wwPDB X-ray Structure Validation Summary Report (i)

Sep 13, 2022 – 10:22 pm BST

PDB ID	:	7Q6I
Title	:	Vibrio maritimus FtsA 1-396 ATP and FtsN 1-29, bent tetramers in double filament arrangement
Authors	:	Nierhaus, T.; Kureisaite-Ciziene, D.; Lowe, J.
Deposited on	:	2021-11-07
Resolution	:	3.60 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:

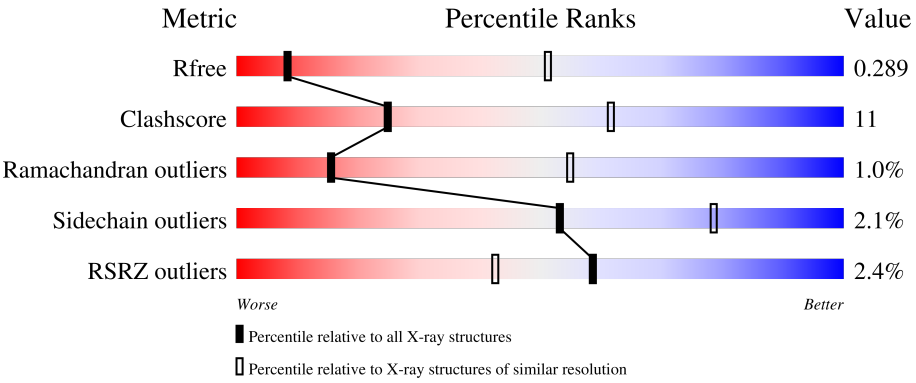
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	396	71% 25%
1	B	396	73% 23%
1	C	396	73% 23%
1	D	396	71% 19% 9%
1	E	396	73% 23%

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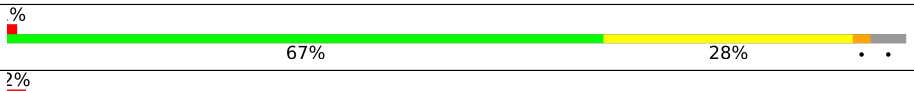
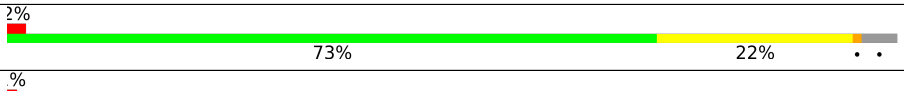
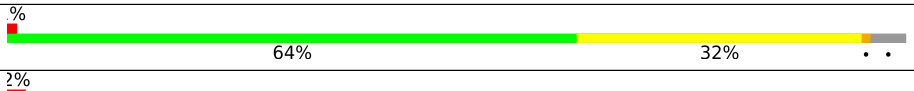
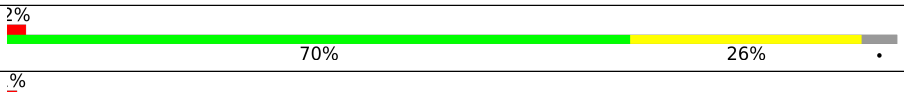
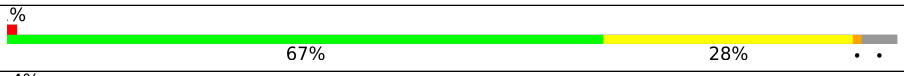
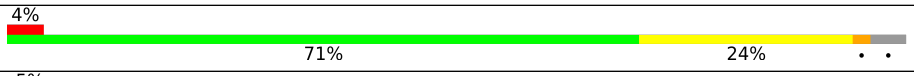
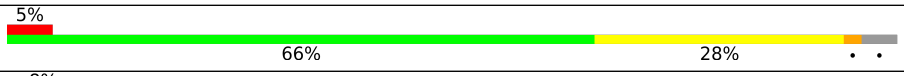
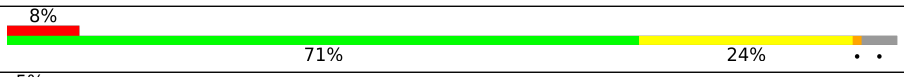
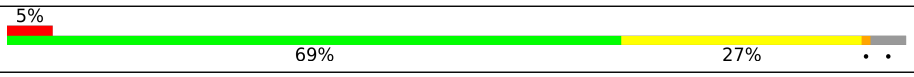
Mol	Chain	Length	Quality of chain
1	F	396	
1	G	396	
1	H	396	
1	I	396	
1	J	396	
1	K	396	
1	L	396	
1	M	396	
1	N	396	
1	O	396	
1	P	396	
2	X	37	
2	Y	37	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 46262 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.

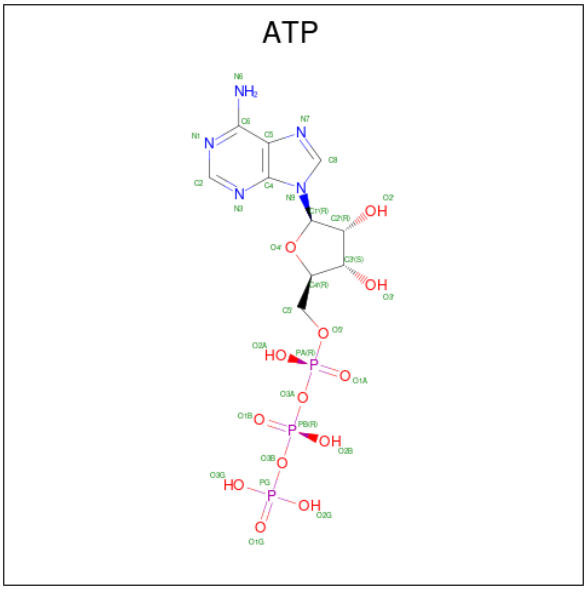
- Molecule 1 is a protein called Cell division protein FtsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	B	383	Total	C	N	O	S	0	0	0
			2871	1780	505	572	14			
1	C	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	D	362	Total	C	N	O	S	0	0	0
			2717	1690	475	538	14			
1	E	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	F	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	G	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	H	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	I	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	J	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	K	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	L	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	M	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	N	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	O	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			
1	P	382	Total	C	N	O	S	0	0	0
			2863	1776	504	569	14			

- Molecule 2 is a protein called Cell division protein FtsN (polyAla model).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	8	Total	C	N	O	0	0	0
			40	24	8	8			
2	Y	8	Total	C	N	O	0	0	0
			40	24	8	8			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	N	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	O	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

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

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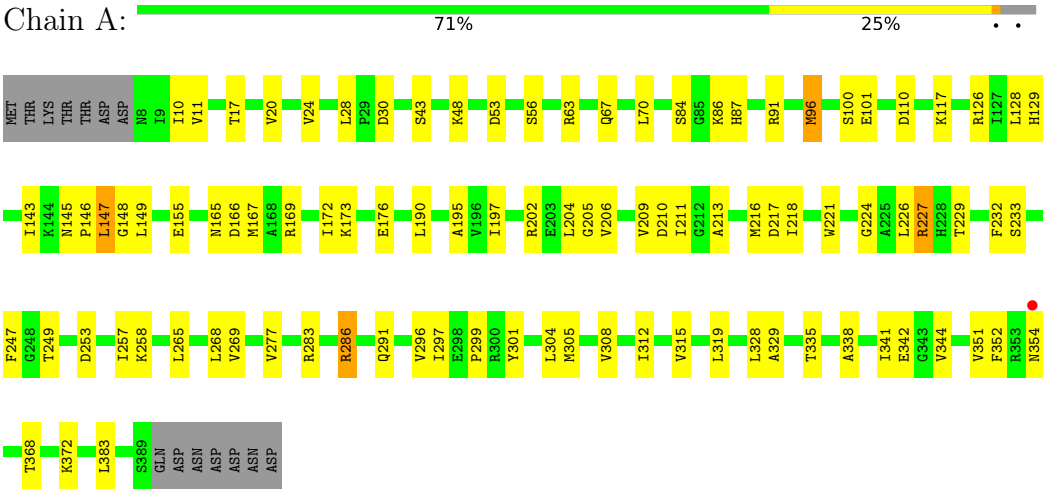
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0
4	N	1	Total Mg 1 1	0	0
4	O	1	Total Mg 1 1	0	0
4	P	1	Total Mg 1 1	0	0

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.

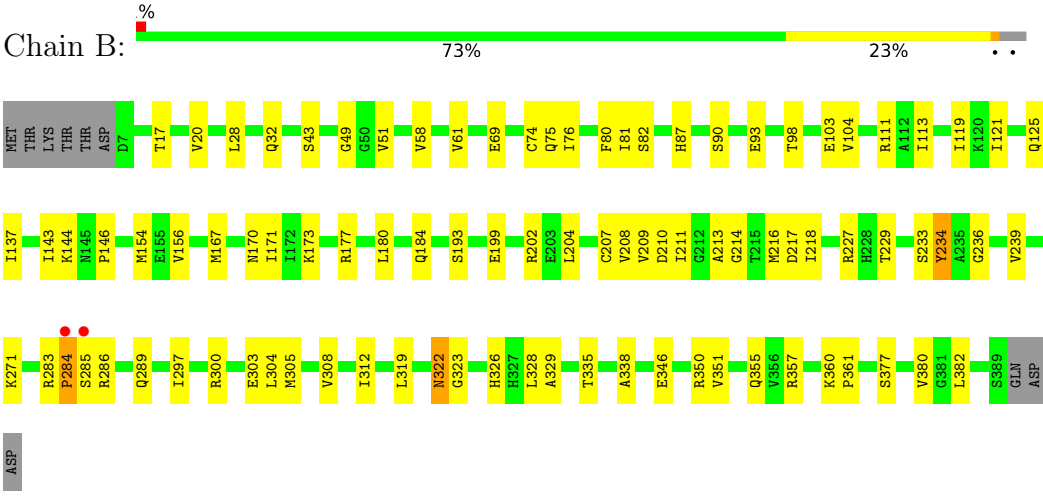
• Molecule 1: Cell division protein FtsA

Chain A:



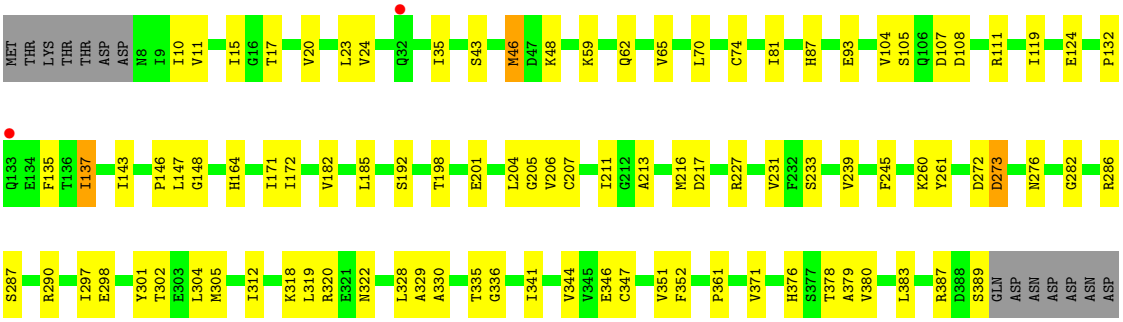
• Molecule 1: Cell division protein FtsA

Chain B:



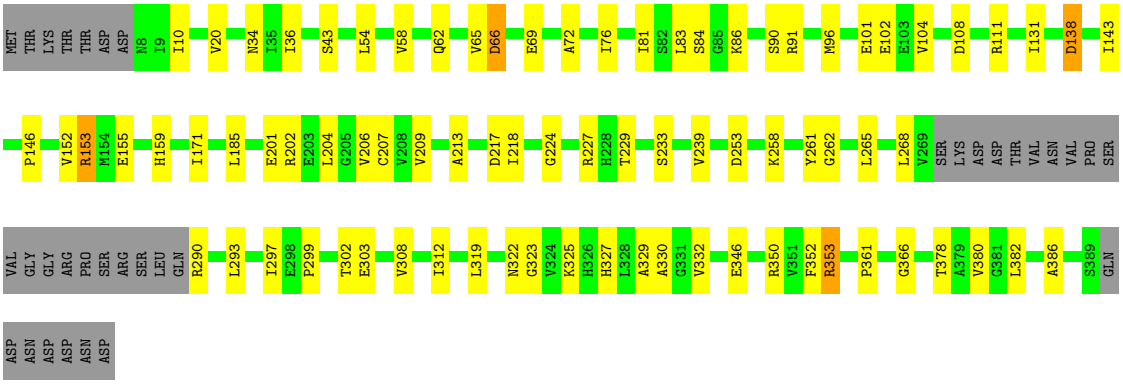
• Molecule 1: Cell division protein FtsA

Chain C:



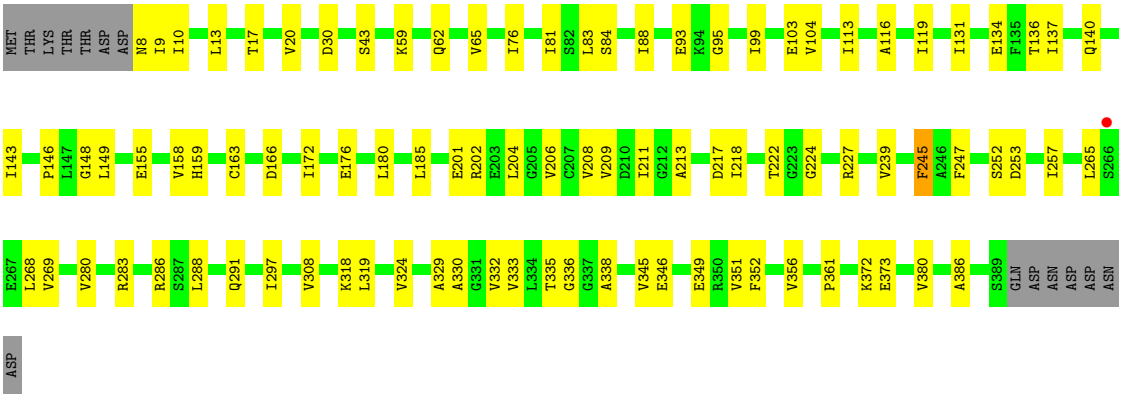
• Molecule 1: Cell division protein FtsA

Chain D:



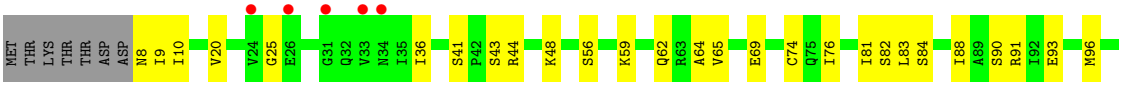
• Molecule 1: Cell division protein FtsA

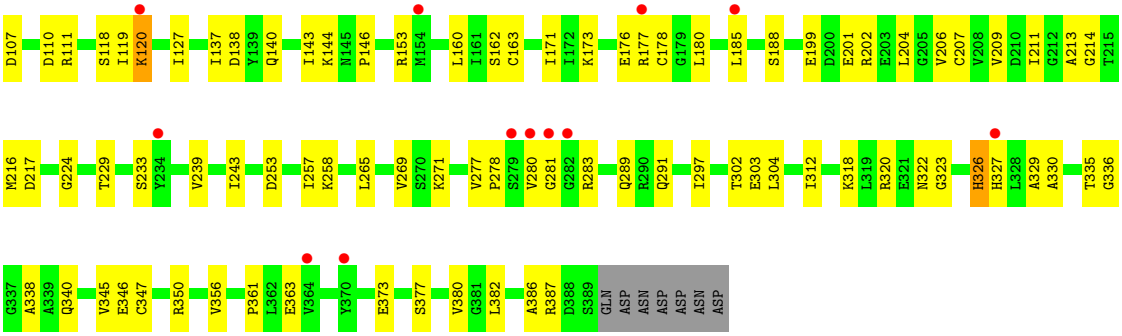
Chain E:



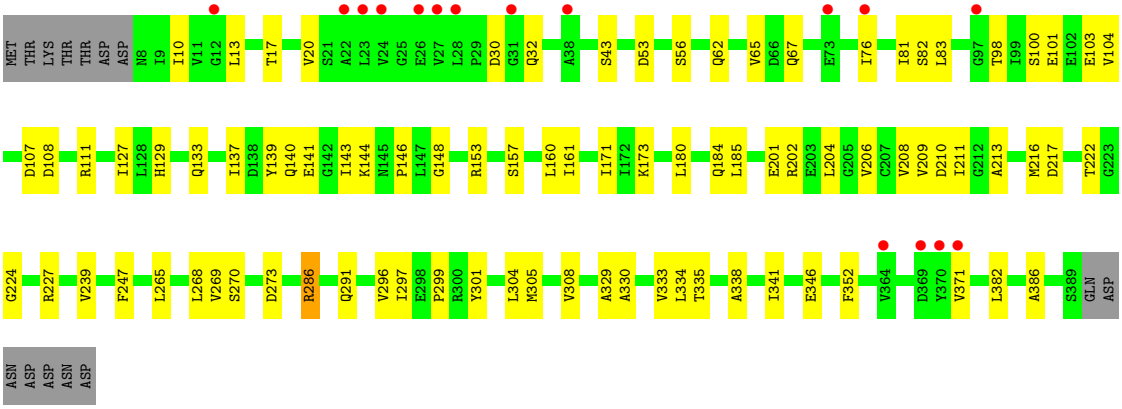
• Molecule 1: Cell division protein FtsA

Chain F:

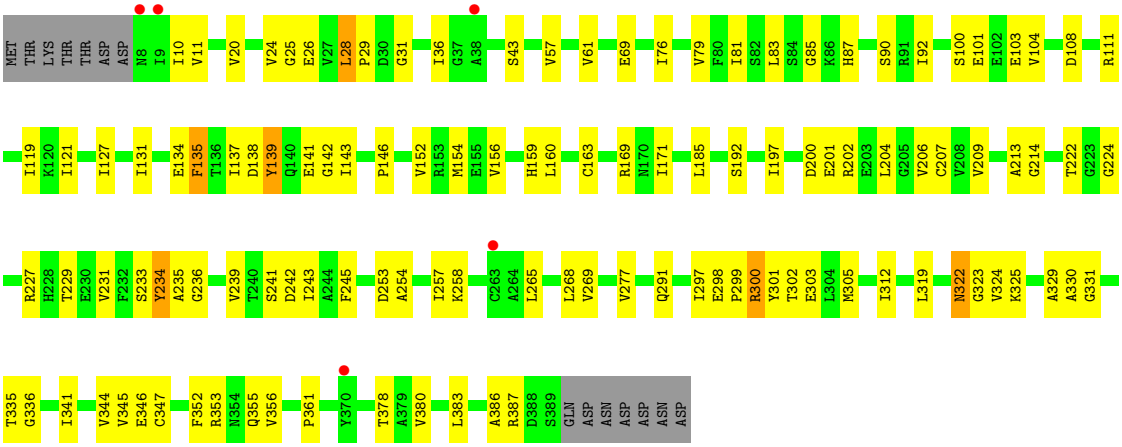




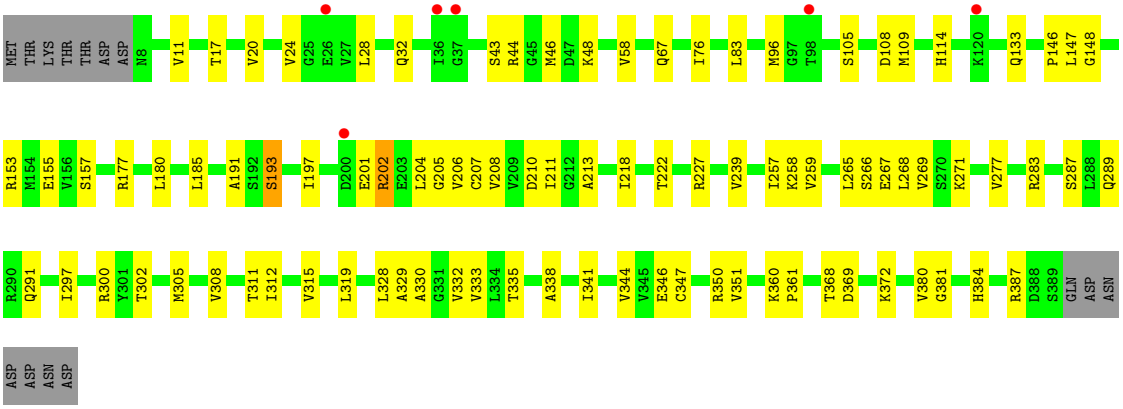
• Molecule 1: Cell division protein FtsA



• Molecule 1: Cell division protein FtsA

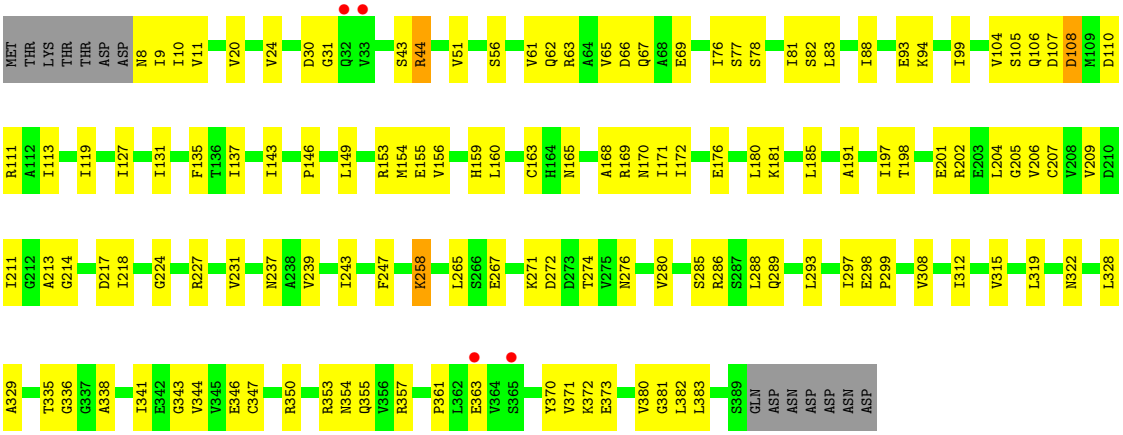


• Molecule 1: Cell division protein FtsA



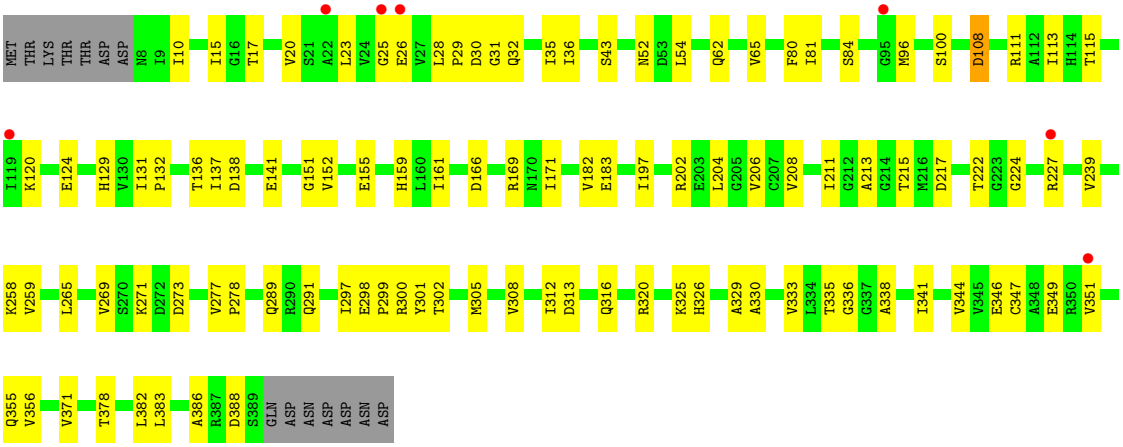
• Molecule 1: Cell division protein FtsA

Chain J:



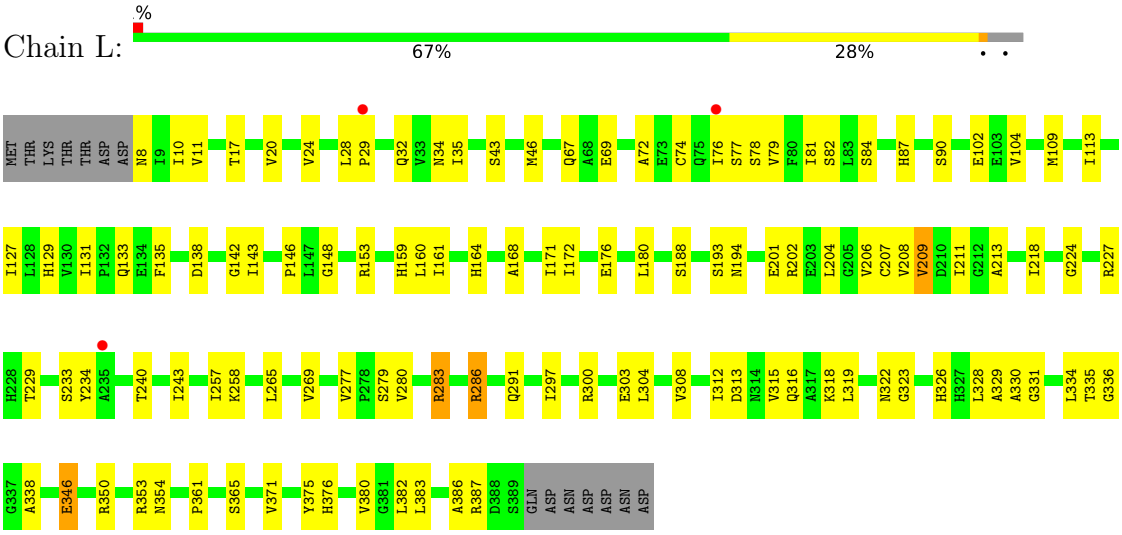
• Molecule 1: Cell division protein FtsA

Chain K:



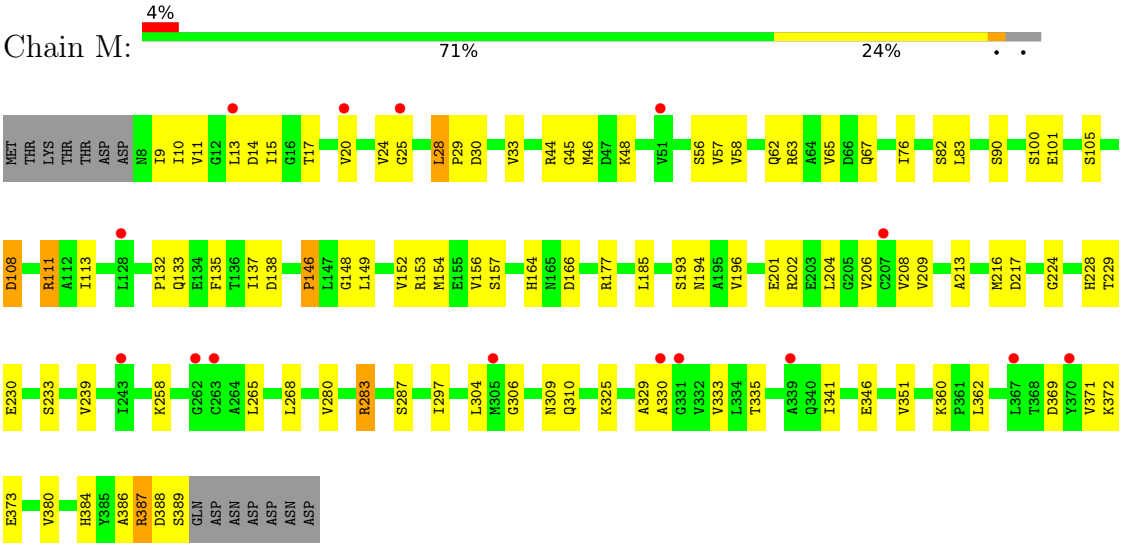
• Molecule 1: Cell division protein FtsA

Chain L:



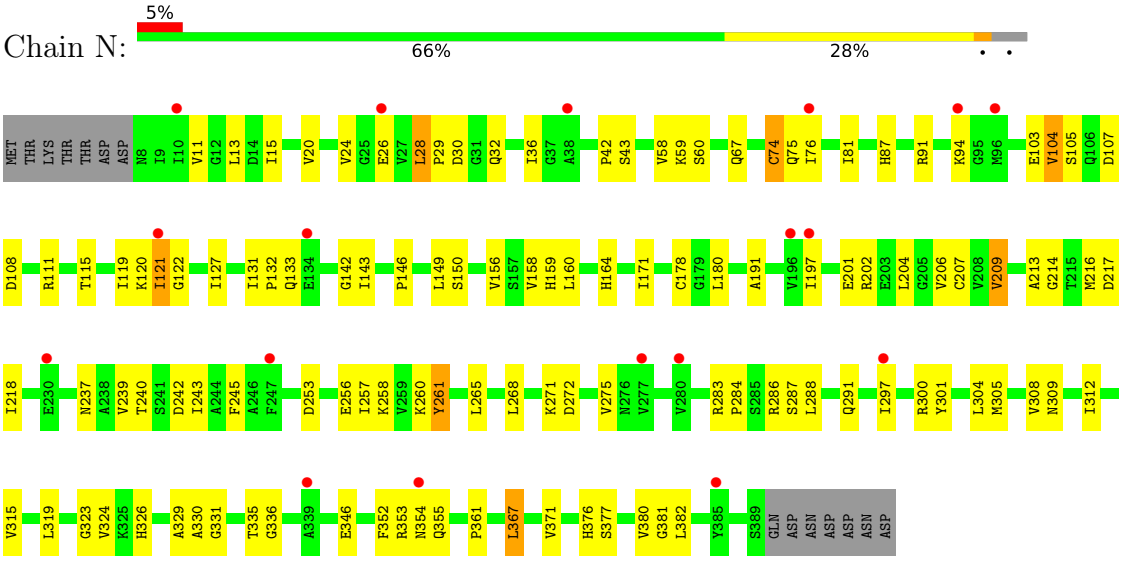
• Molecule 1: Cell division protein FtsA

Chain M:



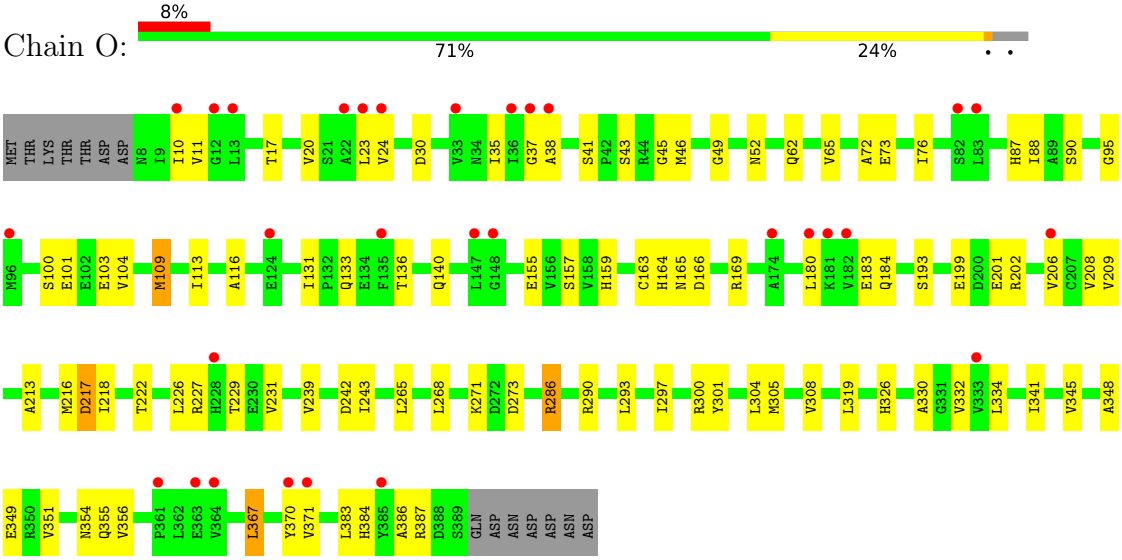
• Molecule 1: Cell division protein FtsA

Chain N:



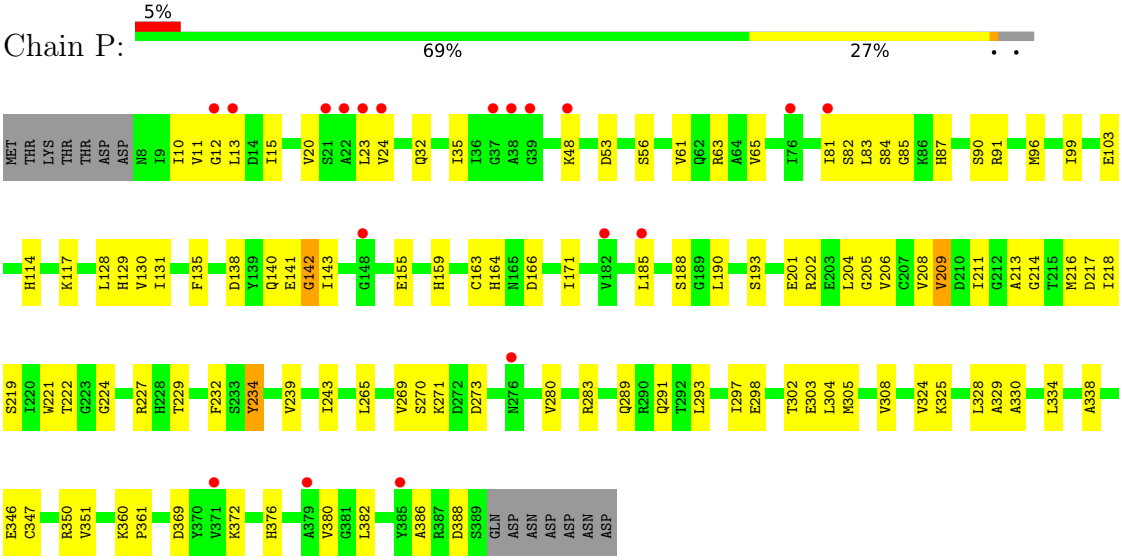
• Molecule 1: Cell division protein FtsA

Chain O:



• Molecule 1: Cell division protein FtsA

Chain P:

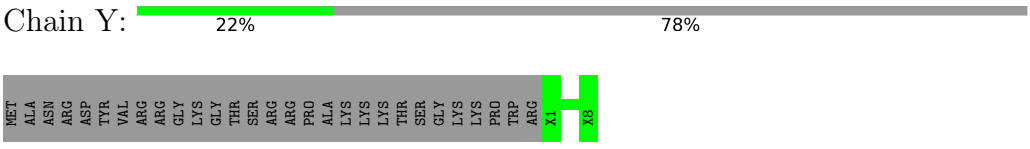


• Molecule 2: Cell division protein FtsN (polyAla model)

Chain X:

• Molecule 2: Cell division protein FtsN (polyAla model)

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.69Å 119.99Å 329.79Å 90.00° 93.76° 90.00°	Depositor
Resolution (Å)	49.88 – 3.60 73.35 – 3.56	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.88-3.60) 99.2 (73.35-3.56)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.20rc1_4392, REFMAC 5.8.0230	Depositor
R, R_{free}	0.241 , 0.287 0.242 , 0.289	Depositor DCC
R_{free} test set	4439 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	110.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	46262	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: 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	0.25	0/2898	0.52	0/3921
1	B	0.25	0/2906	0.52	0/3932
1	C	0.25	0/2898	0.51	0/3921
1	D	0.26	0/2749	0.52	0/3717
1	E	0.25	0/2898	0.50	0/3921
1	F	0.25	0/2898	0.53	0/3921
1	G	0.25	0/2898	0.51	0/3921
1	H	0.27	0/2898	0.55	1/3921 (0.0%)
1	I	0.26	0/2898	0.54	0/3921
1	J	0.26	0/2898	0.53	0/3921
1	K	0.25	0/2898	0.51	0/3921
1	L	0.26	0/2898	0.52	0/3921
1	M	0.25	0/2898	0.53	1/3921 (0.0%)
1	N	0.26	0/2898	0.57	2/3921 (0.1%)
1	O	0.27	0/2898	0.55	1/3921 (0.0%)
1	P	0.27	0/2898	0.56	0/3921
All	All	0.26	0/46227	0.53	5/62543 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	28	LEU	CA-CB-CG	8.49	134.84	115.30
1	N	367	LEU	CA-CB-CG	7.82	133.29	115.30
1	N	28	LEU	CA-CB-CG	6.69	130.68	115.30
1	O	367	LEU	CA-CB-CG	6.11	129.35	115.30
1	H	28	LEU	CA-CB-CG	5.78	128.59	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2863	0	2872	65	0
1	B	2871	0	2879	53	3
1	C	2863	0	2875	61	0
1	D	2717	0	2728	50	1
1	E	2863	0	2875	57	0
1	F	2863	0	2875	67	0
1	G	2863	0	2873	49	0
1	H	2863	0	2875	73	1
1	I	2863	0	2873	52	0
1	J	2863	0	2873	86	0
1	K	2863	0	2875	71	0
1	L	2863	0	2873	65	2
1	M	2863	0	2875	66	1
1	N	2863	0	2875	79	0
1	O	2863	0	2875	72	0
1	P	2863	0	2872	61	2
2	X	40	0	11	1	0
2	Y	40	0	11	0	0
3	A	31	0	11	1	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	D	31	0	12	2	0
3	E	31	0	12	0	0
3	F	31	0	12	2	0
3	G	31	0	11	2	0
3	H	31	0	12	2	0
3	I	31	0	11	1	0
3	J	31	0	11	2	0
3	K	31	0	12	1	0
3	L	31	0	11	1	0
3	M	31	0	12	3	0
3	N	31	0	12	1	0
3	O	31	0	12	2	0
3	P	31	0	11	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
All	All	46262	0	46051	995	5

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 11.

The worst 5 of 995 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:M:28:LEU:HD12	1:M:29:PRO:HD2	1.51	0.92
1:L:11:VAL:HG12	1:L:24:VAL:HG12	1.52	0.91
1:M:11:VAL:HG11	1:M:76:ILE:HD11	1.58	0.84
1:H:302:THR:OG1	1:H:347:CYS:SG	2.36	0.83
1:H:239:VAL:HG13	1:H:258:LYS:HE2	1.59	0.82

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:153:ARG:NH2	1:P:114:HIS:O[1_465]	1.98	0.22
1:B:303:GLU:OE1	1:L:233:SER:OG[1_455]	2.11	0.09
1:B:233:SER:OG	1:L:303:GLU:OE1[1_455]	2.14	0.06
1:B:285:SER:OG	1:D:253:ASP:OD2[1_545]	2.14	0.06
1:H:233:SER:OG	1:P:303:GLU:OE1[1_455]	2.19	0.01

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	380/396 (96%)	355 (93%)	24 (6%)	1 (0%)	41 75
1	B	381/396 (96%)	352 (92%)	24 (6%)	5 (1%)	12 50
1	C	380/396 (96%)	354 (93%)	24 (6%)	2 (0%)	29 68
1	D	358/396 (90%)	333 (93%)	21 (6%)	4 (1%)	14 53
1	E	380/396 (96%)	355 (93%)	25 (7%)	0	100 100
1	F	380/396 (96%)	352 (93%)	22 (6%)	6 (2%)	9 46
1	G	380/396 (96%)	356 (94%)	24 (6%)	0	100 100
1	H	380/396 (96%)	344 (90%)	27 (7%)	9 (2%)	6 37
1	I	380/396 (96%)	359 (94%)	20 (5%)	1 (0%)	41 75
1	J	380/396 (96%)	350 (92%)	24 (6%)	6 (2%)	9 46
1	K	380/396 (96%)	355 (93%)	24 (6%)	1 (0%)	41 75
1	L	380/396 (96%)	348 (92%)	26 (7%)	6 (2%)	9 46
1	M	380/396 (96%)	353 (93%)	23 (6%)	4 (1%)	14 53
1	N	380/396 (96%)	347 (91%)	25 (7%)	8 (2%)	7 40
1	O	380/396 (96%)	356 (94%)	24 (6%)	0	100 100
1	P	380/396 (96%)	351 (92%)	21 (6%)	8 (2%)	7 40
All	All	6059/6336 (96%)	5620 (93%)	378 (6%)	61 (1%)	15 55

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	B	322	ASN
1	D	322	ASN
1	F	138	ASP
1	F	322	ASN

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	315/329 (96%)	306 (97%)	9 (3%)	42	72
1	B	316/329 (96%)	309 (98%)	7 (2%)	52	77
1	C	315/329 (96%)	307 (98%)	8 (2%)	47	75
1	D	297/329 (90%)	291 (98%)	6 (2%)	55	79
1	E	315/329 (96%)	313 (99%)	2 (1%)	86	94
1	F	315/329 (96%)	310 (98%)	5 (2%)	62	83
1	G	315/329 (96%)	308 (98%)	7 (2%)	52	77
1	H	315/329 (96%)	308 (98%)	7 (2%)	52	77
1	I	315/329 (96%)	305 (97%)	10 (3%)	39	70
1	J	315/329 (96%)	308 (98%)	7 (2%)	52	77
1	K	315/329 (96%)	310 (98%)	5 (2%)	62	83
1	L	315/329 (96%)	307 (98%)	8 (2%)	47	75
1	M	315/329 (96%)	310 (98%)	5 (2%)	62	83
1	N	315/329 (96%)	308 (98%)	7 (2%)	52	77
1	O	315/329 (96%)	309 (98%)	6 (2%)	57	80
1	P	315/329 (96%)	311 (99%)	4 (1%)	69	86
All	All	5023/5264 (95%)	4920 (98%)	103 (2%)	53	78

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	266	SER
1	K	301	TYR
1	P	63	ARG
1	I	300	ARG
1	J	155	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	140	GLN
1	G	62	GLN
1	M	309	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	F	501	4	26,33,33	0.58	0	31,52,52	0.78	2 (6%)
3	ATP	M	501	4	26,33,33	0.58	0	31,52,52	0.81	2 (6%)
3	ATP	L	501	4	26,33,33	0.59	0	31,52,52	0.83	2 (6%)
3	ATP	J	501	4	26,33,33	0.58	0	31,52,52	0.85	3 (9%)
3	ATP	C	501	4	26,33,33	0.58	0	31,52,52	0.76	2 (6%)
3	ATP	A	501	4	26,33,33	0.57	0	31,52,52	0.79	2 (6%)
3	ATP	G	501	4	26,33,33	0.58	0	31,52,52	0.81	2 (6%)
3	ATP	P	501	4	26,33,33	0.59	0	31,52,52	0.83	2 (6%)
3	ATP	D	501	4	26,33,33	0.59	0	31,52,52	0.79	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ATP	E	501	4	26,33,33	0.57	0	31,52,52	0.78	2 (6%)
3	ATP	N	501	4	26,33,33	0.59	0	31,52,52	0.79	2 (6%)
3	ATP	I	501	4	26,33,33	0.59	0	31,52,52	0.82	2 (6%)
3	ATP	K	501	4	26,33,33	0.57	0	31,52,52	0.78	2 (6%)
3	ATP	O	501	4	26,33,33	0.58	0	31,52,52	0.80	2 (6%)
3	ATP	B	501	4	26,33,33	0.58	0	31,52,52	0.84	2 (6%)
3	ATP	H	501	4	26,33,33	0.59	0	31,52,52	0.82	2 (6%)

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	F	501	4	-	0/18/38/38	0/3/3/3
3	ATP	M	501	4	-	4/18/38/38	0/3/3/3
3	ATP	L	501	4	-	3/18/38/38	0/3/3/3
3	ATP	J	501	4	-	2/18/38/38	0/3/3/3
3	ATP	C	501	4	-	4/18/38/38	0/3/3/3
3	ATP	A	501	4	-	5/18/38/38	0/3/3/3
3	ATP	G	501	4	-	3/18/38/38	0/3/3/3
3	ATP	P	501	4	-	2/18/38/38	0/3/3/3
3	ATP	D	501	4	-	3/18/38/38	0/3/3/3
3	ATP	E	501	4	-	8/18/38/38	0/3/3/3
3	ATP	N	501	4	-	0/18/38/38	0/3/3/3
3	ATP	I	501	4	-	1/18/38/38	0/3/3/3
3	ATP	K	501	4	-	8/18/38/38	0/3/3/3
3	ATP	O	501	4	-	3/18/38/38	0/3/3/3
3	ATP	B	501	4	-	1/18/38/38	0/3/3/3
3	ATP	H	501	4	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	501	ATP	C5-C6-N6	2.41	124.01	120.35
3	O	501	ATP	C5-C6-N6	2.34	123.92	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	501	ATP	C5-C6-N6	2.32	123.88	120.35
3	F	501	ATP	C5-C6-N6	2.32	123.87	120.35
3	N	501	ATP	C5-C6-N6	2.32	123.87	120.35

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	ATP	C5'-O5'-PA-O1A
3	C	501	ATP	C5'-O5'-PA-O2A
3	D	501	ATP	PB-O3B-PG-O2G
3	E	501	ATP	PB-O3B-PG-O3G
3	E	501	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

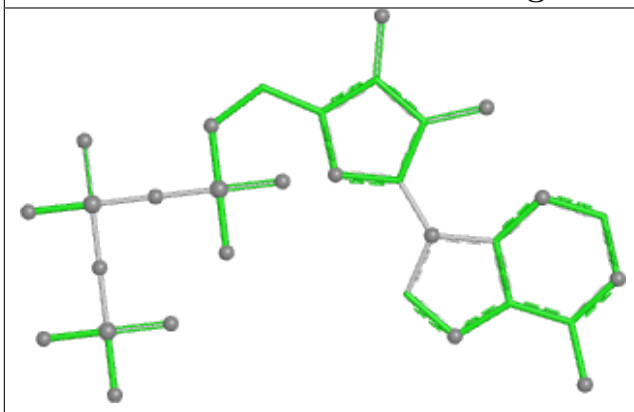
14 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	ATP	2	0
3	M	501	ATP	3	0
3	L	501	ATP	1	0
3	J	501	ATP	2	0
3	A	501	ATP	1	0
3	G	501	ATP	2	0
3	P	501	ATP	1	0
3	D	501	ATP	2	0
3	N	501	ATP	1	0
3	I	501	ATP	1	0
3	K	501	ATP	1	0
3	O	501	ATP	2	0
3	B	501	ATP	1	0
3	H	501	ATP	2	0

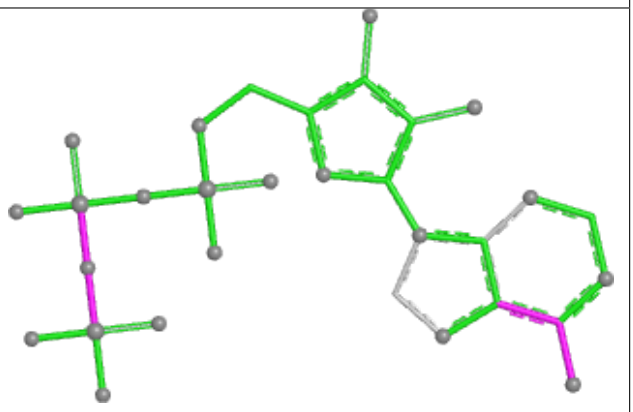
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

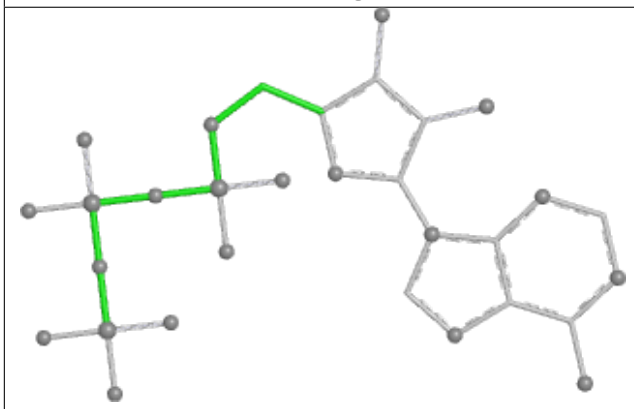
Ligand ATP F 501



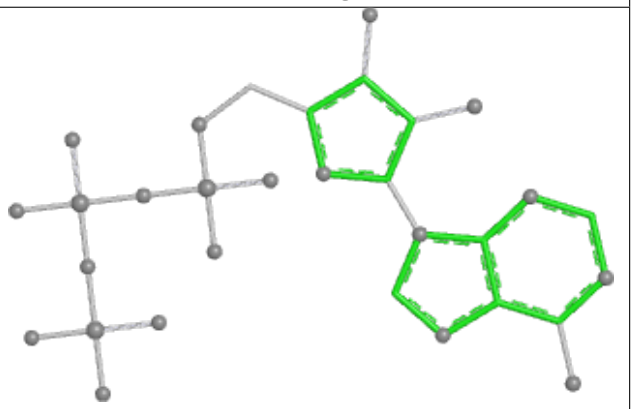
Bond lengths



Bond angles

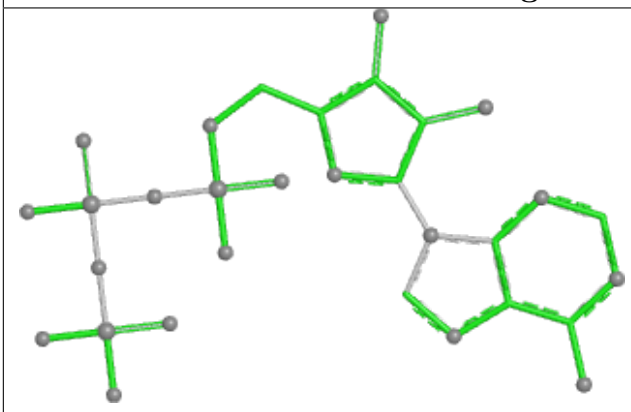


Torsions



Rings

Ligand ATP M 501



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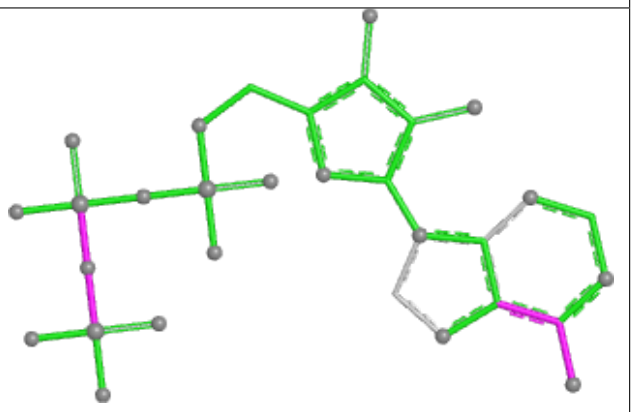
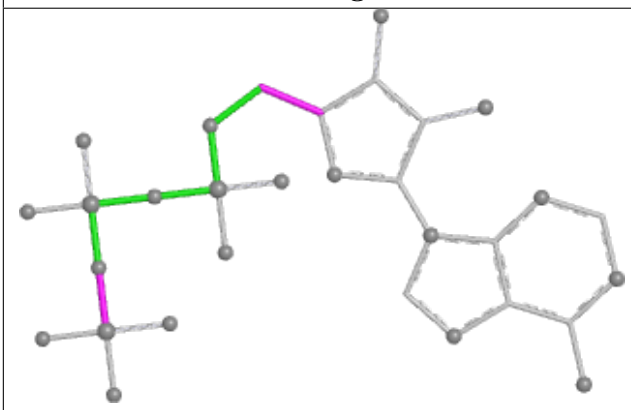


Bond angles



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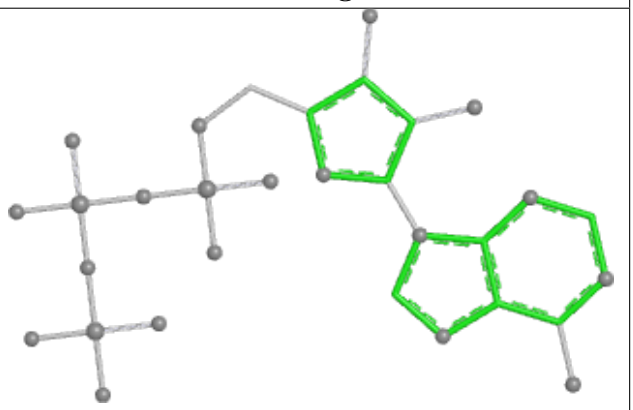
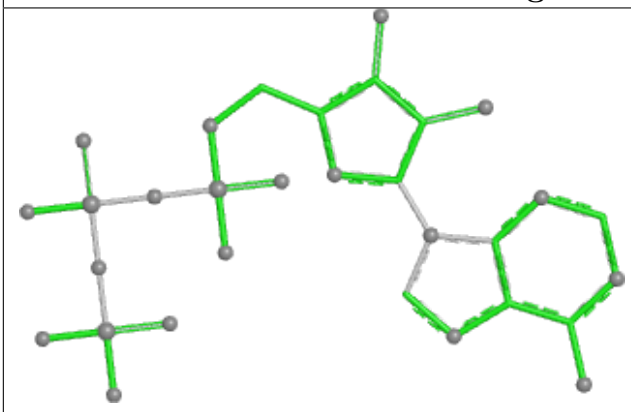
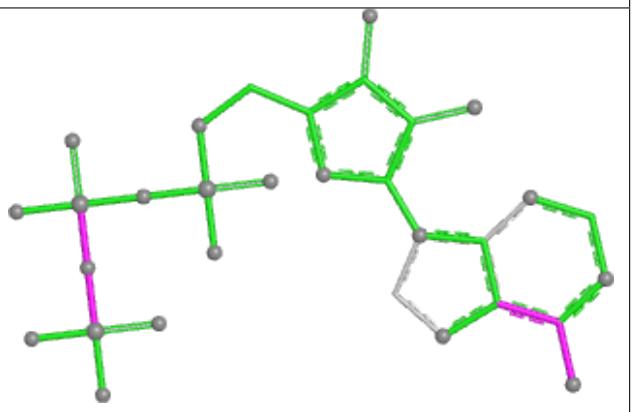


Rings

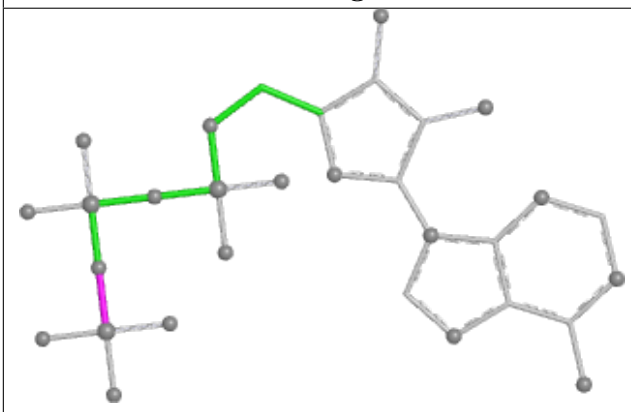
Ligand ATP L 501



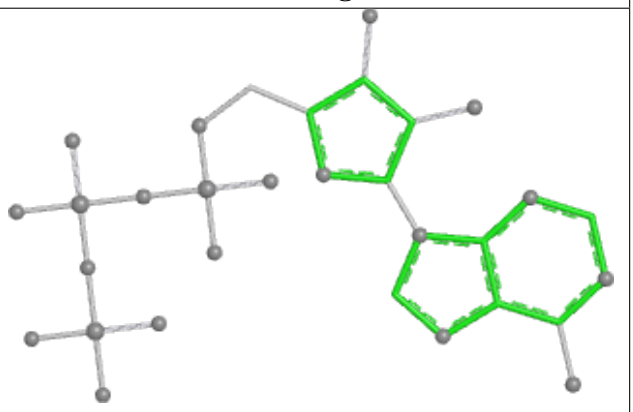
Bond lengths



Bond angles

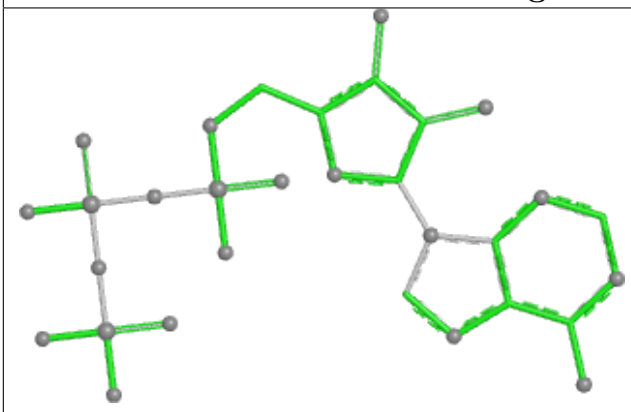


Torsions



Rings

Ligand ATP J 501



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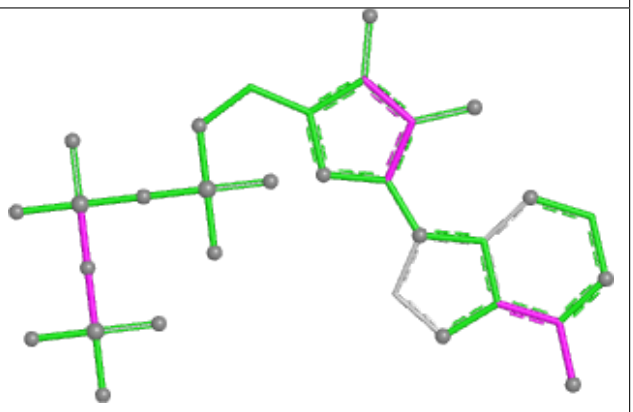
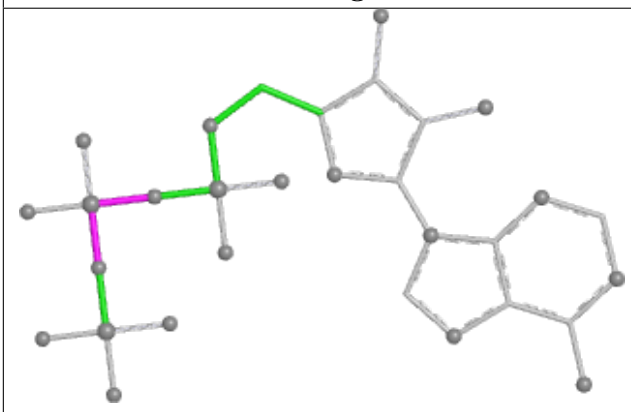
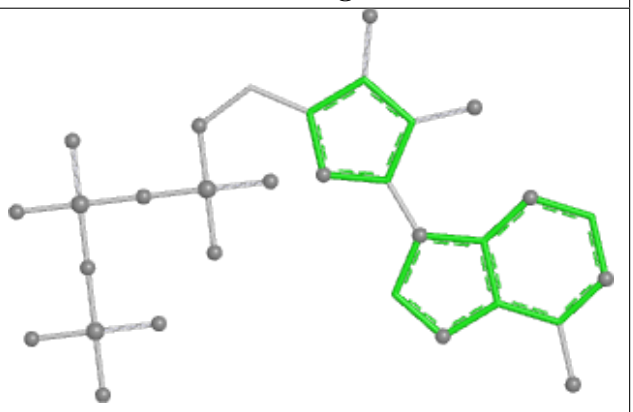


Bond angles

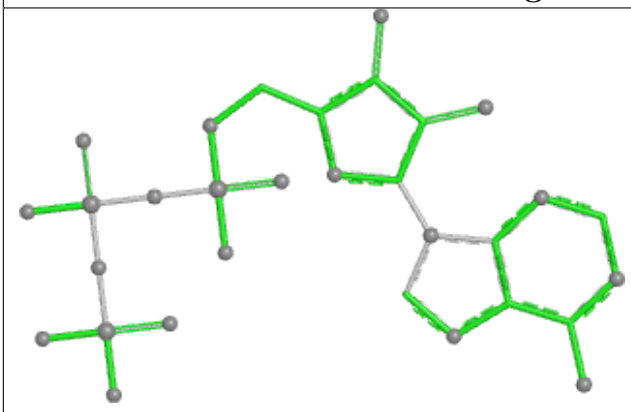


Torsions

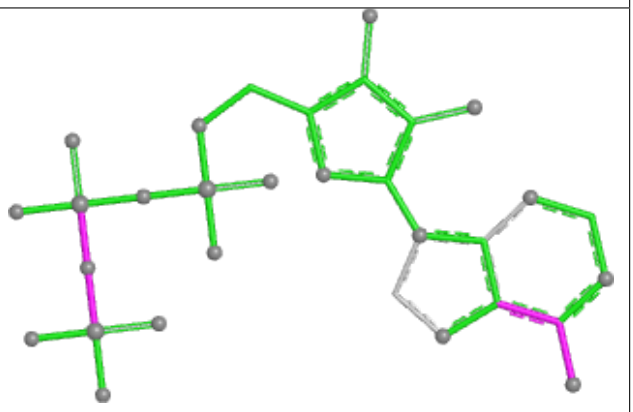


Rings

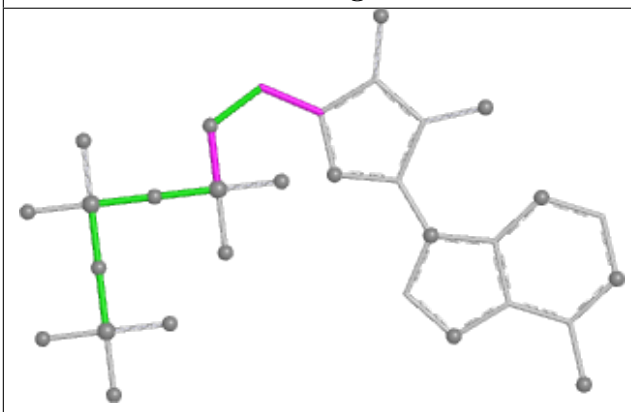
Ligand ATP C 501



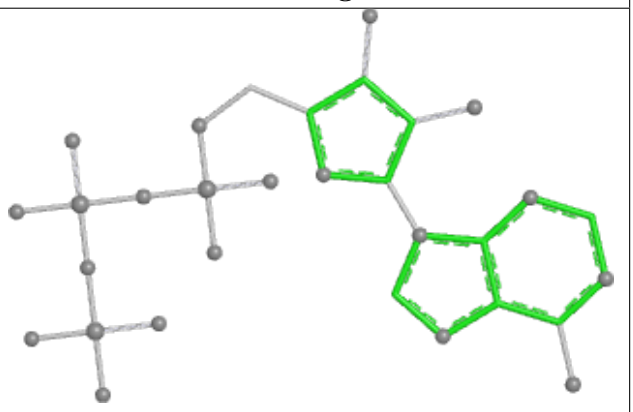
Bond lengths



Bond angles

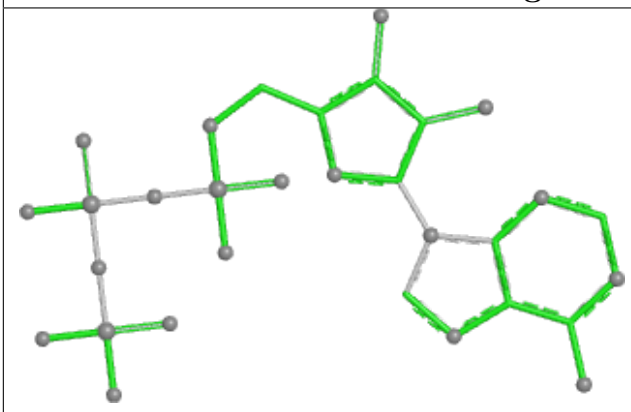


Torsions



Rings

Ligand ATP A 501



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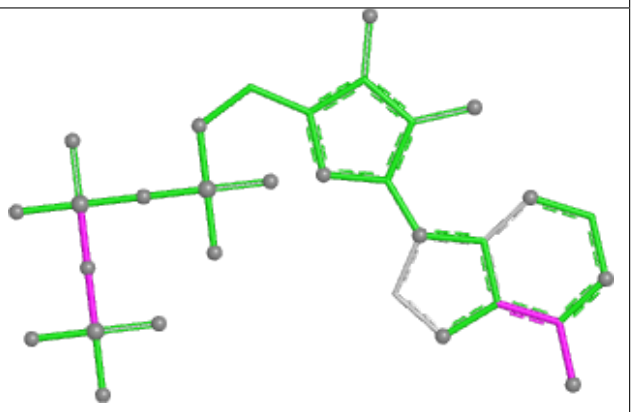
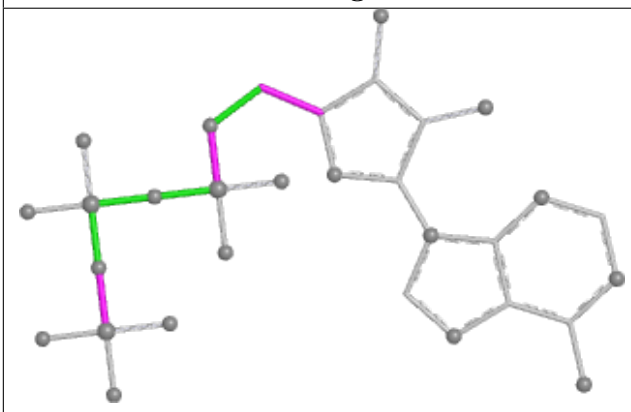
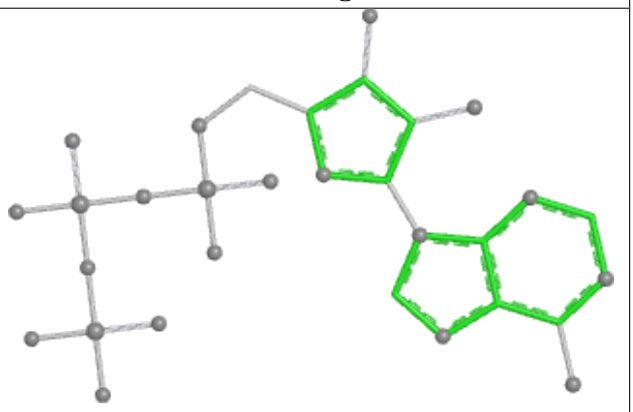


Bond angles

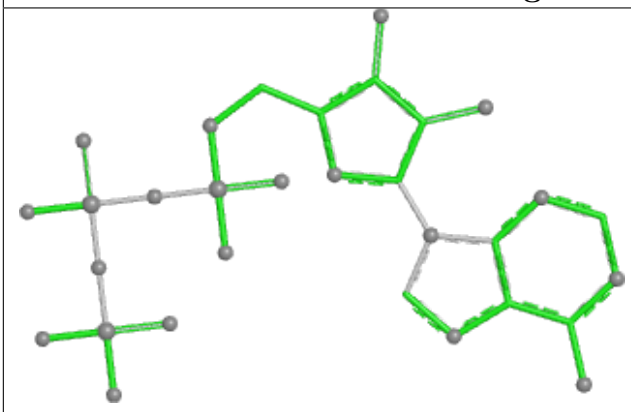


Torsions

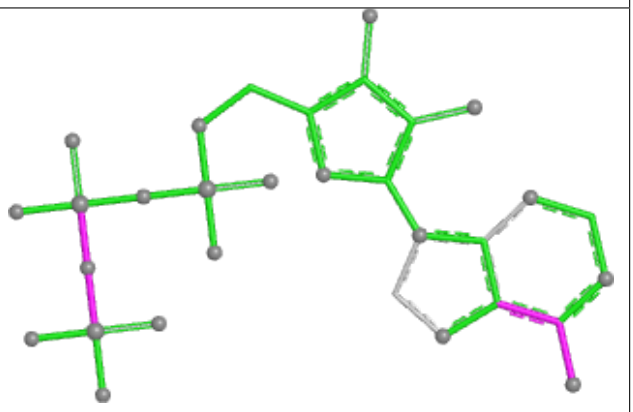


Rings

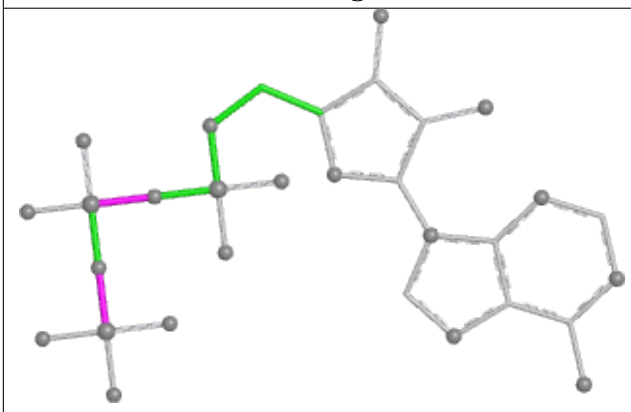
Ligand ATP G 501



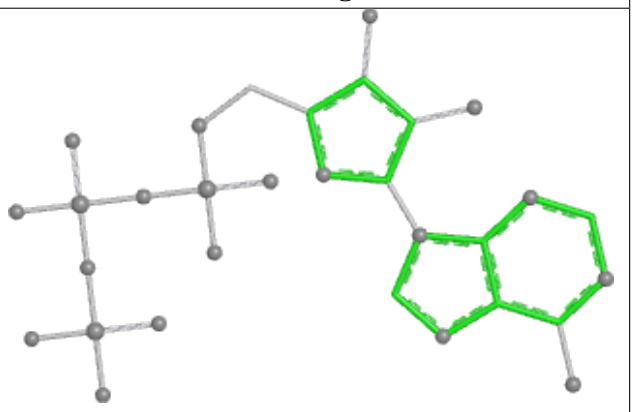
Bond lengths



Bond angles

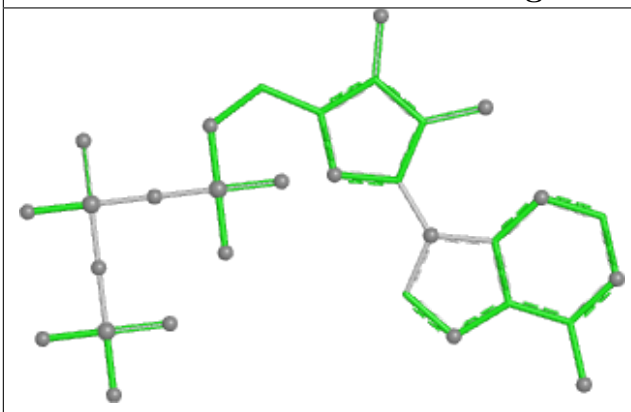


Torsions

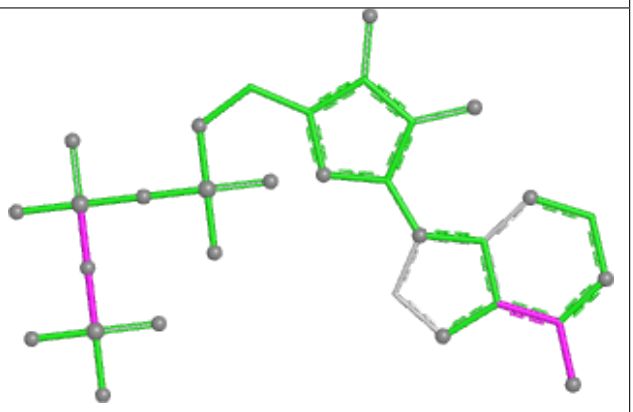


Rings

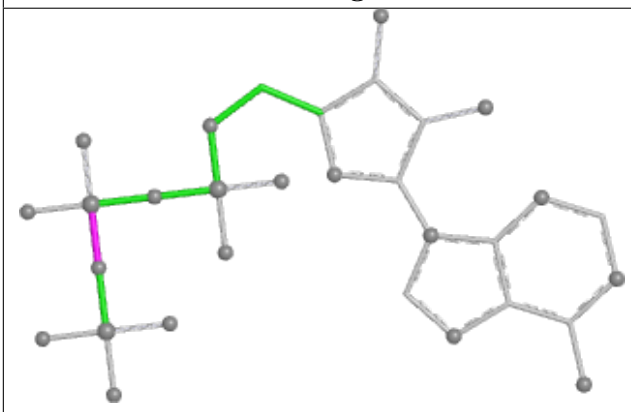
Ligand ATP P 501



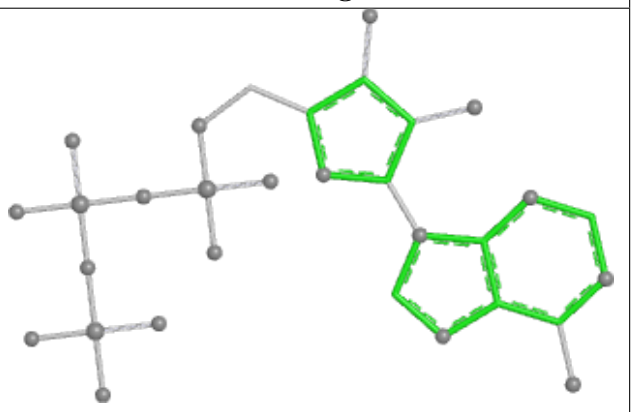
Bond lengths



Bond angles

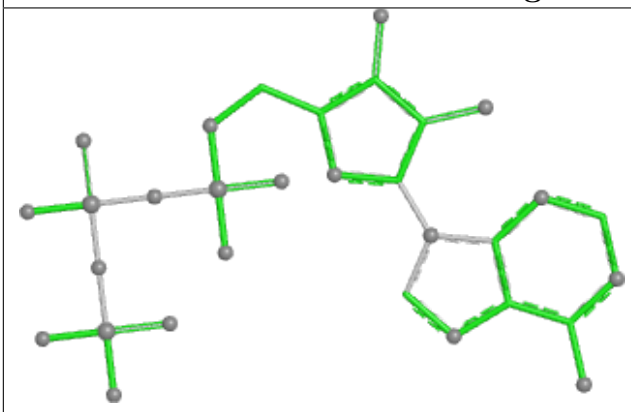


Torsions

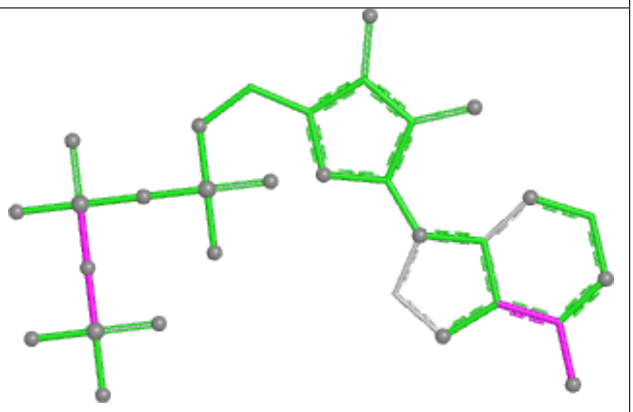


Rings

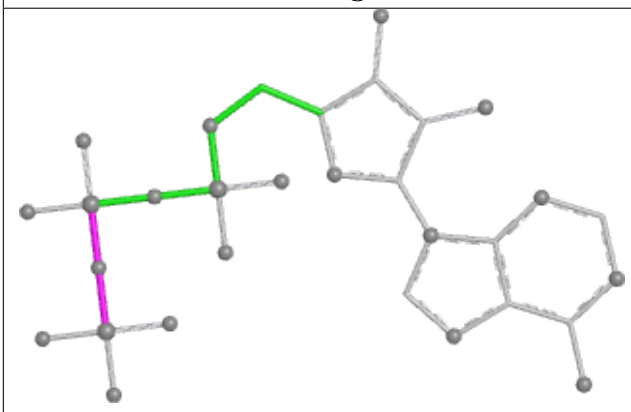
Ligand ATP D 501



Bond lengths



Bond angles



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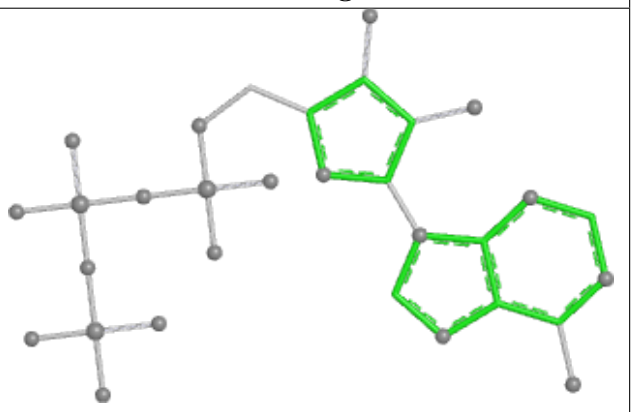
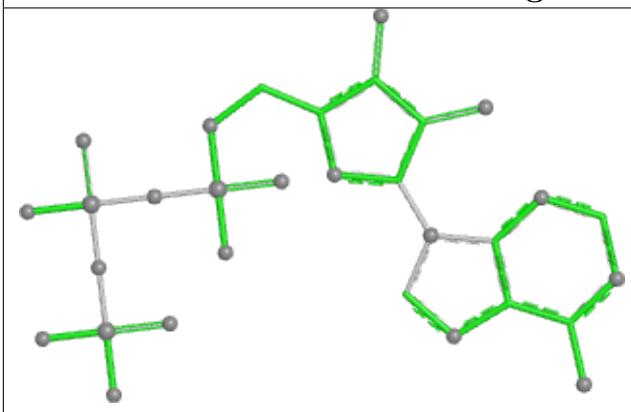
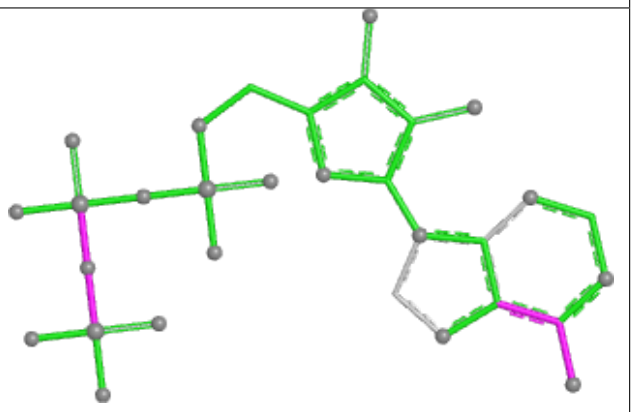


Rings

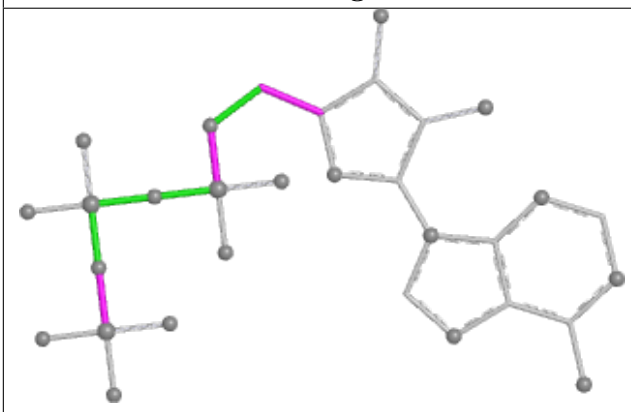
Ligand ATP E 501



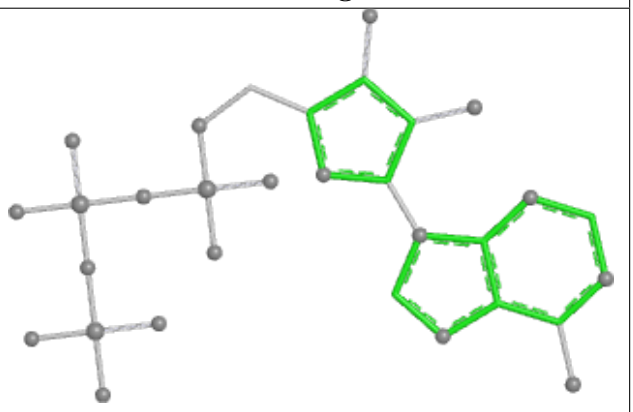
Bond lengths



Bond angles

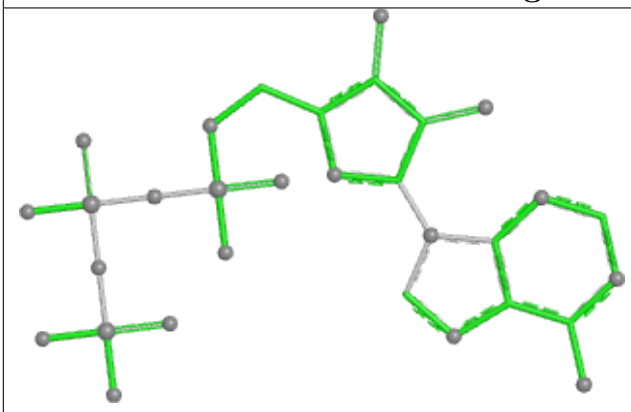


Torsions

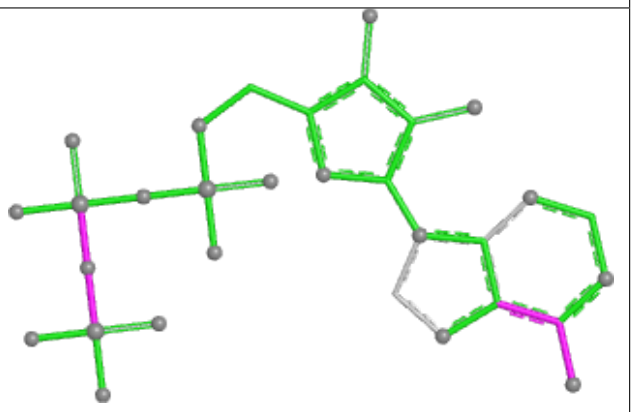


Rings

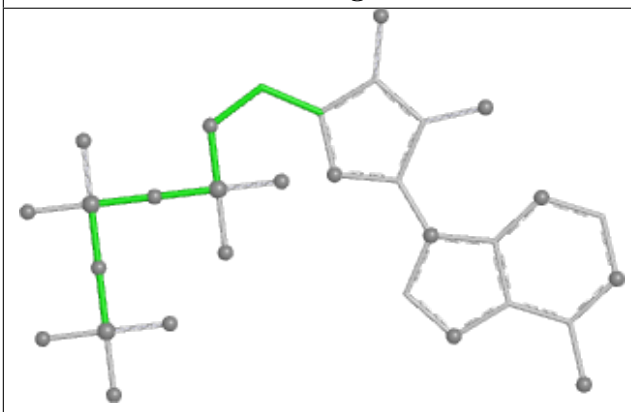
Ligand ATP N 501



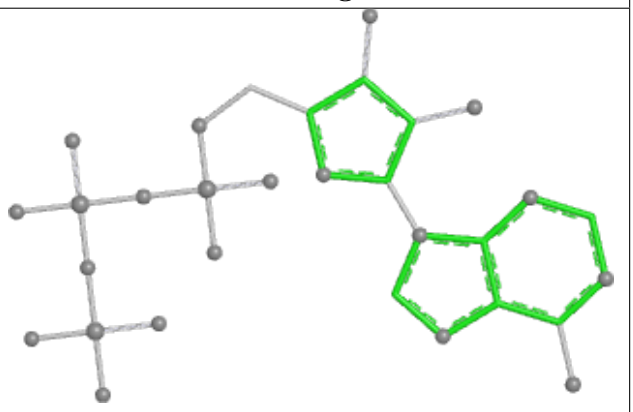
Bond lengths



Bond angles

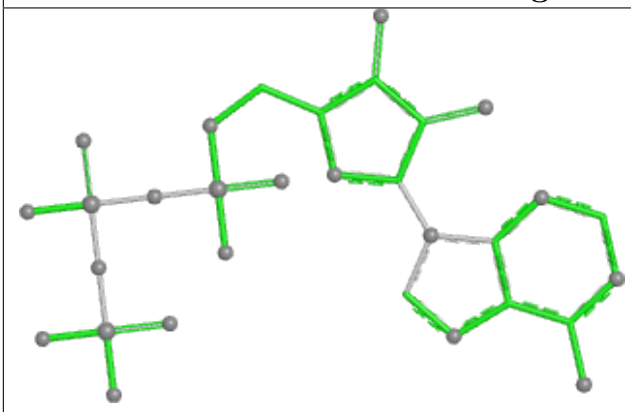


Torsions

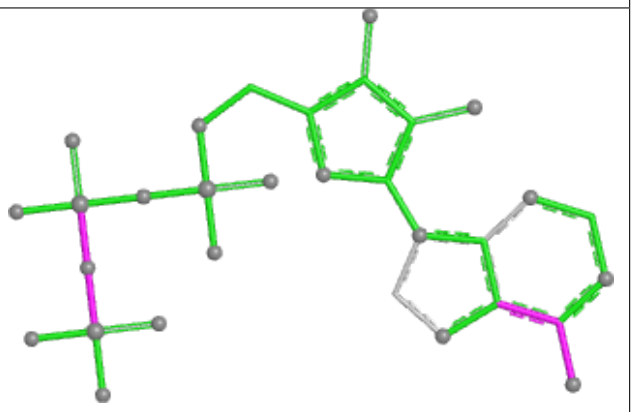


Rings

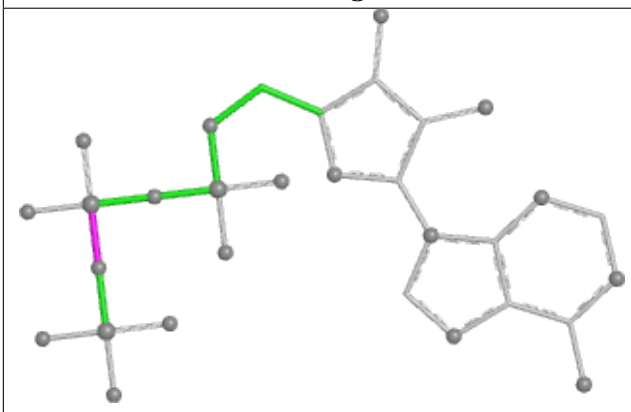
Ligand ATP I 501



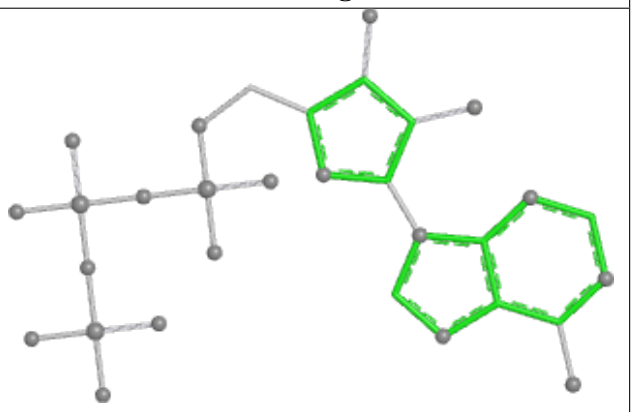
Bond lengths



Bond angles

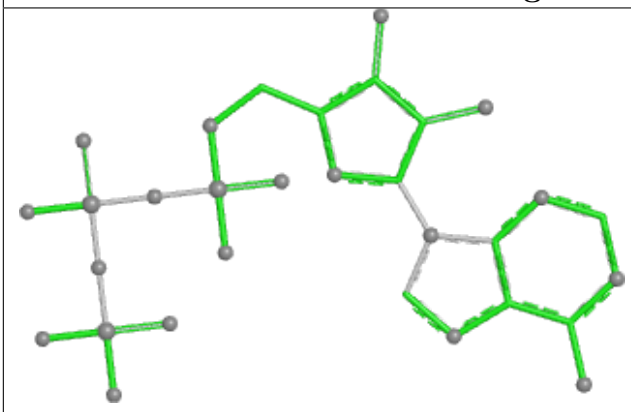


Torsions

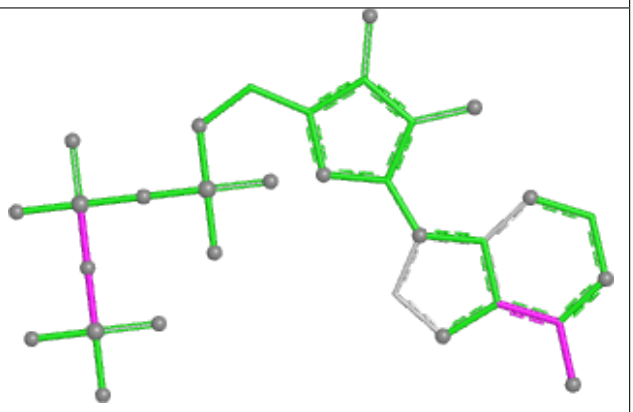


Rings

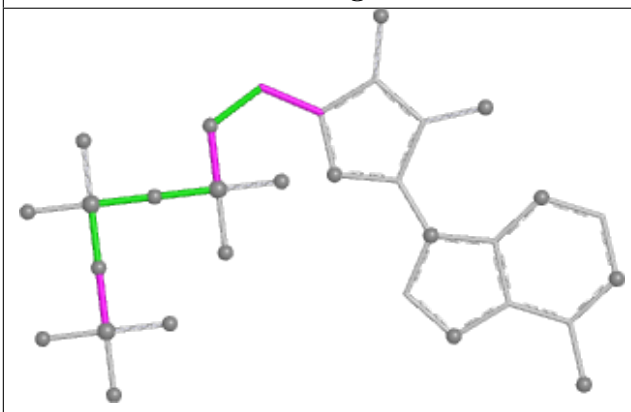
Ligand ATP K 501



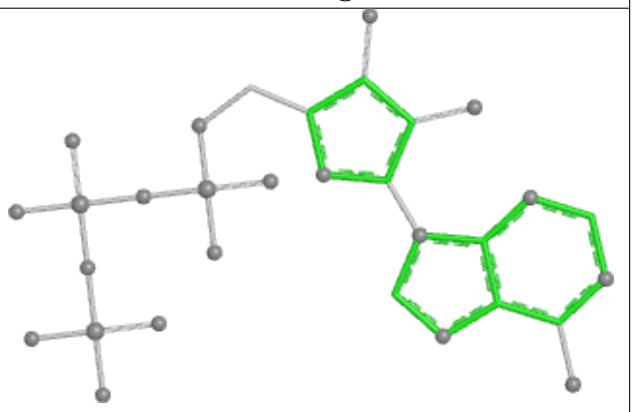
Bond lengths



Bond angles

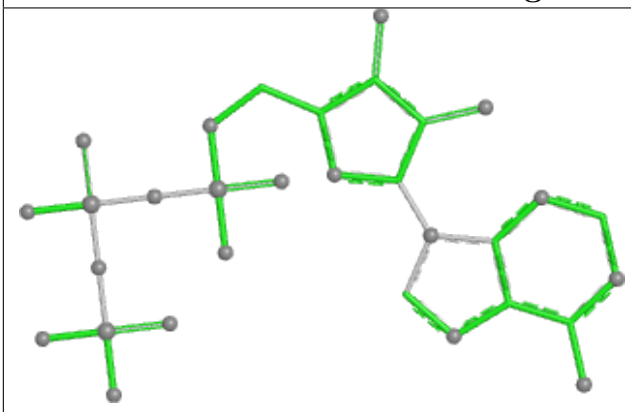


Torsions

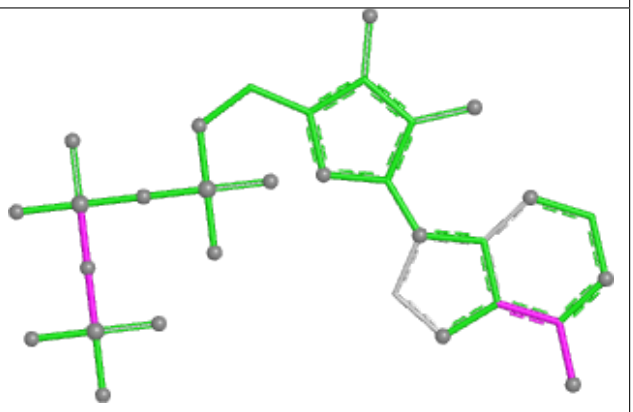


Rings

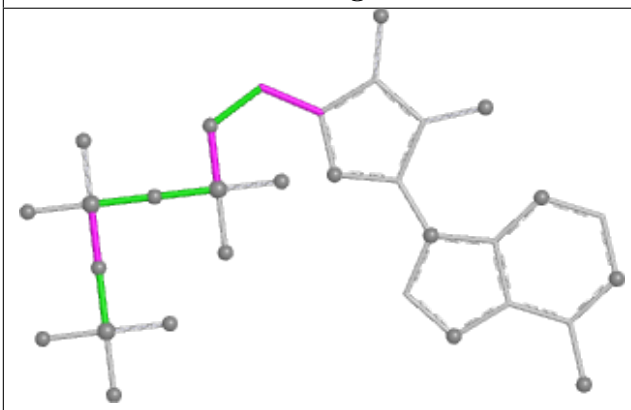
Ligand ATP O 501



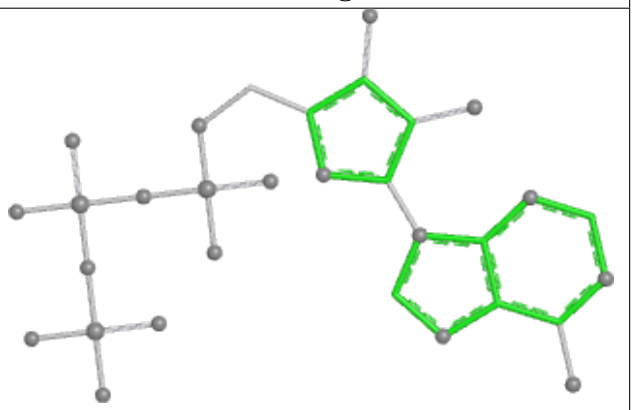
Bond lengths



Bond angles

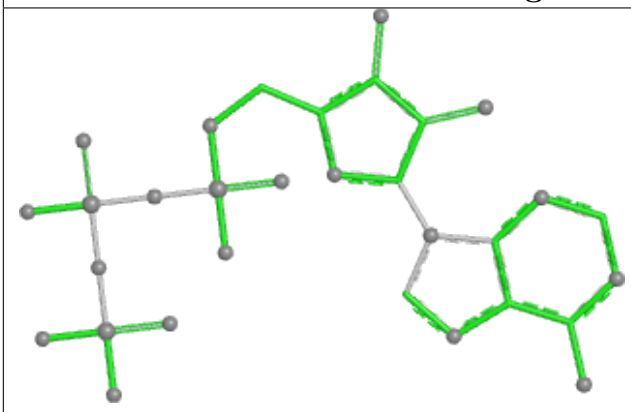


Torsions

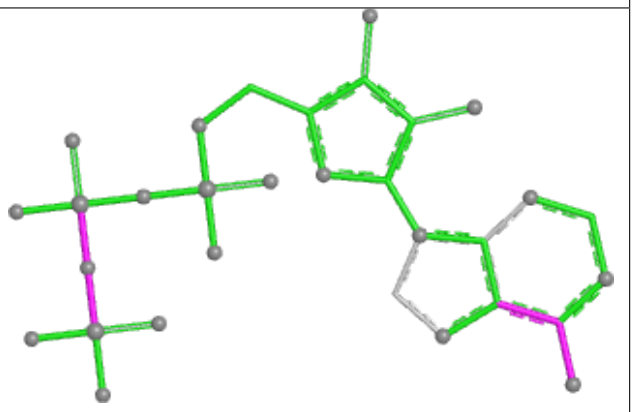


Rings

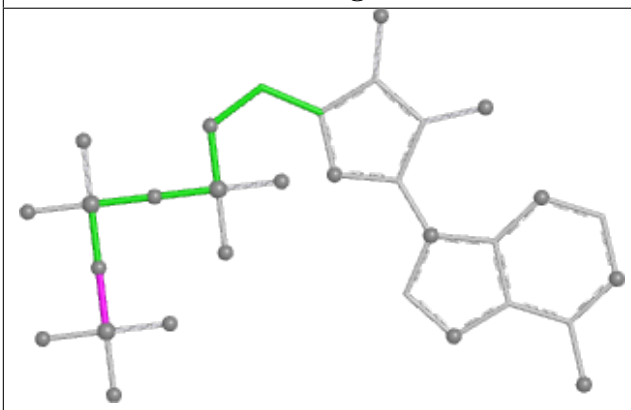
Ligand ATP B 501



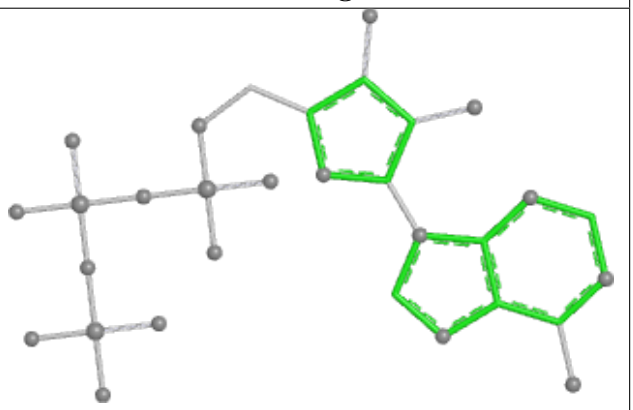
Bond lengths



Bond angles

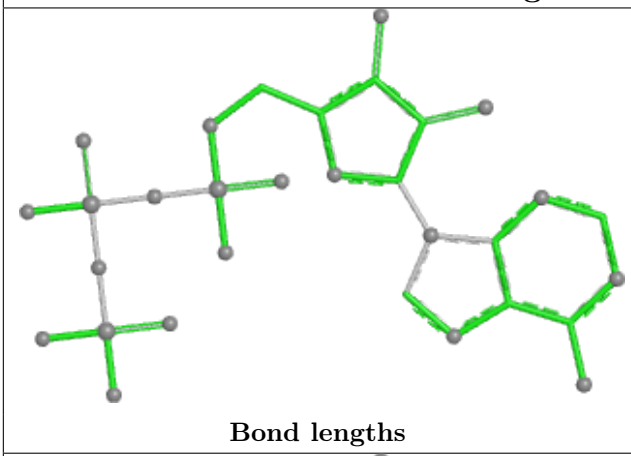


Torsions

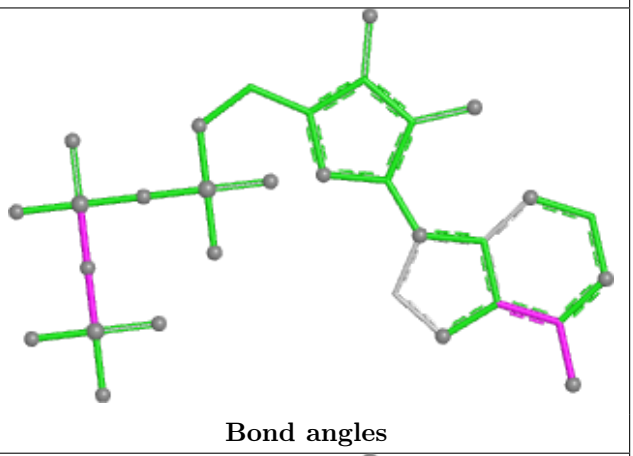


Rings

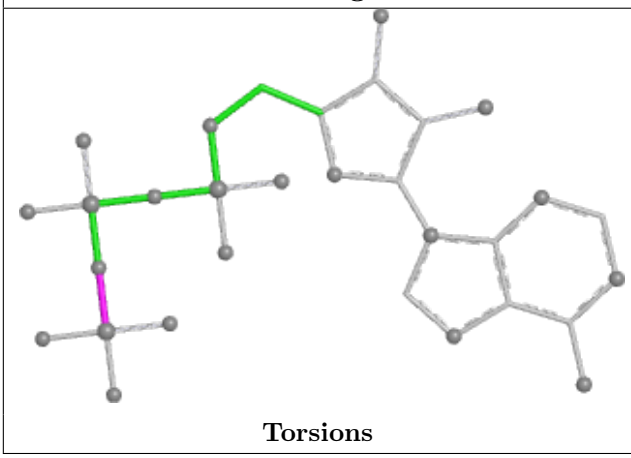
Ligand ATP H 501



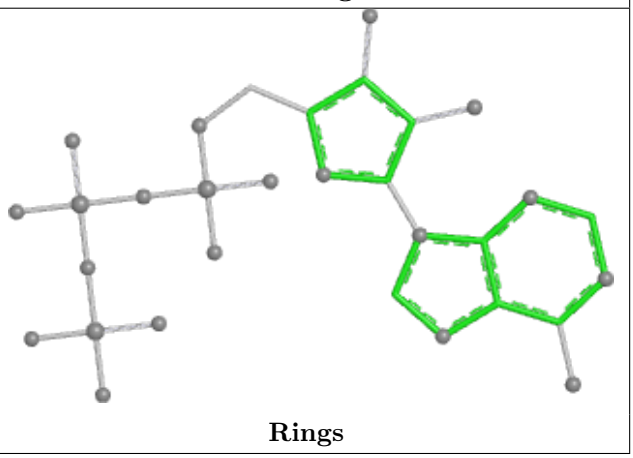
Bond lengths



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	382/396 (96%)	0.00	1 (0%) 94 88	56, 83, 116, 143	0
1	B	383/396 (96%)	0.09	2 (0%) 91 83	64, 90, 148, 712	0
1	C	382/396 (96%)	0.06	2 (0%) 91 83	56, 87, 122, 165	0
1	D	362/396 (91%)	0.01	0 100 100	51, 86, 125, 157	0
1	E	382/396 (96%)	0.17	1 (0%) 94 88	70, 102, 142, 176	0
1	F	382/396 (96%)	0.38	17 (4%) 33 21	71, 112, 157, 189	0
1	G	382/396 (96%)	0.31	16 (4%) 36 23	78, 117, 163, 213	0
1	H	382/396 (96%)	0.23	5 (1%) 77 63	72, 109, 147, 187	0
1	I	382/396 (96%)	0.18	6 (1%) 72 57	73, 113, 146, 169	0
1	J	382/396 (96%)	0.19	4 (1%) 82 70	74, 110, 147, 175	0
1	K	382/396 (96%)	0.23	7 (1%) 68 53	74, 116, 162, 194	0
1	L	382/396 (96%)	0.18	3 (0%) 86 75	71, 105, 150, 189	0
1	M	382/396 (96%)	0.34	15 (3%) 39 25	105, 150, 180, 194	0
1	N	382/396 (96%)	0.47	18 (4%) 31 19	97, 133, 164, 184	0
1	O	382/396 (96%)	0.57	30 (7%) 12 7	103, 142, 170, 198	0
1	P	382/396 (96%)	0.34	19 (4%) 28 18	99, 134, 173, 190	0
2	X	0/37	-	-	-	-
2	Y	0/37	-	-	-	-
All	All	6093/6410 (95%)	0.24	146 (2%) 59 42	51, 113, 162, 712	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	22	ALA	7.5
1	P	38	ALA	6.7
1	O	38	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	285	SER	5.1
1	P	148	GLY	4.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	P	502	1/1	0.77	0.32	86,86,86,86	0
4	MG	O	502	1/1	0.79	0.21	94,94,94,94	0
3	ATP	M	501	31/31	0.85	0.27	125,154,159,164	0
3	ATP	K	501	31/31	0.87	0.25	80,106,113,123	0
3	ATP	O	501	31/31	0.87	0.22	115,141,149,149	0
4	MG	I	502	1/1	0.88	0.33	57,57,57,57	0
4	MG	C	502	1/1	0.89	0.33	56,56,56,56	0
4	MG	J	502	1/1	0.89	0.30	55,55,55,55	0
3	ATP	F	501	31/31	0.90	0.25	69,91,109,111	0
4	MG	E	502	1/1	0.90	0.24	52,52,52,52	0
3	ATP	P	501	31/31	0.90	0.21	97,109,132,149	0
4	MG	F	502	1/1	0.91	0.32	56,56,56,56	0
3	ATP	H	501	31/31	0.91	0.24	76,90,99,106	0
3	ATP	I	501	31/31	0.91	0.23	81,102,118,129	0
3	ATP	E	501	31/31	0.91	0.24	62,92,105,121	0
3	ATP	C	501	31/31	0.91	0.27	57,66,86,92	0
3	ATP	L	501	31/31	0.92	0.21	60,87,109,115	0
3	ATP	J	501	31/31	0.92	0.26	71,85,102,116	0
3	ATP	N	501	31/31	0.92	0.20	87,107,118,122	0
3	ATP	B	501	31/31	0.92	0.29	63,74,91,95	0
3	ATP	A	501	31/31	0.93	0.24	56,68,86,87	0

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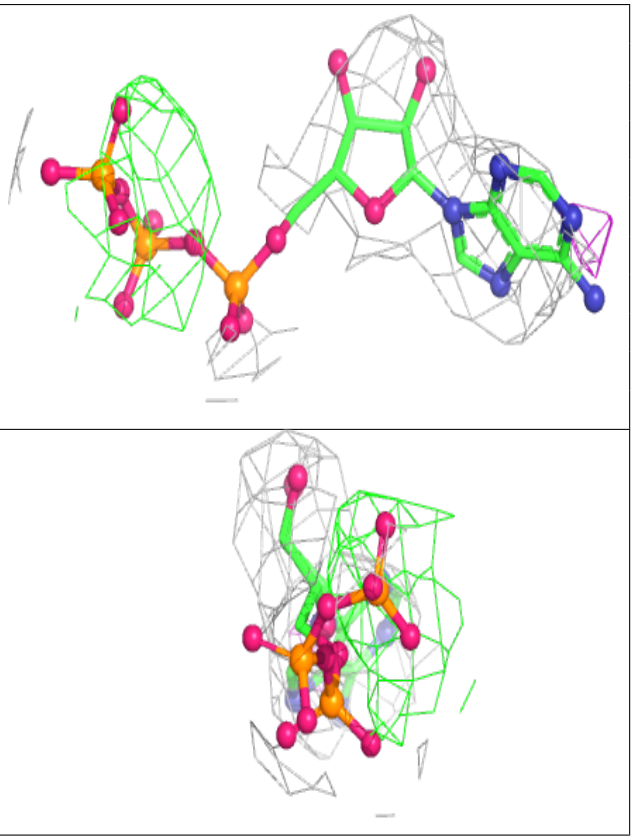
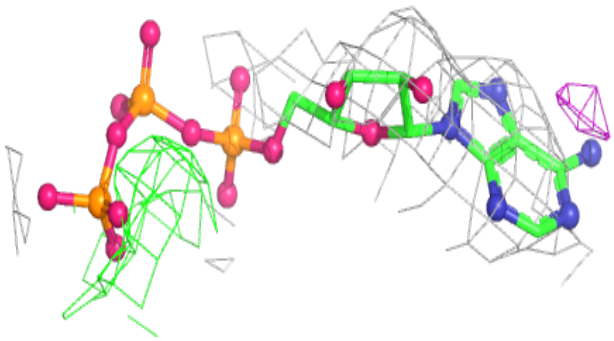
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	K	502	1/1	0.93	0.38	83,83,83,83	0
4	MG	L	502	1/1	0.93	0.33	43,43,43,43	0
3	ATP	G	501	31/31	0.93	0.18	80,106,118,122	0
4	MG	D	502	1/1	0.93	0.43	58,58,58,58	0
4	MG	N	502	1/1	0.94	0.25	81,81,81,81	0
3	ATP	D	501	31/31	0.94	0.27	53,71,88,92	0
4	MG	M	502	1/1	0.94	0.29	92,92,92,92	0
4	MG	A	502	1/1	0.96	0.32	41,41,41,41	0
4	MG	H	502	1/1	0.97	0.29	67,67,67,67	0
4	MG	B	502	1/1	0.97	0.42	39,39,39,39	0
4	MG	G	502	1/1	0.97	0.24	80,80,80,80	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 M 501:

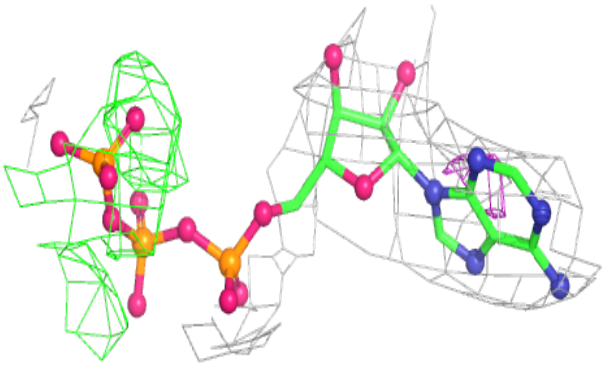
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

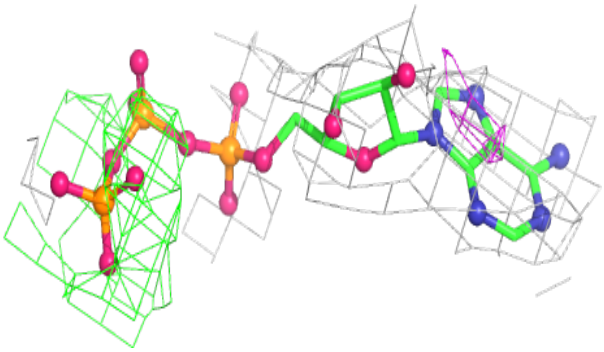


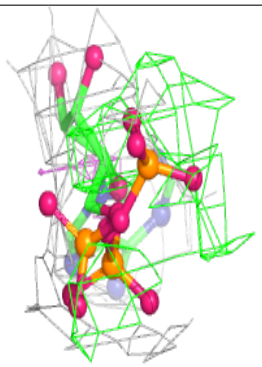


Electron density around ATP K 501:

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

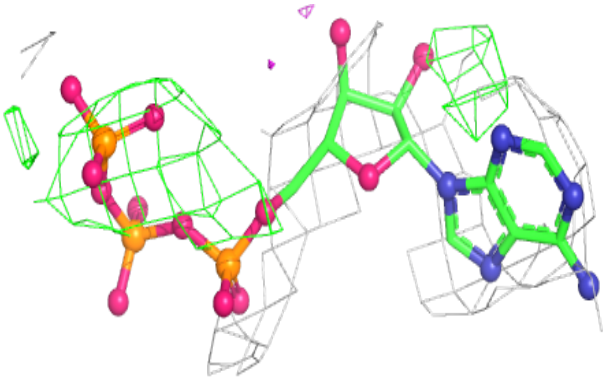


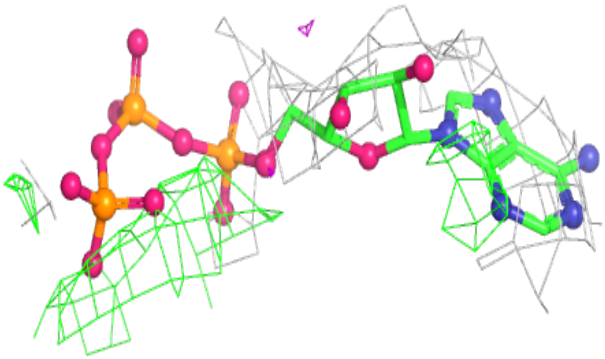


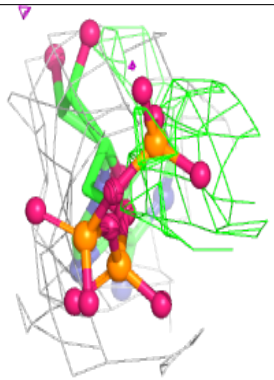


Electron density around ATP O 501:

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

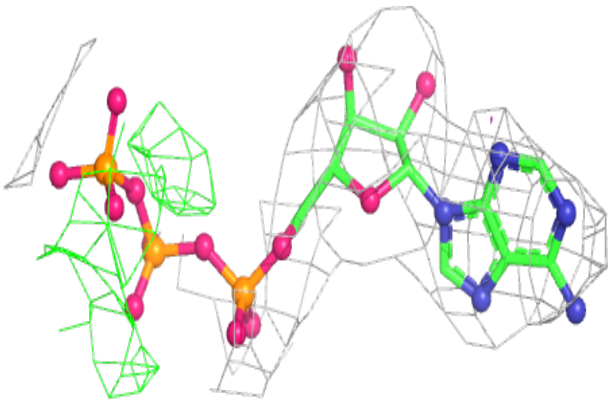


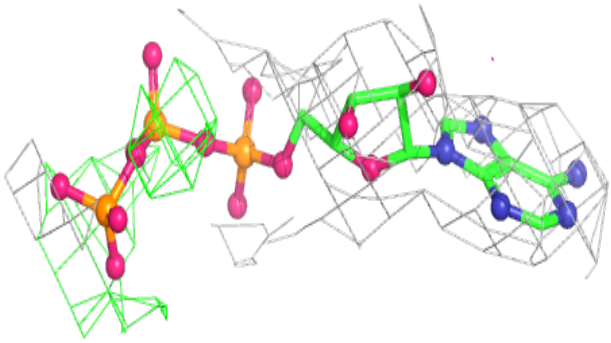


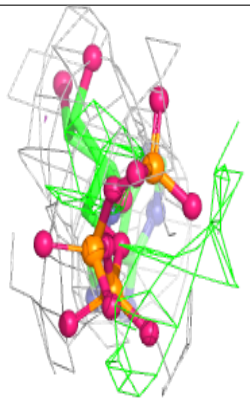


Electron density around ATP F 501:

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

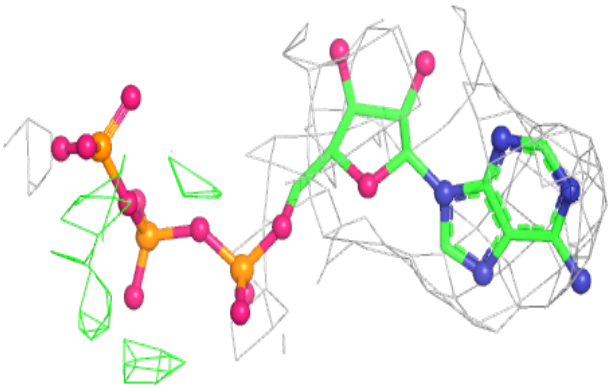


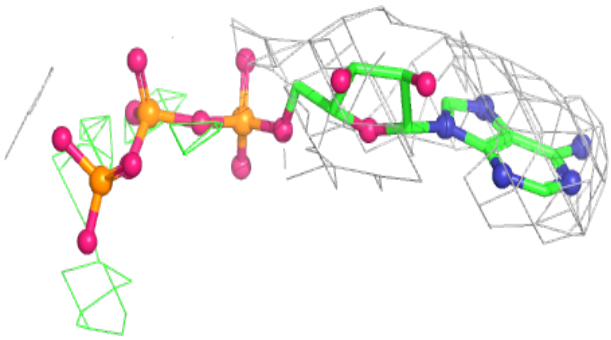


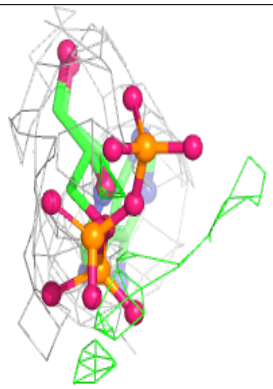


Electron density around ATP P 501:

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

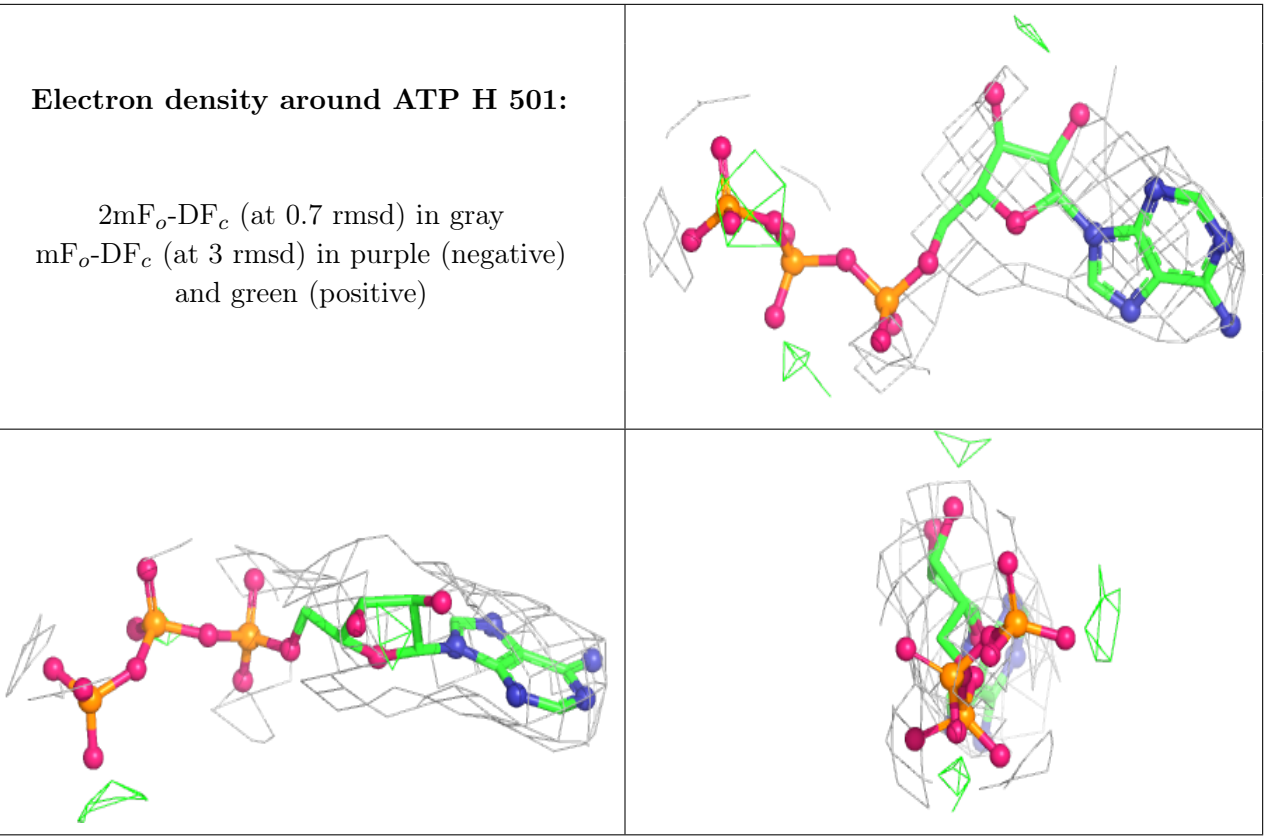






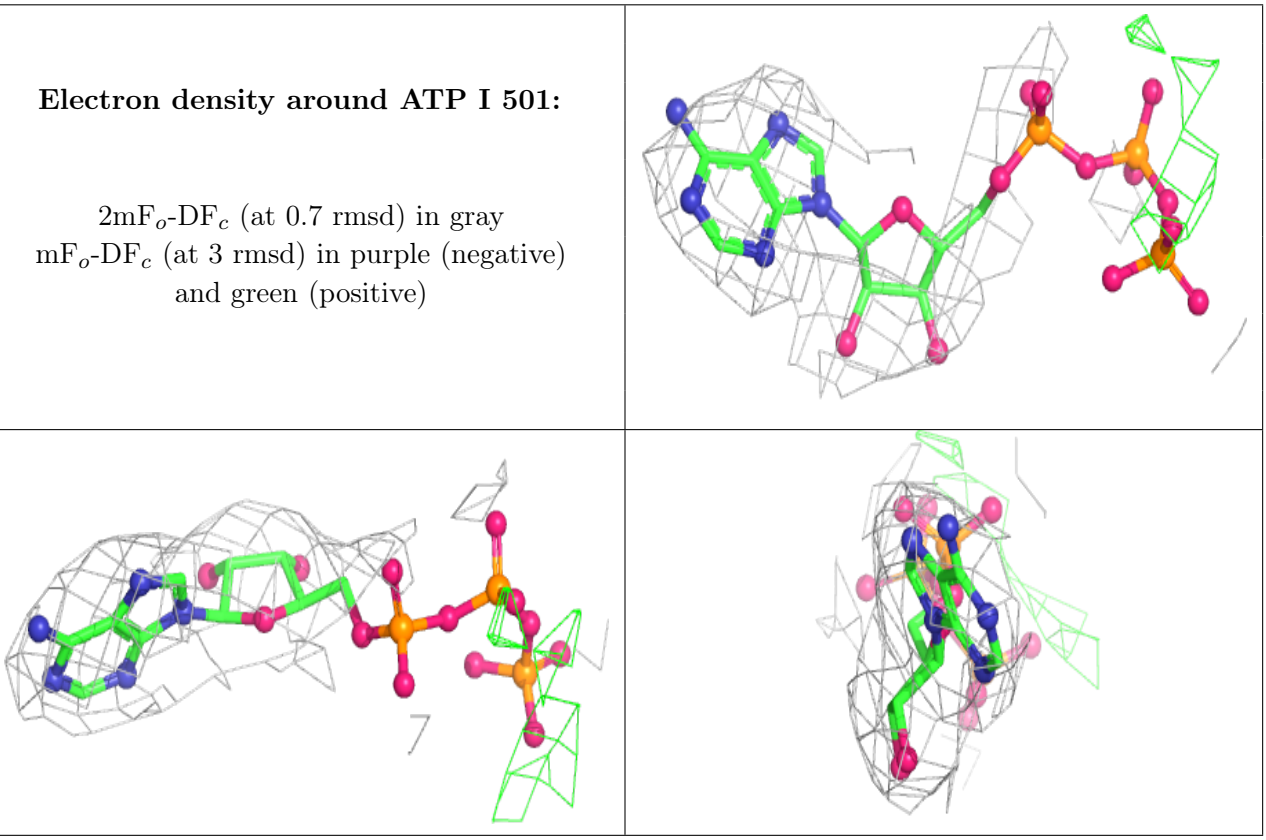
Electron density around ATP H 501:

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



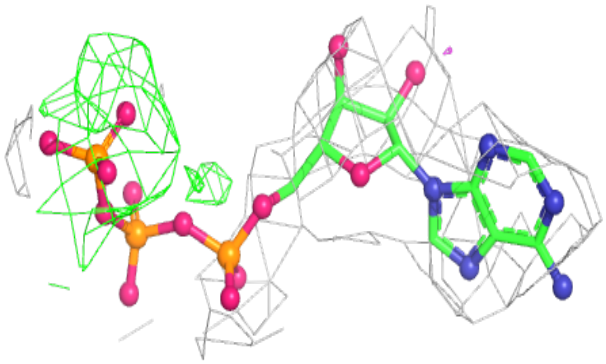
Electron density around ATP I 501:

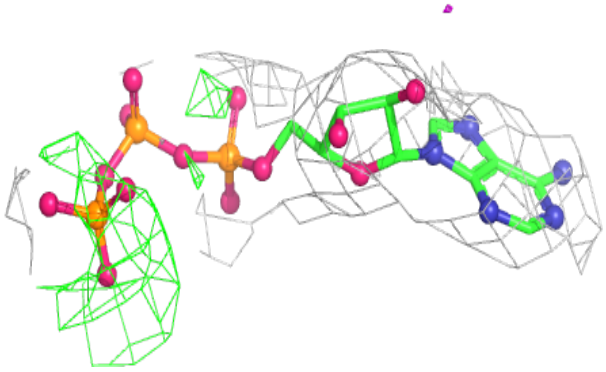
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

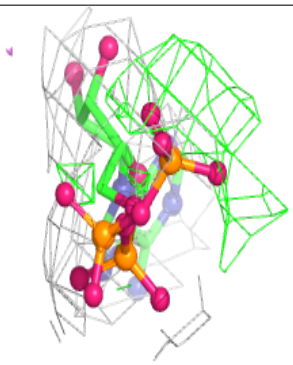


Electron density around ATP E 501:

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

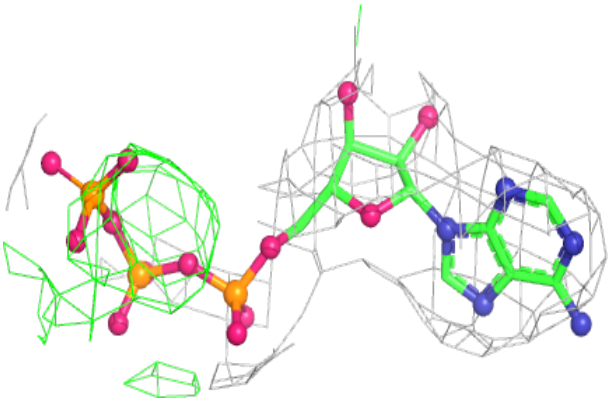


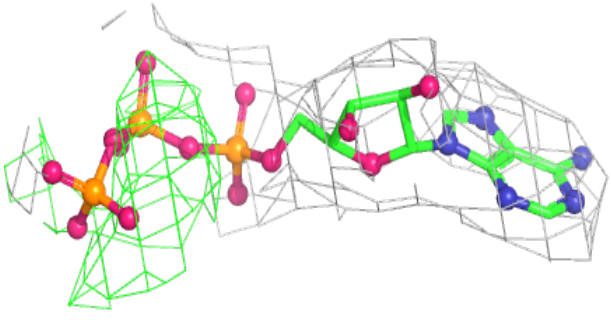


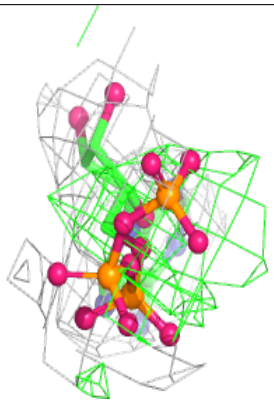


Electron density around ATP C 501:

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

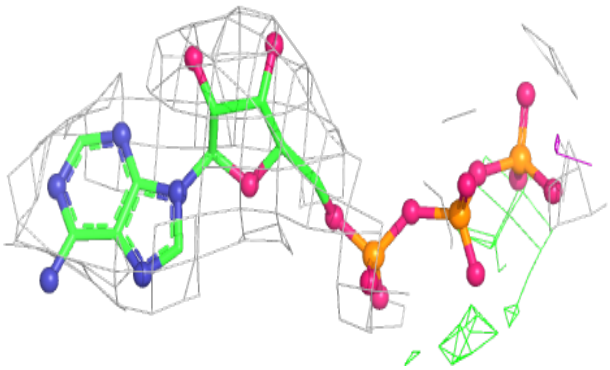


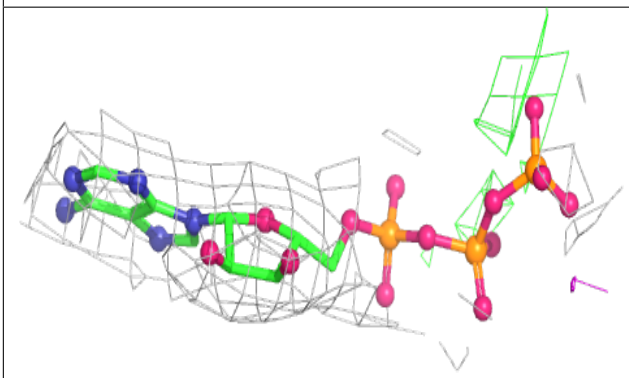


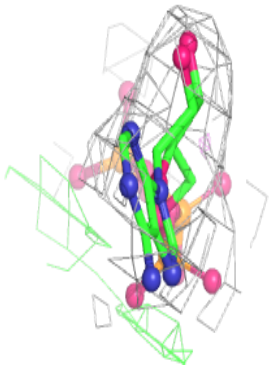


Electron density around ATP L 501:

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

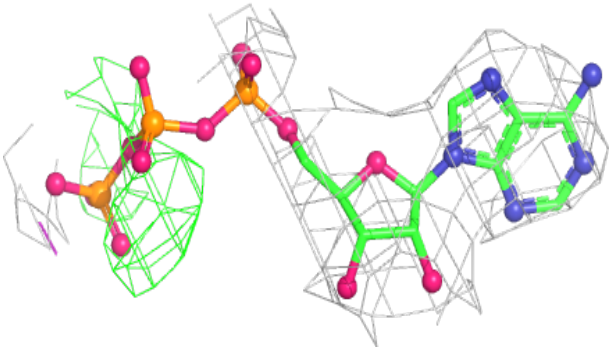


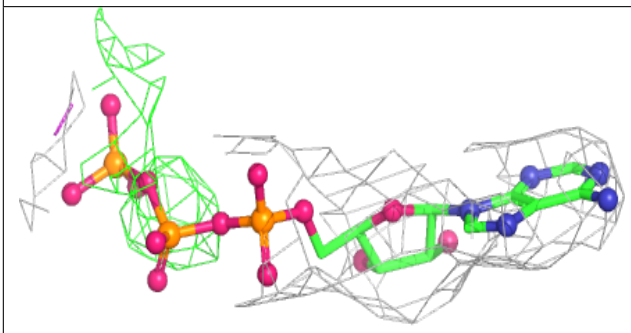


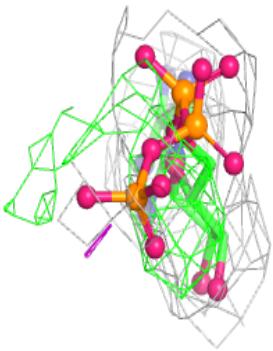


Electron density around ATP J 501:

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

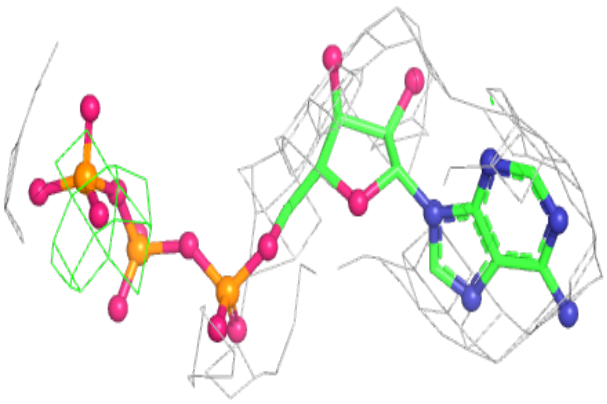


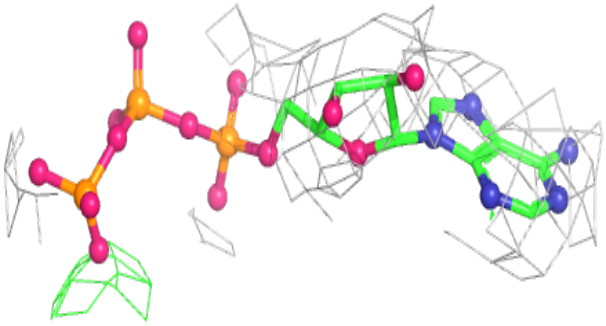


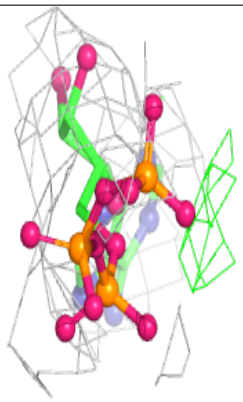


Electron density around ATP N 501:

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

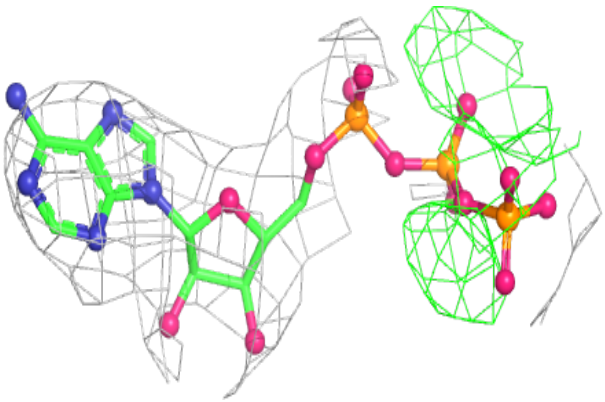


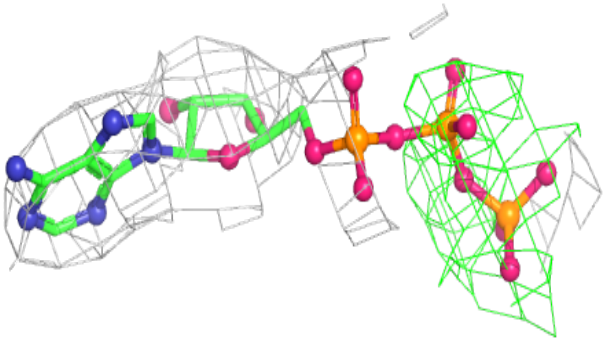


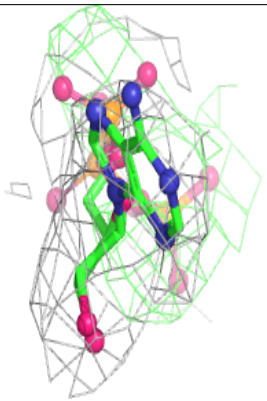


Electron density around ATP B 501:

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

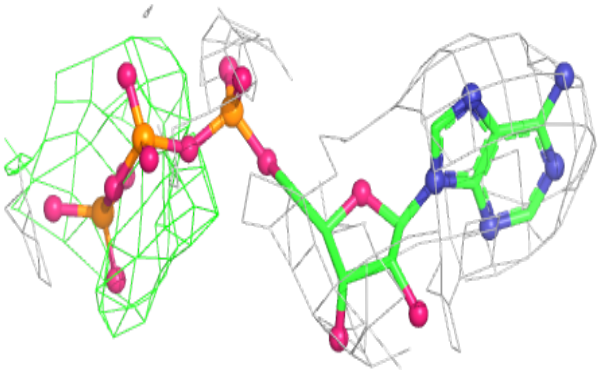


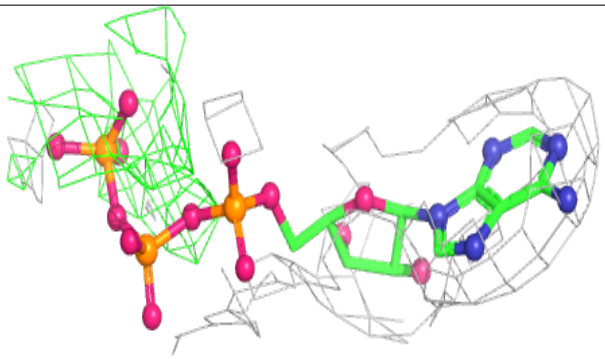


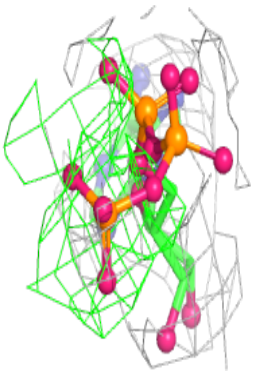


Electron density around ATP A 501:

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

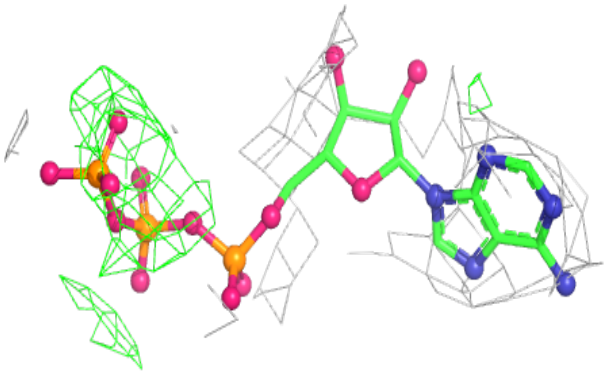


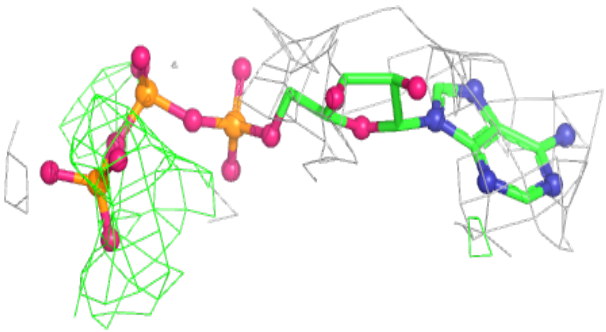


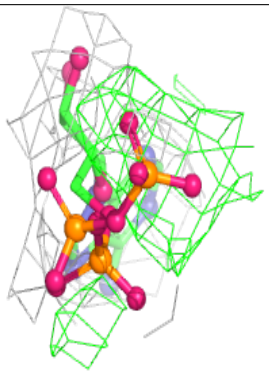


Electron density around ATP G 501:

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

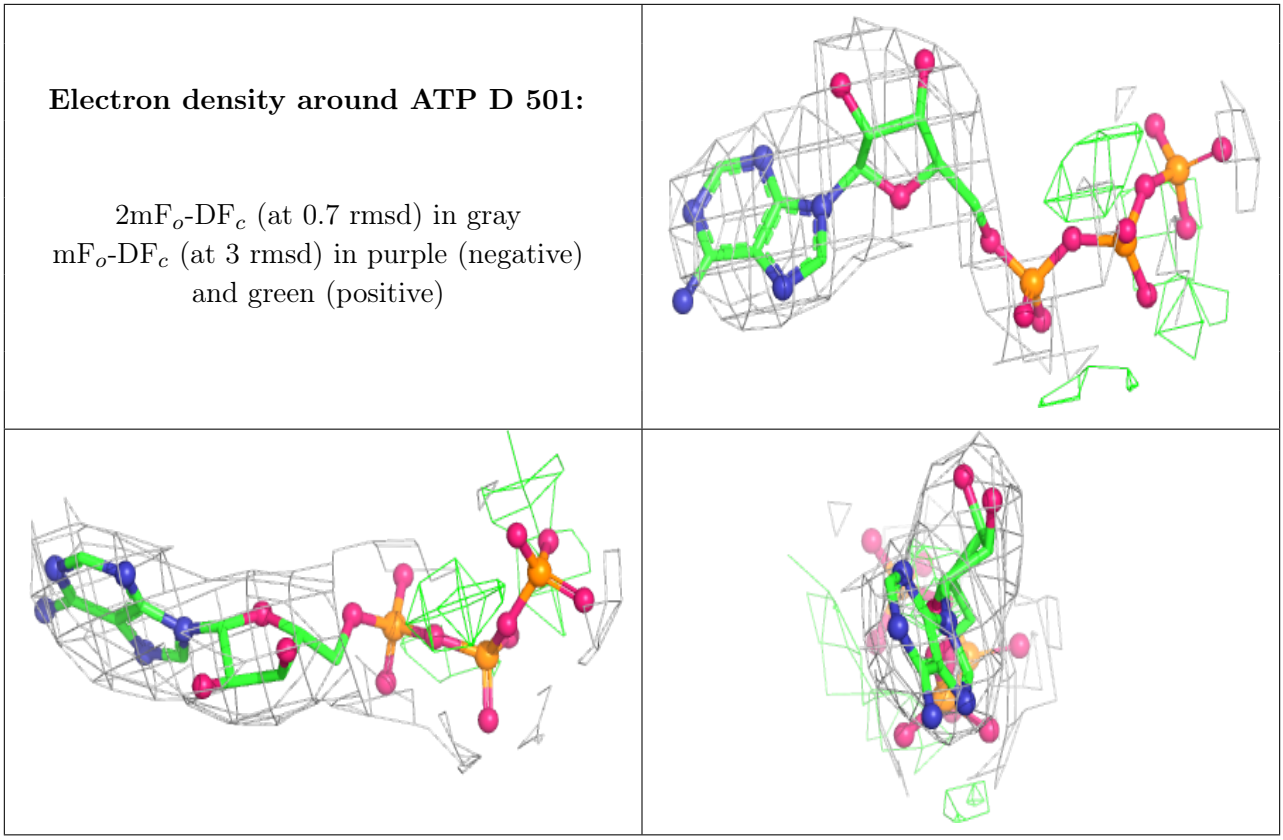






Electron density around ATP D 501:

$2mF_o$-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

There are no such residues in this entry.