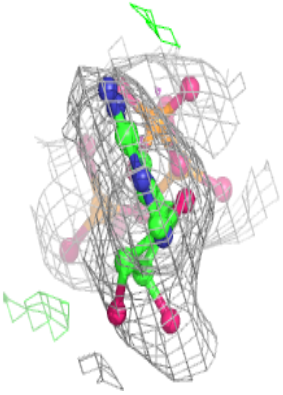


Electron density around ATP E 601:

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

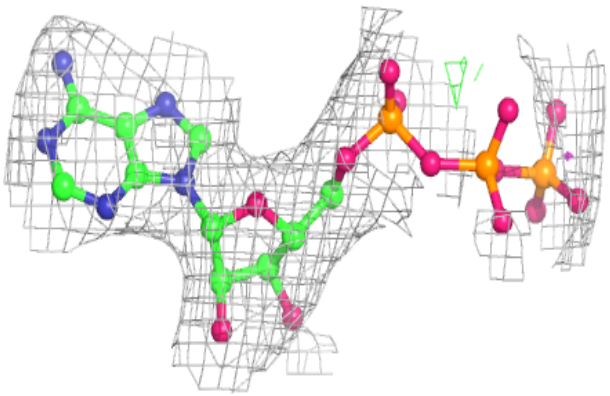


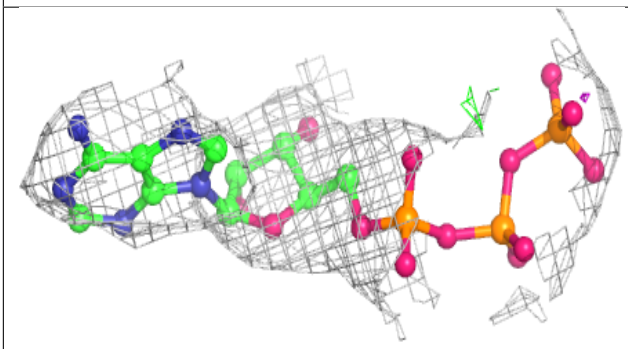


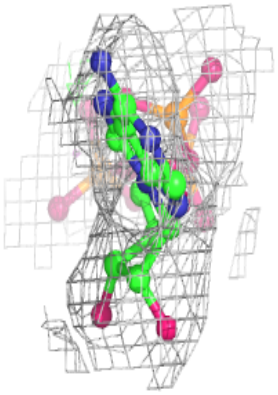


Electron density around ATP L 602:

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

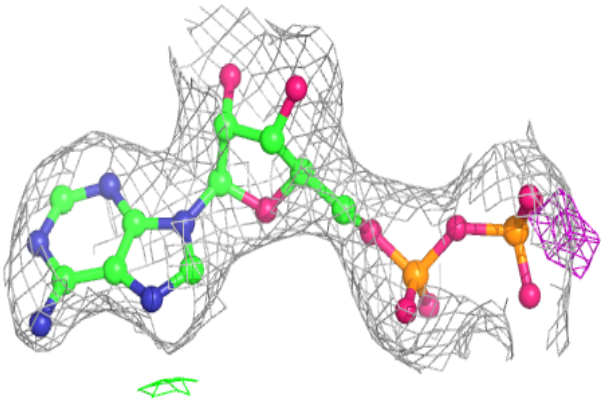


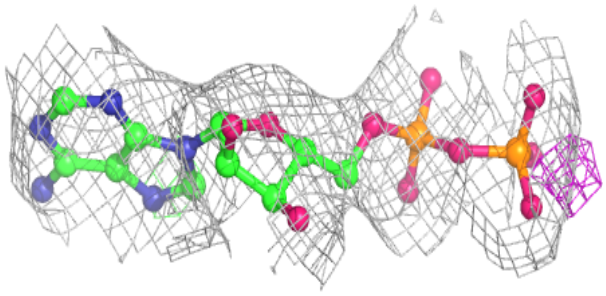


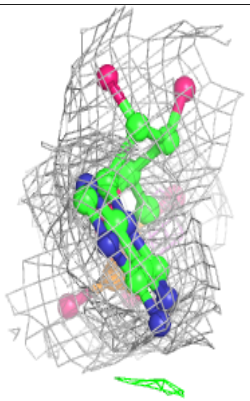


Electron density around ADP I 602:

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

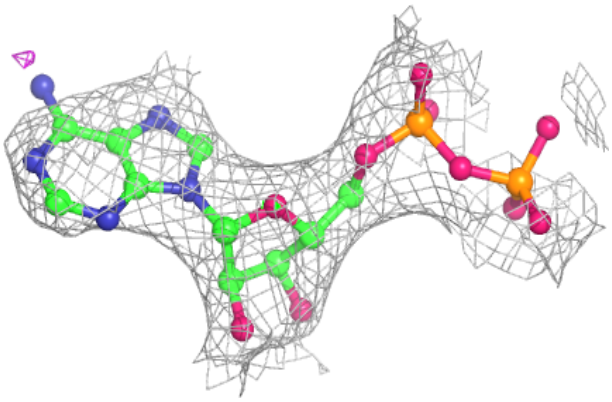


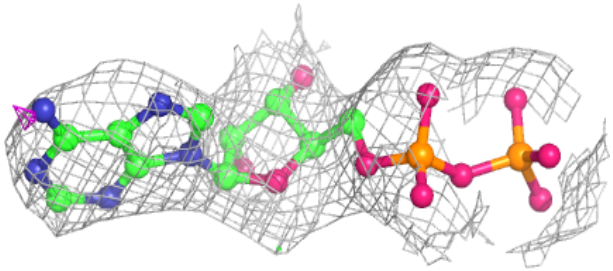


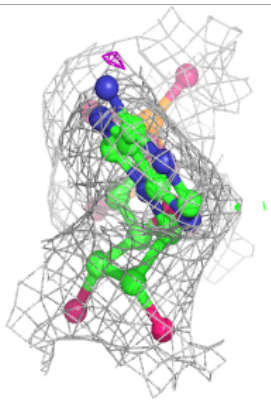


Electron density around ADP D 602:

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

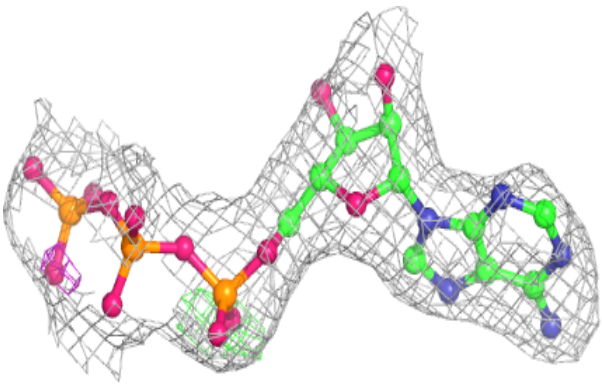


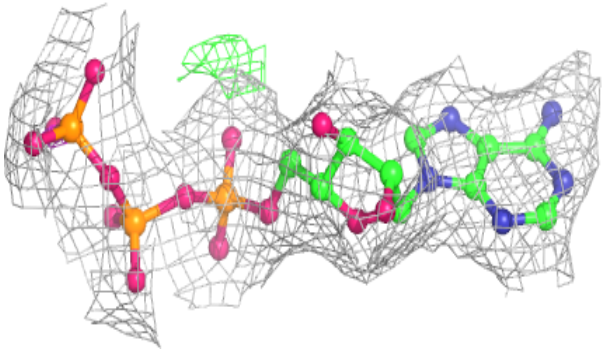


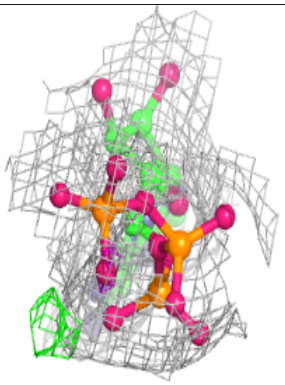


Electron density around ATP J 701:

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

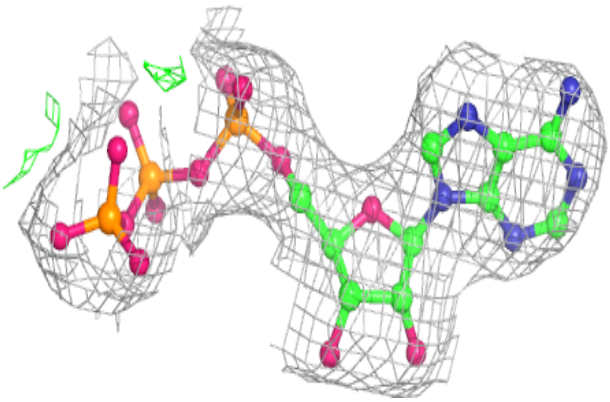


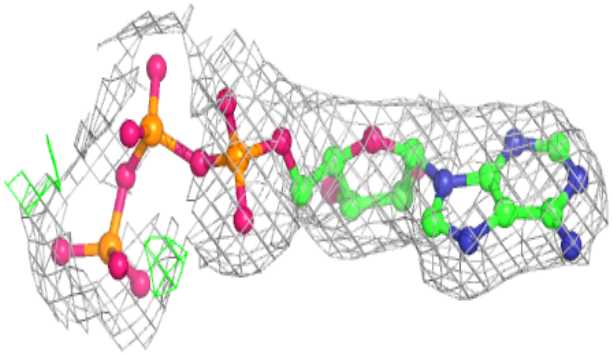


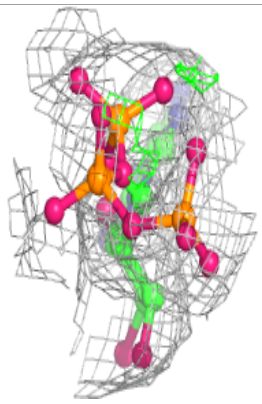


Electron density around ATP B 701:

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

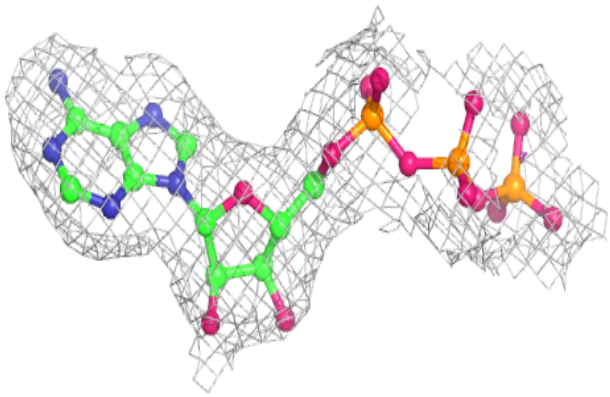


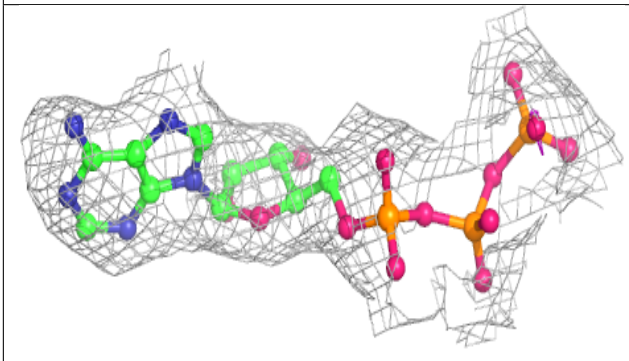


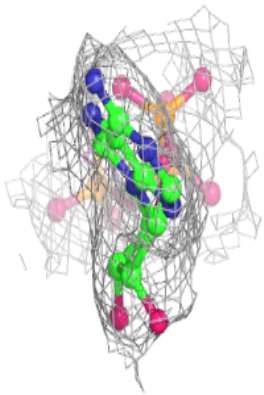


Electron density around ATP E 602:

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

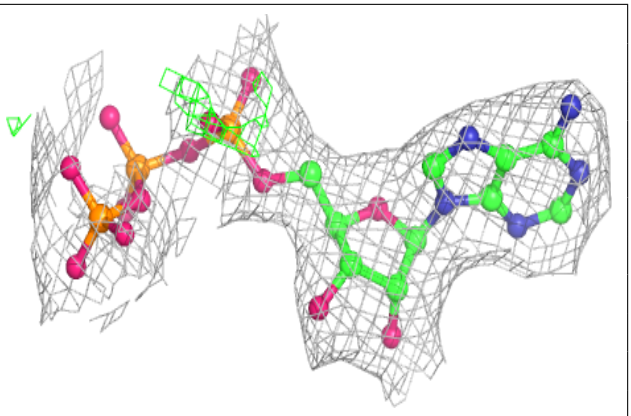


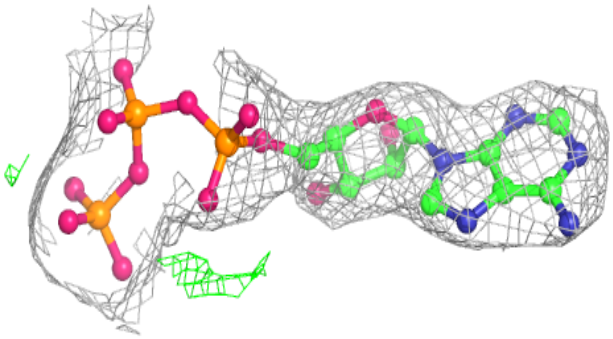


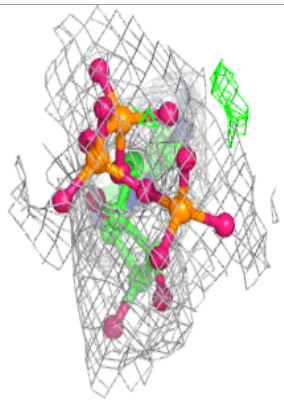


Electron density around ATP F 602:

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

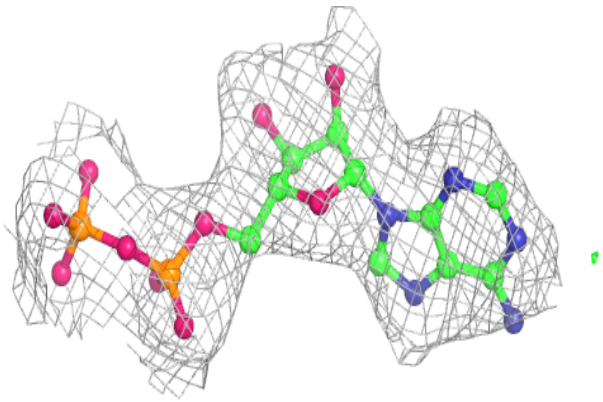


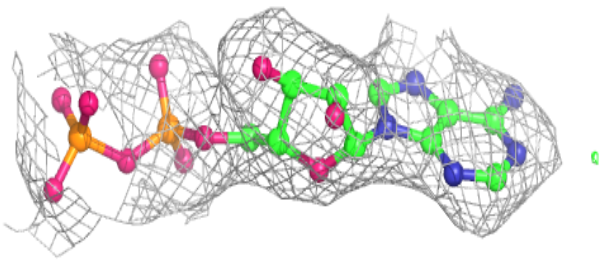


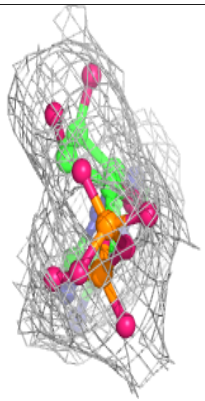


Electron density around ADP I 601:

$2mF_o$-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.