



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 08:42 am BST

PDB ID : 4N1A
Title : Thermomonospora curvata EccC (ATPases 2 and 3) in complex with a signal sequence peptide
Authors : Dovala, D.L.; Bendebury, A.; Cox, J.S.; Stroud, R.M.; Rosenberg, O.S.
Deposited on : 2013-10-03
Resolution : 3.24 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 : 2.11
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) : 2.11

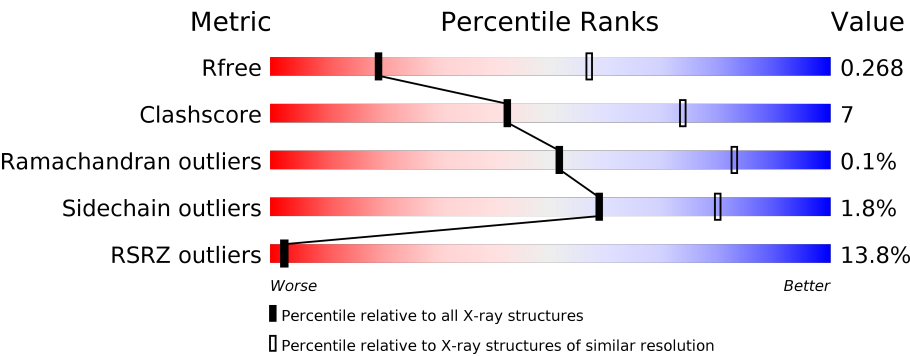
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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 on 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	589	<div><div></div><div>80%14%6%</div></div>
1	B	589	<div><div></div><div>78%15%6%</div></div>
1	C	589	<div><div>%</div><div>79%14%6%</div></div>
1	E	589	<div><div>51%</div><div>78%16%6%</div></div>
2	G	23	<div><div></div><div>17%13%70%</div></div>
2	H	23	<div><div></div><div>17%. . 74%</div></div>

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Mol	Chain	Length	Quality of chain
2	J	23	
2	K	23	

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
4	MG	E	1402	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17460 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 divisionFtsK/SpoIIIE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4298	2712	762	814	10			
1	B	553	Total	C	N	O	S	0	0	0
			4229	2671	738	810	10			
1	C	554	Total	C	N	O	S	0	0	0
			4247	2682	744	811	10			
1	E	555	Total	C	N	O	S	0	0	0
			4292	2709	759	814	10			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	MET	-	EXPRESSION TAG	UNP D1A4G7
A	728	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	729	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	730	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	731	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	732	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	733	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	734	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	735	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	736	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	737	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	738	SER	-	EXPRESSION TAG	UNP D1A4G7
A	739	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	740	PHE	-	EXPRESSION TAG	UNP D1A4G7
A	741	SER	-	EXPRESSION TAG	UNP D1A4G7
A	742	ILE	-	EXPRESSION TAG	UNP D1A4G7
A	743	ASP	-	EXPRESSION TAG	UNP D1A4G7
A	744	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	745	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	746	SER	-	EXPRESSION TAG	UNP D1A4G7
A	747	LEU	-	EXPRESSION TAG	UNP D1A4G7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	748	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	749	VAL	-	EXPRESSION TAG	UNP D1A4G7
A	750	LEU	-	EXPRESSION TAG	UNP D1A4G7
A	751	PHE	-	EXPRESSION TAG	UNP D1A4G7
A	752	GLN	-	EXPRESSION TAG	UNP D1A4G7
A	753	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	754	PRO	-	EXPRESSION TAG	UNP D1A4G7
A	755	SER	-	EXPRESSION TAG	UNP D1A4G7
A	756	SER	-	EXPRESSION TAG	UNP D1A4G7
A	757	PRO	-	EXPRESSION TAG	UNP D1A4G7
A	758	SER	-	EXPRESSION TAG	UNP D1A4G7
B	727	MET	-	EXPRESSION TAG	UNP D1A4G7
B	728	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	729	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	730	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	731	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	732	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	733	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	734	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	735	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	736	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	737	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	738	SER	-	EXPRESSION TAG	UNP D1A4G7
B	739	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	740	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	741	SER	-	EXPRESSION TAG	UNP D1A4G7
B	742	ILE	-	EXPRESSION TAG	UNP D1A4G7
B	743	ASP	-	EXPRESSION TAG	UNP D1A4G7
B	744	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	745	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	746	SER	-	EXPRESSION TAG	UNP D1A4G7
B	747	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	748	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	749	VAL	-	EXPRESSION TAG	UNP D1A4G7
B	750	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	751	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	752	GLN	-	EXPRESSION TAG	UNP D1A4G7
B	753	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	754	PRO	-	EXPRESSION TAG	UNP D1A4G7
B	755	SER	-	EXPRESSION TAG	UNP D1A4G7
B	756	SER	-	EXPRESSION TAG	UNP D1A4G7
B	757	PRO	-	EXPRESSION TAG	UNP D1A4G7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	758	SER	-	EXPRESSION TAG	UNP D1A4G7
C	727	MET	-	EXPRESSION TAG	UNP D1A4G7
C	728	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	729	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	730	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	731	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	732	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	733	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	734	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	735	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	736	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	737	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	738	SER	-	EXPRESSION TAG	UNP D1A4G7
C	739	GLU	-	EXPRESSION TAG	UNP D1A4G7
C	740	PHE	-	EXPRESSION TAG	UNP D1A4G7
C	741	SER	-	EXPRESSION TAG	UNP D1A4G7
C	742	ILE	-	EXPRESSION TAG	UNP D1A4G7
C	743	ASP	-	EXPRESSION TAG	UNP D1A4G7
C	744	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	745	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	746	SER	-	EXPRESSION TAG	UNP D1A4G7
C	747	LEU	-	EXPRESSION TAG	UNP D1A4G7
C	748	GLU	-	EXPRESSION TAG	UNP D1A4G7
C	749	VAL	-	EXPRESSION TAG	UNP D1A4G7
C	750	LEU	-	EXPRESSION TAG	UNP D1A4G7
C	751	PHE	-	EXPRESSION TAG	UNP D1A4G7
C	752	GLN	-	EXPRESSION TAG	UNP D1A4G7
C	753	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	754	PRO	-	EXPRESSION TAG	UNP D1A4G7
C	755	SER	-	EXPRESSION TAG	UNP D1A4G7
C	756	SER	-	EXPRESSION TAG	UNP D1A4G7
C	757	PRO	-	EXPRESSION TAG	UNP D1A4G7
C	758	SER	-	EXPRESSION TAG	UNP D1A4G7
E	727	MET	-	EXPRESSION TAG	UNP D1A4G7
E	728	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	729	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	730	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	731	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	732	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	733	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	734	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	735	HIS	-	EXPRESSION TAG	UNP D1A4G7

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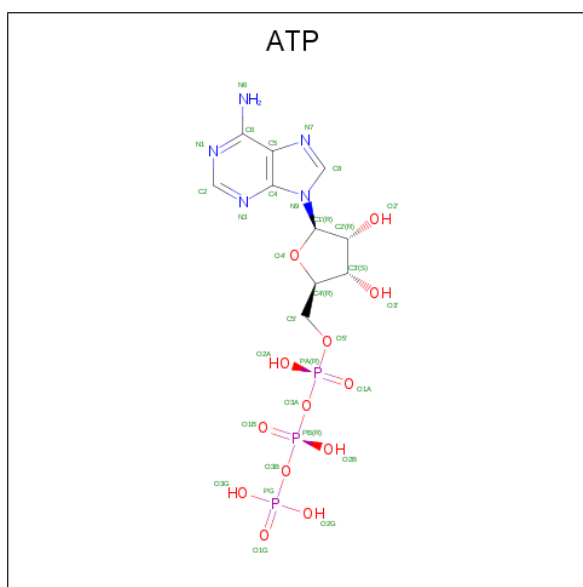
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Chain	Residue	Modelled	Actual	Comment	Reference
E	736	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	737	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	738	SER	-	EXPRESSION TAG	UNP D1A4G7
E	739	GLU	-	EXPRESSION TAG	UNP D1A4G7
E	740	PHE	-	EXPRESSION TAG	UNP D1A4G7
E	741	SER	-	EXPRESSION TAG	UNP D1A4G7
E	742	ILE	-	EXPRESSION TAG	UNP D1A4G7
E	743	ASP	-	EXPRESSION TAG	UNP D1A4G7
E	744	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	745	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	746	SER	-	EXPRESSION TAG	UNP D1A4G7
E	747	LEU	-	EXPRESSION TAG	UNP D1A4G7
E	748	GLU	-	EXPRESSION TAG	UNP D1A4G7
E	749	VAL	-	EXPRESSION TAG	UNP D1A4G7
E	750	LEU	-	EXPRESSION TAG	UNP D1A4G7
E	751	PHE	-	EXPRESSION TAG	UNP D1A4G7
E	752	GLN	-	EXPRESSION TAG	UNP D1A4G7
E	753	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	754	PRO	-	EXPRESSION TAG	UNP D1A4G7
E	755	SER	-	EXPRESSION TAG	UNP D1A4G7
E	756	SER	-	EXPRESSION TAG	UNP D1A4G7
E	757	PRO	-	EXPRESSION TAG	UNP D1A4G7
E	758	SER	-	EXPRESSION TAG	UNP D1A4G7

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	0	0	0
			56	35	12	9			
2	H	6	Total	C	N	O	0	0	0
			48	31	10	7			
2	J	7	Total	C	N	O	0	0	0
			50	32	9	9			
2	K	6	Total	C	N	O	0	0	0
			45	29	8	8			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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

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

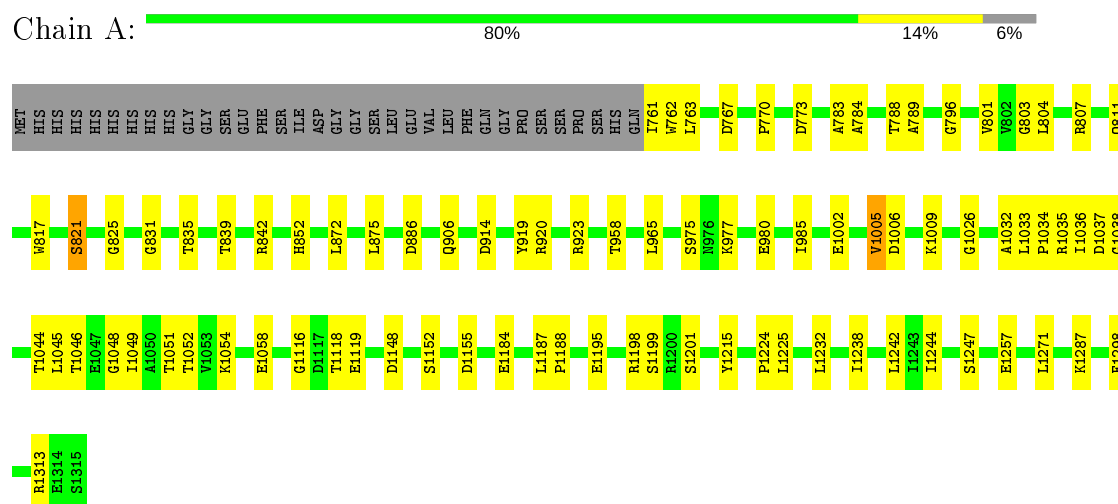
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		

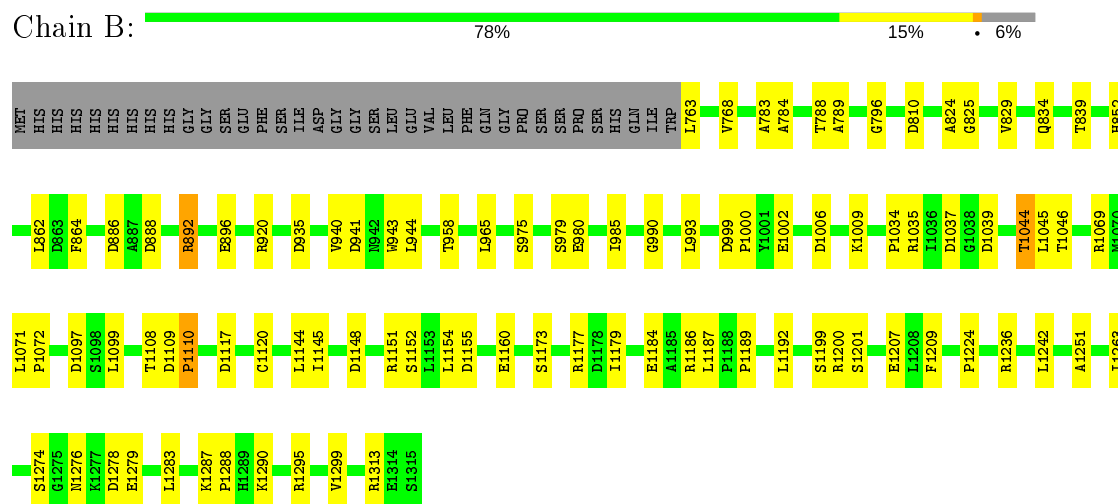
3 Residue-property plots

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

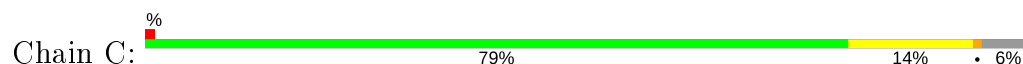
- Molecule 1: Cell divisionFtsK/SpoIIIE

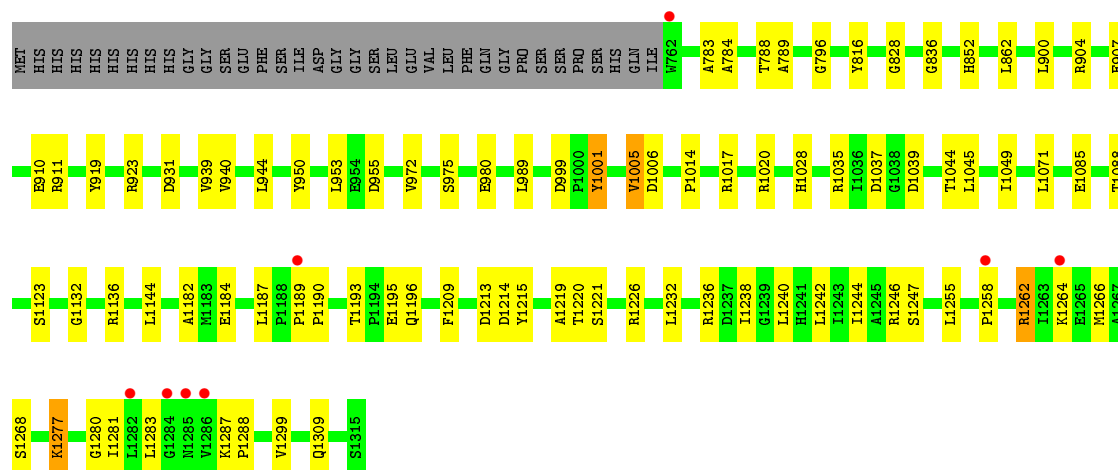


- Molecule 1: Cell divisionFtsK/SpoIIIE

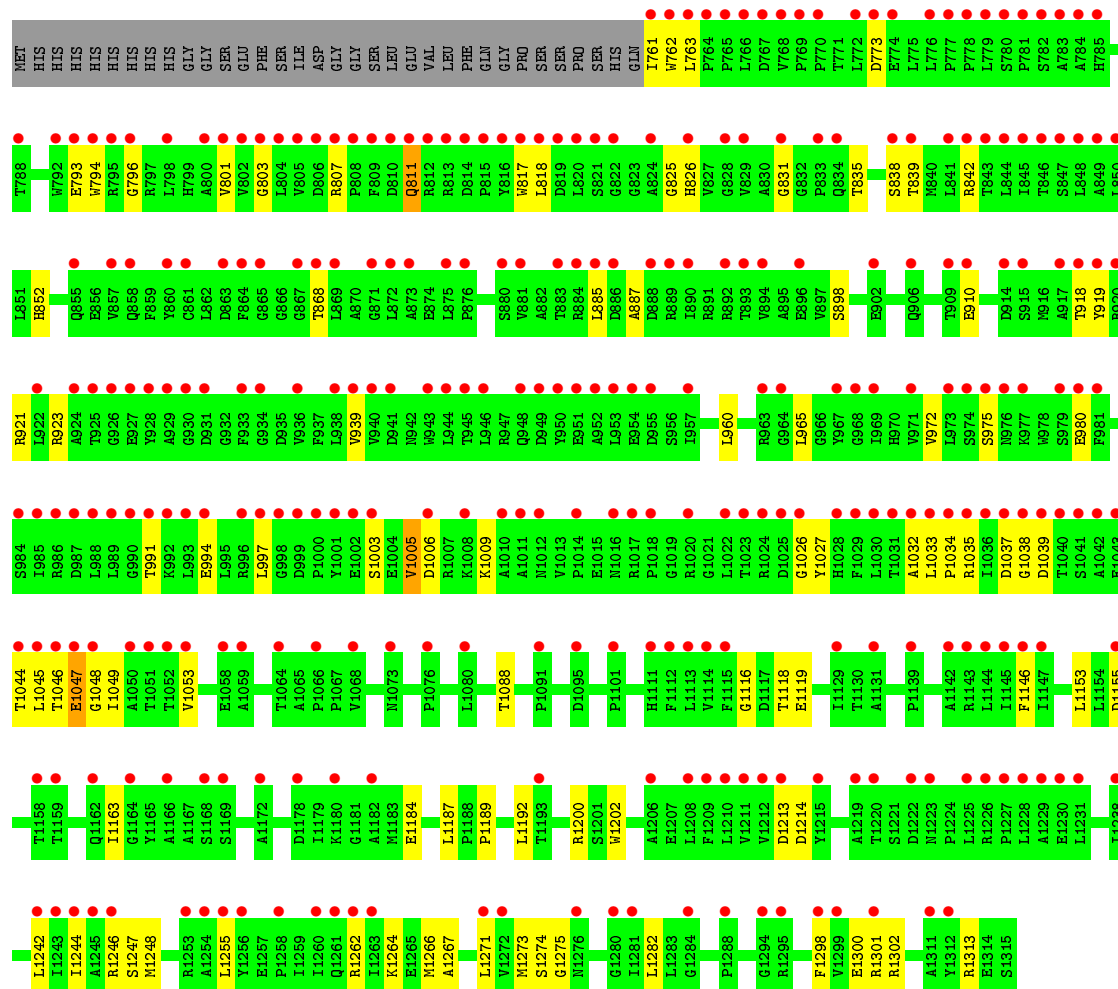
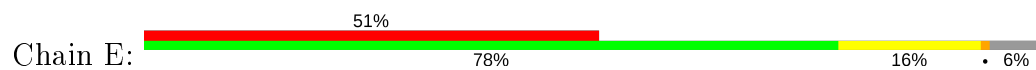


- Molecule 1: Cell divisionFtsK/SpoIIIE





• Molecule 1: Cell divisionFtsK/SpoIIIE



• Molecule 2: Uncharacterized protein

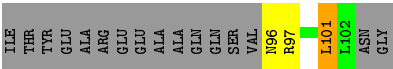




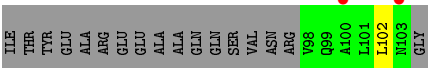
● Molecule 2: Uncharacterized protein



● Molecule 2: Uncharacterized protein



● Molecule 2: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	216.15Å 216.15Å 186.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 3.24 48.33 – 3.24	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.15-3.24) 100.0 (48.33-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.266 0.229 , 0.268	Depositor DCC
R_{free} test set	2000 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17460	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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 [i](#)

5.1 Standard geometry [i](#)

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	0/4395	0.40	0/5984
1	B	0.26	0/4324	0.43	1/5895 (0.0%)
1	C	0.20	0/4344	0.40	0/5924
1	E	0.28	0/4389	0.47	1/5977 (0.0%)
2	G	0.22	0/55	0.41	0/73
2	H	0.21	0/47	0.39	0/62
2	J	0.22	0/49	0.38	0/66
2	K	0.28	0/44	0.54	0/59
All	All	0.25	0/17647	0.43	2/24040 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	768	VAL	C-N-CD	5.94	140.87	128.40
1	E	1033	LEU	C-N-CD	5.73	140.44	128.40

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	4298	0	4268	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4229	0	4164	57	0
1	C	4247	0	4175	60	0
1	E	4292	0	4257	73	0
2	G	56	0	62	2	0
2	H	48	0	56	2	0
2	J	50	0	51	3	0
2	K	45	0	49	1	0
3	A	62	0	24	1	0
3	B	62	0	24	3	0
3	C	62	0	24	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
5	B	1	0	0	0	0
All	All	17460	0	17154	238	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 7.

The worst 5 of 238 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1035:ARG:NH2	1:E:1037:ASP:OD2	1.80	1.13
1:E:1044:THR:HA	1:E:1047:GLU:OE2	1.56	0.98
1:C:1264:LYS:NZ	1:C:1268:SER:O	2.01	0.93
1:E:763:LEU:HD21	1:E:811:GLN:HA	1.57	0.86
1:E:1044:THR:CA	1:E:1047:GLU:OE2	2.24	0.85

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	553/589 (94%)	535 (97%)	18 (3%)	0	100	100
1	B	551/589 (94%)	524 (95%)	26 (5%)	1 (0%)	47	78
1	C	552/589 (94%)	515 (93%)	37 (7%)	0	100	100
1	E	553/589 (94%)	536 (97%)	16 (3%)	1 (0%)	47	78
2	G	5/23 (22%)	5 (100%)	0	0	100	100
2	H	4/23 (17%)	4 (100%)	0	0	100	100
2	J	5/23 (22%)	5 (100%)	0	0	100	100
2	K	4/23 (17%)	2 (50%)	2 (50%)	0	100	100
All	All	2227/2448 (91%)	2126 (96%)	99 (4%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	886	ASP
1	E	1005	VAL

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	455/485 (94%)	450 (99%)	5 (1%)	73	87
1	B	445/485 (92%)	436 (98%)	9 (2%)	55	78
1	C	446/485 (92%)	434 (97%)	12 (3%)	44	73
1	E	454/485 (94%)	451 (99%)	3 (1%)	84	92
2	G	6/18 (33%)	5 (83%)	1 (17%)	2	9
2	H	5/18 (28%)	3 (60%)	2 (40%)	0	0
2	J	5/18 (28%)	4 (80%)	1 (20%)	1	5
2	K	5/18 (28%)	5 (100%)	0	100	100
All	All	1821/2012 (90%)	1788 (98%)	33 (2%)	59	80

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	816	TYR
1	C	1001	TYR
1	E	811	GLN
1	C	911	ARG
1	C	955	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	99	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	A	1401	4	26,33,33	0.94	1 (3%)	31,52,52	1.56	5 (16%)
3	ATP	C	1401	4	26,33,33	0.94	1 (3%)	31,52,52	1.58	5 (16%)
3	ATP	B	1401	4	26,33,33	0.94	1 (3%)	31,52,52	1.52	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	1402	4	26,33,33	0.95	1 (3%)	31,52,52	1.54	5 (16%)
3	ATP	C	1402	4	26,33,33	0.93	1 (3%)	31,52,52	1.56	5 (16%)
3	ATP	A	1402	4	26,33,33	0.94	1 (3%)	31,52,52	1.61	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1401	4	-	2/18/38/38	0/3/3/3
3	ATP	C	1401	4	-	2/18/38/38	0/3/3/3
3	ATP	B	1401	4	-	0/18/38/38	0/3/3/3
3	ATP	B	1402	4	-	0/18/38/38	0/3/3/3
3	ATP	C	1402	4	-	0/18/38/38	0/3/3/3
3	ATP	A	1402	4	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1401	ATP	C5-C4	2.52	1.47	1.40
3	B	1402	ATP	C5-C4	2.52	1.47	1.40
3	C	1401	ATP	C5-C4	2.51	1.47	1.40
3	A	1402	ATP	C5-C4	2.51	1.47	1.40
3	B	1401	ATP	C5-C4	2.49	1.47	1.40

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	ATP	PB-O3B-PG	-3.79	119.82	132.83
3	C	1401	ATP	PB-O3B-PG	-3.71	120.08	132.83
3	A	1402	ATP	PA-O3A-PB	-3.69	120.15	132.83
3	A	1401	ATP	PA-O3A-PB	-3.67	120.24	132.83
3	C	1402	ATP	PB-O3B-PG	-3.66	120.26	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1401	ATP	PA-O3A-PB-O1B

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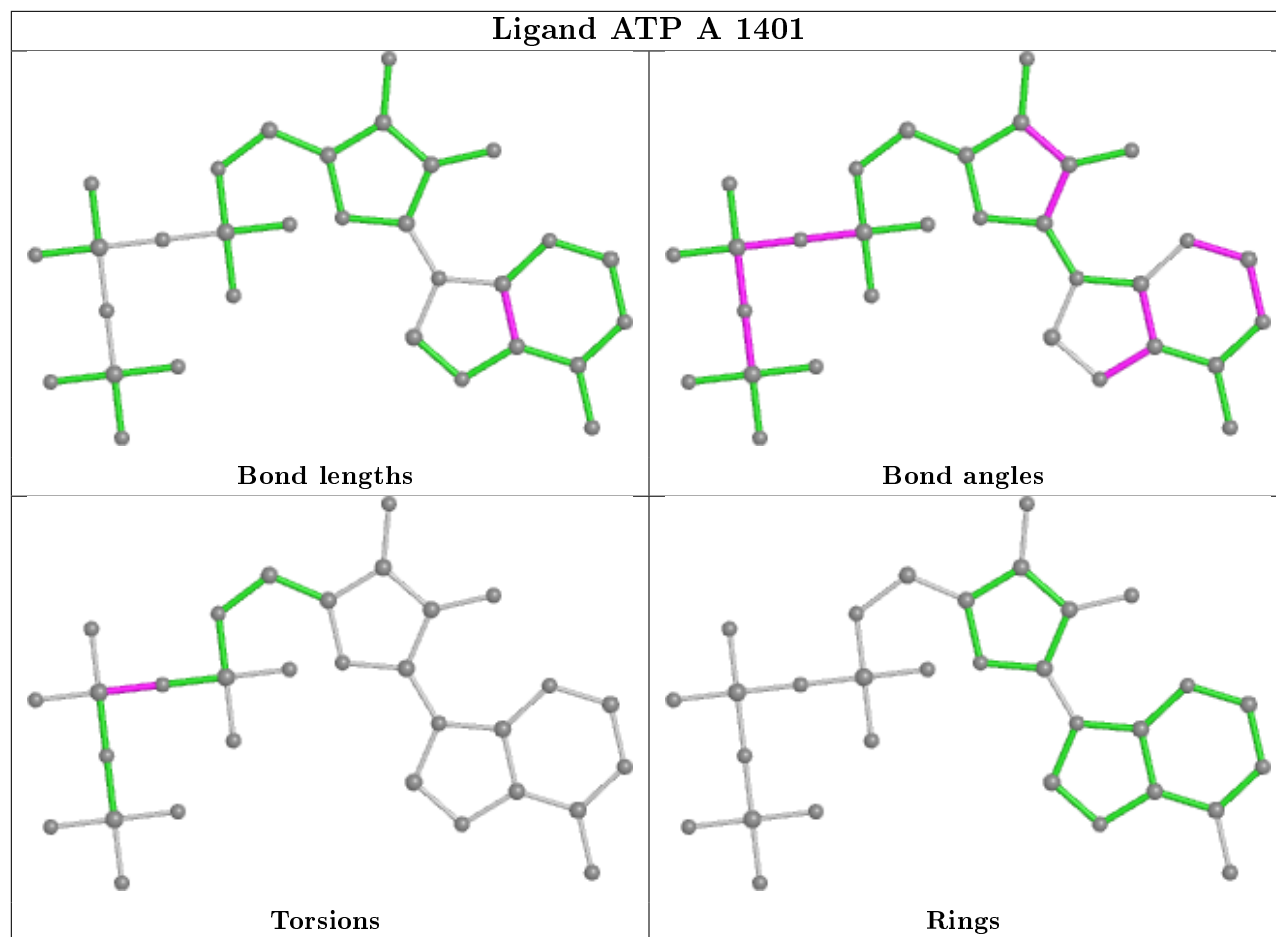
Mol	Chain	Res	Type	Atoms
3	C	1401	ATP	PA-O3A-PB-O1B
3	A	1401	ATP	PA-O3A-PB-O2B
3	C	1401	ATP	PA-O3A-PB-O2B

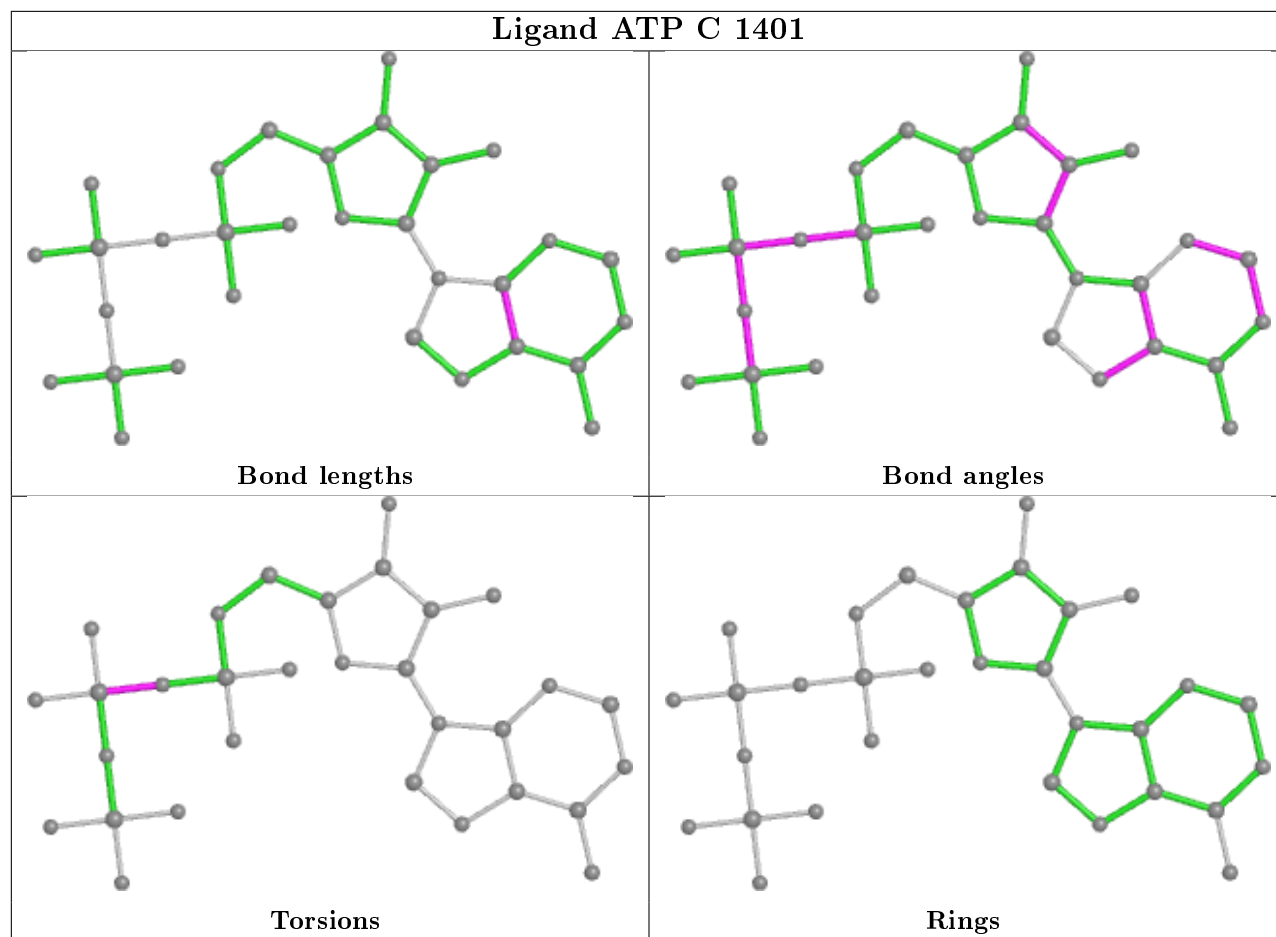
There are no ring outliers.

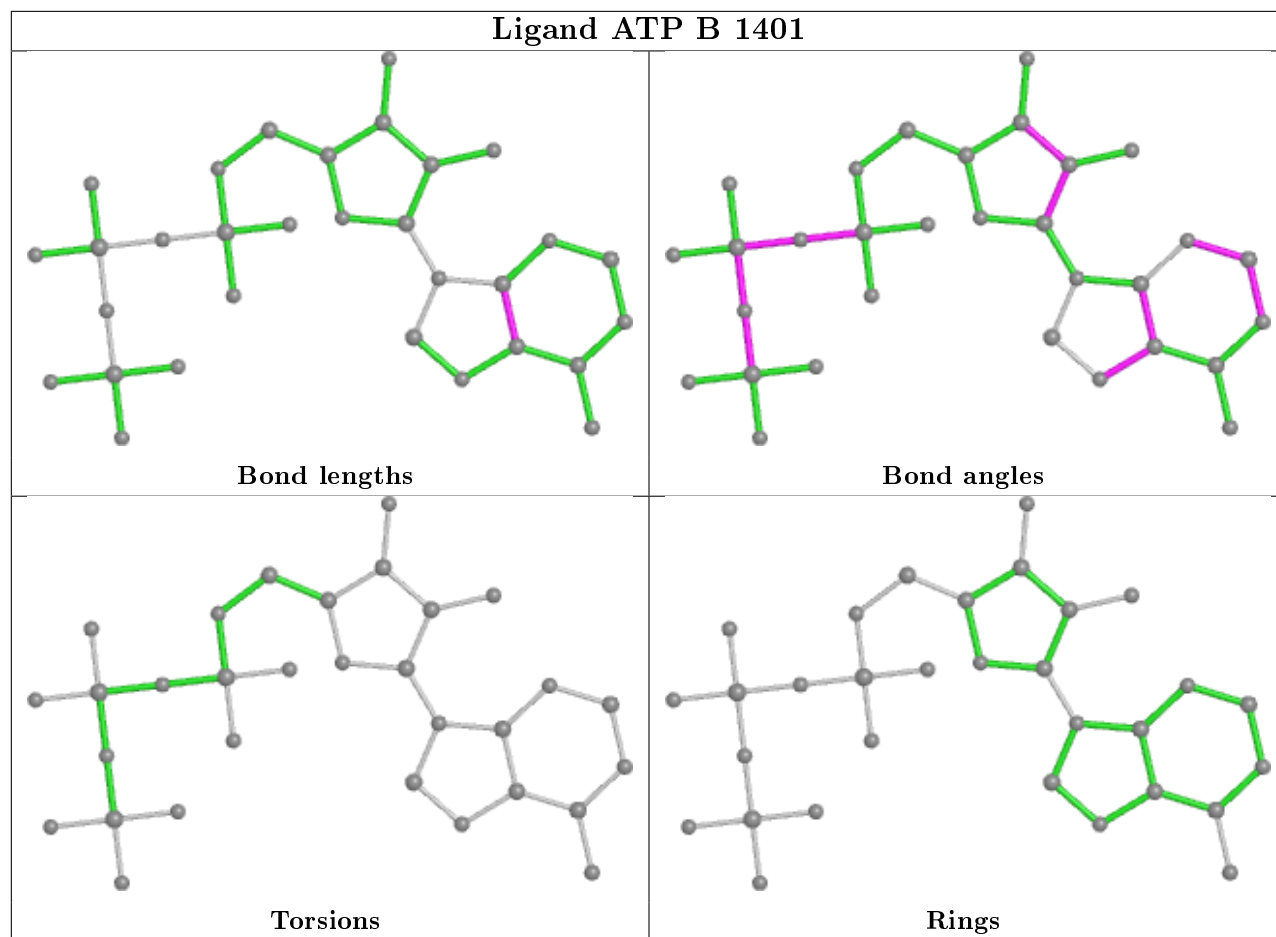
4 monomers are involved in 6 short contacts:

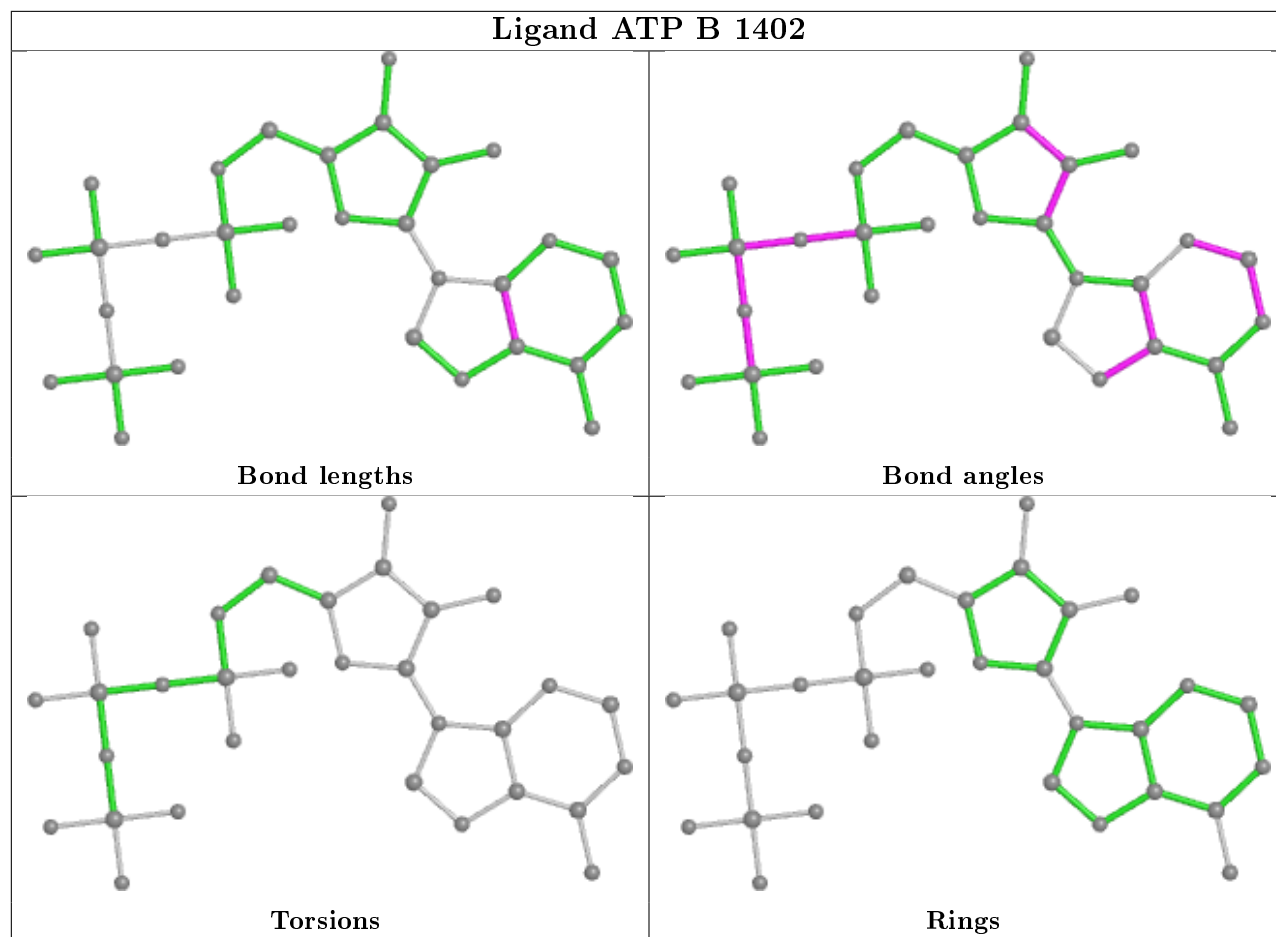
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1401	ATP	1	0
3	C	1401	ATP	1	0
3	B	1401	ATP	3	0
3	C	1402	ATP	1	0

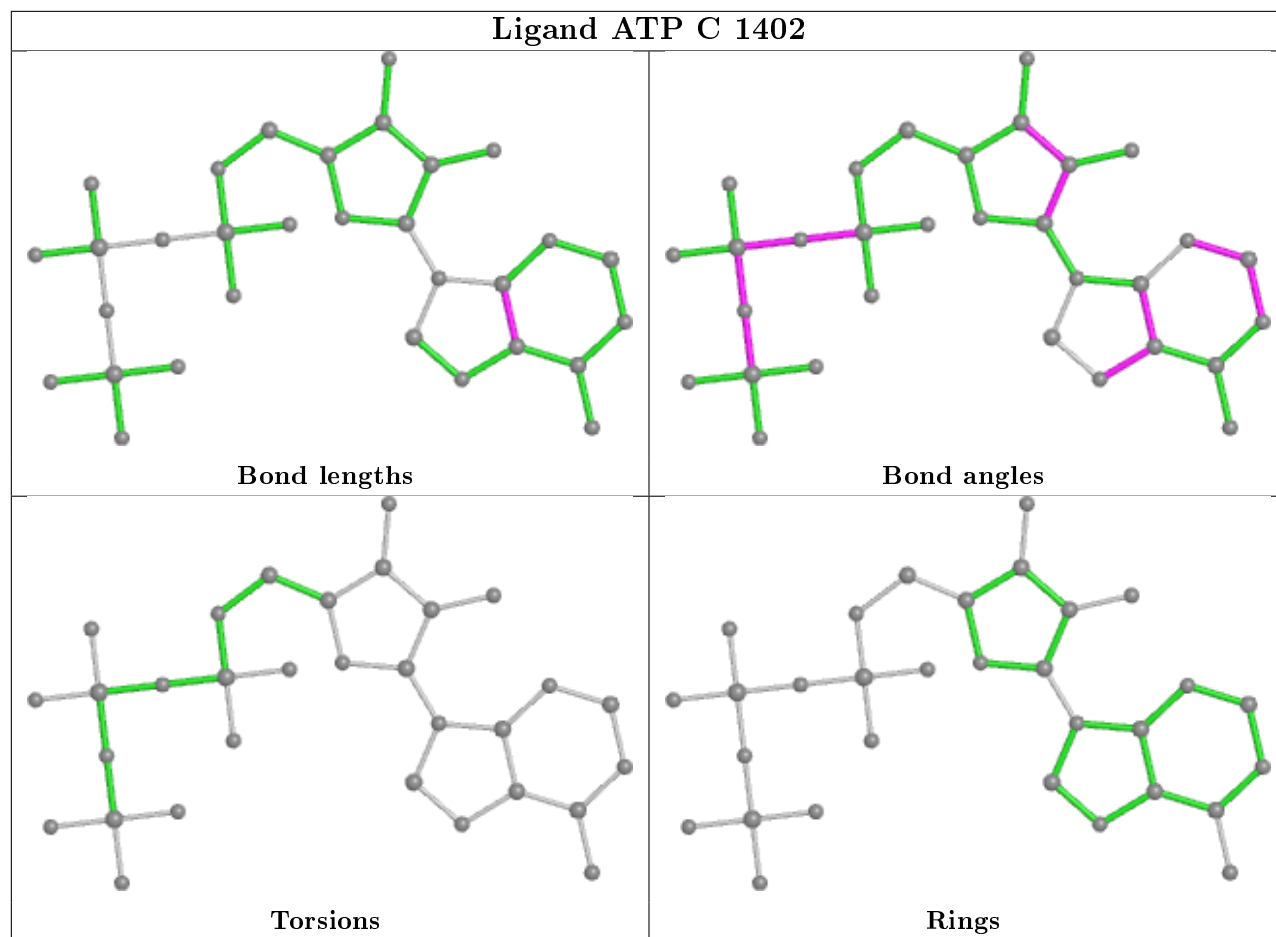
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

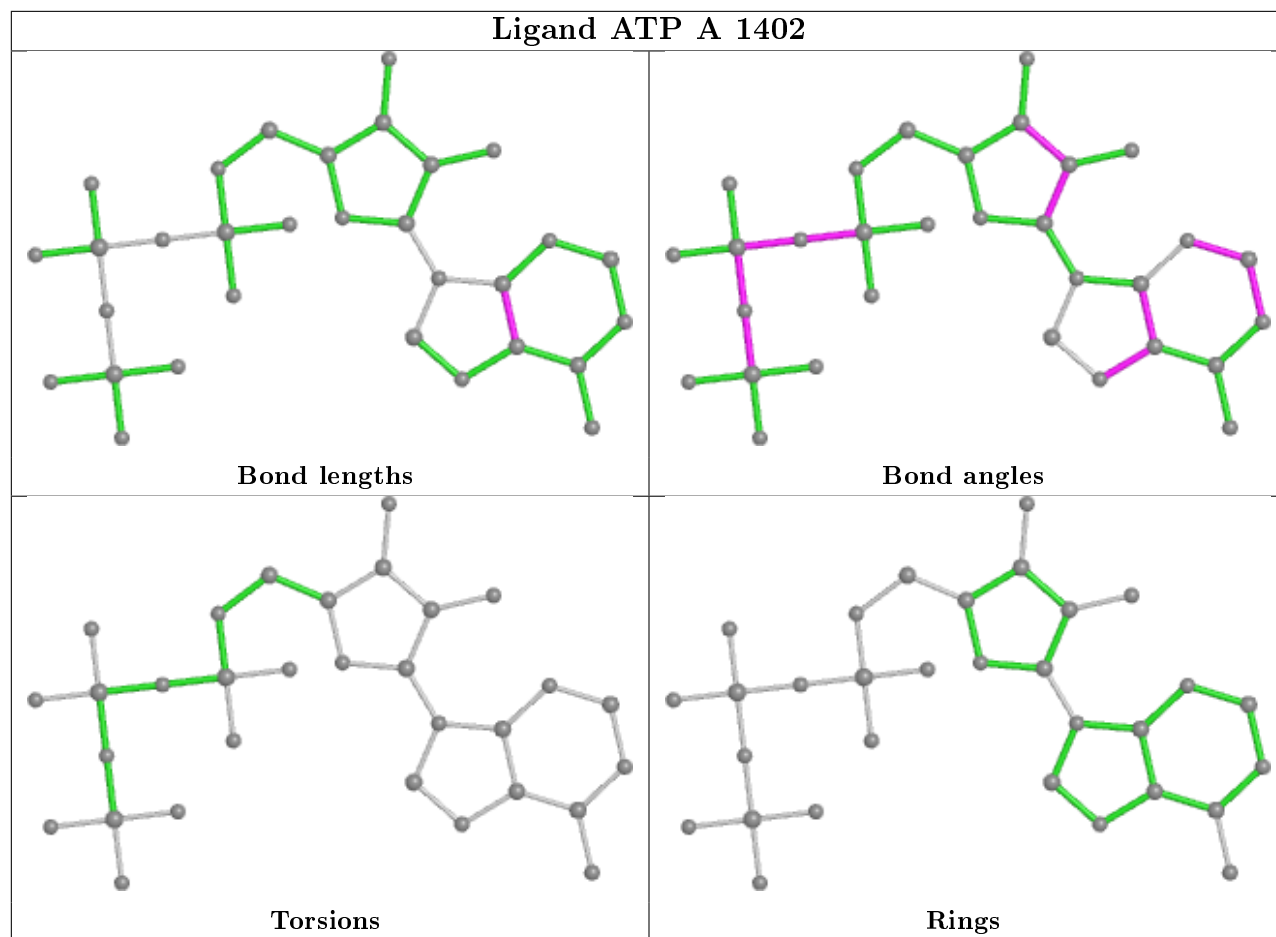












5.7 Other polymers [i](#)

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, 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	555/589 (94%)	-0.35	0 100 100	25, 48, 78, 103	0
1	B	553/589 (93%)	-0.33	0 100 100	29, 55, 90, 122	0
1	C	554/589 (94%)	-0.08	8 (1%) 75 66	43, 84, 137, 177	0
1	E	555/589 (94%)	2.40	299 (53%) 0 0	122, 187, 222, 279	0
2	G	7/23 (30%)	-0.29	0 100 100	64, 66, 92, 95	0
2	H	6/23 (26%)	-0.03	0 100 100	96, 102, 122, 128	0
2	J	7/23 (30%)	0.02	0 100 100	102, 110, 118, 124	0
2	K	6/23 (26%)	1.55	2 (33%) 0 0	136, 159, 170, 175	0
All	All	2243/2448 (91%)	0.41	309 (13%) 2 2	25, 72, 205, 279	0

The worst 5 of 309 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	767	ASP	10.2
1	E	801	VAL	9.2
1	E	816	TYR	8.3
1	E	934	GLY	8.3
1	E	988	LEU	7.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

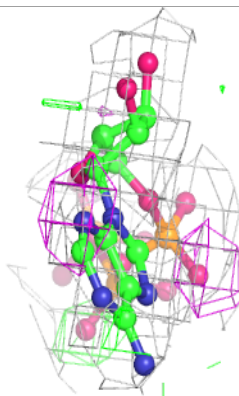
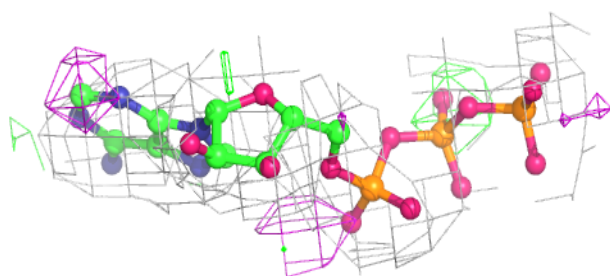
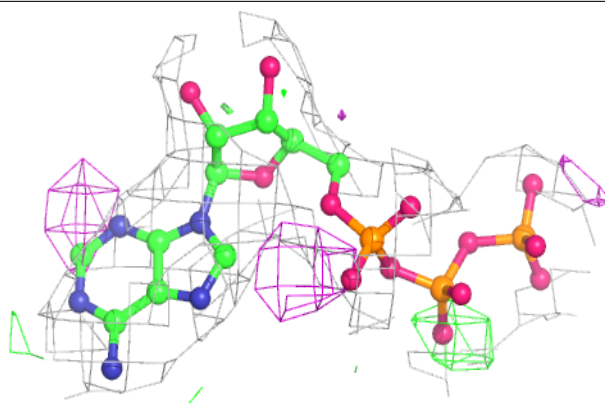
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	E	1402	1/1	-0.28	0.65	286,286,286,286	0
4	MG	E	1401	1/1	0.06	0.40	204,204,204,204	0
3	ATP	B	1402	31/31	0.94	0.19	43,58,78,120	0
3	ATP	C	1402	31/31	0.95	0.17	54,68,77,83	0
4	MG	C	1403	1/1	0.96	0.19	55,55,55,55	0
3	ATP	B	1401	31/31	0.96	0.19	28,44,68,79	0
3	ATP	C	1401	31/31	0.96	0.17	35,60,79,88	0
4	MG	B	1403	1/1	0.96	0.21	48,48,48,48	0
3	ATP	A	1401	31/31	0.97	0.17	38,62,77,82	0
4	MG	A	1404	1/1	0.97	0.23	45,45,45,45	0
3	ATP	A	1402	31/31	0.97	0.17	24,39,57,88	0
4	MG	A	1403	1/1	0.97	0.40	43,43,43,43	0
4	MG	C	1404	1/1	0.97	0.22	45,45,45,45	0
4	MG	B	1404	1/1	0.99	0.19	34,34,34,34	0

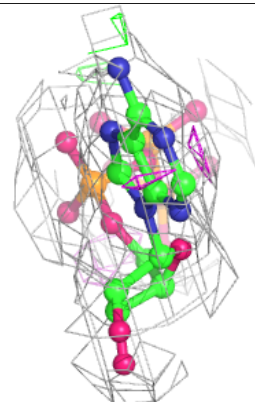
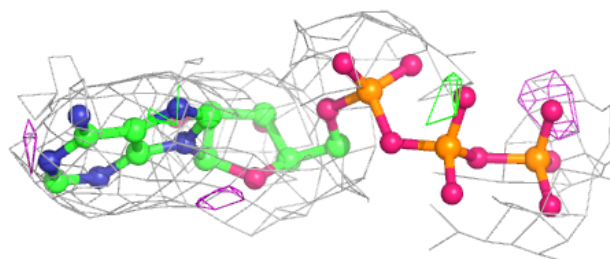
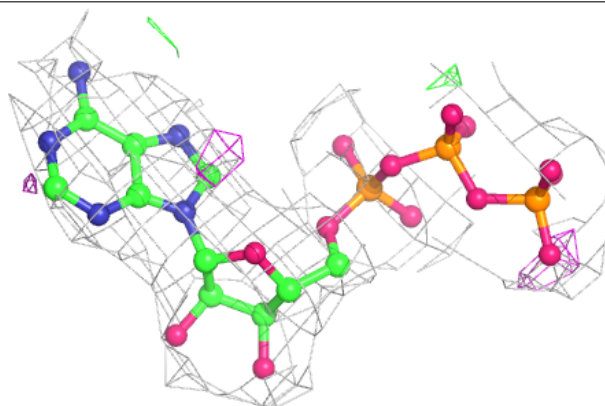
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 1402:

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

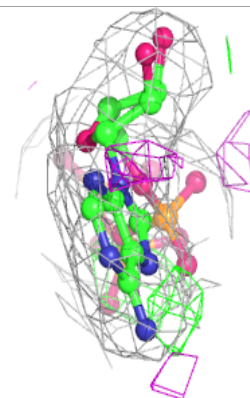
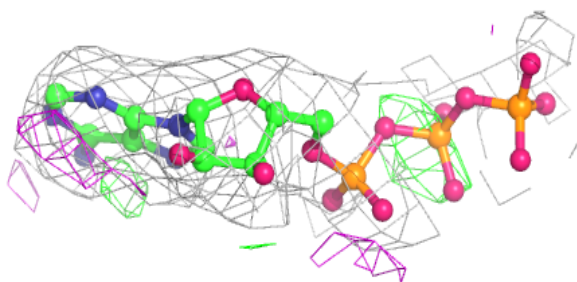
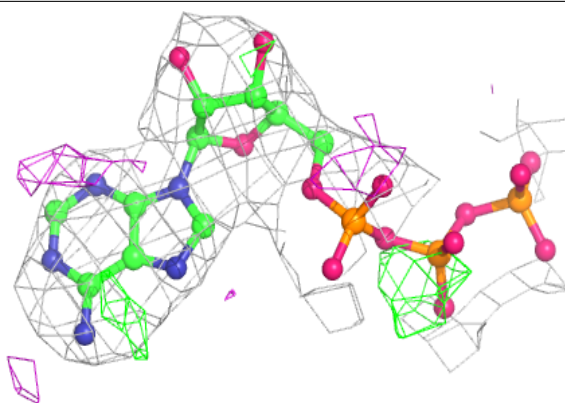
**Electron density around ATP C 1402:**

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

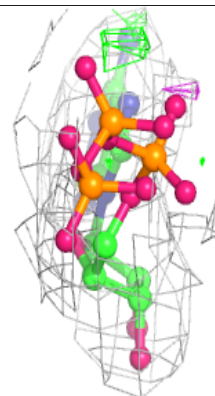
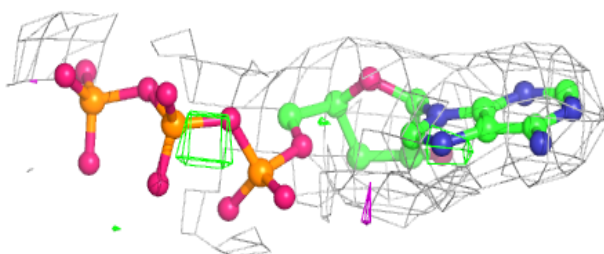
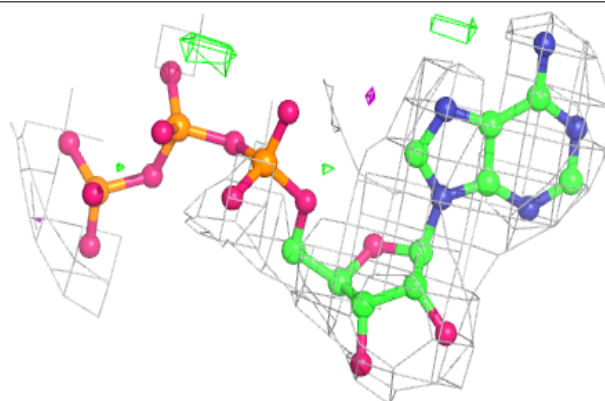


Electron density around ATP B 1401:

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

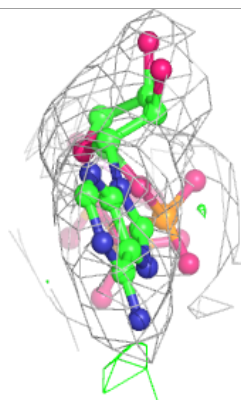
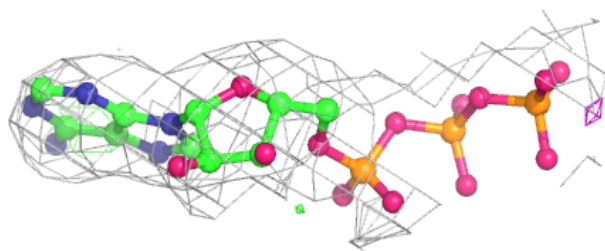
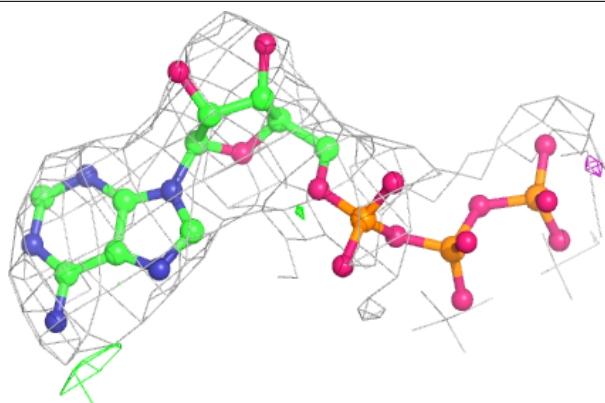
**Electron density around ATP C 1401:**

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

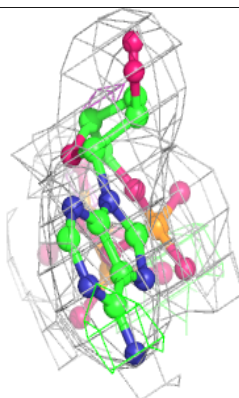
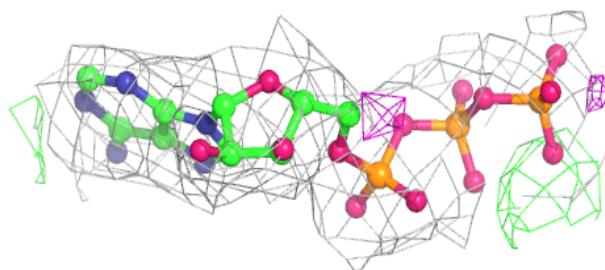
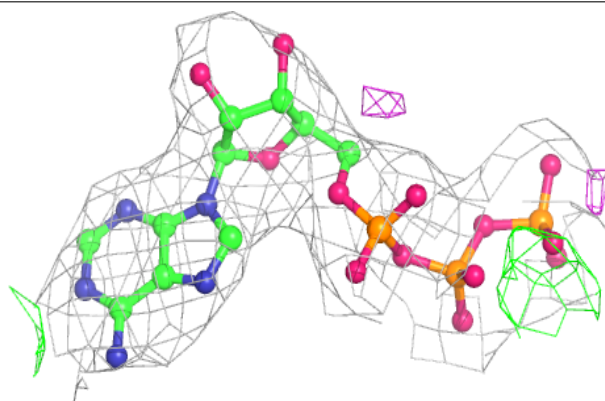


Electron density around ATP A 1401:

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

**Electron density around ATP A 1402:**

$2mF_o-DF_c$ (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.