



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2021 – 04:32 PM EDT

PDB ID : 3K0E
Title : Crystal structure of the phosphorylation-site mutant T426N of the KaiC circadian clock protein
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on : 2009-09-24
Resolution : 3.20 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 ⓘ symbol.

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	:	2.23.2
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)	:	2.23.2

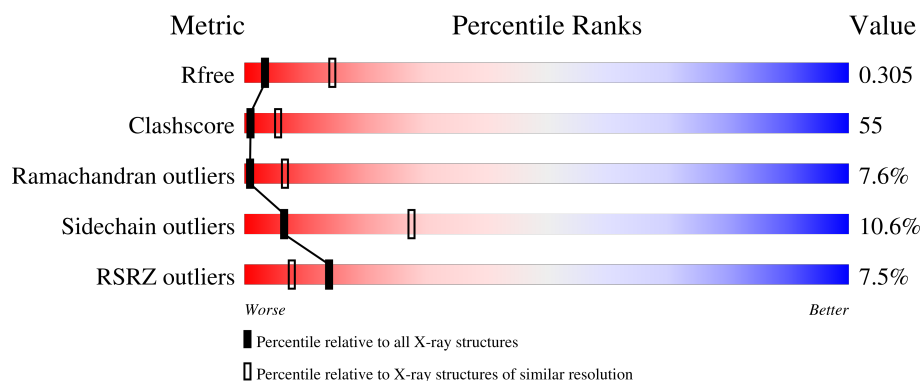
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>12%</div> <div>29% 57% 11% . .</div> </div>
1	B	519	<div> <div>7%</div> <div>27% 54% 13% . 5%</div> </div>
1	C	519	<div> <div>5%</div> <div>29% 53% 12% . 6%</div> </div>
1	D	519	<div> <div>4%</div> <div>30% 52% 11% . 7%</div> </div>
1	E	519	<div> <div>6%</div> <div>31% 55% 9% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	519	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	D	431	-	-	X	-
1	TPO	F	432	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23897 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
			3994	2509	702	766	2	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3879	2439	679	744	2	15			
1	C	488	Total	C	N	O	P	S	0	0	0
			3855	2425	675	738	2	15			
1	D	485	Total	C	N	O	P	S	0	0	0
			3831	2411	672	731	2	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3887	2445	680	745	2	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3994	2509	702	766	2	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	ASN	THR	engineered mutation	UNP Q79PF4
B	426	ASN	THR	engineered mutation	UNP Q79PF4
C	426	ASN	THR	engineered mutation	UNP Q79PF4
D	426	ASN	THR	engineered mutation	UNP Q79PF4
E	426	ASN	THR	engineered mutation	UNP Q79PF4
F	426	ASN	THR	engineered mutation	UNP Q79PF4

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Mg	0	0
			4	4		
2	B	4	Total	Mg	0	0
			4	4		
2	C	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	3	Total Mg 3 3	0	0
2	E	2	Total Mg 2 2	0	0
2	F	3	Total Mg 3 3	0	0

-
- The image displays the chemical structure of Adenosine Triphosphate (ATP). The structure consists of an adenine base (a purine ring system with an amino group at N6) linked to a ribose sugar, which is in turn linked to a chain of three phosphate groups. The atoms are labeled with IDs: N1, N6, C1, C2, C3, C4, C5, C6, C7, C8, N3, N7, N9, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801, O802, O803, O804, O805, O8

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0	0



WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

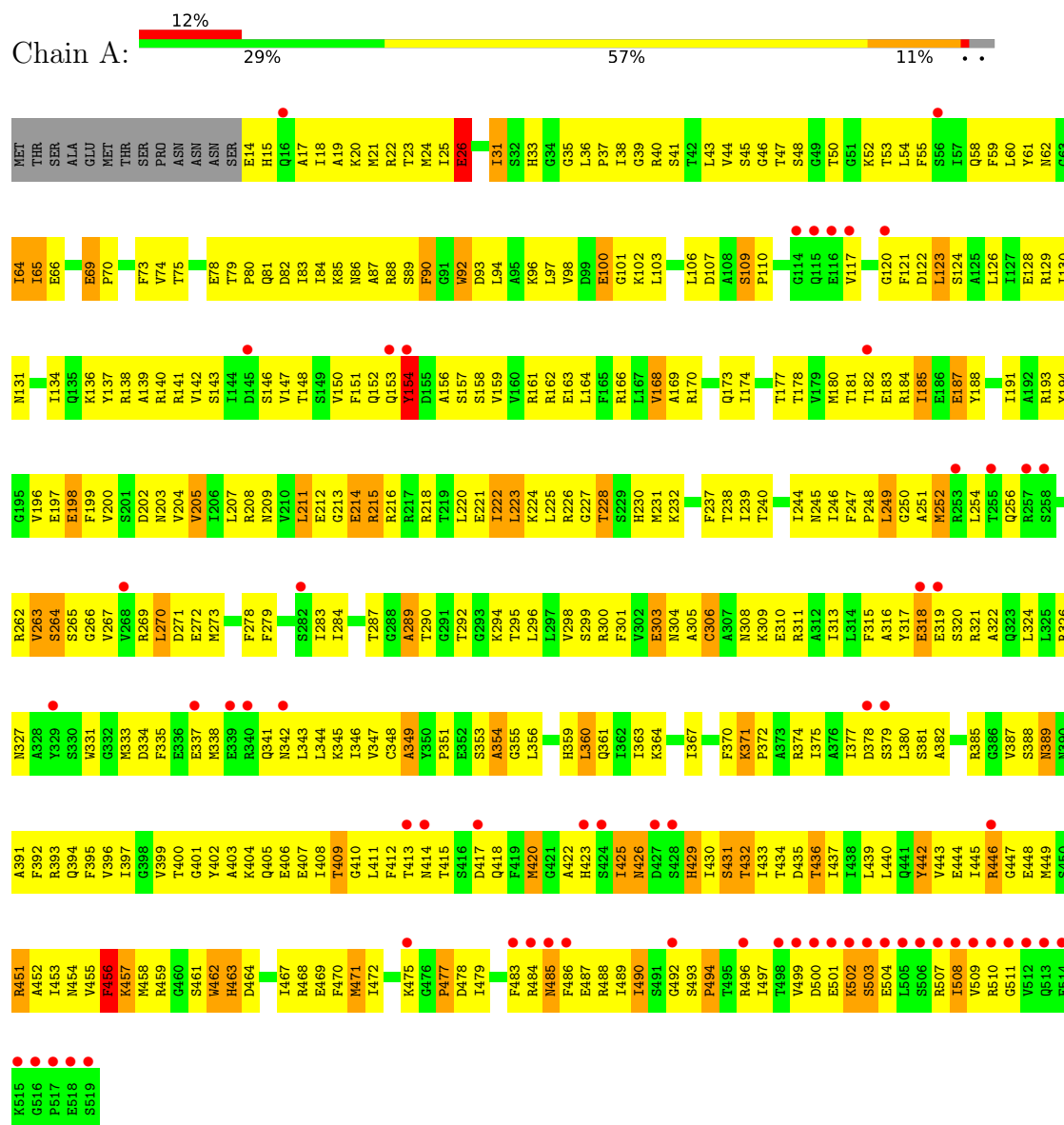
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	4	Total	O	0	0
			4	4		
4	C	6	Total	O	0	0
			6	6		
4	D	19	Total	O	0	0
			19	19		
4	E	11	Total	O	0	0
			11	11		
4	F	17	Total	O	0	0
			17	17		

3 Residue-property plots

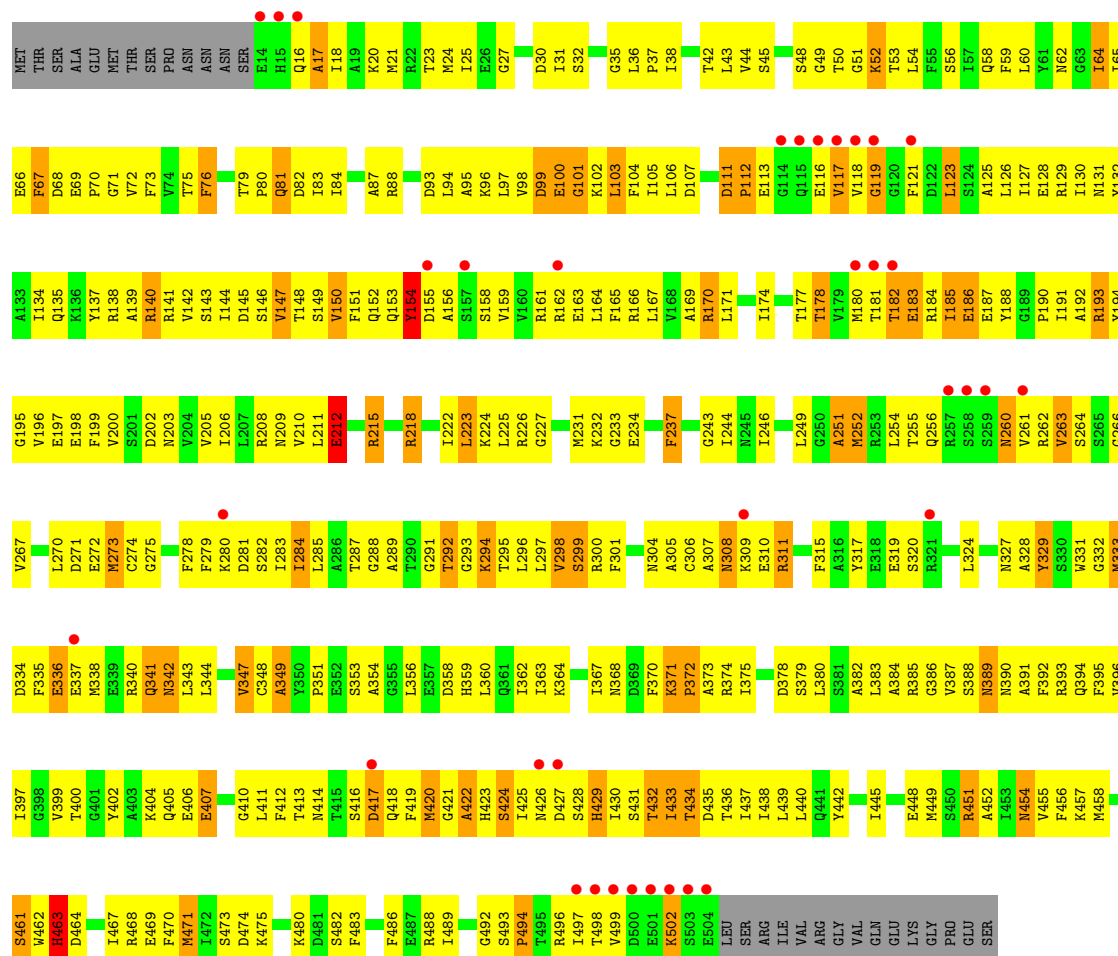
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

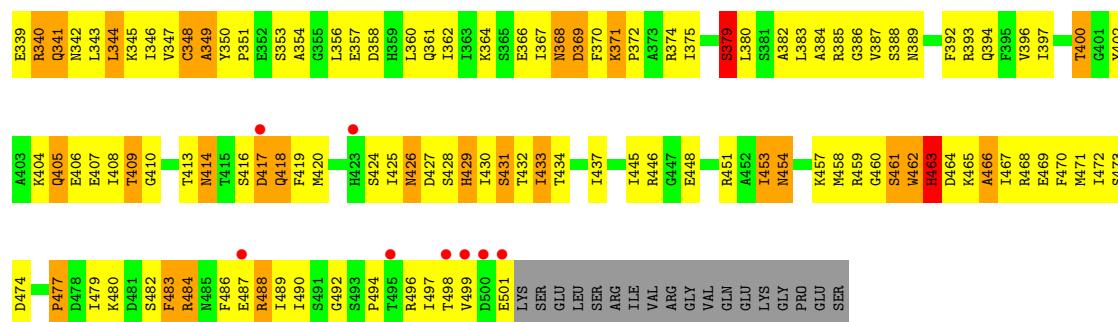
• Molecule 1: Circadian clock protein kinase KaiC



• Molecule 1: Circadian clock protein kinase KaiC



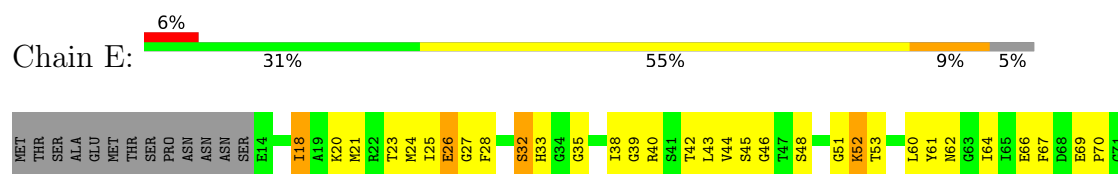


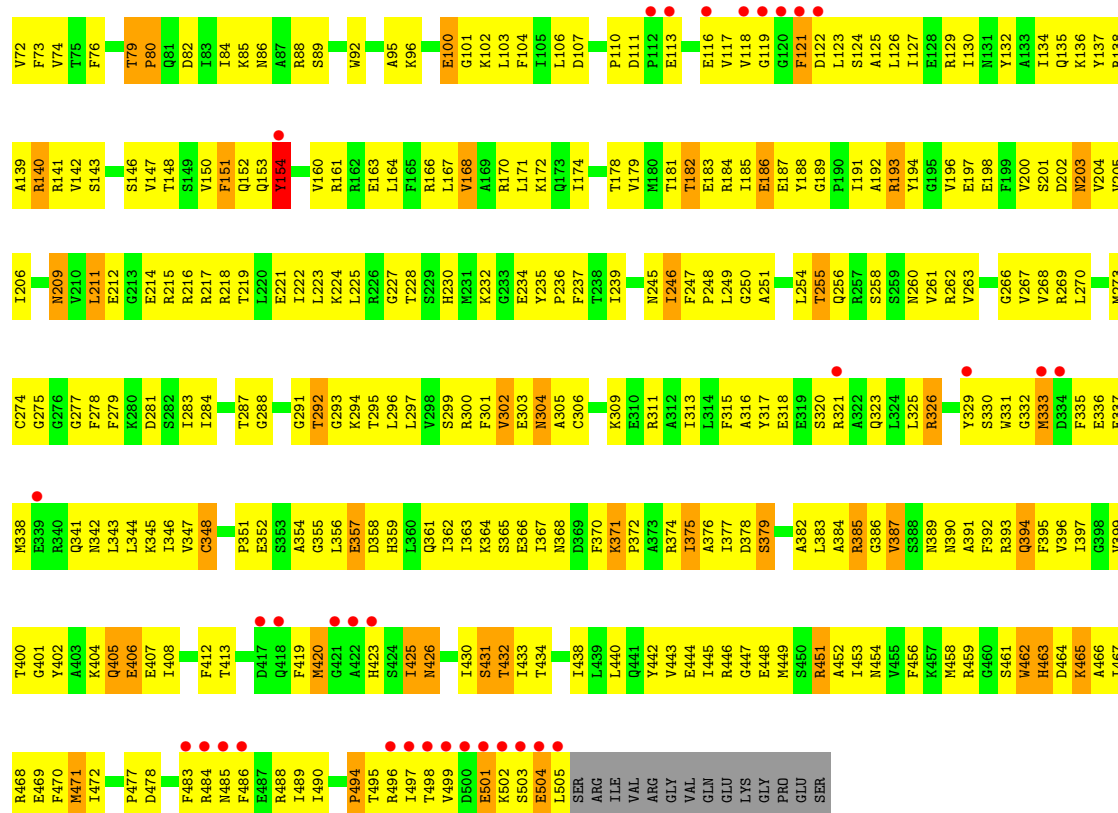


• Molecule 1: Circadian clock protein kinase KaiC

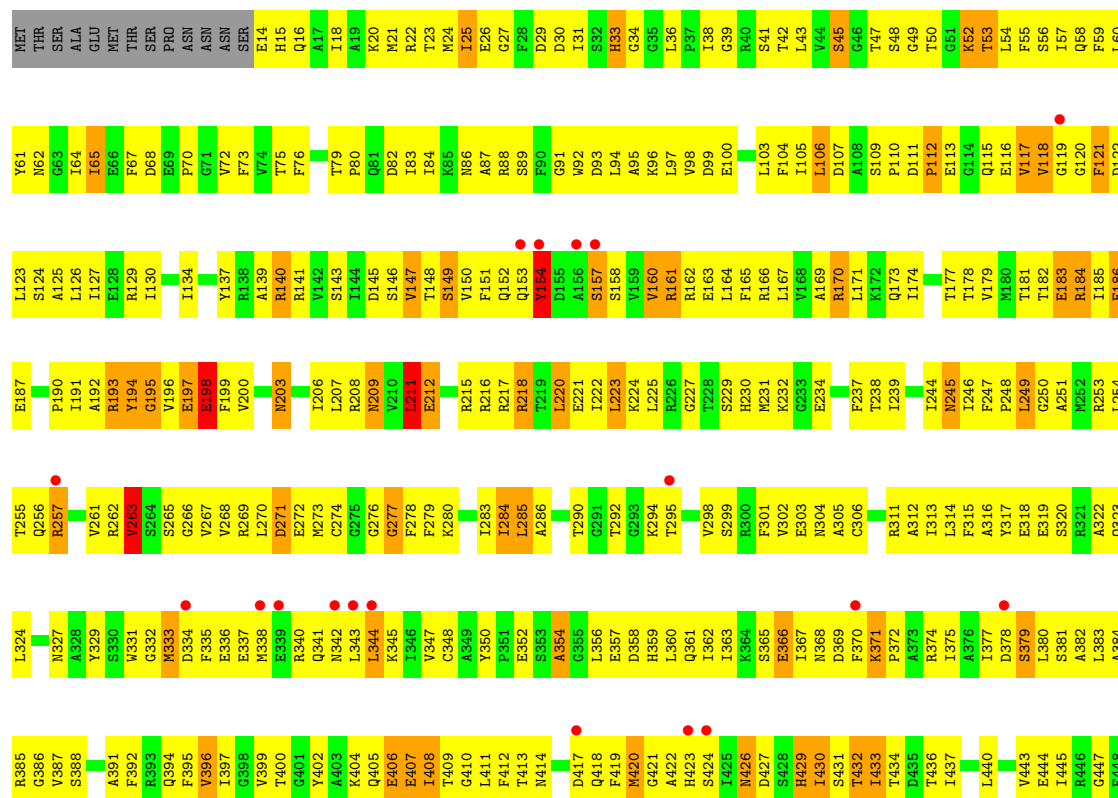


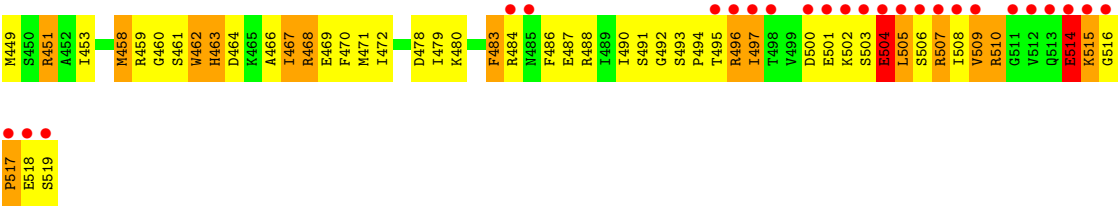
• Molecule 1: Circadian clock protein kinase KaiC





● Molecule 1: Circadian clock protein kinase KaiC





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.50Å 135.83Å 204.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.89 – 3.17	Depositor EDS
% Data completeness (in resolution range)	85.3 (30.00-3.20) 91.4 (29.89-3.17)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.320 0.233 , 0.305	Depositor DCC
R_{free} test set	5782 reflections (9.50%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23897	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: TPO, SEP, ATP, 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	0.40	0/4038	0.67	0/5438
1	B	0.39	0/3922	0.64	0/5283
1	C	0.43	0/3898	0.69	0/5252
1	D	0.50	0/3874	0.73	0/5219
1	E	0.48	0/3930	0.72	0/5294
1	F	0.46	0/4038	0.71	1/5438 (0.0%)
All	All	0.45	0/23700	0.70	1/31924 (0.0%)

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	C	0	1
1	D	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	25	ILE	N-CA-C	-5.53	96.06	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	235	TYR	Sidechain
1	D	132	TYR	Sidechain
1	E	188	TYR	Sidechain

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	3994	0	3982	450	0
1	B	3879	0	3859	442	0
1	C	3855	0	3836	442	0
1	D	3831	0	3816	453	0
1	E	3887	0	3870	428	0
1	F	3994	0	3982	550	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
3	A	62	0	24	2	0
3	B	62	0	24	7	0
3	C	62	0	24	5	0
3	D	62	0	24	8	0
3	E	62	0	24	9	0
3	F	62	0	24	4	0
4	A	8	0	0	2	0
4	B	4	0	0	2	0
4	C	6	0	0	2	0
4	D	19	0	0	17	0
4	E	11	0	0	3	0
4	F	17	0	0	9	0
All	All	23897	0	23489	2615	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 55.

The worst 5 of 2615 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:A:24:MET:HB2	1:A:62:ASN:HD22	1.14	1.13
1:B:147:VAL:HG11	1:B:180:MET:HE2	1.29	1.13
1:D:211:LEU:HB2	1:D:216:ARG:HD3	1.18	1.11
1:F:191:ILE:CB	1:F:198:GLU:HG3	1.82	1.09
1:B:379:SER:H	1:B:413:THR:HB	1.14	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/519 (97%)	369 (74%)	97 (19%)	36 (7%)	1	7
1	B	487/519 (94%)	351 (72%)	94 (19%)	42 (9%)	1	4
1	C	484/519 (93%)	361 (75%)	90 (19%)	33 (7%)	1	9
1	D	481/519 (93%)	372 (77%)	77 (16%)	32 (7%)	1	9
1	E	488/519 (94%)	369 (76%)	93 (19%)	26 (5%)	2	15
1	F	502/519 (97%)	363 (72%)	85 (17%)	54 (11%)	0	2
All	All	2944/3114 (94%)	2185 (74%)	536 (18%)	223 (8%)	1	7

5 of 223 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	154	TYR
1	A	463	HIS
1	B	17	ALA
1	B	48	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/442 (97%)	387 (90%)	43 (10%)	7	30
1	B	417/442 (94%)	375 (90%)	42 (10%)	7	29
1	C	414/442 (94%)	360 (87%)	54 (13%)	4	19
1	D	411/442 (93%)	362 (88%)	49 (12%)	5	22
1	E	418/442 (95%)	380 (91%)	38 (9%)	9	34
1	F	430/442 (97%)	388 (90%)	42 (10%)	8	31
All	All	2520/2652 (95%)	2252 (89%)	268 (11%)	6	27

5 of 268 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	56	SER
1	F	170	ARG
1	F	430	ILE
1	C	178	THR
1	C	140	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	209	ASN
1	F	304	ASN
1	C	203	ASN
1	C	152	GLN
1	F	342	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	D	432	1	8,10,11	0.98	0	10,14,16	1.42	2 (20%)
1	SEP	E	431	1	8,9,10	1.52	1 (12%)	8,12,14	1.31	1 (12%)
1	TPO	A	432	1	8,10,11	1.00	0	10,14,16	1.62	2 (20%)
1	SEP	B	431	1	8,9,10	1.57	1 (12%)	8,12,14	1.03	0
1	TPO	C	432	1	8,10,11	1.07	0	10,14,16	1.29	1 (10%)
1	TPO	F	432	1	8,10,11	1.05	0	10,14,16	1.66	3 (30%)
1	SEP	C	431	1	8,9,10	1.64	1 (12%)	8,12,14	4.21	2 (25%)
1	SEP	F	431	1	8,9,10	1.52	1 (12%)	8,12,14	1.40	1 (12%)
1	SEP	D	431	1	8,9,10	1.52	1 (12%)	8,12,14	0.86	0
1	TPO	E	432	1	8,10,11	0.96	0	10,14,16	1.57	2 (20%)
1	SEP	A	431	1	8,9,10	1.52	1 (12%)	8,12,14	0.94	0
1	TPO	B	432	1	8,10,11	1.06	0	10,14,16	1.57	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	D	432	1	-	4/9/11/13	-
1	SEP	E	431	1	-	1/5/8/10	-
1	TPO	A	432	1	-	3/9/11/13	-
1	SEP	B	431	1	-	0/5/8/10	-
1	TPO	C	432	1	-	5/9/11/13	-
1	TPO	F	432	1	-	2/9/11/13	-
1	SEP	C	431	1	-	1/5/8/10	-
1	SEP	F	431	1	-	0/5/8/10	-
1	SEP	D	431	1	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	E	432	1	-	1/9/11/13	-
1	SEP	A	431	1	-	0/5/8/10	-
1	TPO	B	432	1	-	4/9/11/13	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	431	SEP	P-O1P	3.46	1.61	1.50
1	B	431	SEP	P-O1P	3.42	1.61	1.50
1	D	431	SEP	P-O1P	3.33	1.61	1.50
1	E	431	SEP	P-O1P	3.32	1.61	1.50
1	F	431	SEP	P-O1P	3.30	1.61	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	431	SEP	OG-CB-CA	10.13	118.01	108.14
1	C	431	SEP	P-OG-CB	-5.77	102.40	118.30
1	A	432	TPO	P-OG1-CB	-4.04	111.01	123.21
1	E	432	TPO	P-OG1-CB	-3.91	111.39	123.21
1	F	432	TPO	P-OG1-CB	-3.87	111.52	123.21

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	432	TPO	C-CA-CB-CG2
1	B	432	TPO	CG2-CB-OG1-P

There are no ring outliers.

9 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	432	TPO	1	0
1	E	431	SEP	2	0
1	A	432	TPO	1	0
1	F	432	TPO	13	0
1	C	431	SEP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	431	SEP	6	0
1	E	432	TPO	2	0
1	A	431	SEP	3	0
1	B	432	TPO	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 20 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ATP	E	903	2	26,33,33	1.26	4 (15%)	31,52,52	1.91	9 (29%)
3	ATP	D	903	2	26,33,33	1.31	2 (7%)	31,52,52	1.82	6 (19%)
3	ATP	A	901	2	26,33,33	1.33	4 (15%)	31,52,52	1.79	7 (22%)
3	ATP	A	903	2	26,33,33	1.35	4 (15%)	31,52,52	1.74	6 (19%)
3	ATP	B	903	2	26,33,33	1.35	4 (15%)	31,52,52	1.71	4 (12%)
3	ATP	B	901	2	26,33,33	1.16	2 (7%)	31,52,52	1.84	5 (16%)
3	ATP	F	903	2	26,33,33	1.21	1 (3%)	31,52,52	1.87	7 (22%)
3	ATP	C	901	2	26,33,33	1.32	4 (15%)	31,52,52	1.72	5 (16%)
3	ATP	C	903	2	26,33,33	1.24	3 (11%)	31,52,52	1.83	5 (16%)
3	ATP	F	901	2	26,33,33	1.32	3 (11%)	31,52,52	1.81	7 (22%)
3	ATP	D	901	2	26,33,33	1.29	2 (7%)	31,52,52	1.75	5 (16%)
3	ATP	E	901	2	26,33,33	1.25	2 (7%)	31,52,52	1.76	6 (19%)

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	E	903	2	-	7/18/38/38	0/3/3/3
3	ATP	D	903	2	-	7/18/38/38	0/3/3/3
3	ATP	A	901	2	-	7/18/38/38	0/3/3/3
3	ATP	A	903	2	-	8/18/38/38	0/3/3/3
3	ATP	B	903	2	-	9/18/38/38	0/3/3/3
3	ATP	B	901	2	-	8/18/38/38	0/3/3/3
3	ATP	F	903	2	-	7/18/38/38	0/3/3/3
3	ATP	C	901	2	-	5/18/38/38	0/3/3/3
3	ATP	C	903	2	-	9/18/38/38	0/3/3/3
3	ATP	F	901	2	-	7/18/38/38	0/3/3/3
3	ATP	D	901	2	-	7/18/38/38	0/3/3/3
3	ATP	E	901	2	-	7/18/38/38	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	903	ATP	C2-N3	4.29	1.39	1.32
3	F	901	ATP	C2-N3	4.26	1.39	1.32
3	A	903	ATP	C2-N3	4.23	1.38	1.32
3	E	901	ATP	C2-N3	4.14	1.38	1.32
3	B	903	ATP	C2-N3	4.06	1.38	1.32

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	903	ATP	N3-C2-N1	-6.14	119.09	128.68
3	D	901	ATP	N3-C2-N1	-5.71	119.75	128.68
3	C	901	ATP	N3-C2-N1	-5.59	119.95	128.68
3	A	903	ATP	N3-C2-N1	-5.55	120.00	128.68
3	B	901	ATP	N3-C2-N1	-5.53	120.03	128.68

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	PB-O3A-PA-O5'
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	O4'-C4'-C5'-O5'

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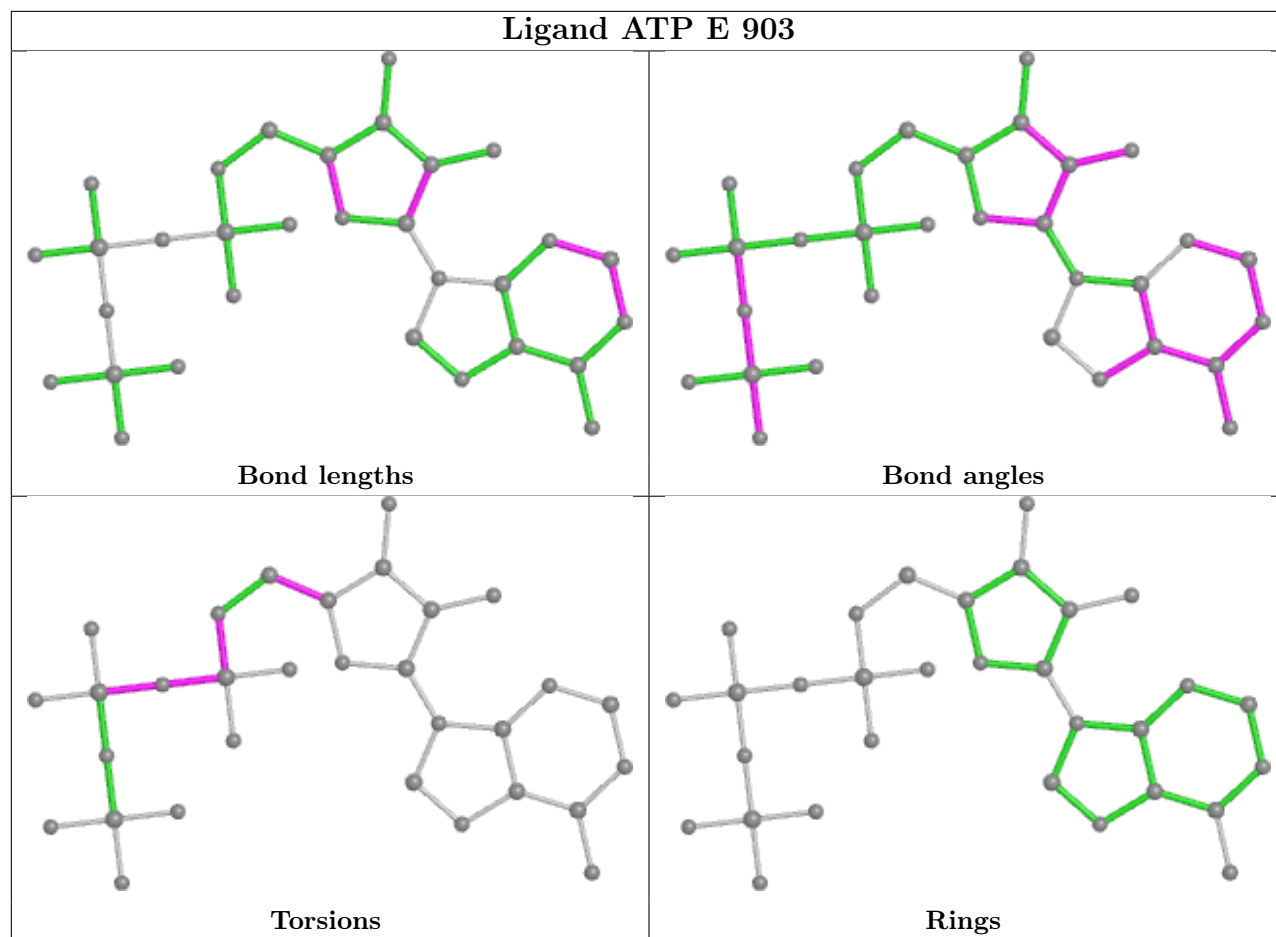
Mol	Chain	Res	Type	Atoms
3	A	901	ATP	C3'-C4'-C5'-O5'
3	A	903	ATP	C5'-O5'-PA-O1A

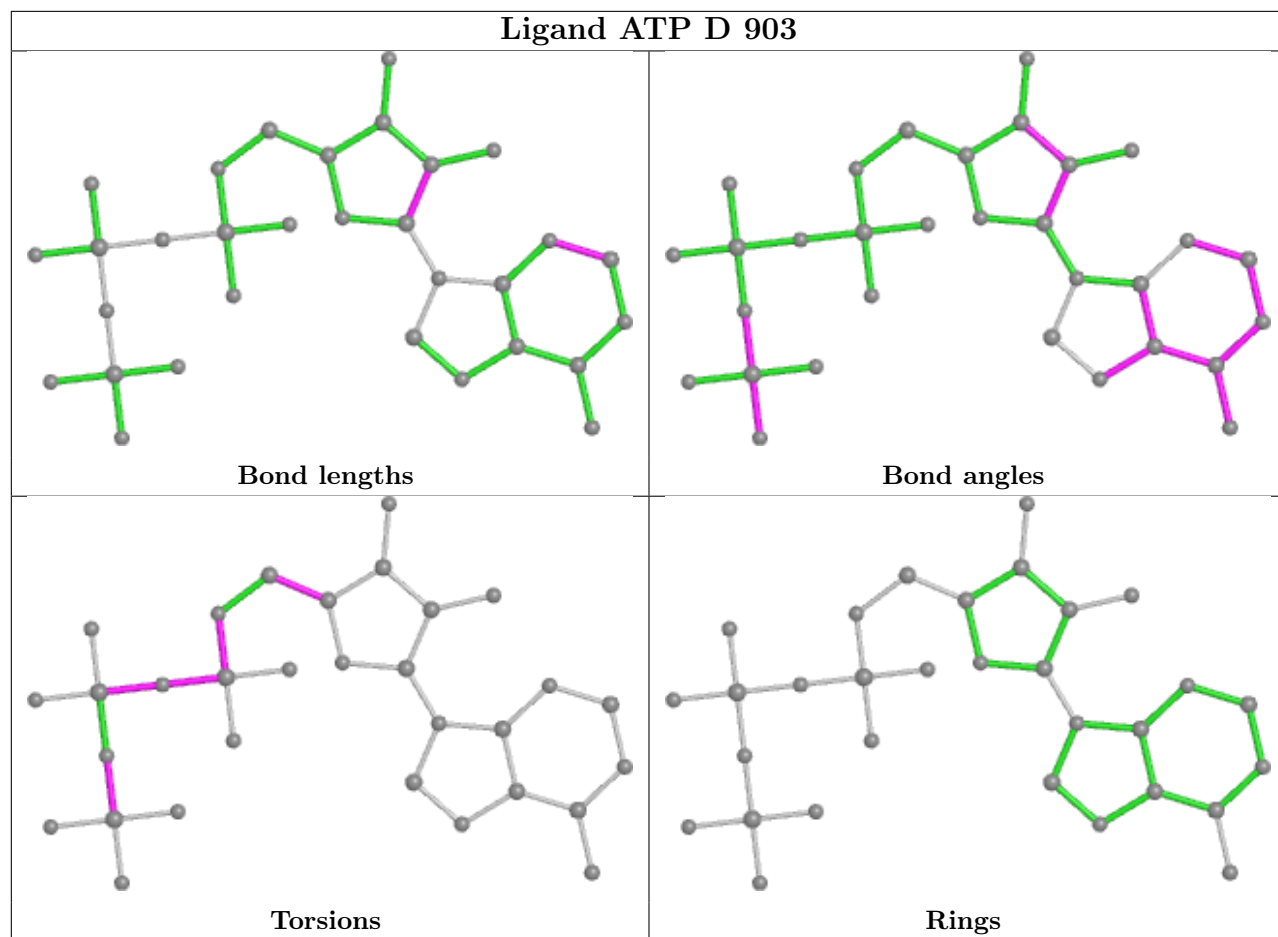
There are no ring outliers.

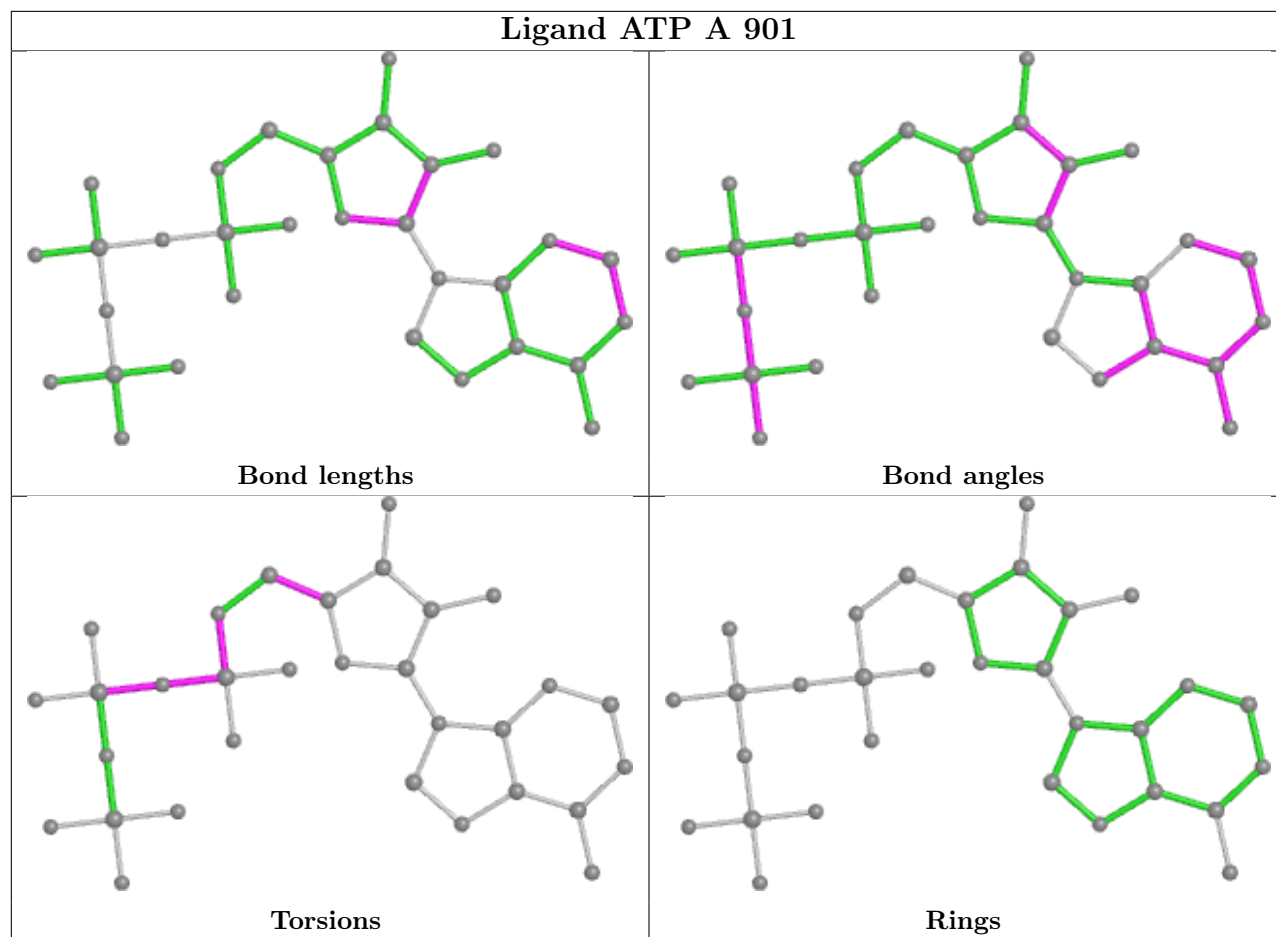
11 monomers are involved in 35 short contacts:

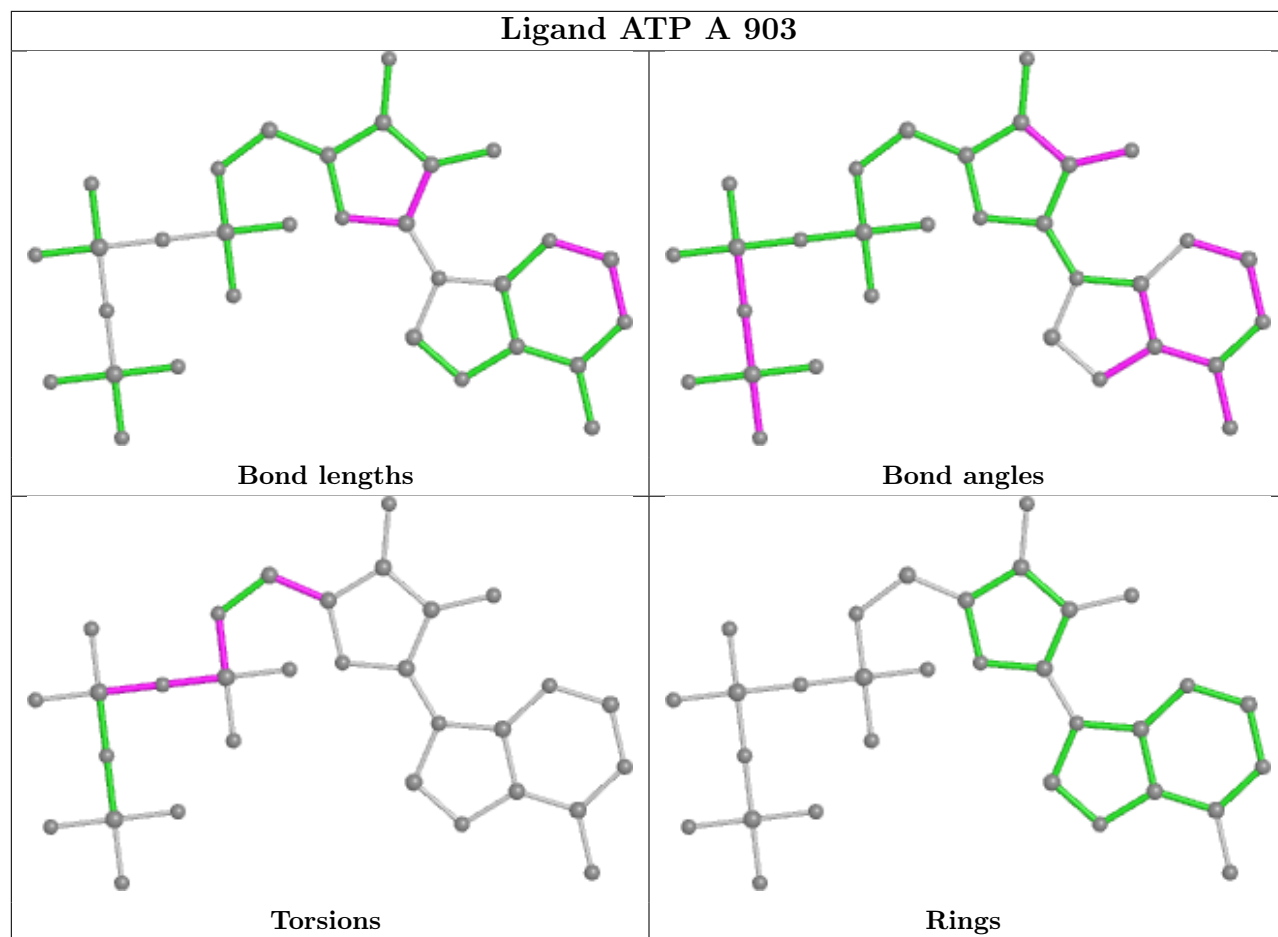
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	903	ATP	3	0
3	D	903	ATP	3	0
3	A	903	ATP	2	0
3	B	903	ATP	4	0
3	B	901	ATP	3	0
3	F	903	ATP	3	0
3	C	901	ATP	3	0
3	C	903	ATP	2	0
3	F	901	ATP	1	0
3	D	901	ATP	5	0
3	E	901	ATP	6	0

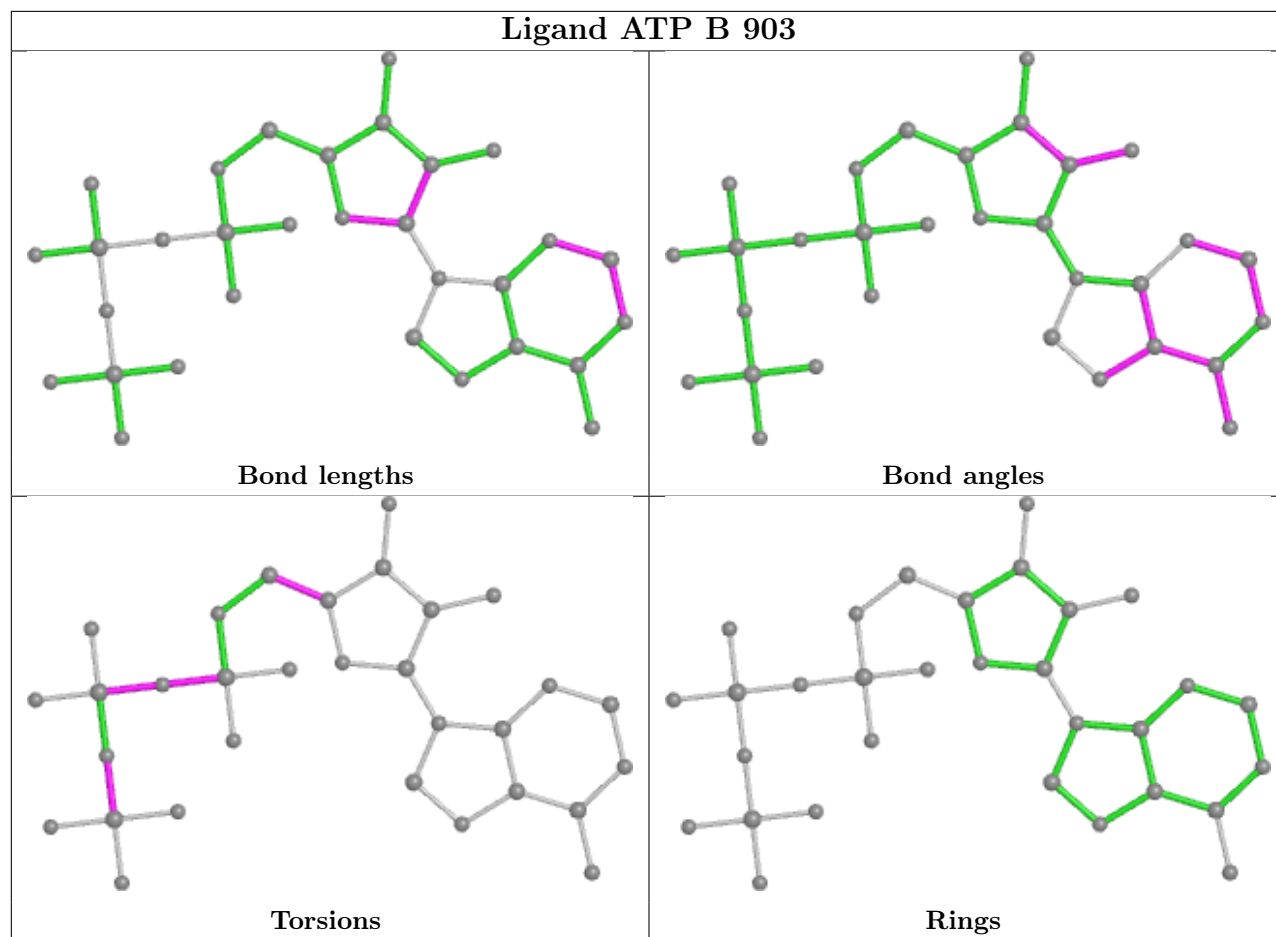
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

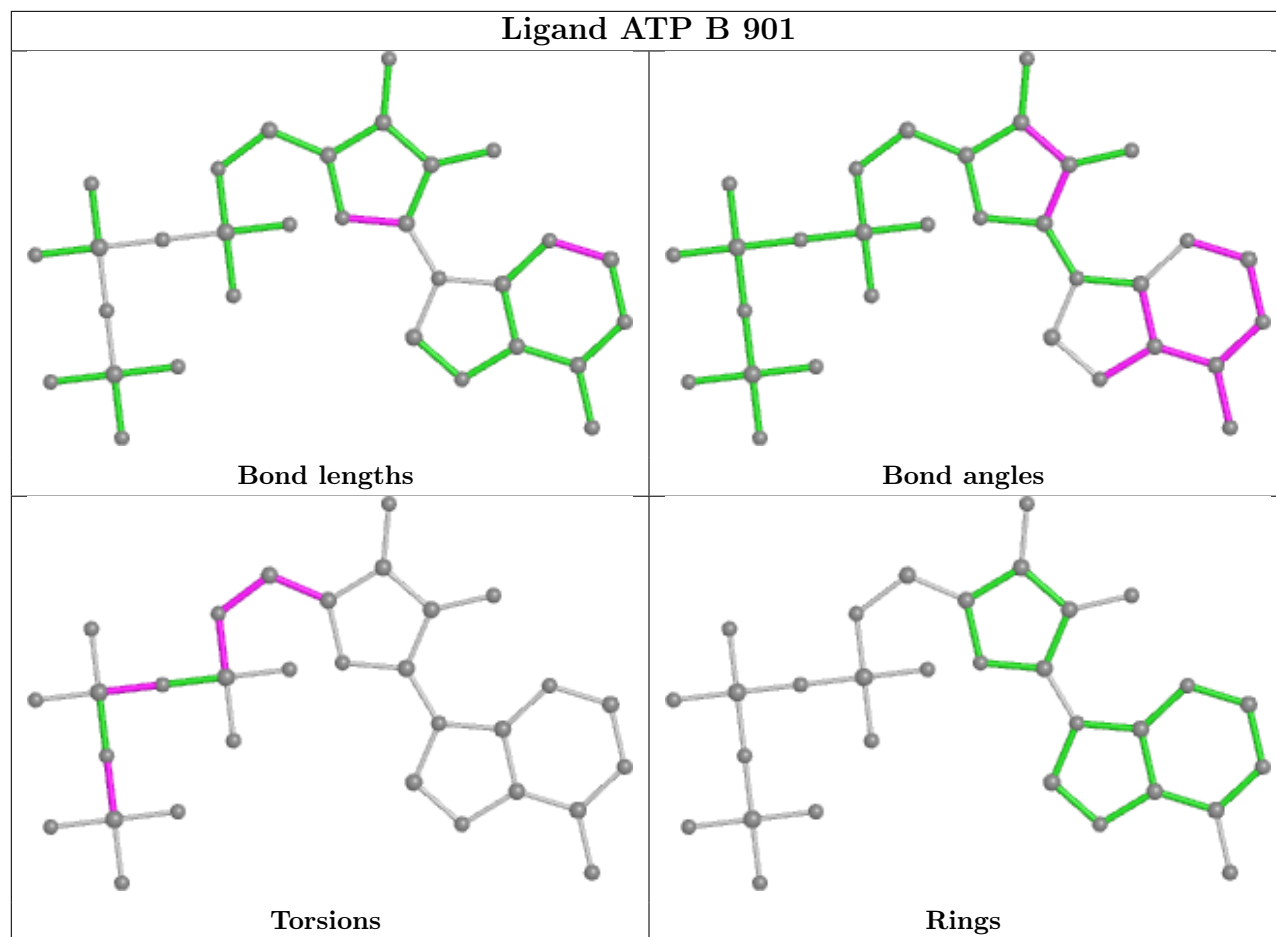




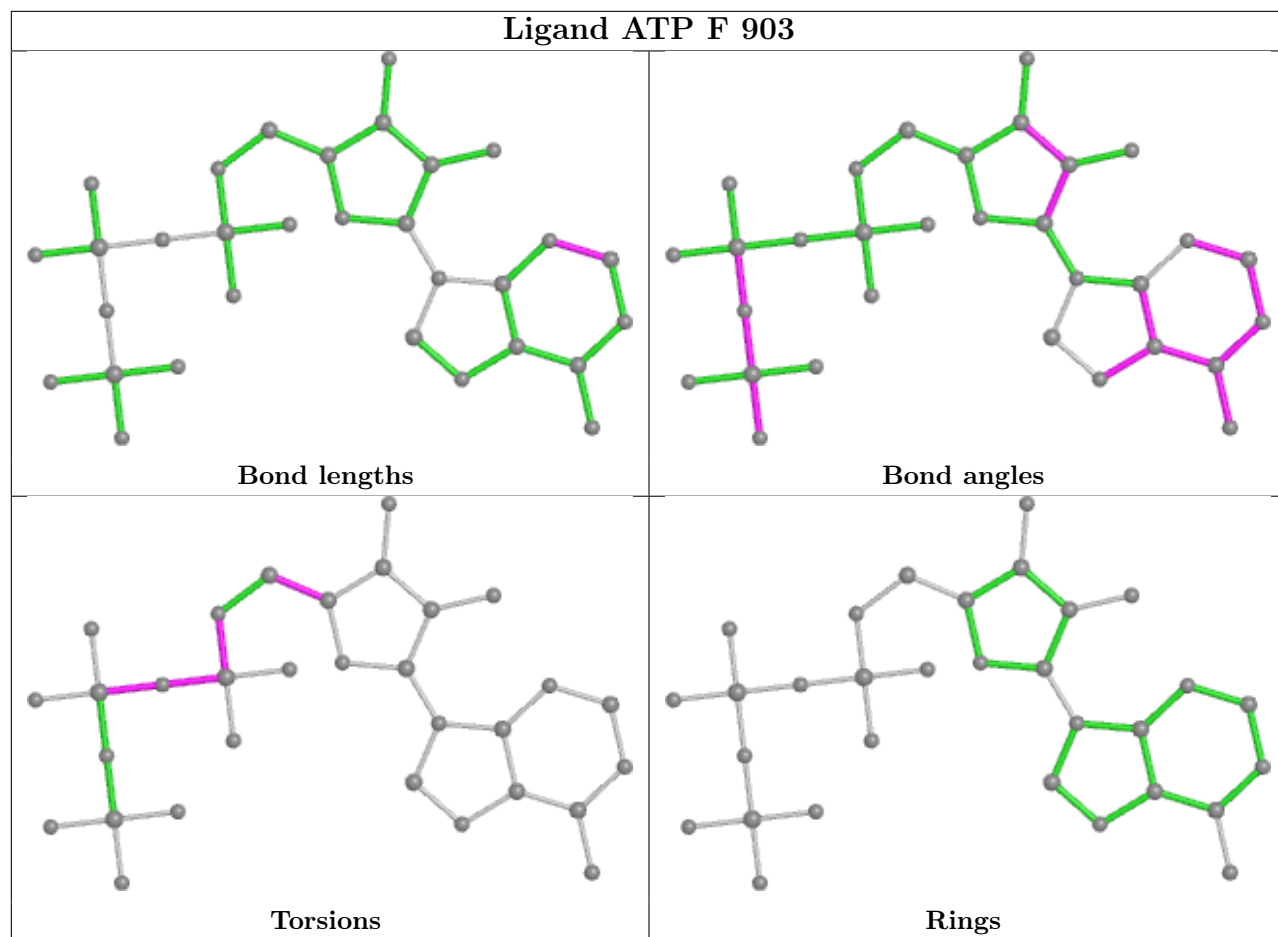


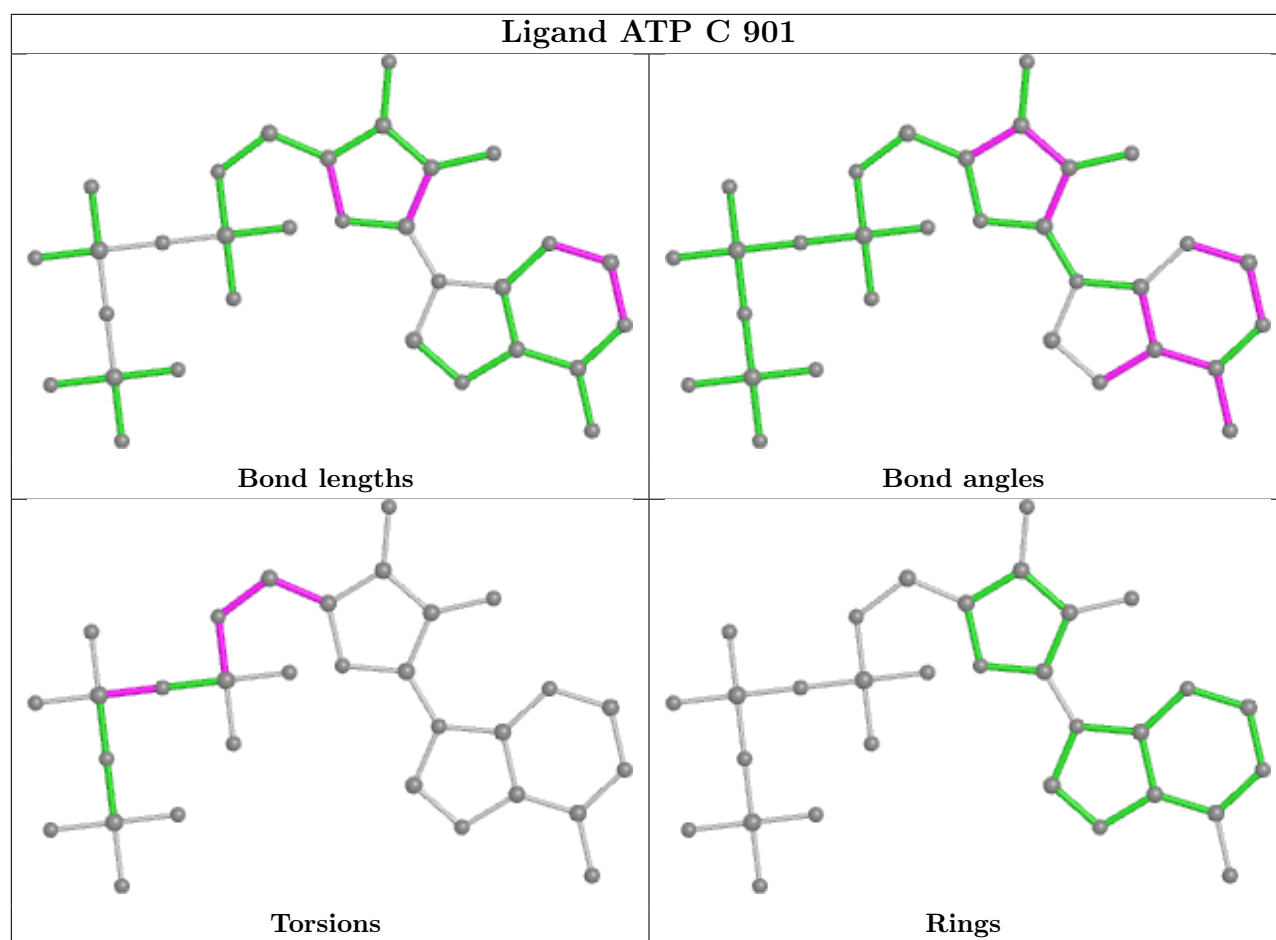


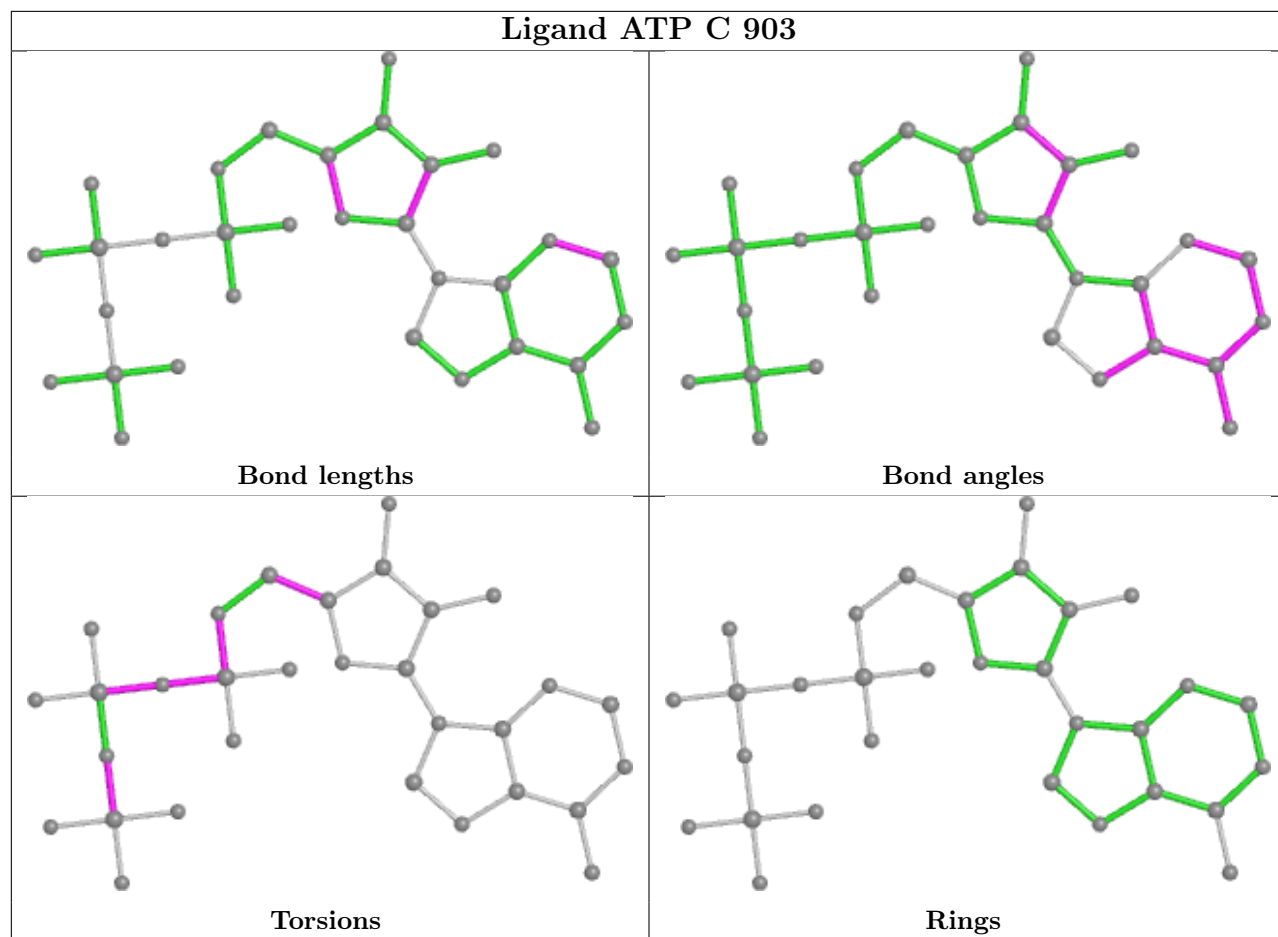




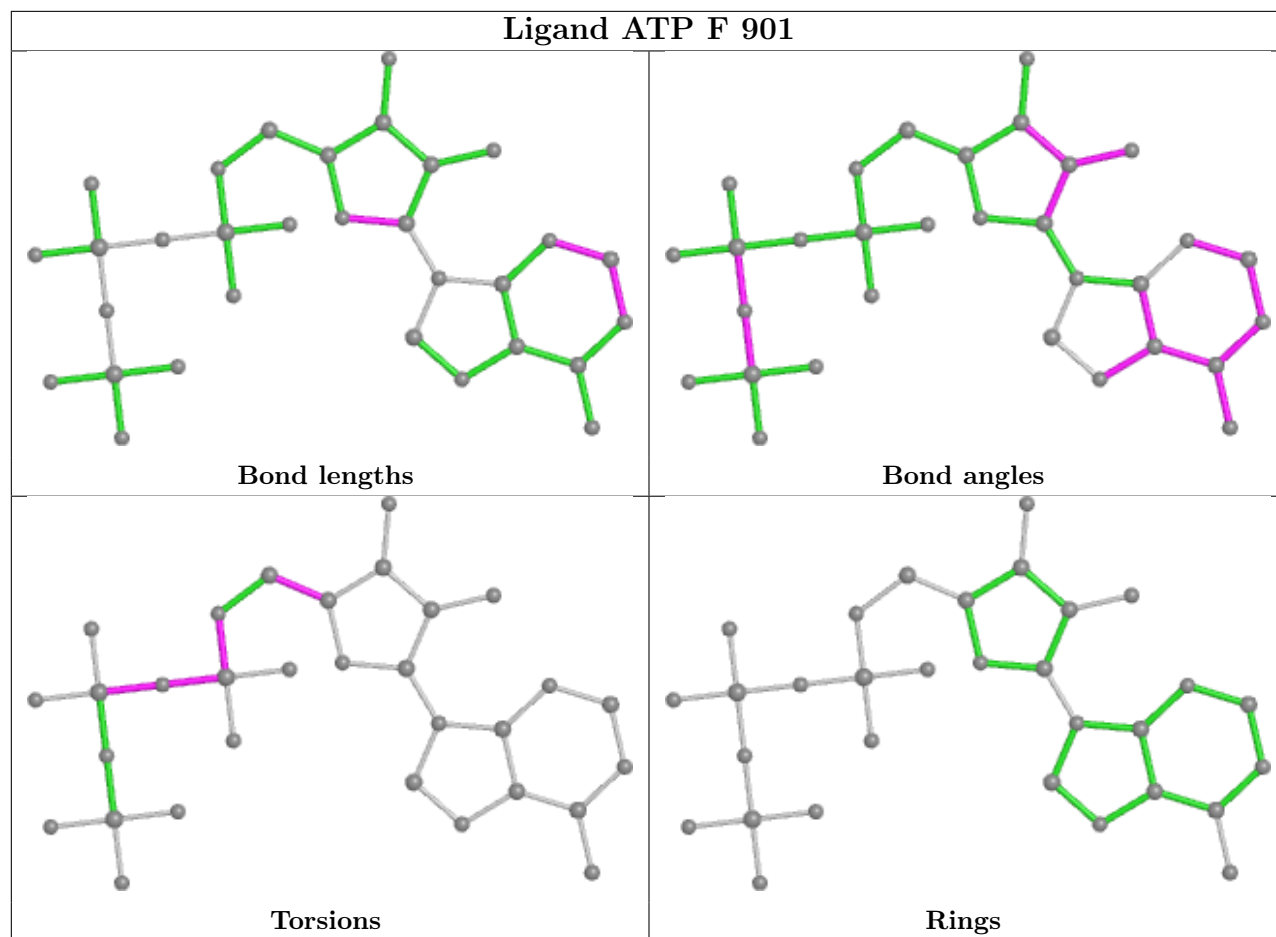
Ligand ATP F 903

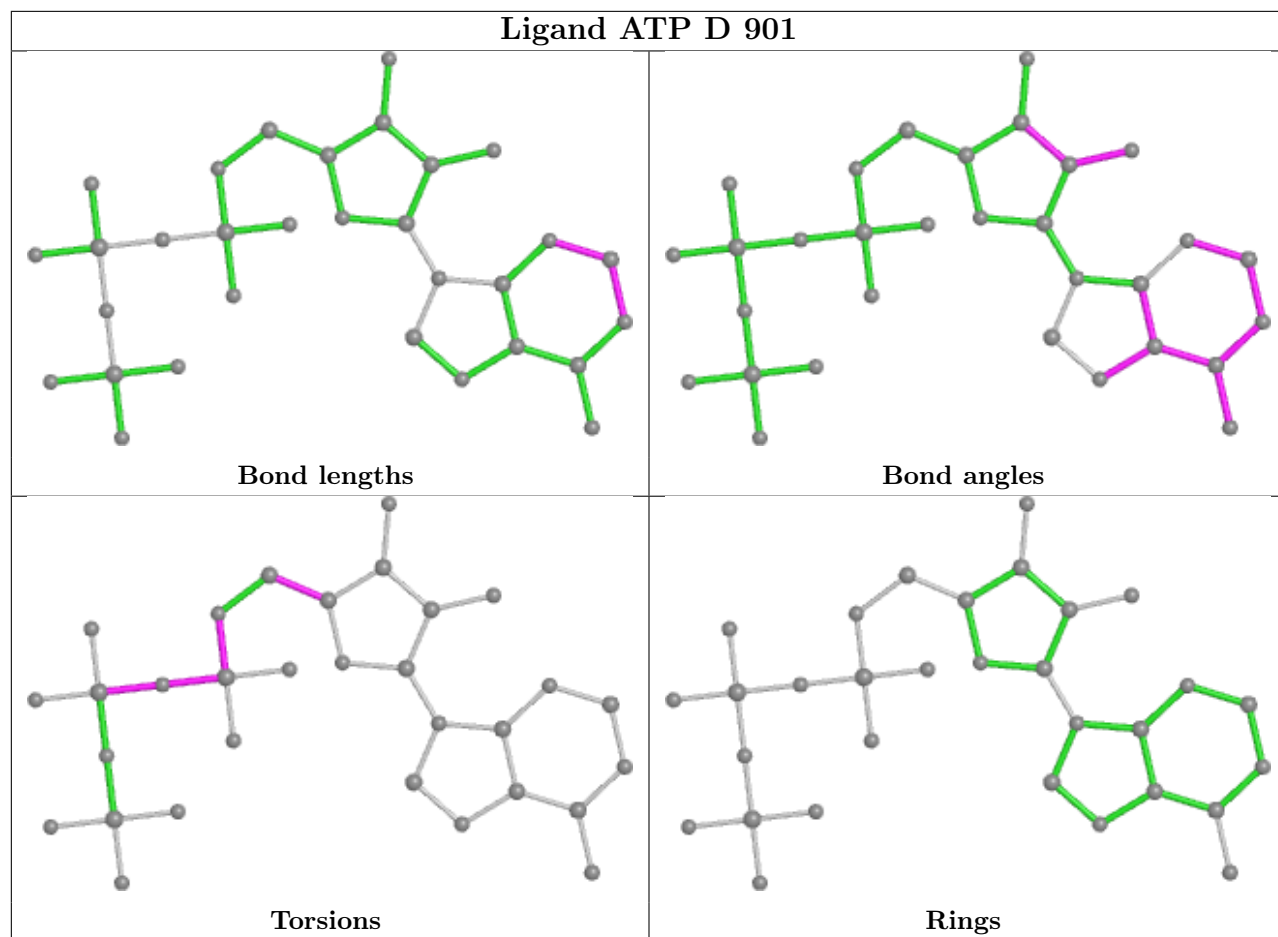


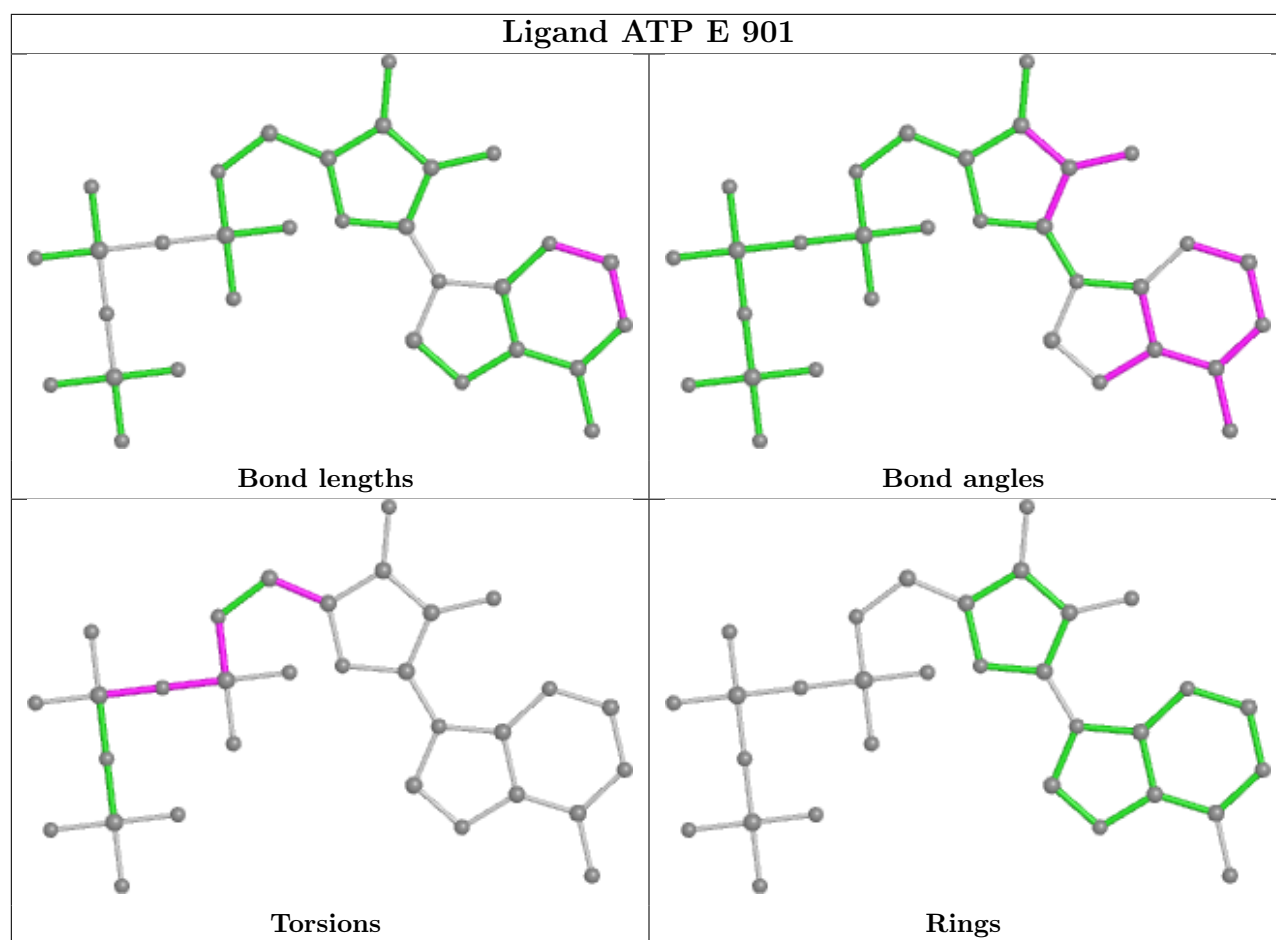




Ligand ATP F 901







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	504/519 (97%)	0.46	63 (12%) 3 2	29, 92, 154, 184	0
1	B	489/519 (94%)	0.24	35 (7%) 15 9	47, 95, 151, 185	0
1	C	486/519 (93%)	0.07	28 (5%) 23 13	34, 74, 144, 176	0
1	D	483/519 (93%)	-0.14	21 (4%) 35 22	11, 59, 123, 150	0
1	E	490/519 (94%)	0.04	33 (6%) 17 10	10, 70, 137, 179	0
1	F	504/519 (97%)	0.24	43 (8%) 10 6	15, 84, 154, 175	0
All	All	2956/3114 (94%)	0.16	223 (7%) 14 8	10, 80, 147, 185	0

The worst 5 of 223 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	517	PRO	9.0
1	A	519	SER	8.5
1	F	423	HIS	8.1
1	A	503	SER	7.7
1	A	516	GLY	7.5

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	431	10/11	0.67	0.26	109,115,120,121	0
1	SEP	C	431	10/11	0.72	0.38	96,106,119,119	0
1	SEP	F	431	10/11	0.76	0.31	104,110,117,117	0
1	SEP	D	431	10/11	0.79	0.24	96,105,117,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	B	431	10/11	0.81	0.35	129,136,148,148	0
1	SEP	E	431	10/11	0.88	0.21	89,93,102,104	0
1	TPO	B	432	11/12	0.89	0.35	120,127,130,130	0
1	TPO	A	432	11/12	0.91	0.23	106,109,114,114	0
1	TPO	F	432	11/12	0.92	0.24	97,99,101,103	0
1	TPO	C	432	11/12	0.94	0.24	83,88,91,92	0
1	TPO	E	432	11/12	0.94	0.18	73,80,83,84	0
1	TPO	D	432	11/12	0.95	0.25	77,82,83,89	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	801	1/1	0.83	0.25	42,42,42,42	0
3	ATP	F	901	31/31	0.85	0.31	103,116,121,121	0
2	MG	C	801	1/1	0.86	0.14	17,17,17,17	0
3	ATP	A	901	31/31	0.89	0.27	83,93,100,100	0
3	ATP	B	903	31/31	0.89	0.24	68,74,79,79	0
2	MG	D	802	1/1	0.89	0.29	15,15,15,15	0
3	ATP	A	903	31/31	0.90	0.23	65,68,74,75	0
2	MG	A	701	1/1	0.90	0.16	27,27,27,27	0
3	ATP	C	903	31/31	0.90	0.29	52,56,76,78	0
3	ATP	E	901	31/31	0.90	0.25	74,92,98,98	0
2	MG	C	701	1/1	0.90	0.68	49,49,49,49	0
2	MG	B	802	1/1	0.91	0.16	57,57,57,57	0
3	ATP	D	903	31/31	0.91	0.30	29,35,62,63	0
3	ATP	C	901	31/31	0.92	0.20	56,59,63,64	0
2	MG	F	802	1/1	0.92	0.67	92,92,92,92	0
3	ATP	D	901	31/31	0.92	0.27	68,73,80,80	0
3	ATP	B	901	31/31	0.93	0.20	69,77,80,82	0
2	MG	B	701	1/1	0.93	0.68	93,93,93,93	0
2	MG	D	520	1/1	0.93	0.54	12,12,12,12	0
2	MG	E	801	1/1	0.93	0.44	44,44,44,44	0

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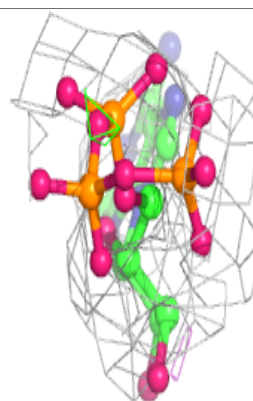
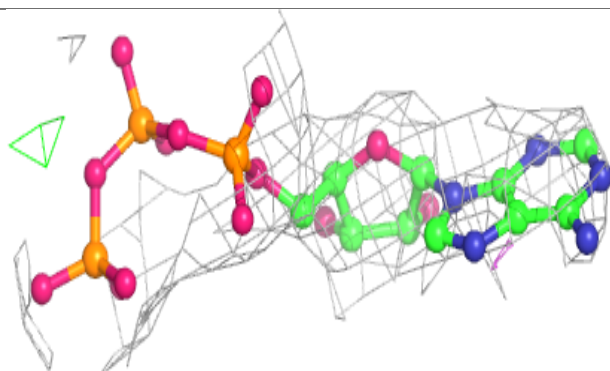
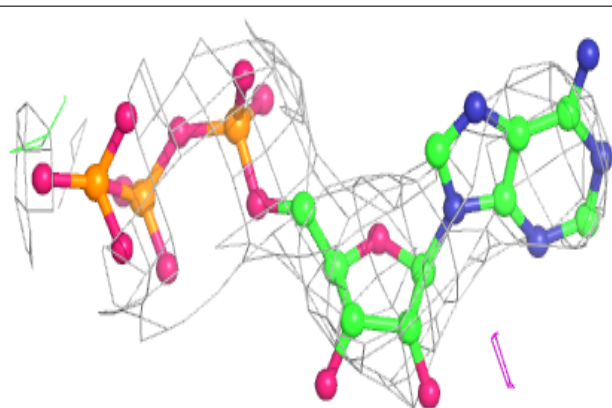
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ATP	F	903	31/31	0.94	0.23	38,43,47,48	0
2	MG	B	702	1/1	0.95	0.46	61,61,61,61	0
3	ATP	E	903	31/31	0.95	0.21	22,35,50,53	0
2	MG	E	702	1/1	0.96	0.24	56,56,56,56	0
2	MG	B	801	1/1	0.97	0.28	88,88,88,88	0
2	MG	D	801	1/1	0.97	0.11	48,48,48,48	0
2	MG	F	701	1/1	0.97	0.64	67,67,67,67	0
2	MG	C	702	1/1	0.97	0.34	50,50,50,50	0
2	MG	A	802	1/1	0.97	0.21	66,66,66,66	0
2	MG	C	802	1/1	0.98	0.18	105,105,105,105	0
2	MG	F	520	1/1	0.98	0.23	82,82,82,82	0
2	MG	A	702	1/1	0.99	0.23	7,7,7,7	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.

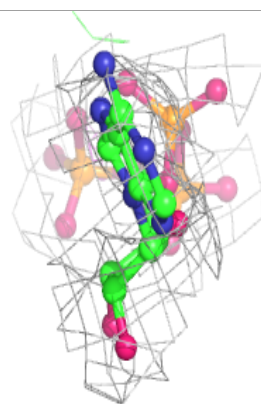
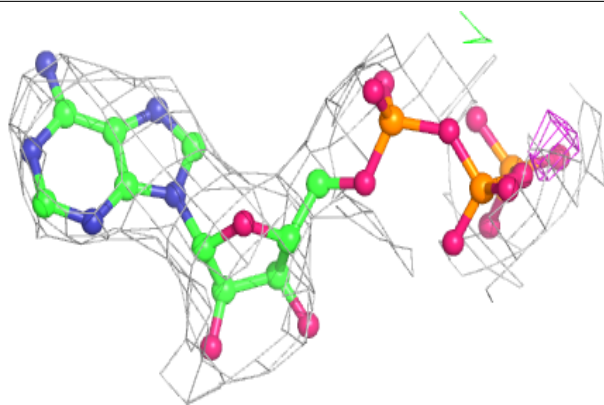
Electron density around ATP F 901:

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

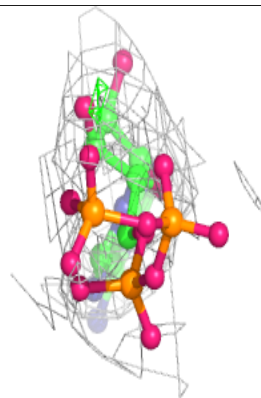
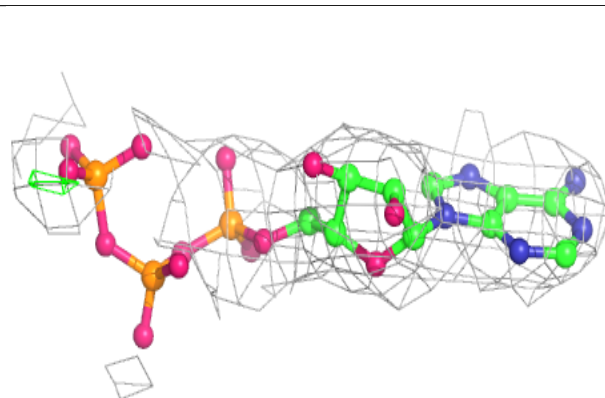
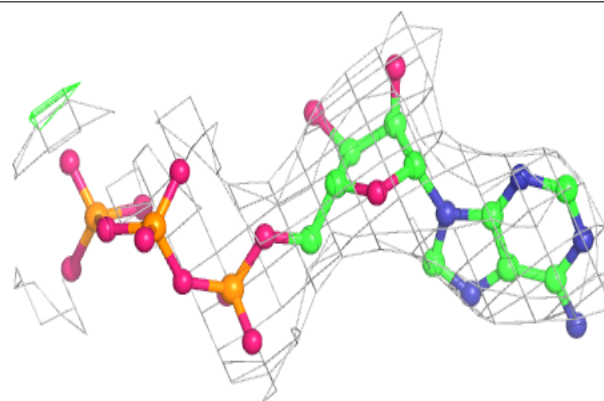


Electron density around ATP A 901:

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

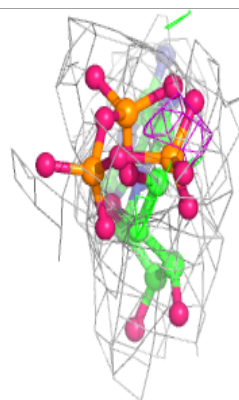
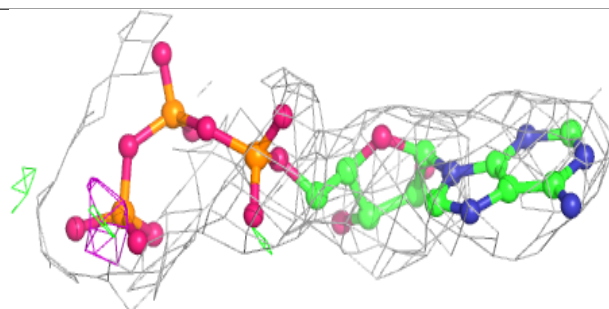
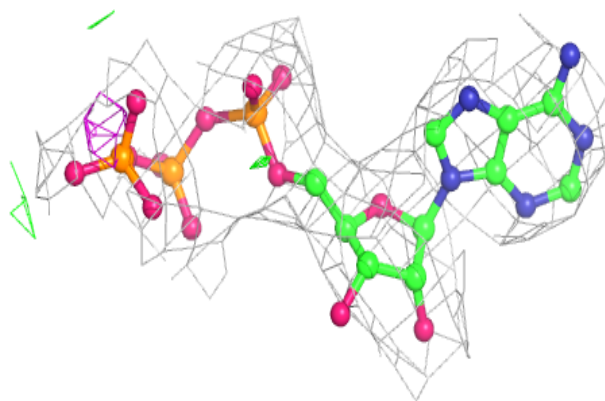
**Electron density around ATP B 903:**

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

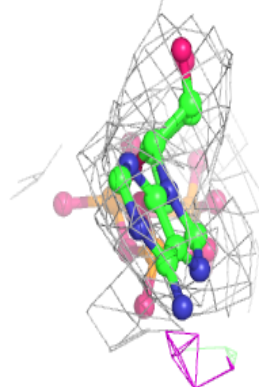
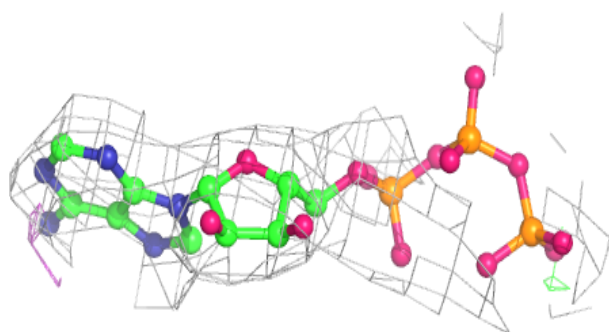
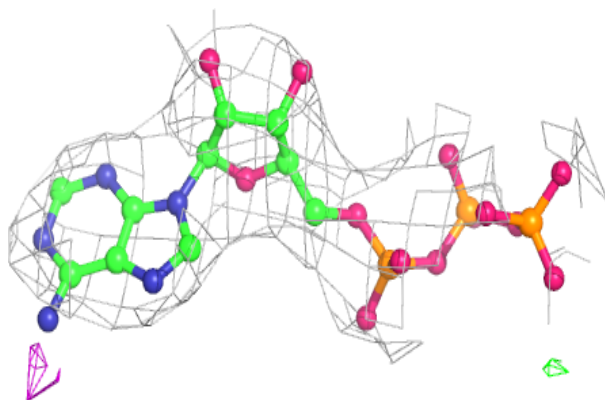


Electron density around ATP A 903:

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

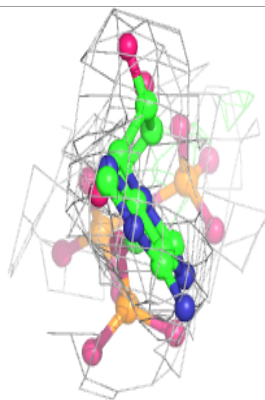
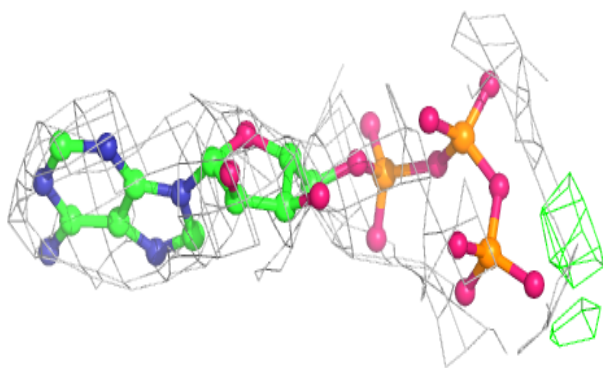
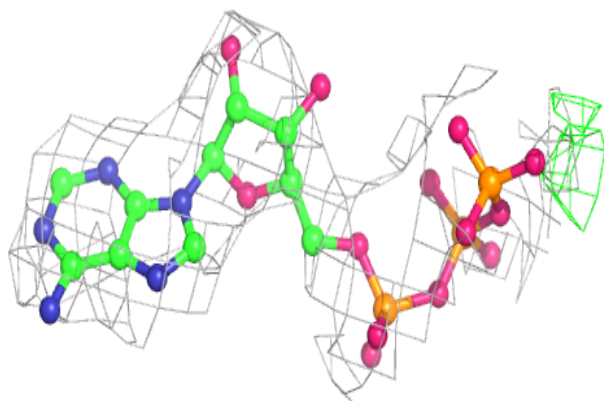
**Electron density around ATP C 903:**

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

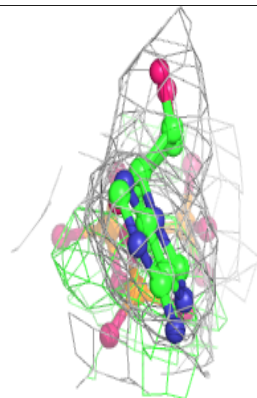
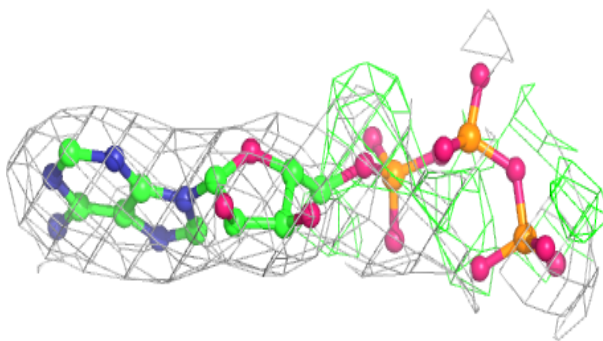
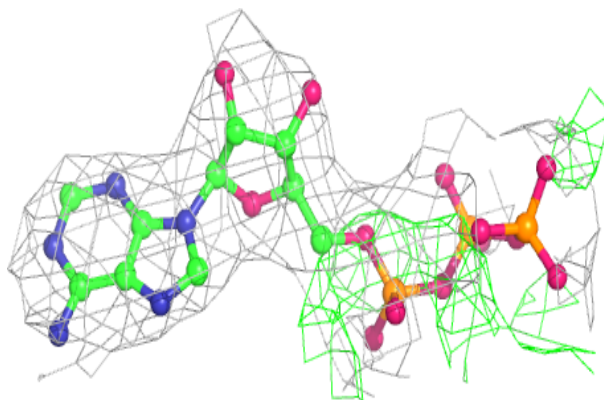


Electron density around ATP E 901:

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

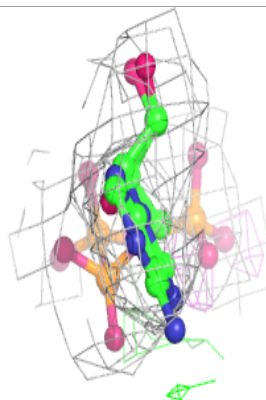
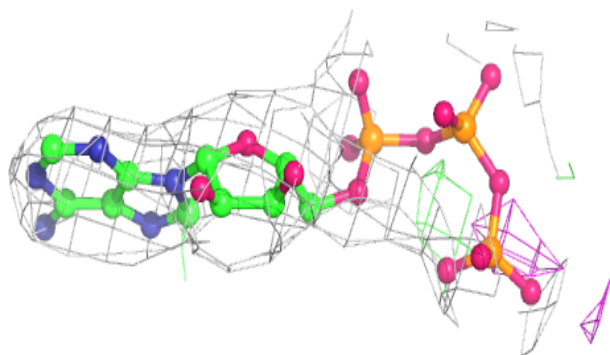
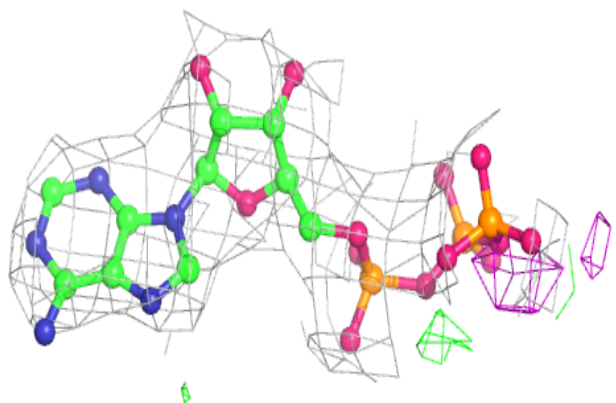
**Electron density around ATP D 903:**

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

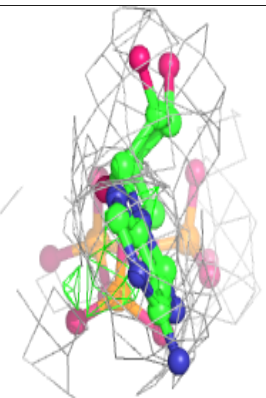
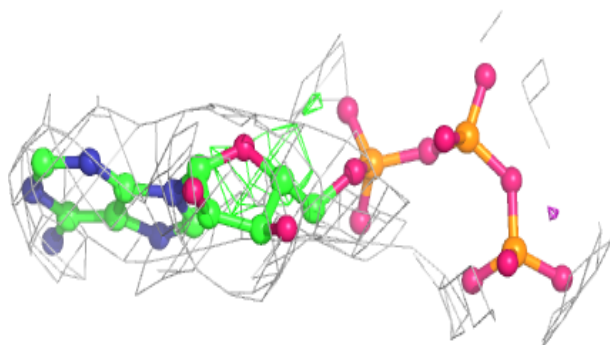
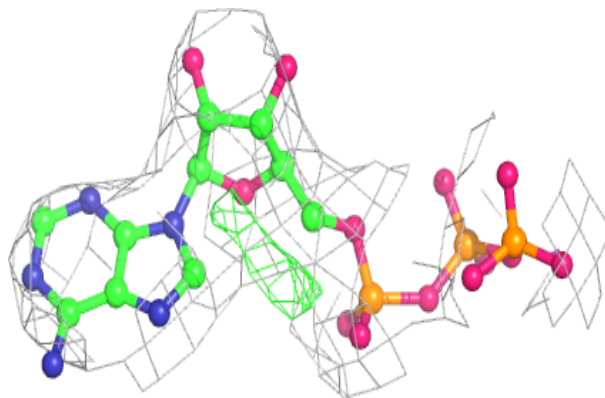


Electron density around ATP C 901:

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

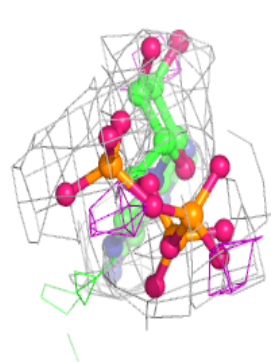
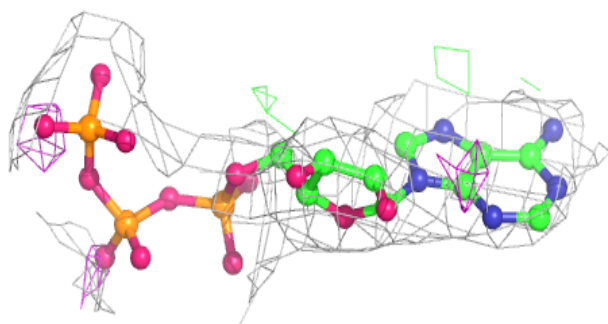
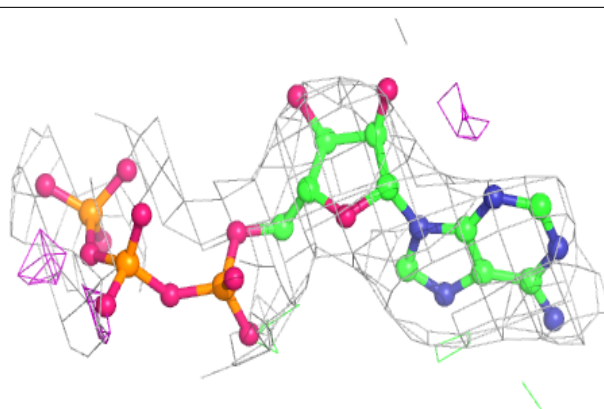
**Electron density around ATP D 901:**

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

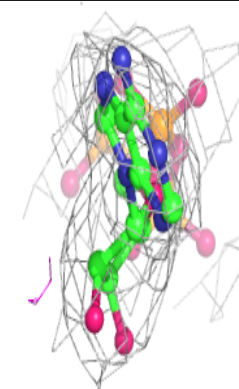
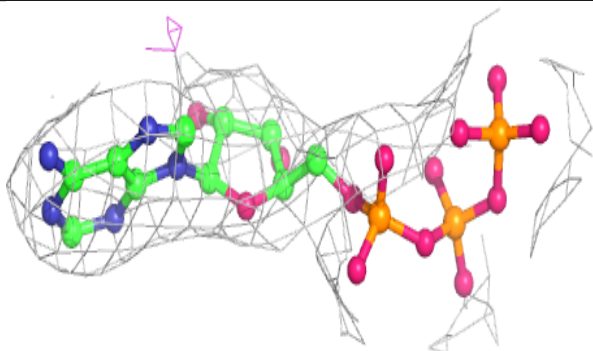
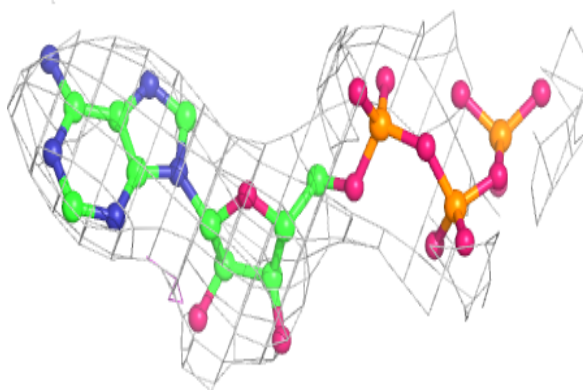


Electron density around ATP B 901:

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

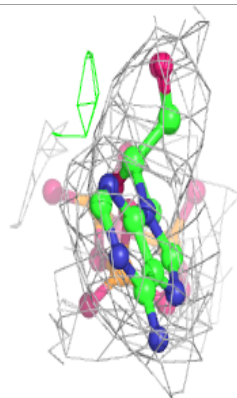
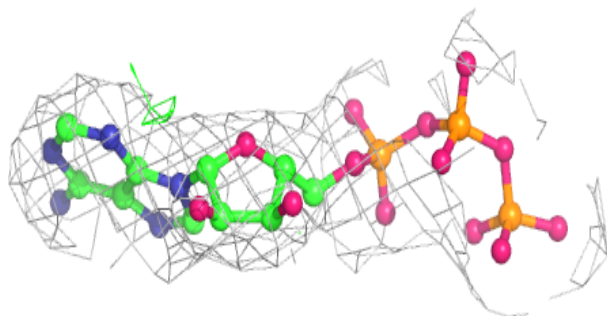
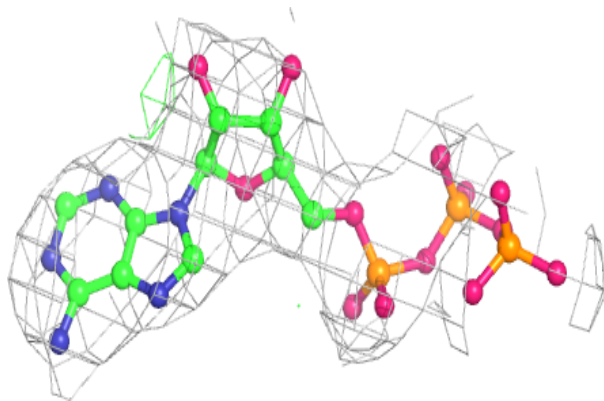
**Electron density around ATP F 903:**

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



Electron density around ATP E 903:

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.