Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:37 AM BST

PDB ID	:	4YB7
Title	:	Adenosine triphosphate phosphoribosyltransferase from Campylobacter jejuni in complex with ATP
Authors	:	Mittelstaedt, G.; Moggre, G.-J.; Parker, E.J.
Deposited on	:	2015-02-18
Resolution	:	2.20 Å(reported)

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

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

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

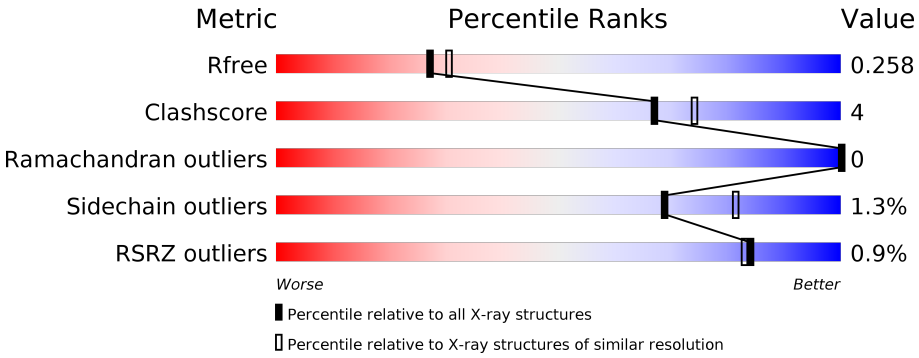
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	300	92% 6% •
1	B	300	89% 10% •
1	C	300	% 86% 12% ••
1	D	300	% 91% 7% •
1	E	300	% 90% 8% •
1	F	300	89% 7% ••

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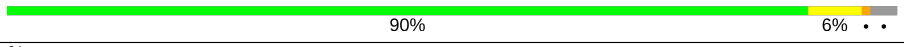
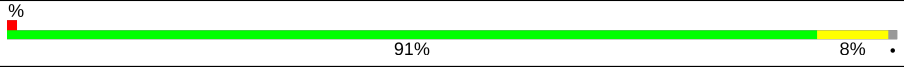
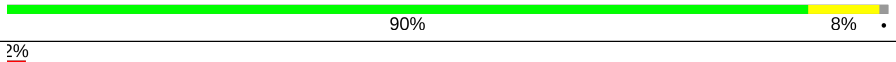
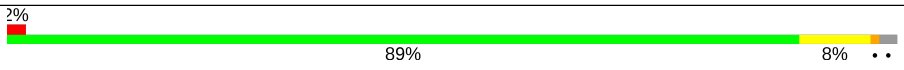
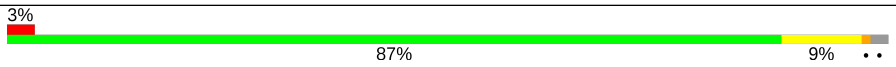
Mol	Chain	Length	Quality of chain
1	G	300	
1	H	300	
1	I	300	
1	J	300	
1	K	300	
1	L	300	

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
3	PO4	J	302	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26987 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 ATP phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	296	Total	C	N	O	S	0	0	0
			2228	1418	381	416	13			
1	C	294	Total	C	N	O	S	0	1	0
			2198	1399	376	409	14			
1	D	294	Total	C	N	O	S	0	0	0
			2168	1381	370	404	13			
1	E	295	Total	C	N	O	S	0	0	0
			2203	1395	377	418	13			
1	I	292	Total	C	N	O	S	0	0	0
			2169	1377	376	403	13			
1	K	294	Total	C	N	O	S	0	1	0
			2168	1380	369	405	14			
1	A	296	Total	C	N	O	S	0	0	0
			2202	1404	379	406	13			
1	F	293	Total	C	N	O	S	0	1	0
			2191	1389	375	413	14			
1	G	292	Total	C	N	O	S	0	0	0
			2149	1364	365	407	13			
1	H	296	Total	C	N	O	S	5	0	0
			2162	1372	372	405	13			
1	J	296	Total	C	N	O	S	0	0	0
			2218	1409	379	417	13			
1	L	293	Total	C	N	O	S	0	1	0
			2148	1360	368	406	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP Q5HSJ4
C	0	GLY	-	expression tag	UNP Q5HSJ4
D	0	GLY	-	expression tag	UNP Q5HSJ4
E	0	GLY	-	expression tag	UNP Q5HSJ4
I	0	GLY	-	expression tag	UNP Q5HSJ4

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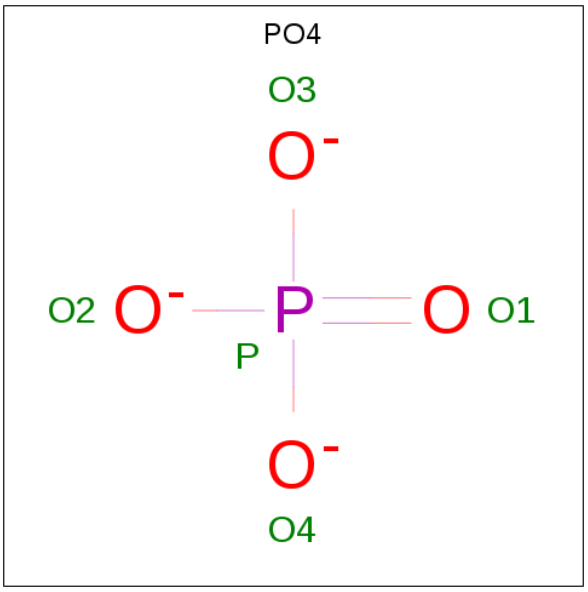
Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP Q5HSJ4
A	0	GLY	-	expression tag	UNP Q5HSJ4
F	0	GLY	-	expression tag	UNP Q5HSJ4
G	0	GLY	-	expression tag	UNP Q5HSJ4
H	0	GLY	-	expression tag	UNP Q5HSJ4
J	0	GLY	-	expression tag	UNP Q5HSJ4
L	0	GLY	-	expression tag	UNP Q5HSJ4

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

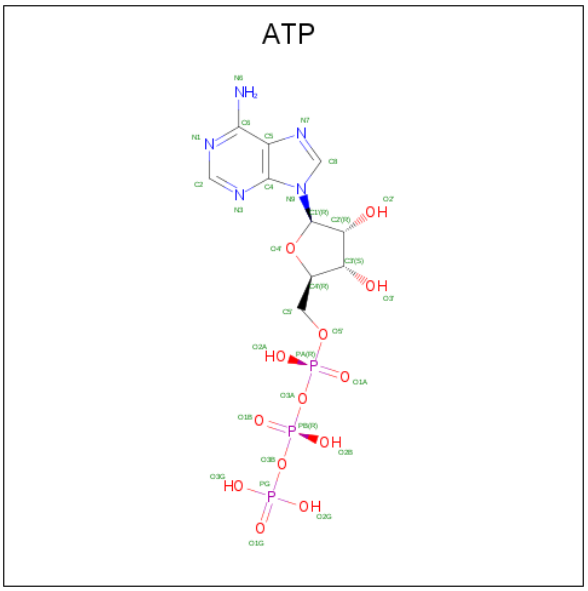
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0
2	F	1	Total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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



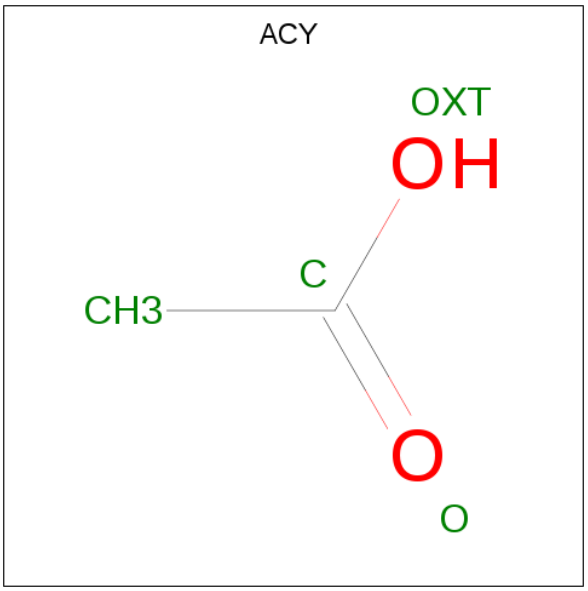
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	I	1	Total O P 5 4 1	0	0
3	J	1	Total O P 5 4 1	0	0

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



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

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	52	Total O 52 52	0	0
6	C	44	Total O 44 44	0	0
6	D	31	Total O 31 31	0	0
6	E	19	Total O 19 19	0	0
6	I	22	Total O 22 22	0	0
6	K	15	Total O 15 15	0	0
6	A	68	Total O 68 68	0	0
6	F	29	Total O 29 29	0	0
6	G	34	Total O 34 34	0	0
6	H	12	Total O 12 12	0	0
6	J	26	Total O 26 26	0	0

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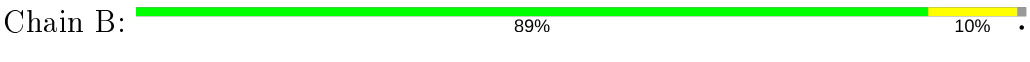
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	13	Total	O	0	0
			13	13		

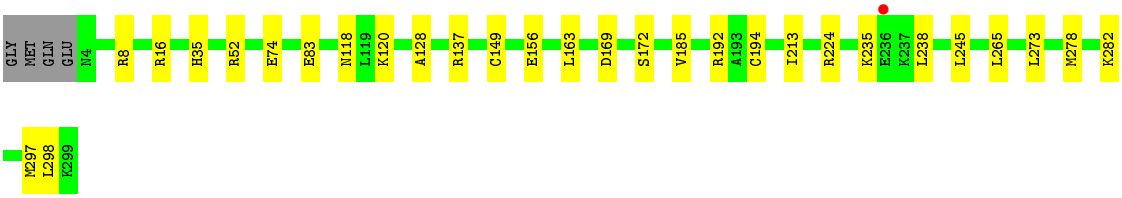
3 Residue-property plots (i)

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: ATP phosphoribosyltransferase

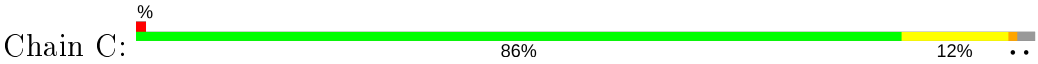
Chain B:

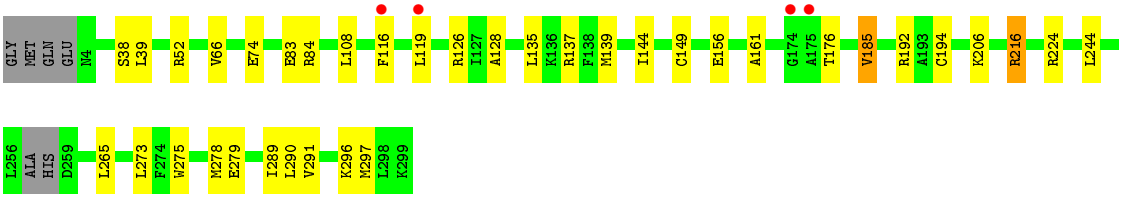




- Molecule 1: ATP phosphoribosyltransferase

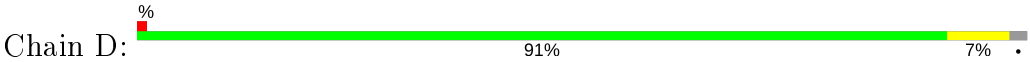
Chain C:

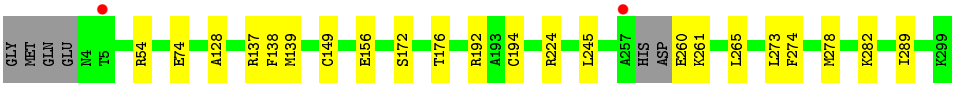




- Molecule 1: ATP phosphoribosyltransferase

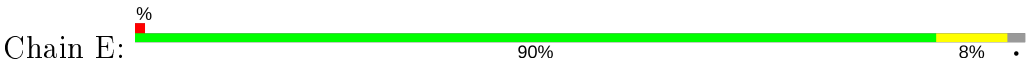
Chain D:

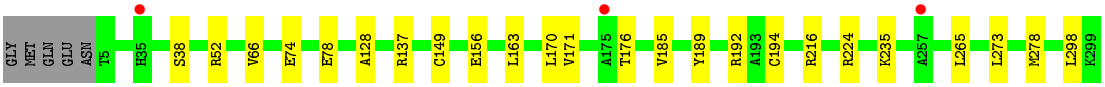




- Molecule 1: ATP phosphoribosyltransferase

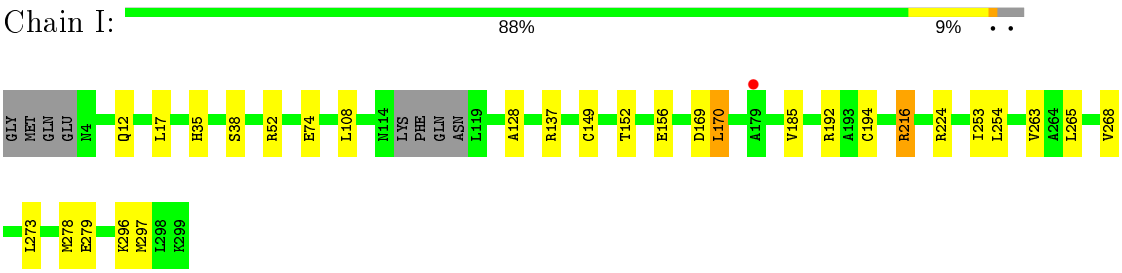
Chain E:





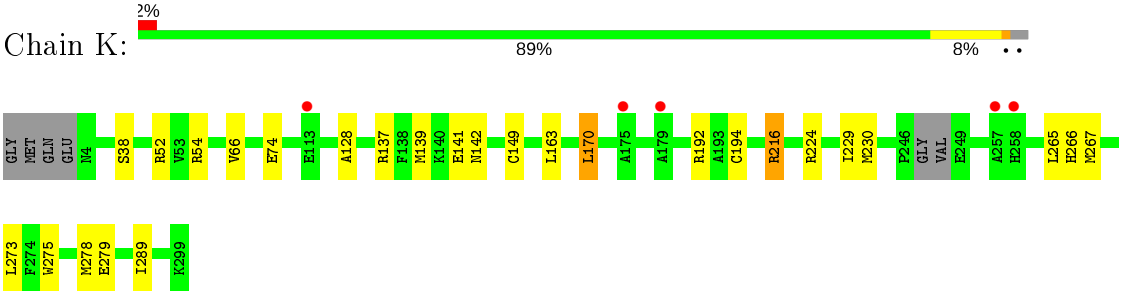
- Molecule 1: ATP phosphoribosyltransferase

Chain I:



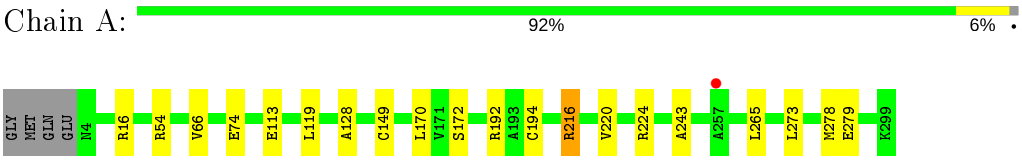
• Molecule 1: ATP phosphoribosyltransferase

Chain K:



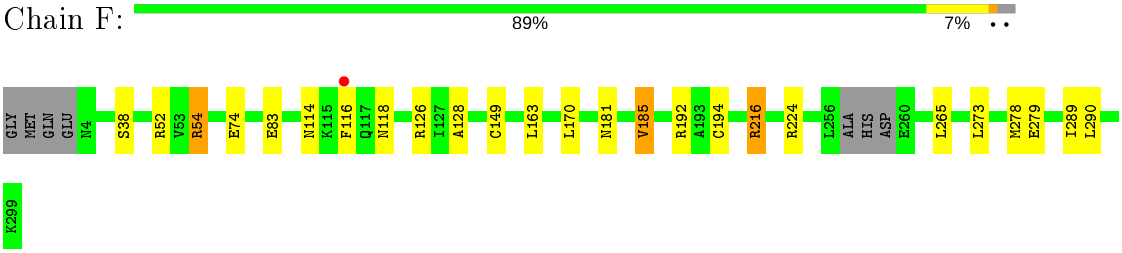
• Molecule 1: ATP phosphoribosyltransferase

Chain A:



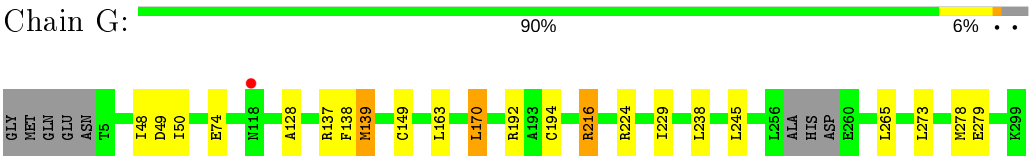
• Molecule 1: ATP phosphoribosyltransferase

Chain F:



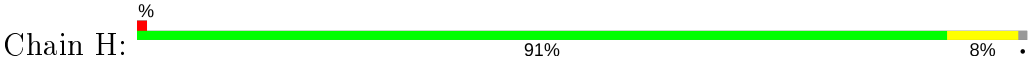
• Molecule 1: ATP phosphoribosyltransferase

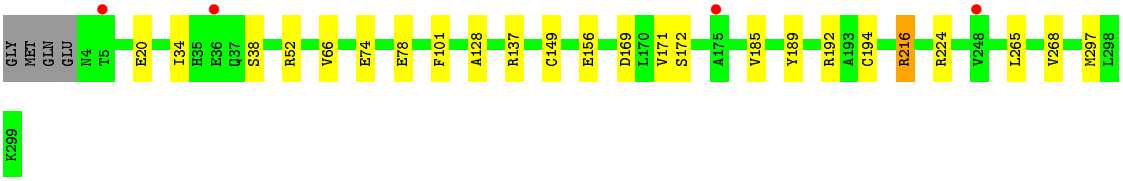
Chain G:



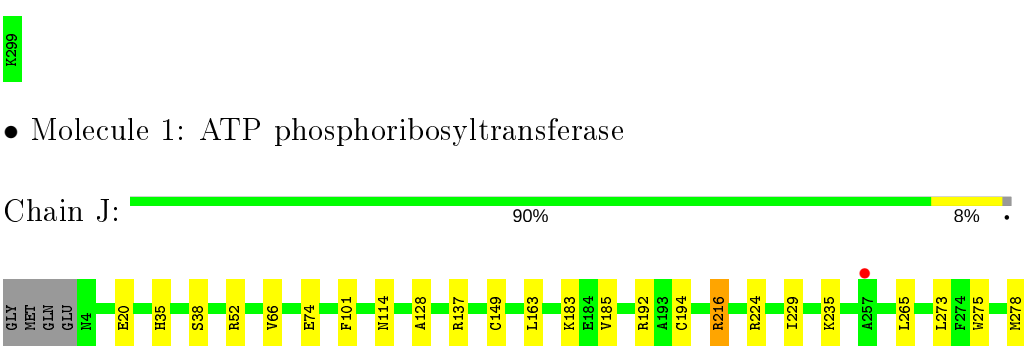
• Molecule 1: ATP phosphoribosyltransferase

Chain H:

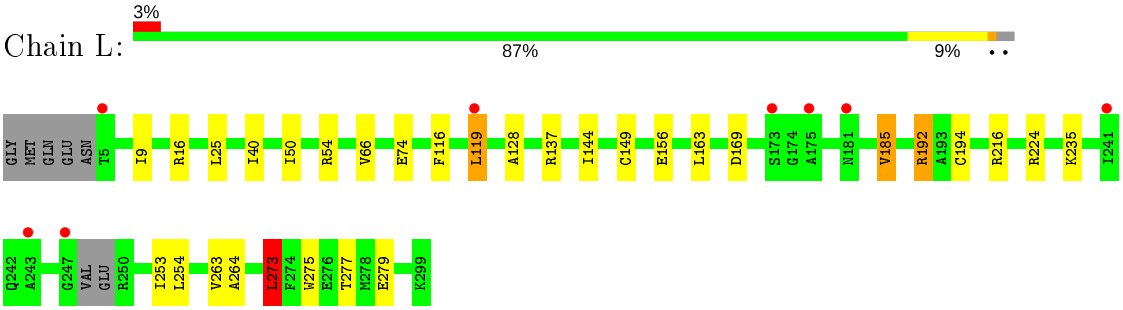




• Molecule 1: ATP phosphoribosyltransferase



• Molecule 1: ATP phosphoribosyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	91.67Å 91.83Å 154.90Å 101.11° 95.21° 118.14°	Depositor
Resolution (Å)	50.00 – 2.20 48.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.20) 98.1 (48.06-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.231 , 0.254 0.235 , 0.258	Depositor DCC
R_{free} test set	10624 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.053 for k,h,-h-k-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26987	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: PO4, ACY, 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	0.49	0/2229	0.79	4/3020 (0.1%)
1	B	0.49	0/2257	0.75	6/3055 (0.2%)
1	C	0.48	0/2225	0.85	10/3011 (0.3%)
1	D	0.45	0/2195	0.78	6/2977 (0.2%)
1	E	0.44	0/2231	0.82	8/3026 (0.3%)
1	F	0.44	0/2216	0.78	8/2997 (0.3%)
1	G	0.44	0/2174	0.85	9/2950 (0.3%)
1	H	0.41	0/2190	0.80	9/2974 (0.3%)
1	I	0.47	0/2197	0.82	7/2976 (0.2%)
1	J	0.44	0/2247	0.80	8/3042 (0.3%)
1	K	0.44	0/2194	0.82	9/2975 (0.3%)
1	L	0.46	0/2174	0.83	10/2952 (0.3%)
All	All	0.45	0/26529	0.81	94/35955 (0.3%)

There are no bond length outliers.

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	ARG	NE-CZ-NH2	-14.79	112.91	120.30
1	I	192	ARG	NE-CZ-NH2	-14.55	113.03	120.30
1	J	192	ARG	NE-CZ-NH2	-14.34	113.13	120.30
1	H	192	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	A	192	ARG	NE-CZ-NH1	13.90	127.25	120.30
1	G	192	ARG	NE-CZ-NH2	13.90	127.25	120.30
1	F	192	ARG	NE-CZ-NH2	13.87	127.23	120.30
1	C	192	ARG	NE-CZ-NH2	13.82	127.21	120.30
1	D	192	ARG	NE-CZ-NH2	-13.80	113.40	120.30
1	H	192	ARG	NE-CZ-NH1	13.77	127.19	120.30
1	J	192	ARG	NE-CZ-NH1	13.75	127.17	120.30
1	I	192	ARG	NE-CZ-NH1	13.74	127.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	224	ARG	NE-CZ-NH1	-13.54	113.53	120.30
1	L	192	ARG	NE-CZ-NH2	13.52	127.06	120.30
1	E	192	ARG	NE-CZ-NH2	13.48	127.04	120.30
1	K	192	ARG	NE-CZ-NH2	13.44	127.02	120.30
1	D	192	ARG	NE-CZ-NH1	13.21	126.90	120.30
1	C	192	ARG	NE-CZ-NH1	-12.99	113.80	120.30
1	F	192	ARG	NE-CZ-NH1	-12.96	113.82	120.30
1	G	224	ARG	NE-CZ-NH2	12.71	126.65	120.30
1	G	192	ARG	NE-CZ-NH1	-12.68	113.96	120.30
1	E	192	ARG	NE-CZ-NH1	-12.54	114.03	120.30
1	L	192	ARG	NE-CZ-NH1	-12.44	114.08	120.30
1	K	192	ARG	NE-CZ-NH1	-12.44	114.08	120.30
1	B	192	ARG	NE-CZ-NH2	11.45	126.02	120.30
1	C	137	ARG	NE-CZ-NH2	11.39	125.99	120.30
1	E	137	ARG	NE-CZ-NH2	11.27	125.94	120.30
1	B	192	ARG	NE-CZ-NH1	-11.23	114.69	120.30
1	H	137	ARG	NE-CZ-NH2	11.21	125.90	120.30
1	J	137	ARG	NE-CZ-NH2	11.21	125.90	120.30
1	G	137	ARG	NE-CZ-NH2	10.85	125.73	120.30
1	E	216	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	B	137	ARG	NE-CZ-NH2	10.69	125.64	120.30
1	D	137	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	I	137	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	E	216	ARG	NE-CZ-NH2	9.52	125.06	120.30
1	I	137	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	137	ARG	NE-CZ-NH1	-9.33	115.64	120.30
1	B	137	ARG	NE-CZ-NH1	-9.26	115.67	120.30
1	H	137	ARG	NE-CZ-NH1	-9.21	115.69	120.30
1	L	137	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	E	137	ARG	NE-CZ-NH1	-9.13	115.73	120.30
1	I	216	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	K	54	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	L	137	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	C	216	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	D	137	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	K	137	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	G	137	ARG	NE-CZ-NH1	-8.79	115.91	120.30
1	K	137	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	K	216	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	H	216	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	J	137	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	D	224	ARG	NE-CZ-NH2	-8.58	116.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	216	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	216	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	G	216	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	F	126	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	L	216	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	J	216	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	C	126	ARG	NE-CZ-NH2	8.25	124.43	120.30
1	L	273	LEU	CB-CG-CD1	7.55	123.84	111.00
1	I	216	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	K	216	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	D	224	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	L	224	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	224	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	L	224	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	C	216	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	C	224	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	H	216	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	G	216	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	J	224	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	K	224	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	F	224	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	H	224	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	F	216	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	F	224	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	J	216	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	L	216	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	216	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	E	224	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	K	224	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	224	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	F	54	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	I	224	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	E	224	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	J	224	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	C	244	LEU	CB-CG-CD2	5.99	121.18	111.00
1	G	139	MET	CG-SD-CE	-5.76	90.98	100.20
1	H	224	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	224	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	H	34	ILE	O-C-N	-5.05	114.62	122.70
1	L	119	LEU	CB-CG-CD2	5.02	119.53	111.00

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	2202	0	2219	16	0
1	B	2228	0	2247	24	0
1	C	2198	0	2200	30	0
1	D	2168	0	2142	28	0
1	E	2203	0	2185	11	1
1	F	2191	0	2190	15	1
1	G	2149	0	2110	21	0
1	H	2162	0	2109	17	0
1	I	2169	0	2159	21	0
1	J	2218	0	2210	23	1
1	K	2168	0	2131	16	1
1	L	2148	0	2087	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	E	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	2	0
4	C	31	0	12	0	0
4	D	31	0	12	2	0
4	E	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	31	0	12	0	0
4	G	31	0	12	1	0
4	H	31	0	12	0	0
4	I	31	0	12	1	0
4	J	31	0	12	2	0
4	K	31	0	12	1	0
4	L	31	0	12	2	0
5	J	4	0	3	0	0
6	A	68	0	0	2	0
6	B	52	0	0	1	0
6	C	44	0	0	2	0
6	D	31	0	0	3	0
6	E	19	0	0	0	0
6	F	29	0	0	1	0
6	G	34	0	0	0	0
6	H	12	0	0	0	0
6	I	22	0	0	0	0
6	J	26	0	0	2	0
6	K	15	0	0	0	0
6	L	13	0	0	0	0
All	All	26987	0	26136	207	2

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 4.

All (207) 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:D:138:PHE:HD2	1:D:139:MET:HE2	1.09	1.18
1:K:139:MET:O	1:K:142:ASN:O	1.68	1.12
1:E:156:GLU:OE1	1:E:176:THR:HG21	1.50	1.11
1:B:245:LEU:HD21	1:B:273:LEU:HD11	1.28	1.10
1:D:138:PHE:CD2	1:D:139:MET:CE	2.38	1.07
1:D:138:PHE:CD2	1:D:139:MET:HE2	1.89	1.06
1:H:20:GLU:OE1	1:H:101:PHE:HB2	1.59	1.02
1:E:156:GLU:OE1	1:E:176:THR:CG2	2.11	0.98
1:L:253:ILE:CG2	1:L:263:VAL:HG11	1.96	0.94
1:J:20:GLU:OE1	1:J:101:PHE:HB2	1.66	0.94
1:D:156:GLU:HG3	1:D:176:THR:HG22	1.47	0.94
1:D:138:PHE:HD2	1:D:139:MET:CE	1.77	0.88
1:B:245:LEU:CD2	1:B:273:LEU:HD11	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:302:ATP:O1G	6:D:421:HOH:O	1.92	0.87
1:D:138:PHE:CE2	1:D:139:MET:CE	2.57	0.86
1:H:20:GLU:OE1	1:H:101:PHE:CB	2.23	0.85
1:B:83:GLU:OE2	6:B:430:HOH:O	1.98	0.81
1:G:229:ILE:HD13	1:G:245:LEU:HD21	1.63	0.81
1:C:206:LYS:NZ	6:C:416:HOH:O	2.11	0.81
1:K:38:SER:O	1:K:52:ARG:NH2	2.13	0.80
1:D:156:GLU:HG3	1:D:176:THR:CG2	2.12	0.80
1:H:20:GLU:OE1	1:H:101:PHE:CD2	2.36	0.79
1:L:156:GLU:OE2	1:L:169:ASP:OD2	2.01	0.78
1:L:253:ILE:HG22	1:L:263:VAL:HG11	1.65	0.78
1:H:156:GLU:OE1	1:H:169:ASP:OD2	2.00	0.77
1:H:20:GLU:OE1	1:H:101:PHE:CG	2.38	0.76
1:J:163:LEU:CD2	1:L:66:VAL:CG1	2.63	0.76
1:B:235:LYS:HD2	1:A:243:ALA:HB1	1.67	0.76
1:J:20:GLU:OE1	1:J:101:PHE:CB	2.34	0.76
1:D:245:LEU:HD11	1:D:273:LEU:HD11	1.68	0.75
1:A:74:GLU:HG3	1:A:194:CYS:SG	2.27	0.75
1:J:74:GLU:HG3	1:J:194:CYS:SG	2.28	0.74
1:D:138:PHE:CE2	1:D:139:MET:HE3	2.22	0.74
1:C:74:GLU:HG3	1:C:194[A]:CYS:SG	2.27	0.74
1:G:245:LEU:HD11	1:G:273:LEU:HD11	1.69	0.74
1:K:74:GLU:HG3	1:K:194[A]:CYS:SG	2.28	0.73
1:H:38:SER:O	1:H:52:ARG:NE	2.20	0.73
1:I:74:GLU:HG3	1:I:194:CYS:SG	2.28	0.73
1:H:74:GLU:HG3	1:H:194:CYS:SG	2.28	0.73
1:F:74:GLU:HG3	1:F:194[B]:CYS:SG	2.29	0.73
1:L:253:ILE:HG23	1:L:263:VAL:HG11	1.70	0.73
1:L:74:GLU:HG3	1:L:194[B]:CYS:SG	2.29	0.72
1:D:74:GLU:HG3	1:D:194:CYS:SG	2.30	0.72
1:E:74:GLU:HG3	1:E:194:CYS:SG	2.29	0.72
1:G:74:GLU:HG3	1:G:194:CYS:SG	2.30	0.71
1:F:279:GLU:OE2	1:H:216:ARG:HD2	1.89	0.71
1:B:74:GLU:HG3	1:B:194:CYS:SG	2.31	0.70
1:D:260:GLU:HG2	1:D:261:LYS:H	1.55	0.70
1:C:296:LYS:HD3	1:K:278:MET:HE2	1.74	0.69
1:C:279:GLU:OE2	1:I:216:ARG:HD2	1.93	0.68
1:I:253:ILE:CG2	1:I:263:VAL:HG21	2.23	0.68
1:C:296:LYS:HB3	1:K:278:MET:HE1	1.75	0.67
1:G:163:LEU:CD2	1:H:66:VAL:CG1	2.73	0.67
1:A:216:ARG:HD2	1:G:279:GLU:OE2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:253:ILE:HG22	1:I:263:VAL:HG21	1.79	0.65
1:J:163:LEU:HD22	1:L:66:VAL:HG11	1.80	0.64
1:C:296:LYS:HD3	1:K:278:MET:CE	2.27	0.64
1:B:245:LEU:HD21	1:B:273:LEU:CD1	2.17	0.64
1:E:38:SER:O	1:E:52:ARG:NH1	2.32	0.62
1:J:66:VAL:HG11	1:L:163:LEU:CD2	2.30	0.62
1:I:38:SER:O	1:I:52:ARG:NH1	2.33	0.62
1:F:38:SER:O	1:F:52:ARG:NH1	2.33	0.61
1:D:138:PHE:CD2	1:D:139:MET:HE3	2.32	0.61
1:J:38:SER:O	1:J:52:ARG:NH1	2.33	0.61
1:L:235:LYS:HG2	1:L:263:VAL:HG23	1.83	0.61
1:C:38:SER:O	1:C:52:ARG:NH1	2.34	0.60
1:C:290:LEU:HD11	1:I:268:VAL:HG21	1.84	0.60
1:G:163:LEU:CD2	1:H:66:VAL:HG11	2.32	0.60
1:G:50:ILE:HD12	1:G:50:ILE:N	2.17	0.59
1:D:260:GLU:N	1:D:260:GLU:OE1	2.35	0.59
1:I:254:LEU:O	1:I:263:VAL:HG23	2.02	0.59
1:C:108:LEU:HD11	1:C:139:MET:HE1	1.85	0.58
1:C:216:ARG:HD2	1:K:279:GLU:OE2	2.04	0.58
1:G:216:ARG:HG2	1:J:275:TRP:CD2	2.39	0.57
1:G:163:LEU:HD22	1:H:66:VAL:HG11	1.86	0.57
1:B:156:GLU:HG2	1:C:39:LEU:HD11	1.86	0.56
1:J:66:VAL:CG1	1:L:163:LEU:CD2	2.83	0.56
1:G:216:ARG:HD2	1:J:279:GLU:OE2	2.04	0.56
1:K:170:LEU:HD23	4:K:302:ATP:C2	2.40	0.56
1:B:16:ARG:HD3	4:B:303:ATP:C5	2.40	0.55
1:D:54:ARG:HD2	6:D:425:HOH:O	2.05	0.55
1:D:245:LEU:HD11	1:D:273:LEU:CD1	2.35	0.55
1:D:245:LEU:HD21	1:D:273:LEU:HD11	1.88	0.55
1:A:66:VAL:CG1	1:F:163:LEU:CD2	2.85	0.54
1:I:12:GLN:NE2	1:I:17:LEU:H	2.05	0.54
1:E:156:GLU:OE1	1:E:176:THR:HG22	2.05	0.54
1:L:273:LEU:CD2	1:L:277:THR:HB	2.38	0.54
1:I:108:LEU:O	1:I:185:VAL:HG12	2.08	0.54
1:C:216:ARG:HG2	1:K:275:TRP:CD2	2.43	0.54
1:J:20:GLU:OE1	1:J:101:PHE:CG	2.61	0.54
1:J:163:LEU:CD2	1:L:66:VAL:HG11	2.36	0.54
1:C:275:TRP:CD2	1:I:216:ARG:HG2	2.43	0.53
1:C:84:ARG:HD3	6:C:415:HOH:O	2.07	0.53
1:D:138:PHE:HE2	1:D:139:MET:HE3	1.68	0.53
1:J:163:LEU:HD22	1:L:66:VAL:CG1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HB2	6:A:425:HOH:O	2.09	0.53
1:B:156:GLU:HG2	1:C:39:LEU:CD1	2.39	0.53
1:A:54:ARG:NH1	1:F:54:ARG:HH22	2.07	0.53
1:B:298:LEU:HD13	1:D:282:LYS:HG3	1.91	0.53
1:I:254:LEU:O	1:I:263:VAL:CG2	2.56	0.53
1:B:235:LYS:HD2	1:A:243:ALA:CB	2.36	0.52
1:C:289:ILE:O	1:I:297:MET:HA	2.08	0.52
4:J:303:ATP:O2G	6:J:420:HOH:O	2.19	0.52
1:K:230:MET:HG2	1:K:266:HIS:ND1	2.25	0.51
1:B:156:GLU:OE1	1:B:169:ASP:OD2	2.28	0.51
1:A:172:SER:CB	4:A:302:ATP:N6	2.74	0.51
1:B:172:SER:CB	4:B:303:ATP:N6	2.74	0.51
1:L:254:LEU:O	1:L:263:VAL:HG13	2.11	0.51
1:D:138:PHE:CE2	1:D:139:MET:HE1	2.46	0.50
1:G:245:LEU:HD11	1:G:273:LEU:CD1	2.41	0.50
1:D:260:GLU:HG2	1:D:261:LYS:N	2.25	0.50
1:L:273:LEU:HD21	1:L:277:THR:CG2	2.41	0.49
1:C:290:LEU:HD11	1:I:268:VAL:CG2	2.42	0.49
1:D:274:PHE:HB3	6:D:409:HOH:O	2.13	0.49
1:G:50:ILE:CD1	1:G:50:ILE:N	2.76	0.49
1:C:119:LEU:HD23	1:C:144:ILE:HD12	1.94	0.49
4:J:303:ATP:PG	6:J:420:HOH:O	2.69	0.49
1:B:52:ARG:HH11	1:B:52:ARG:HG2	1.78	0.49
1:J:20:GLU:OE1	1:J:101:PHE:CD2	2.66	0.49
1:L:119:LEU:HD23	1:L:144:ILE:CD1	2.43	0.49
1:B:163:LEU:CD2	1:C:66:VAL:CG1	2.90	0.48
1:L:119:LEU:HD23	1:L:144:ILE:HD12	1.94	0.48
1:J:128:ALA:HA	1:J:149:CYS:O	2.14	0.48
1:I:279:GLU:OE2	1:K:216:ARG:HD2	2.14	0.48
1:C:119:LEU:HD23	1:C:144:ILE:CD1	2.43	0.48
1:D:128:ALA:HA	1:D:149:CYS:O	2.14	0.48
1:F:216:ARG:HD2	1:L:279:GLU:OE2	2.11	0.48
1:F:289:ILE:O	1:H:297:MET:HA	2.14	0.48
1:I:128:ALA:HA	1:I:149:CYS:O	2.14	0.47
1:L:128:ALA:HA	1:L:149:CYS:O	2.14	0.47
1:A:16:ARG:HD3	4:A:302:ATP:C5	2.49	0.47
1:F:128:ALA:HA	1:F:149:CYS:O	2.14	0.47
1:E:163:LEU:CD2	1:K:66:VAL:CG1	2.93	0.47
1:G:128:ALA:HA	1:G:149:CYS:O	2.14	0.47
1:L:40:ILE:O	1:L:40:ILE:HG23	2.14	0.47
1:B:163:LEU:CD2	1:C:66:VAL:HG11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LYS:HD3	1:E:298:LEU:CD2	2.44	0.47
1:H:128:ALA:HA	1:H:149:CYS:O	2.14	0.47
1:E:128:ALA:HA	1:E:149:CYS:O	2.15	0.47
1:K:128:ALA:HA	1:K:149:CYS:O	2.14	0.47
1:L:9:ILE:HD13	1:L:25:LEU:HD11	1.96	0.47
1:J:163:LEU:HD23	1:L:66:VAL:CG1	2.45	0.47
1:C:128:ALA:HA	1:C:149:CYS:O	2.15	0.47
1:C:291:VAL:HB	1:I:296:LYS:HB2	1.97	0.47
1:D:172:SER:CB	4:D:302:ATP:N6	2.78	0.47
1:J:66:VAL:HG11	1:L:163:LEU:HD22	1.96	0.47
1:B:118:ASN:HD21	1:B:120:LYS:HB2	1.79	0.47
1:B:128:ALA:HA	1:B:149:CYS:O	2.14	0.46
1:A:66:VAL:HG11	1:F:163:LEU:HD22	1.97	0.46
1:B:8:ARG:NH1	1:C:161:ALA:O	2.42	0.46
1:C:297:MET:HA	1:K:289:ILE:O	2.16	0.46
1:J:114:ASN:O	1:J:183:LYS:NZ	2.42	0.46
1:A:279:GLU:OE2	1:J:216:ARG:HD2	2.16	0.45
1:F:216:ARG:HG2	1:L:275:TRP:CD2	2.51	0.45
1:J:163:LEU:HD23	1:L:66:VAL:HG13	1.98	0.45
1:D:138:PHE:HE2	1:D:139:MET:CE	2.19	0.45
1:A:128:ALA:HA	1:A:149:CYS:O	2.16	0.44
1:D:273:LEU:HD23	1:D:278:MET:SD	2.57	0.44
1:G:48:ILE:HG22	1:G:50:ILE:HD12	1.99	0.44
1:D:156:GLU:CG	1:D:176:THR:CG2	2.91	0.44
1:F:83:GLU:OE2	6:F:428:HOH:O	2.21	0.44
1:L:263:VAL:HG12	1:L:264:ALA:N	2.32	0.44
1:E:66:VAL:CG1	1:K:163:LEU:CD2	2.95	0.44
1:J:66:VAL:CG1	1:L:163:LEU:HD21	2.48	0.44
1:H:78:GLU:OE1	1:H:189:TYR:OH	2.32	0.44
1:L:16:ARG:HD2	4:L:302:ATP:C4	2.52	0.44
1:G:138:PHE:HD1	1:G:139:MET:CE	2.31	0.43
1:C:156:GLU:OE1	1:C:176:THR:HB	2.18	0.43
1:C:273:LEU:HD23	1:C:278:MET:SD	2.59	0.43
1:I:12:GLN:HE22	1:I:17:LEU:H	1.67	0.43
1:G:273:LEU:HD23	1:G:278:MET:SD	2.59	0.43
1:G:49:ASP:C	1:G:50:ILE:HD12	2.39	0.43
1:L:254:LEU:O	1:L:263:VAL:CG1	2.66	0.43
1:F:273:LEU:HD23	1:F:278:MET:SD	2.59	0.43
1:B:238:LEU:HD11	1:B:265:LEU:HD13	2.01	0.43
1:H:171:VAL:CG2	1:H:172:SER:N	2.82	0.43
1:L:54:ARG:NH2	4:L:302:ATP:O3G	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:LEU:HD23	1:E:278:MET:SD	2.59	0.42
1:G:238:LEU:HD23	1:G:238:LEU:HA	1.92	0.42
1:C:108:LEU:HD11	1:C:139:MET:CE	2.49	0.42
1:H:171:VAL:HG22	1:H:172:SER:N	2.35	0.42
1:J:273:LEU:HD23	1:J:278:MET:SD	2.59	0.42
1:L:9:ILE:CG2	1:L:50:ILE:HG13	2.50	0.42
1:A:273:LEU:HD23	1:A:278:MET:SD	2.60	0.41
1:B:273:LEU:HD23	1:B:278:MET:SD	2.59	0.41
1:I:273:LEU:HD23	1:I:278:MET:SD	2.59	0.41
1:A:113:GLU:CB	6:A:414:HOH:O	2.67	0.41
1:A:220:VAL:O	1:A:224:ARG:HG3	2.21	0.41
1:B:297:MET:HA	1:D:289:ILE:O	2.20	0.41
1:F:290:LEU:HD11	1:H:268:VAL:HG21	2.01	0.41
1:G:170:LEU:HD23	4:G:302:ATP:C2	2.54	0.41
1:E:78:GLU:OE1	1:E:189:TYR:OH	2.32	0.41
1:G:48:ILE:HG22	1:G:50:ILE:CD1	2.50	0.41
1:K:229:ILE:HD11	1:K:273:LEU:HD13	2.03	0.41
1:L:116:PHE:CE2	1:L:185:VAL:HG13	2.55	0.41
1:L:9:ILE:O	1:L:9:ILE:HG23	2.21	0.41
1:F:116:PHE:CE2	1:F:185:VAL:HG13	2.56	0.41
1:I:170:LEU:HD23	4:I:303:ATP:C2	2.55	0.41
1:C:135:LEU:HD11	1:C:139:MET:HE3	2.03	0.41
1:D:54:ARG:NH1	1:I:152:THR:HB	2.36	0.41
1:L:273:LEU:HD23	1:L:277:THR:HB	2.01	0.41
1:B:238:LEU:HA	1:B:238:LEU:HD12	1.82	0.40
1:C:116:PHE:CE2	1:C:185:VAL:HG13	2.56	0.40
1:I:156:GLU:OE2	1:I:169:ASP:OD2	2.38	0.40
1:A:54:ARG:NH1	1:F:54:ARG:NH2	2.69	0.40
1:G:138:PHE:CD1	1:G:139:MET:HE1	2.56	0.40
1:J:229:ILE:HD11	1:J:273:LEU:HD13	2.04	0.40

All (2) 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:F:118:ASN:ND2	1:J:235:LYS:O[1_445]	1.72	0.48
1:E:235:LYS:NZ	1:K:141:GLU:OE2[1_655]	2.09	0.11

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	294/300 (98%)	291 (99%)	3 (1%)	0	100	100
1	B	294/300 (98%)	291 (99%)	3 (1%)	0	100	100
1	C	291/300 (97%)	288 (99%)	3 (1%)	0	100	100
1	D	290/300 (97%)	287 (99%)	3 (1%)	0	100	100
1	E	293/300 (98%)	290 (99%)	3 (1%)	0	100	100
1	F	290/300 (97%)	287 (99%)	3 (1%)	0	100	100
1	G	288/300 (96%)	285 (99%)	3 (1%)	0	100	100
1	H	294/300 (98%)	291 (99%)	3 (1%)	0	100	100
1	I	288/300 (96%)	284 (99%)	4 (1%)	0	100	100
1	J	294/300 (98%)	291 (99%)	3 (1%)	0	100	100
1	K	291/300 (97%)	288 (99%)	3 (1%)	0	100	100
1	L	290/300 (97%)	287 (99%)	3 (1%)	0	100	100
All	All	3497/3600 (97%)	3460 (99%)	37 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	227/263 (86%)	225 (99%)	2 (1%)	78	88
1	B	234/263 (89%)	231 (99%)	3 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	228/263 (87%)	225 (99%)	3 (1%)	69 81
1	D	219/263 (83%)	218 (100%)	1 (0%)	88 94
1	E	229/263 (87%)	225 (98%)	4 (2%)	60 74
1	F	228/263 (87%)	223 (98%)	5 (2%)	52 65
1	G	218/263 (83%)	216 (99%)	2 (1%)	78 88
1	H	215/263 (82%)	213 (99%)	2 (1%)	78 88
1	I	223/263 (85%)	220 (99%)	3 (1%)	69 81
1	J	230/263 (88%)	227 (99%)	3 (1%)	69 81
1	K	218/263 (83%)	215 (99%)	3 (1%)	67 80
1	L	215/263 (82%)	212 (99%)	3 (1%)	67 80
All	All	2684/3156 (85%)	2650 (99%)	34 (1%)	69 81

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	HIS
1	B	185	VAL
1	B	213	ILE
1	C	83	GLU
1	C	185	VAL
1	C	265	LEU
1	D	265	LEU
1	E	170	LEU
1	E	171	VAL
1	E	185	VAL
1	E	265	LEU
1	I	35	HIS
1	I	170	LEU
1	I	265	LEU
1	K	170	LEU
1	K	265	LEU
1	K	267	MET
1	A	170	LEU
1	A	265	LEU
1	F	114	ASN
1	F	170	LEU
1	F	181	ASN
1	F	185	VAL

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Mol	Chain	Res	Type
1	F	265	LEU
1	G	170	LEU
1	G	265	LEU
1	H	185	VAL
1	H	265	LEU
1	J	35	HIS
1	J	185	VAL
1	J	265	LEU
1	L	185	VAL
1	L	192	ARG
1	L	273	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	85	GLN
1	B	133	GLN
1	B	145	ASN
1	D	35	HIS
1	D	148	ASN
1	E	85	GLN
1	E	118	ASN
1	E	148	ASN
1	I	12	GLN
1	I	85	GLN
1	I	148	ASN
1	A	80	ASN
1	G	85	GLN
1	G	242	GLN
1	H	148	ASN
1	J	85	GLN
1	J	133	GLN
1	L	133	GLN

5.3.3 RNA

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 31 ligands modelled in this entry, 12 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	G	302	2	26,33,33	1.04	2 (7%)	31,52,52	1.37	3 (9%)
4	ATP	D	302	2	26,33,33	0.96	1 (3%)	31,52,52	1.51	6 (19%)
3	PO4	J	302	-	4,4,4	0.82	0	6,6,6	0.49	0
4	ATP	K	302	2	26,33,33	1.03	2 (7%)	31,52,52	1.46	4 (12%)
4	ATP	H	302	2	26,33,33	0.96	2 (7%)	31,52,52	1.33	3 (9%)
3	PO4	I	302	-	4,4,4	0.85	0	6,6,6	0.44	0
4	ATP	F	302	2	26,33,33	1.18	3 (11%)	31,52,52	1.37	6 (19%)
4	ATP	L	302	2	26,33,33	1.06	2 (7%)	31,52,52	1.44	4 (12%)
4	ATP	A	302	2	26,33,33	1.11	2 (7%)	31,52,52	1.33	3 (9%)
3	PO4	B	302	-	4,4,4	0.83	0	6,6,6	0.54	0
4	ATP	I	303	2	26,33,33	0.95	2 (7%)	31,52,52	1.56	6 (19%)
4	ATP	C	304	2	26,33,33	1.11	3 (11%)	31,52,52	1.54	4 (12%)
4	ATP	E	303	2	26,33,33	1.02	2 (7%)	31,52,52	1.40	6 (19%)
4	ATP	B	303	2	26,33,33	0.99	2 (7%)	31,52,52	1.37	4 (12%)
3	PO4	C	302	-	4,4,4	0.96	0	6,6,6	0.49	0
5	ACY	J	304	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-
3	PO4	E	302	-	4,4,4	0.76	0	6,6,6	0.58	0
4	ATP	J	303	2	26,33,33	0.94	2 (7%)	31,52,52	1.68	7 (22%)
3	PO4	C	303	-	4,4,4	0.87	0	6,6,6	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	G	302	2	-	1/18/38/38	0/3/3/3
4	ATP	D	302	2	-	0/18/38/38	0/3/3/3
4	ATP	F	302	2	-	2/18/38/38	0/3/3/3
4	ATP	K	302	2	-	5/18/38/38	0/3/3/3
4	ATP	H	302	2	-	3/18/38/38	0/3/3/3
4	ATP	L	302	2	-	7/18/38/38	0/3/3/3
4	ATP	A	302	2	-	2/18/38/38	0/3/3/3
4	ATP	I	303	2	-	4/18/38/38	0/3/3/3
4	ATP	C	304	2	-	3/18/38/38	0/3/3/3
4	ATP	E	303	2	-	8/18/38/38	0/3/3/3
4	ATP	B	303	2	-	3/18/38/38	0/3/3/3
4	ATP	J	303	2	-	2/18/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	304	ATP	C2-N3	3.13	1.37	1.32
4	F	302	ATP	C2-N3	2.82	1.36	1.32
4	K	302	ATP	C5-C4	2.69	1.48	1.40
4	B	303	ATP	C2-N3	2.67	1.36	1.32
4	F	302	ATP	O4'-C1'	2.67	1.44	1.41
4	L	302	ATP	C2-N3	2.64	1.36	1.32
4	G	302	ATP	C2-N3	2.61	1.36	1.32
4	E	303	ATP	C5-C4	2.59	1.47	1.40
4	L	302	ATP	C5-C4	2.58	1.47	1.40
4	H	302	ATP	C5-C4	2.56	1.47	1.40
4	E	303	ATP	C2-N3	2.55	1.36	1.32
4	D	302	ATP	C5-C4	2.54	1.47	1.40
4	B	303	ATP	C5-C4	2.52	1.47	1.40
4	G	302	ATP	C5-C4	2.51	1.47	1.40
4	A	302	ATP	C2-N3	2.48	1.36	1.32
4	F	302	ATP	C5-C4	2.46	1.47	1.40
4	A	302	ATP	C5-C4	2.45	1.47	1.40
4	J	303	ATP	C2-N3	2.43	1.36	1.32
4	I	303	ATP	C5-C4	2.41	1.47	1.40
4	I	303	ATP	C2-N3	2.35	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	304	ATP	C5-C4	2.35	1.47	1.40
4	J	303	ATP	C5-C4	2.35	1.47	1.40
5	J	304	ACY	CH3-C	2.26	1.51	1.48
4	K	302	ATP	C2-N3	2.25	1.35	1.32
4	C	304	ATP	C6-C5	2.15	1.51	1.43
4	H	302	ATP	C2-N3	2.06	1.35	1.32

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	303	ATP	PB-O3B-PG	-4.89	116.04	132.83
4	D	302	ATP	N3-C2-N1	-4.25	122.04	128.68
4	H	302	ATP	N3-C2-N1	-4.08	122.30	128.68
4	I	303	ATP	N3-C2-N1	-3.98	122.46	128.68
4	L	302	ATP	N3-C2-N1	-3.97	122.47	128.68
4	K	302	ATP	N3-C2-N1	-3.97	122.47	128.68
4	B	303	ATP	N3-C2-N1	-3.87	122.62	128.68
4	F	302	ATP	N3-C2-N1	-3.86	122.65	128.68
4	G	302	ATP	N3-C2-N1	-3.78	122.76	128.68
4	J	303	ATP	N3-C2-N1	-3.70	122.89	128.68
4	C	304	ATP	N3-C2-N1	-3.67	122.94	128.68
4	A	302	ATP	N3-C2-N1	-3.63	123.00	128.68
4	C	304	ATP	C4-C5-N7	-3.53	105.72	109.40
4	I	303	ATP	C3'-C2'-C1'	3.39	106.08	100.98
4	E	303	ATP	N3-C2-N1	-3.37	123.42	128.68
4	C	304	ATP	C3'-C2'-C1'	3.14	105.71	100.98
4	B	303	ATP	C4-C5-N7	-3.06	106.21	109.40
4	L	302	ATP	C4-C5-N7	-3.05	106.22	109.40
4	G	302	ATP	C4-C5-N7	-3.02	106.25	109.40
4	K	302	ATP	C4-C5-N7	-3.00	106.27	109.40
4	A	302	ATP	C3'-C2'-C1'	2.94	105.40	100.98
4	J	303	ATP	C3'-C2'-C1'	2.89	105.33	100.98
4	G	302	ATP	C3'-C2'-C1'	2.88	105.32	100.98
4	J	303	ATP	C4-C5-N7	-2.71	106.58	109.40
4	E	303	ATP	C3'-C2'-C1'	2.66	104.98	100.98
4	C	304	ATP	O3G-PG-O3B	2.64	113.48	104.64
4	K	302	ATP	C3'-C2'-C1'	2.59	104.87	100.98
4	F	302	ATP	O2A-PA-O1A	2.54	124.78	112.24
4	J	303	ATP	O3G-PG-O2G	2.53	117.30	107.64
4	E	303	ATP	PA-O3A-PB	-2.47	124.35	132.83
4	J	303	ATP	O2A-PA-O1A	2.43	124.26	112.24
4	L	302	ATP	C2'-C3'-C4'	-2.37	98.04	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	302	ATP	C4-C5-N7	-2.36	106.94	109.40
4	E	303	ATP	O3G-PG-O2G	2.34	116.60	107.64
4	D	302	ATP	C3'-C2'-C1'	2.32	104.47	100.98
4	F	302	ATP	O3B-PG-O1G	-2.27	98.58	111.19
4	K	302	ATP	PA-O3A-PB	-2.27	125.03	132.83
4	D	302	ATP	C2-N1-C6	2.25	122.61	118.75
4	I	303	ATP	O2G-PG-O3B	2.23	112.13	104.64
4	D	302	ATP	PB-O3B-PG	-2.22	125.21	132.83
4	B	303	ATP	O2A-PA-O1A	2.21	123.18	112.24
4	B	303	ATP	C3'-C2'-C1'	2.17	104.25	100.98
4	F	302	ATP	PA-O3A-PB	-2.17	125.39	132.83
4	H	302	ATP	O3B-PG-O1G	-2.16	99.18	111.19
4	E	303	ATP	O2A-PA-O1A	2.16	122.94	112.24
4	A	302	ATP	C4-C5-N7	-2.14	107.17	109.40
4	J	303	ATP	O2B-PB-O1B	2.13	122.75	112.24
4	H	302	ATP	C2-N1-C6	2.08	122.31	118.75
4	D	302	ATP	PA-O3A-PB	-2.08	125.69	132.83
4	F	302	ATP	O2G-PG-O3B	2.06	111.53	104.64
4	I	303	ATP	O3G-PG-O2G	2.04	115.43	107.64
4	F	302	ATP	C4-C5-N7	-2.04	107.28	109.40
4	E	303	ATP	N6-C6-N1	2.03	122.79	118.57
4	L	302	ATP	O3G-PG-O2G	2.03	115.39	107.64
4	I	303	ATP	O2A-PA-O1A	2.01	122.18	112.24
4	I	303	ATP	O3B-PG-O1G	-2.01	100.06	111.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	302	ATP	C5'-O5'-PA-O3A
4	K	302	ATP	C5'-O5'-PA-O1A
4	K	302	ATP	O4'-C4'-C5'-O5'
4	K	302	ATP	C3'-C4'-C5'-O5'
4	L	302	ATP	PB-O3B-PG-O3G
4	L	302	ATP	C5'-O5'-PA-O3A
4	E	303	ATP	C5'-O5'-PA-O1A
4	E	303	ATP	C5'-O5'-PA-O3A
4	G	302	ATP	PB-O3B-PG-O1G
4	J	303	ATP	C5'-O5'-PA-O3A
4	I	303	ATP	C5'-O5'-PA-O3A
4	I	303	ATP	PB-O3A-PA-O1A
4	L	302	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	L	302	ATP	C5'-O5'-PA-O2A
4	E	303	ATP	C5'-O5'-PA-O2A
4	E	303	ATP	PG-O3B-PB-O1B
4	A	302	ATP	PB-O3A-PA-O1A
4	H	302	ATP	PG-O3B-PB-O1B
4	K	302	ATP	PG-O3B-PB-O2B
4	F	302	ATP	PG-O3B-PB-O1B
4	L	302	ATP	O4'-C4'-C5'-O5'
4	B	303	ATP	PB-O3B-PG-O2G
4	B	303	ATP	PB-O3B-PG-O3G
4	L	302	ATP	PB-O3B-PG-O2G
4	K	302	ATP	C5'-O5'-PA-O3A
4	E	303	ATP	O4'-C4'-C5'-O5'
4	A	302	ATP	PA-O3A-PB-O1B
4	B	303	ATP	PG-O3B-PB-O2B
4	H	302	ATP	PG-O3B-PB-O2B
4	I	303	ATP	PG-O3B-PB-O2B
4	I	303	ATP	PB-O3A-PA-O2A
4	F	302	ATP	PG-O3B-PB-O2B
4	E	303	ATP	PG-O3B-PB-O2B
4	E	303	ATP	PA-O3A-PB-O1B
4	E	303	ATP	PB-O3A-PA-O2A
4	C	304	ATP	PG-O3B-PB-O2B
4	C	304	ATP	PA-O3A-PB-O1B
4	C	304	ATP	PA-O3A-PB-O2B
4	J	303	ATP	C5'-O5'-PA-O1A
4	L	302	ATP	PB-O3B-PG-O1G

There are no ring outliers.

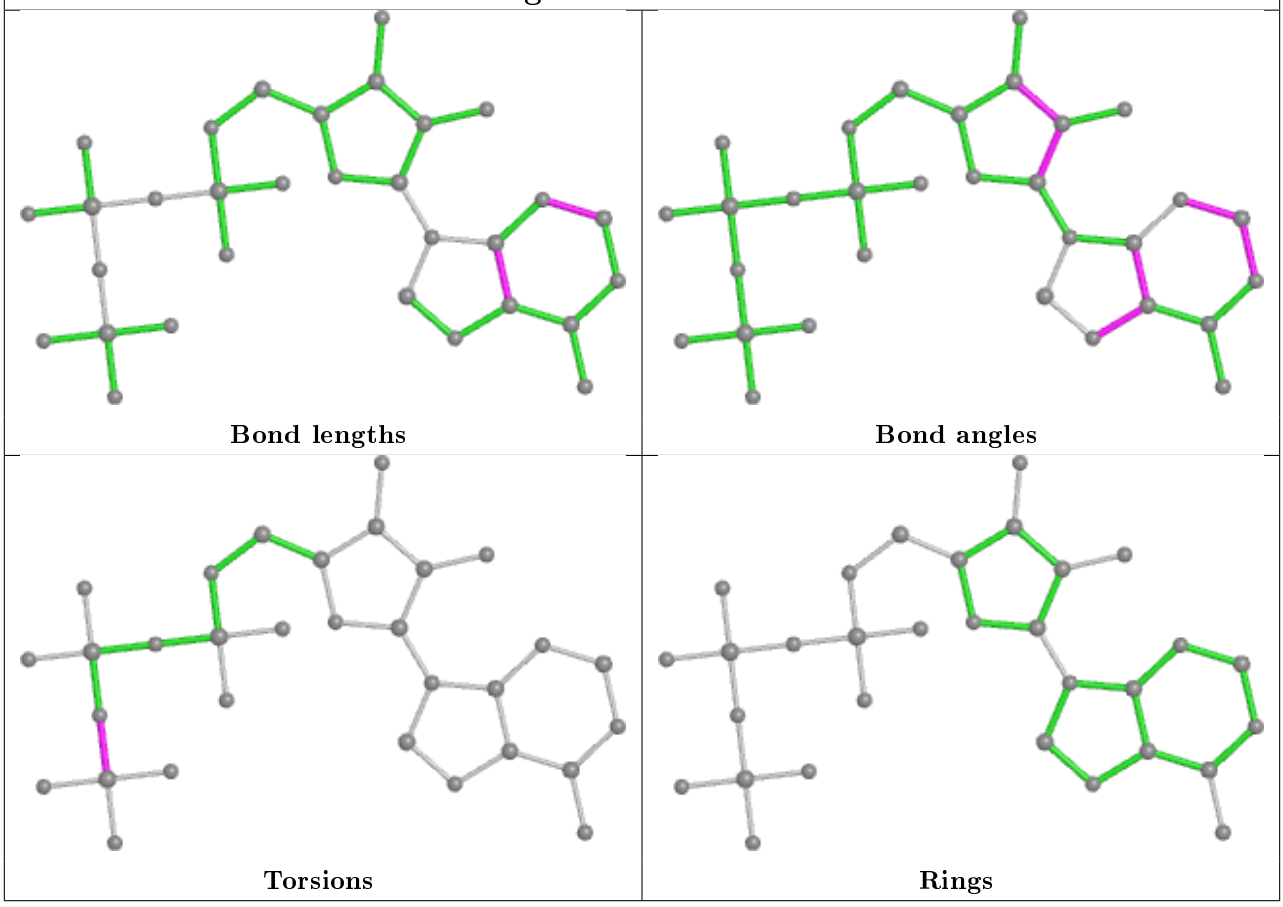
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	302	ATP	1	0
4	D	302	ATP	2	0
4	K	302	ATP	1	0
4	L	302	ATP	2	0
4	A	302	ATP	2	0
4	I	303	ATP	1	0
4	B	303	ATP	2	0
4	J	303	ATP	2	0

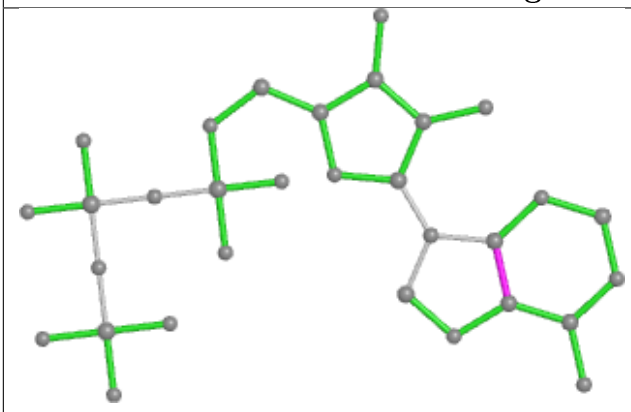
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

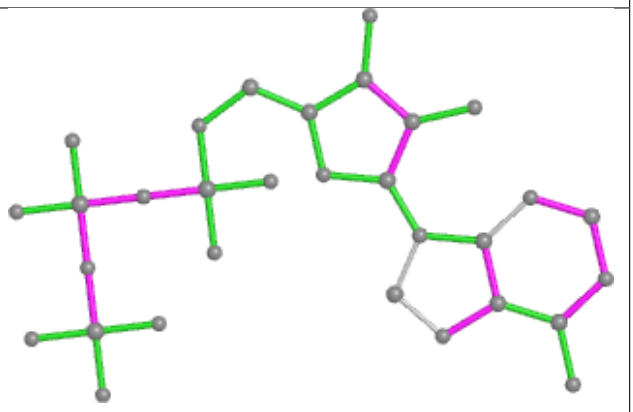
Ligand ATP G 302



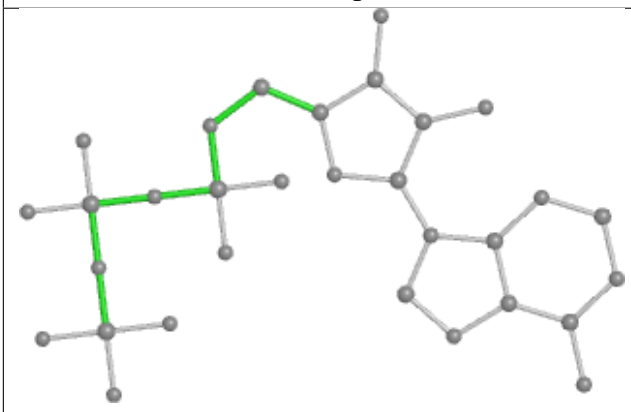
Ligand ATP D 302



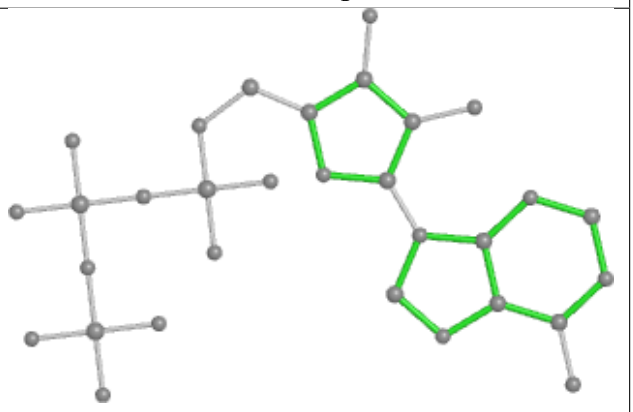
Bond lengths



Bond angles

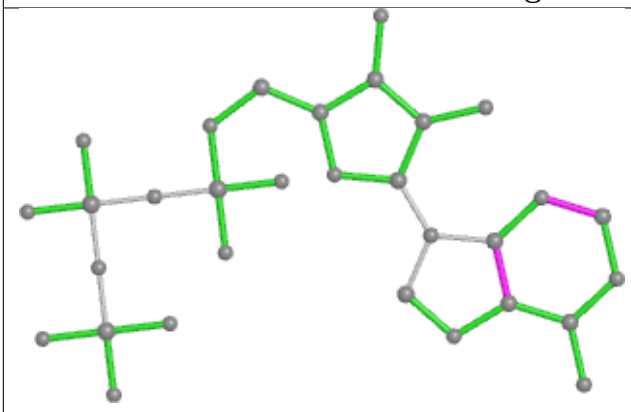


Torsions

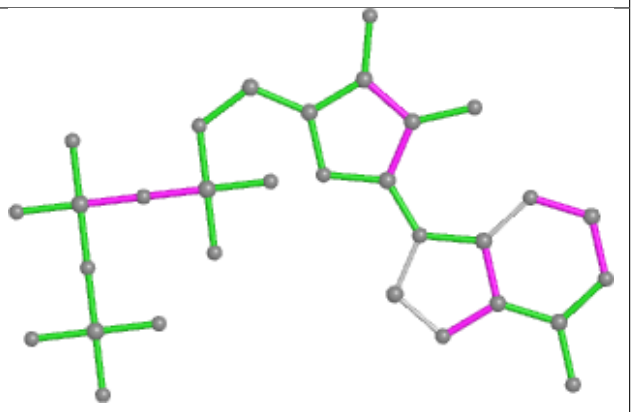


Rings

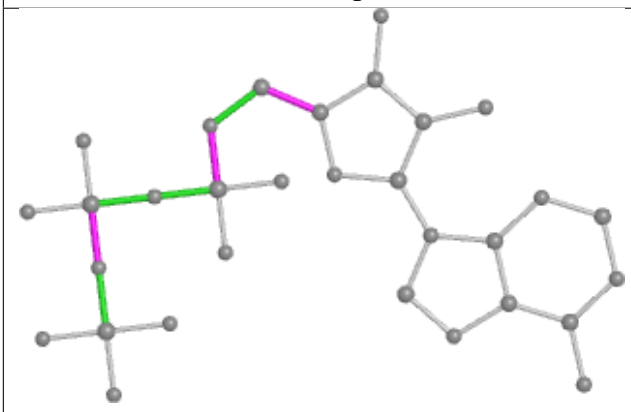
Ligand ATP K 302



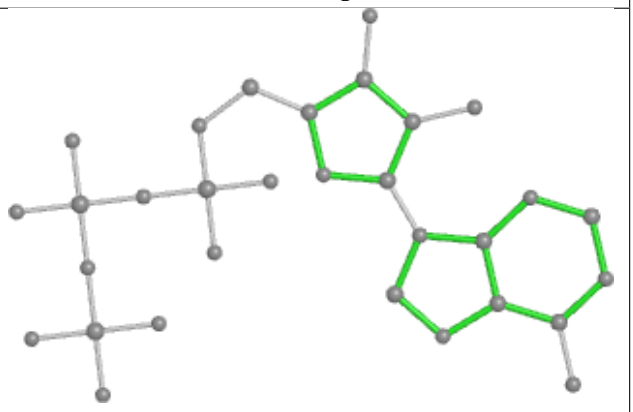
Bond lengths



Bond angles

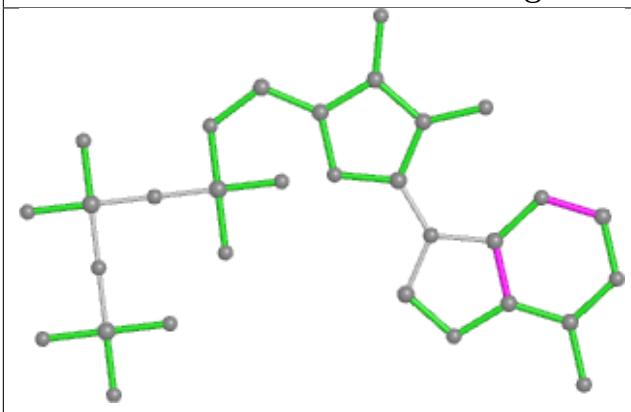


Torsions

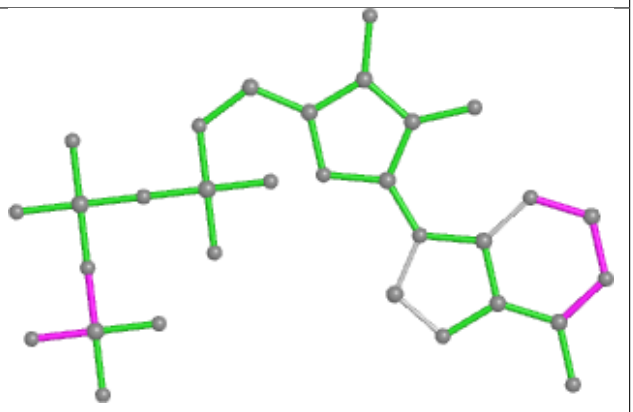


Rings

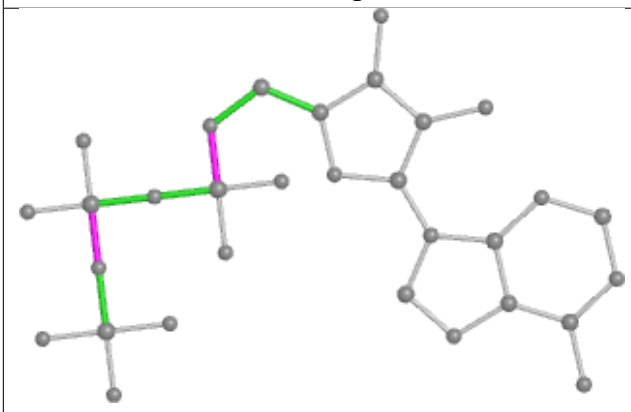
Ligand ATP H 302



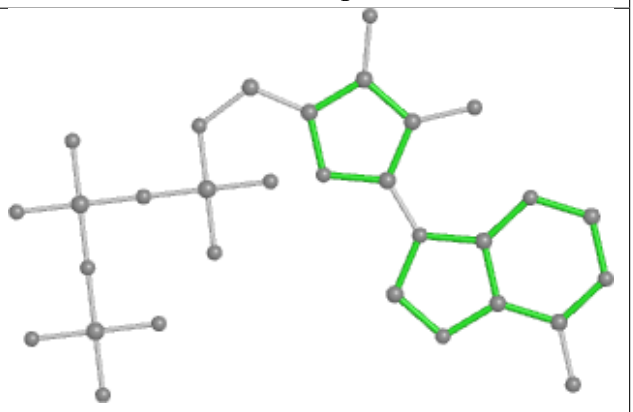
Bond lengths



Bond angles

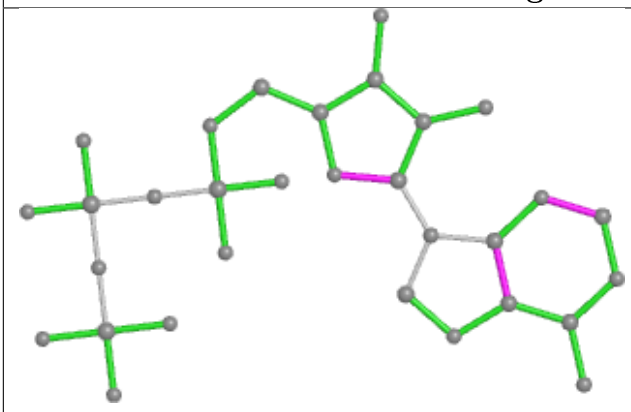


Torsions

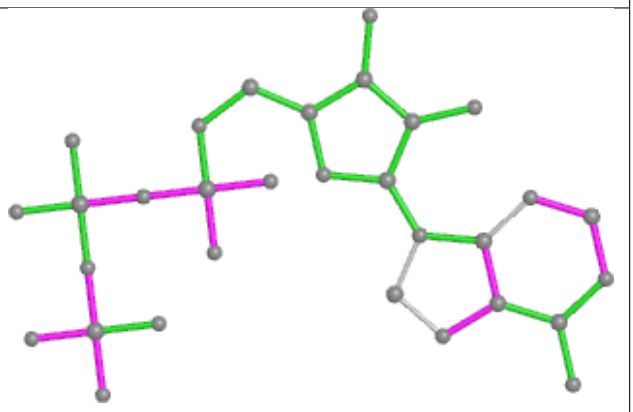


Rings

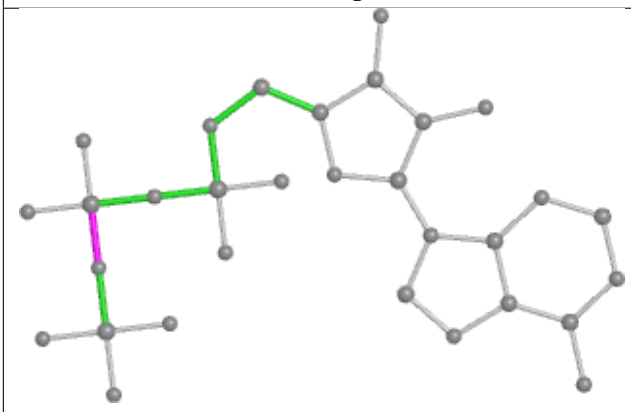
Ligand ATP F 302



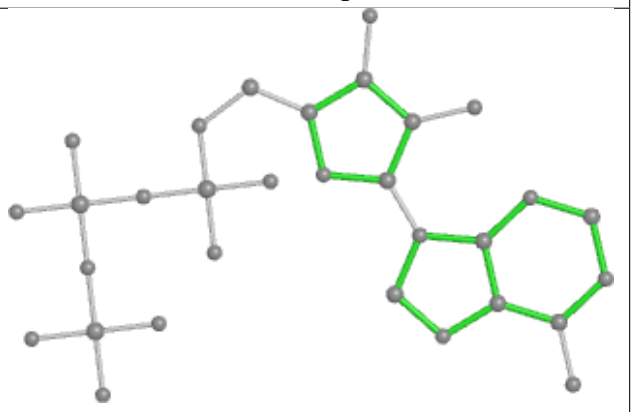
Bond lengths



Bond angles

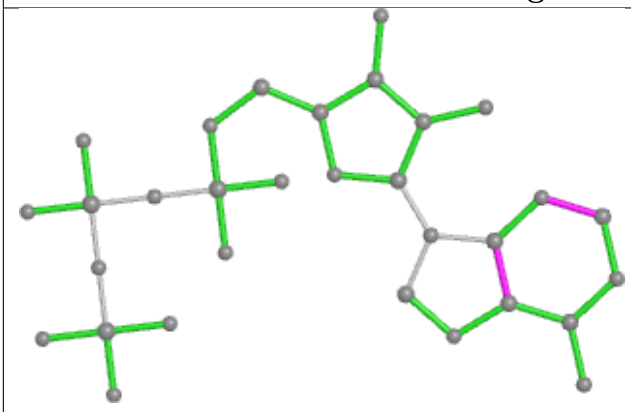


Torsions

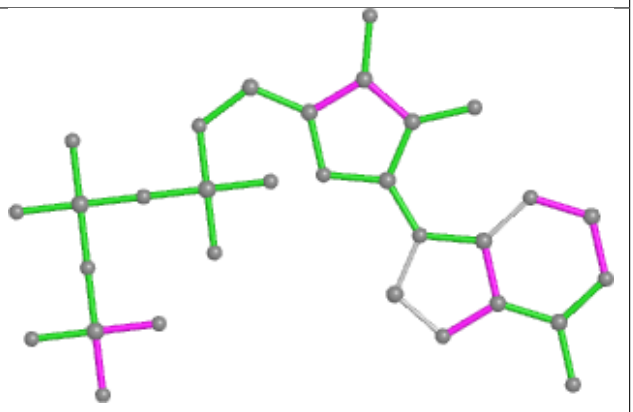


Rings

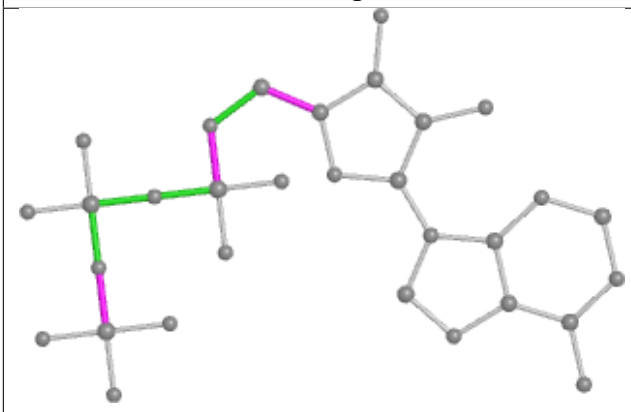
Ligand ATP L 302



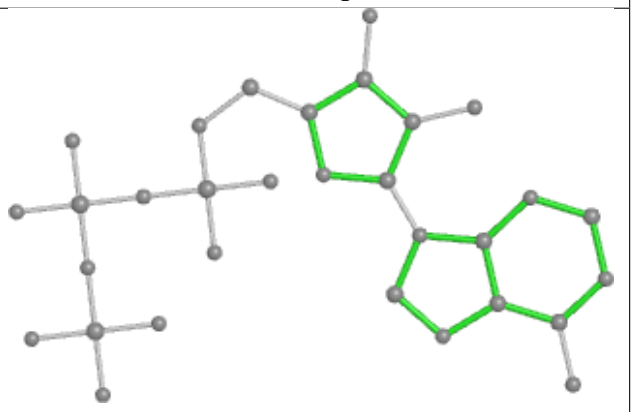
Bond lengths



Bond angles

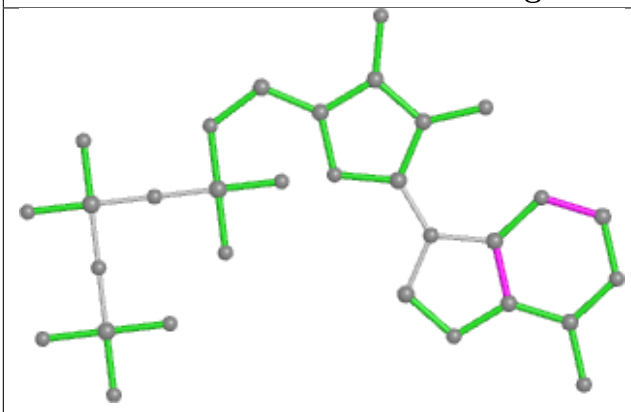


Torsions



Rings

Ligand ATP A 302



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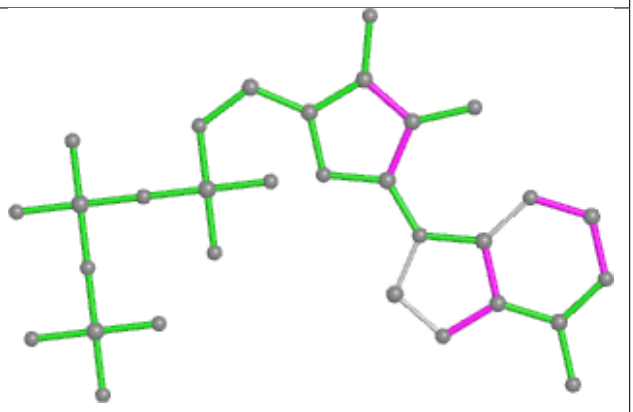
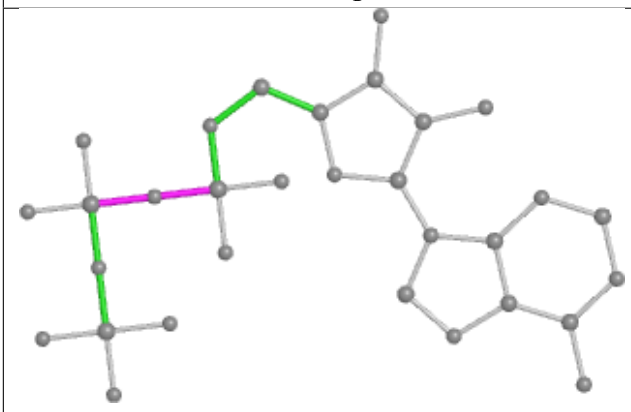
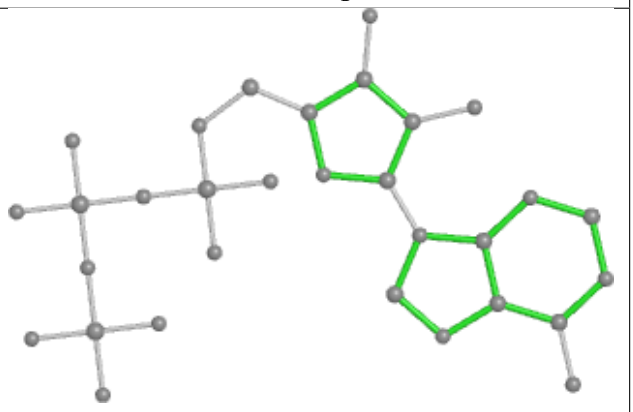


Bond angles

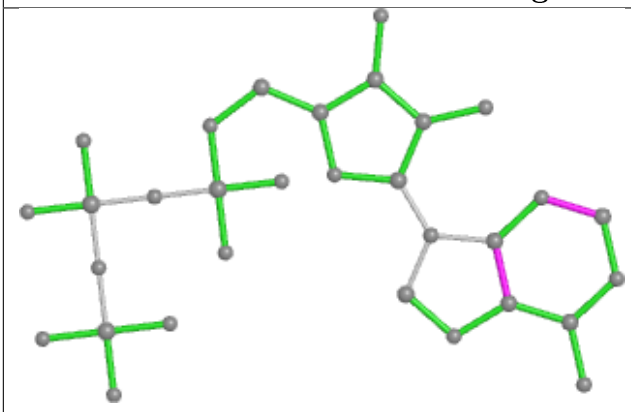


Torsions

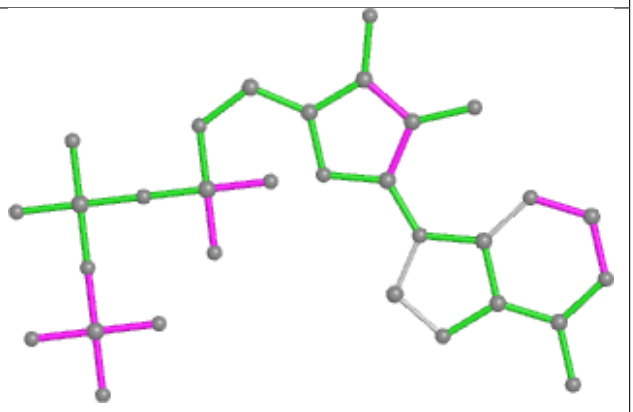


Rings

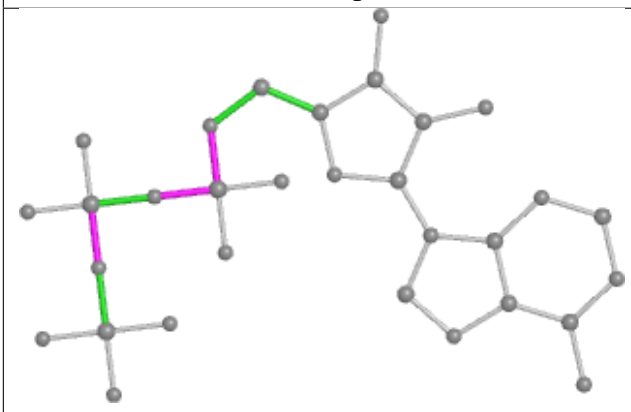
Ligand ATP I 303



Bond lengths



Bond angles



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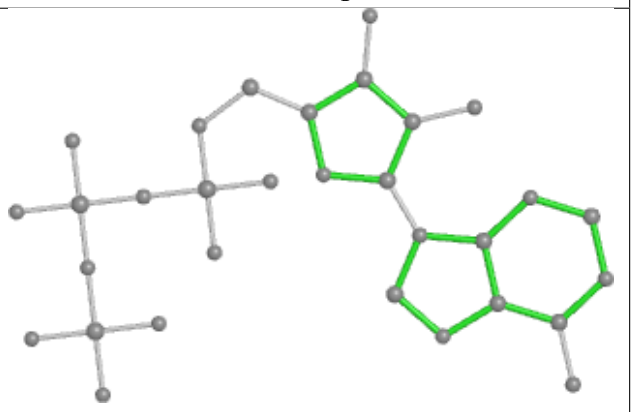
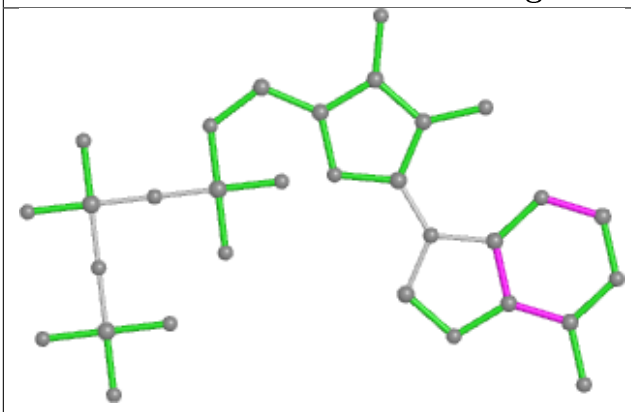
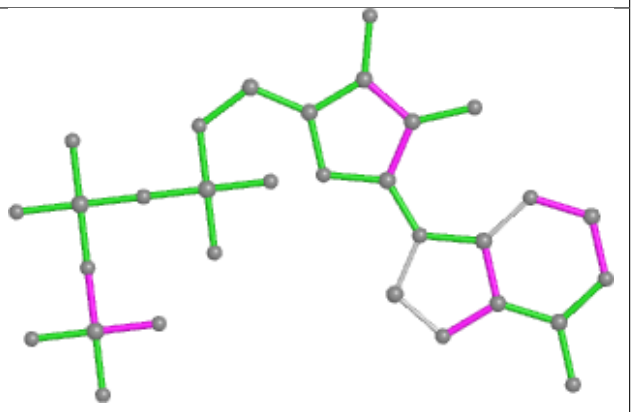


Rings

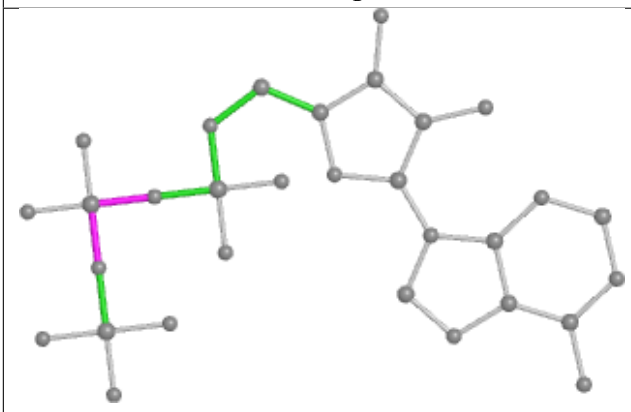
Ligand ATP C 304



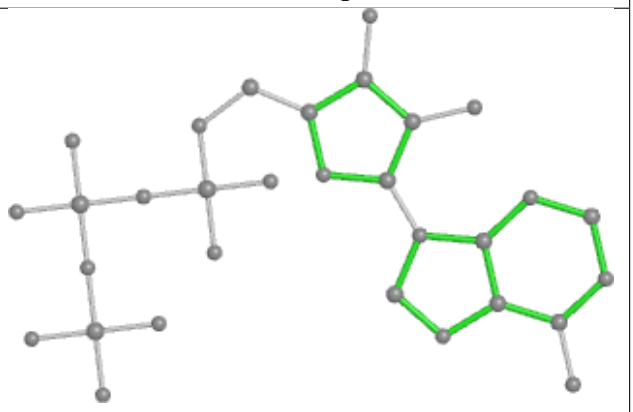
Bond lengths



Bond angles

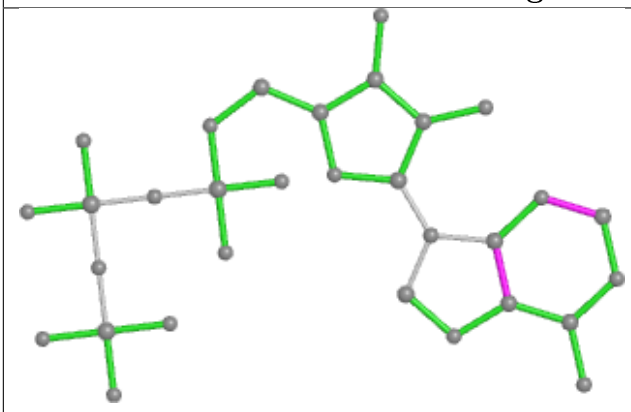


Torsions

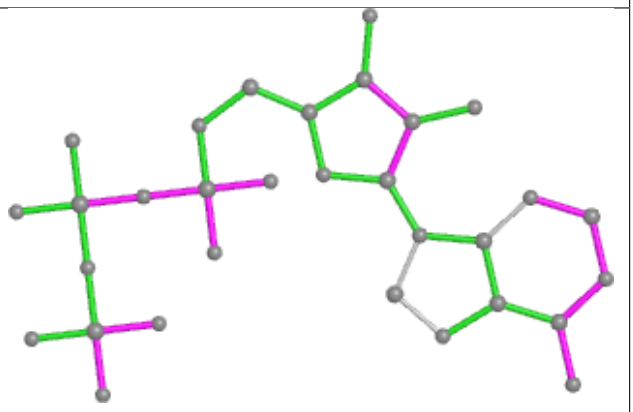


Rings

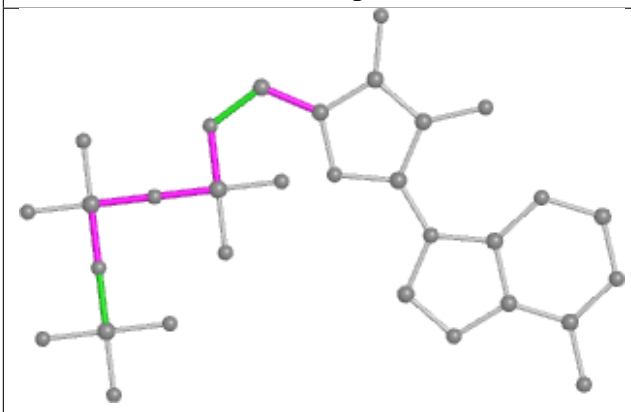
Ligand ATP E 303



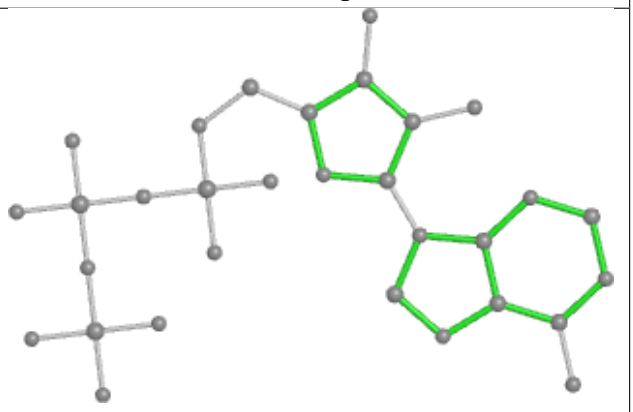
Bond lengths



Bond angles

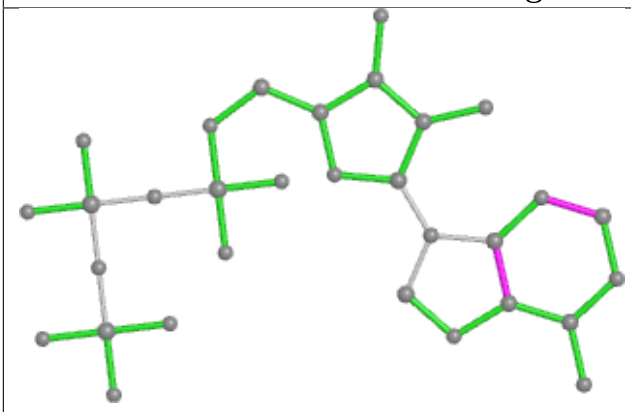


Torsions

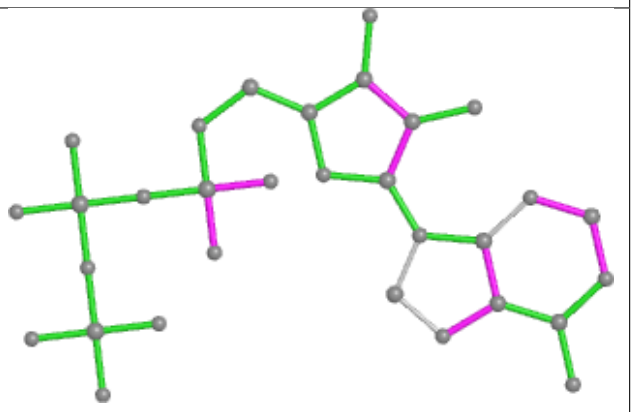


Rings

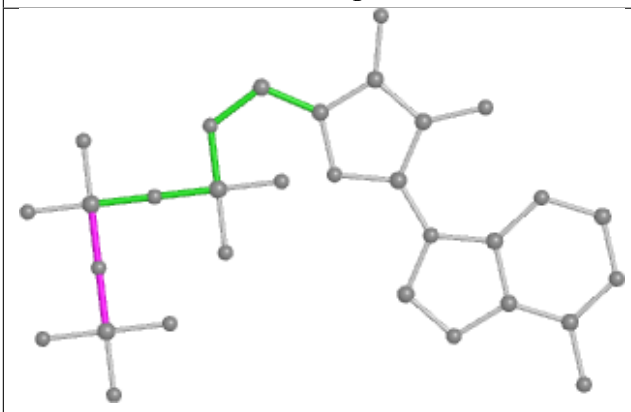
Ligand ATP B 303



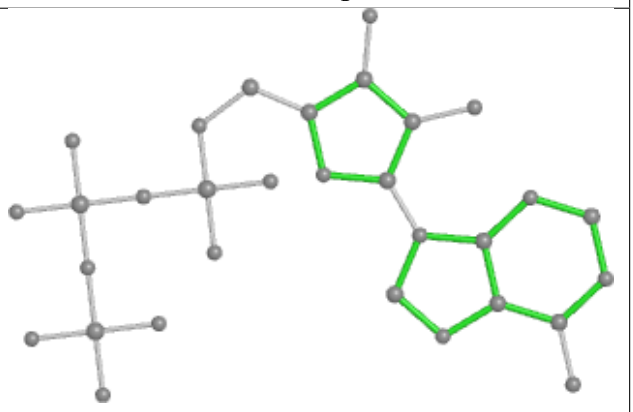
Bond lengths



Bond angles

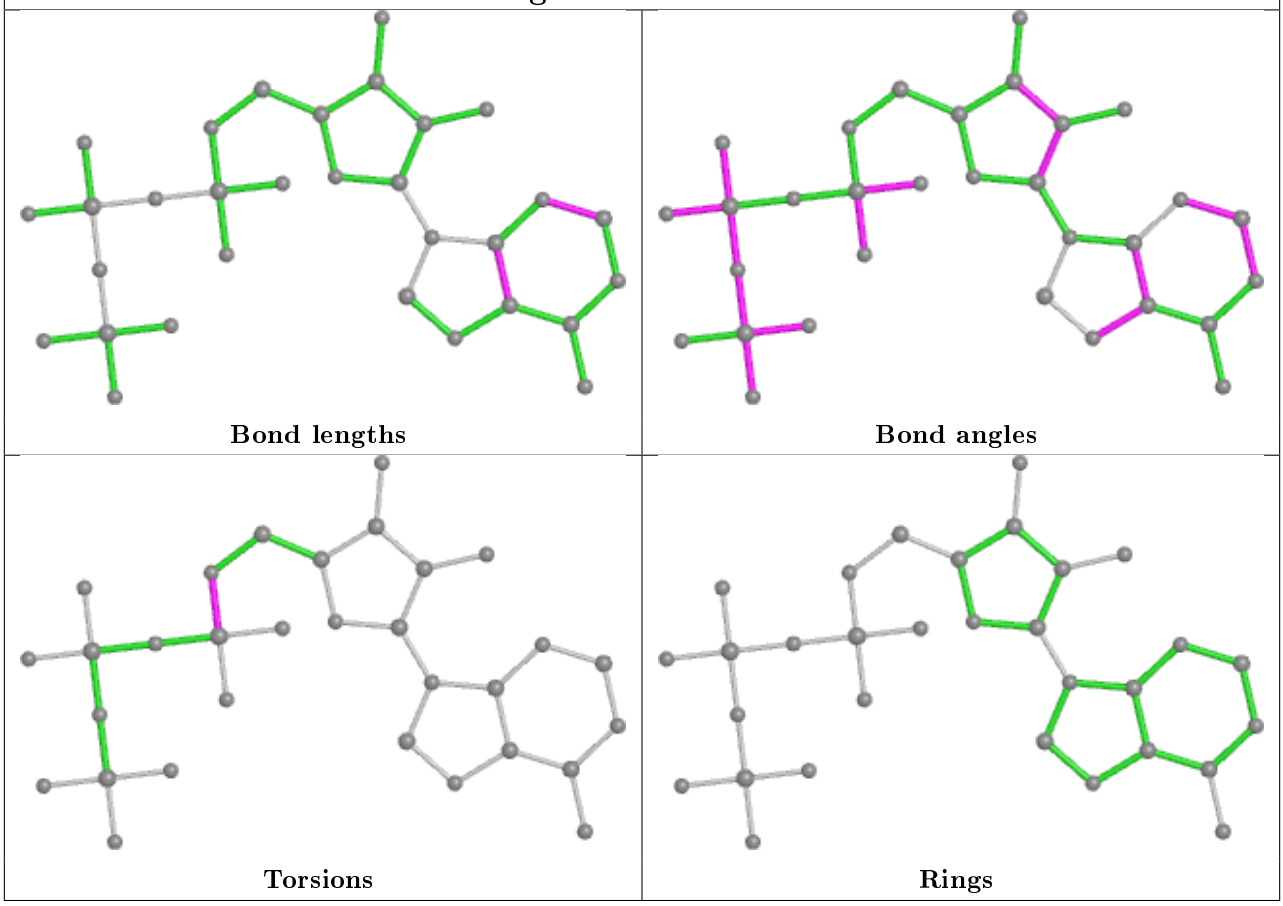


Torsions



Rings

Ligand ATP J 303



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	296/300 (98%)	-0.17	1 (0%)	94	93	18, 35, 64, 92	0
1	B	296/300 (98%)	-0.14	1 (0%)	94	93	18, 38, 72, 92	0
1	C	294/300 (98%)	-0.08	4 (1%)	75	73	19, 39, 77, 94	0
1	D	294/300 (98%)	-0.08	2 (0%)	87	86	23, 43, 79, 99	0
1	E	295/300 (98%)	-0.09	3 (1%)	82	81	23, 49, 79, 100	0
1	F	293/300 (97%)	-0.19	1 (0%)	94	93	21, 42, 69, 85	0
1	G	292/300 (97%)	-0.03	1 (0%)	94	93	23, 44, 77, 99	0
1	H	295/300 (98%)	0.04	4 (1%)	75	73	33, 55, 85, 102	0
1	I	292/300 (97%)	-0.02	1 (0%)	94	93	23, 48, 82, 92	0
1	J	296/300 (98%)	-0.22	1 (0%)	94	93	23, 42, 69, 82	0
1	K	294/300 (98%)	0.00	5 (1%)	70	68	30, 52, 81, 102	0
1	L	293/300 (97%)	0.10	8 (2%)	54	52	28, 52, 82, 91	0
All	All	3530/3600 (98%)	-0.07	32 (0%)	84	83	18, 45, 78, 102	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	257	ALA	3.8
1	K	175	ALA	3.6
1	L	181	ASN	3.4
1	E	175	ALA	3.4
1	B	236	GLU	3.3
1	I	179	ALA	3.2
1	F	116	PHE	3.2
1	H	248	VAL	2.9
1	H	175	ALA	2.9
1	G	118	ASN	2.9
1	J	257	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	5	THR	2.8
1	C	174	GLY	2.8
1	K	257	ALA	2.7
1	L	243	ALA	2.7
1	D	5	THR	2.5
1	L	241	ILE	2.4
1	K	258	HIS	2.4
1	H	5	THR	2.3
1	C	119	LEU	2.3
1	H	36	GLU	2.3
1	L	173	SER	2.2
1	L	175	ALA	2.2
1	E	35	HIS	2.2
1	K	179	ALA	2.2
1	K	113	GLU	2.2
1	C	116	PHE	2.1
1	C	175	ALA	2.1
1	D	257	ALA	2.1
1	A	257	ALA	2.0
1	L	119	LEU	2.0
1	L	247	GLY	2.0

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
3	PO4	E	302	5/5	0.53	0.23	103,108,109,114	0
3	PO4	J	302	5/5	0.55	0.47	128,130,132,136	0

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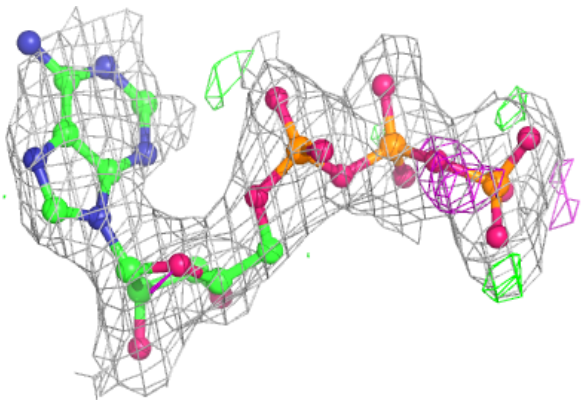
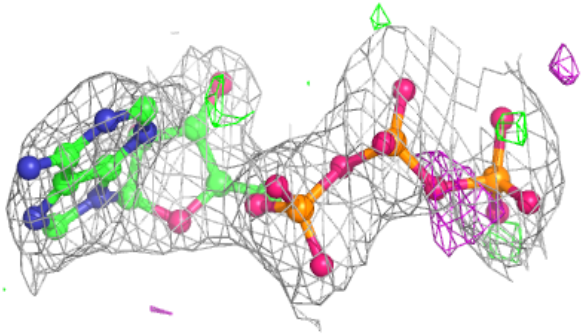
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACY	J	304	4/4	0.59	0.19	56,60,62,65	0
3	PO4	C	303	5/5	0.66	0.18	98,101,108,110	0
3	PO4	I	302	5/5	0.72	0.23	93,96,97,98	0
3	PO4	C	302	5/5	0.85	0.27	92,104,106,111	0
2	MG	L	301	1/1	0.86	0.19	62,62,62,62	0
2	MG	K	301	1/1	0.86	0.12	70,70,70,70	0
2	MG	D	301	1/1	0.88	0.08	49,49,49,49	0
3	PO4	B	302	5/5	0.88	0.16	92,95,99,99	0
4	ATP	L	302	31/31	0.90	0.14	38,55,69,70	0
4	ATP	K	302	31/31	0.92	0.13	39,59,71,76	0
2	MG	B	301	1/1	0.93	0.04	39,39,39,39	0
4	ATP	G	302	31/31	0.93	0.12	37,52,62,68	0
4	ATP	D	302	31/31	0.93	0.16	42,56,70,71	0
4	ATP	E	303	31/31	0.93	0.13	44,54,70,74	0
4	ATP	H	302	31/31	0.93	0.12	45,56,68,72	0
4	ATP	F	302	31/31	0.94	0.11	28,42,58,59	0
2	MG	C	301	1/1	0.94	0.07	45,45,45,45	0
4	ATP	B	303	31/31	0.94	0.12	36,43,53,55	0
4	ATP	I	303	31/31	0.94	0.11	37,48,68,77	0
2	MG	E	301	1/1	0.94	0.09	59,59,59,59	0
4	ATP	A	302	31/31	0.94	0.14	27,45,61,62	0
4	ATP	C	304	31/31	0.94	0.13	28,40,54,56	0
4	ATP	J	303	31/31	0.95	0.12	30,44,60,66	0
2	MG	J	301	1/1	0.95	0.06	42,42,42,42	0
2	MG	I	301	1/1	0.95	0.11	43,43,43,43	0
2	MG	G	301	1/1	0.95	0.05	51,51,51,51	0
2	MG	H	301	1/1	0.97	0.05	55,55,55,55	0
2	MG	F	301	1/1	0.97	0.06	39,39,39,39	0
2	MG	A	301	1/1	0.99	0.07	44,44,44,44	0

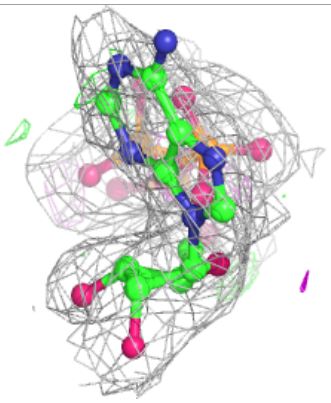
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP L 302:

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

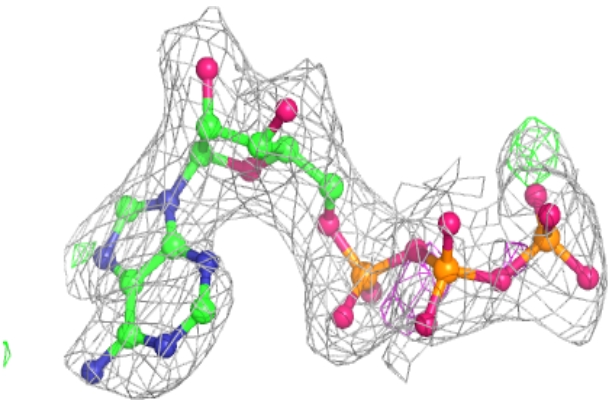


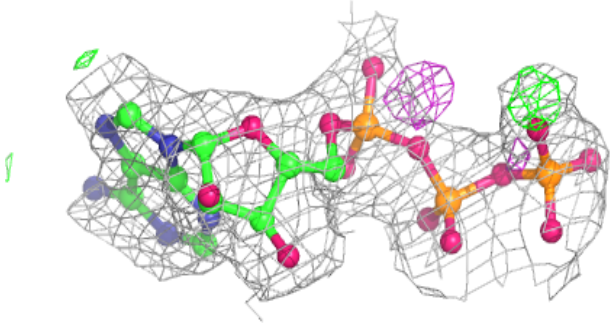


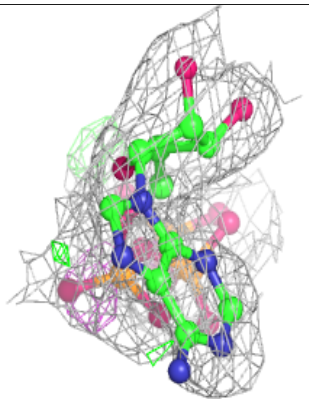


Electron density around ATP K 302:

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

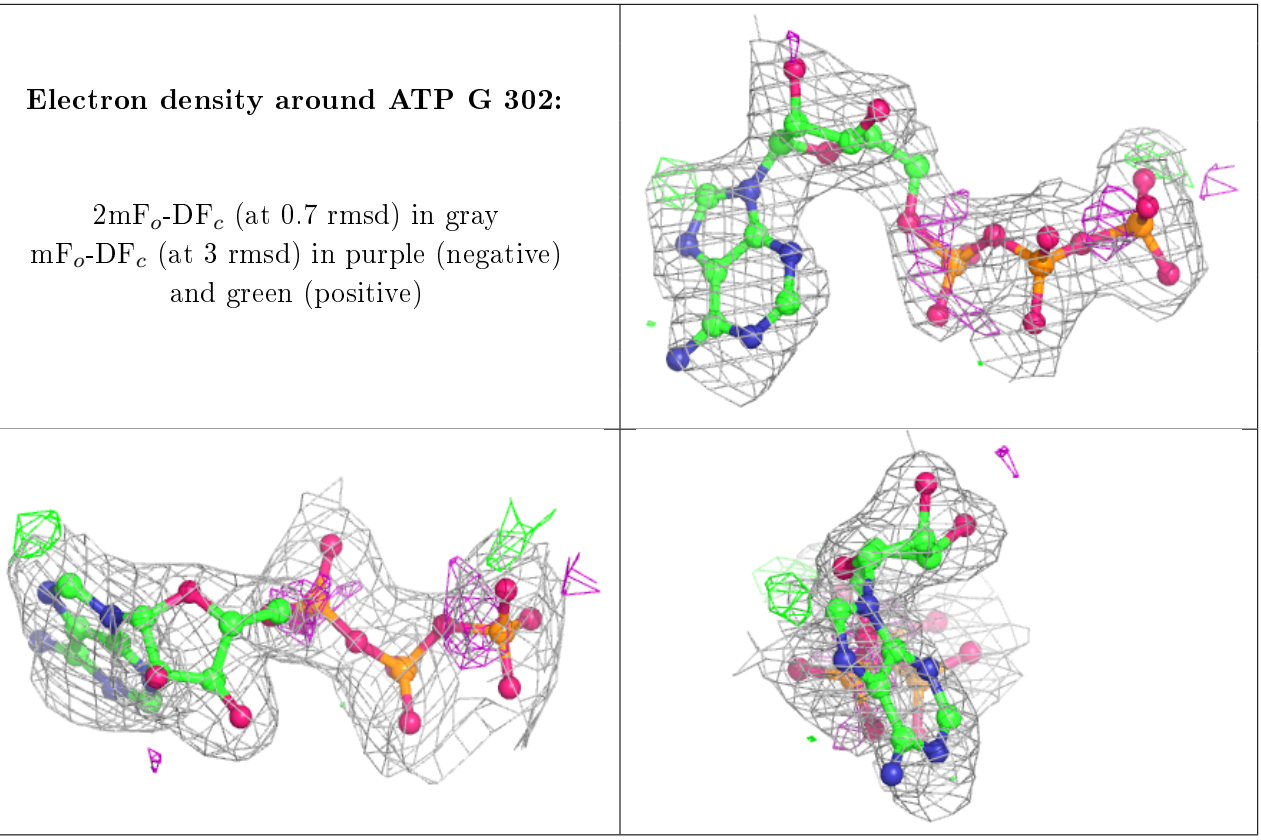






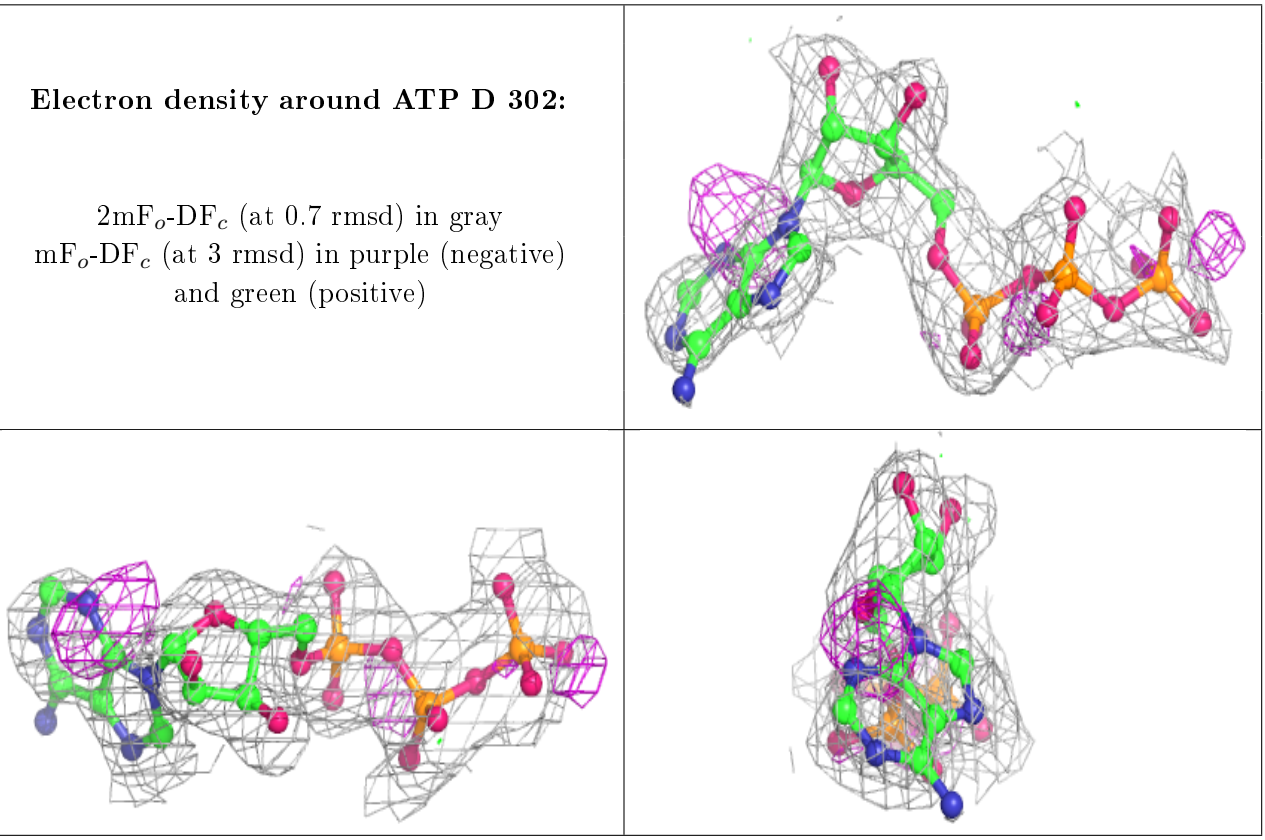
Electron density around ATP G 302:

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



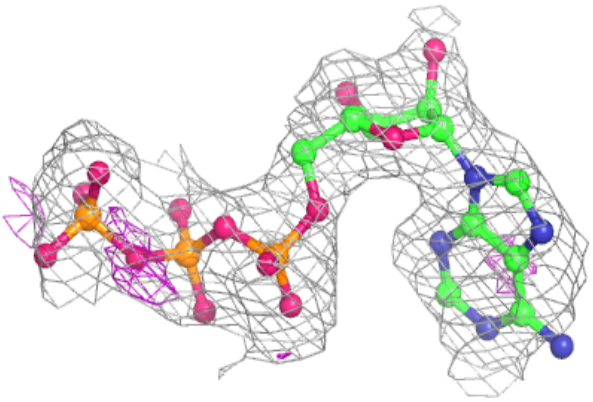
Electron density around ATP D 302:

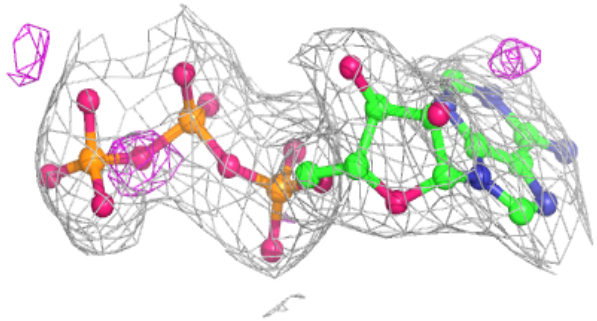
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

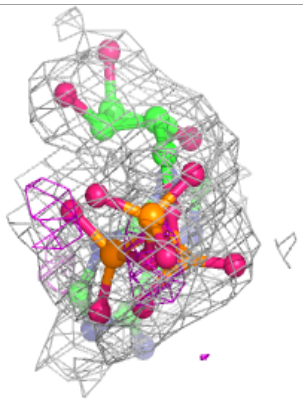


Electron density around ATP E 303:

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

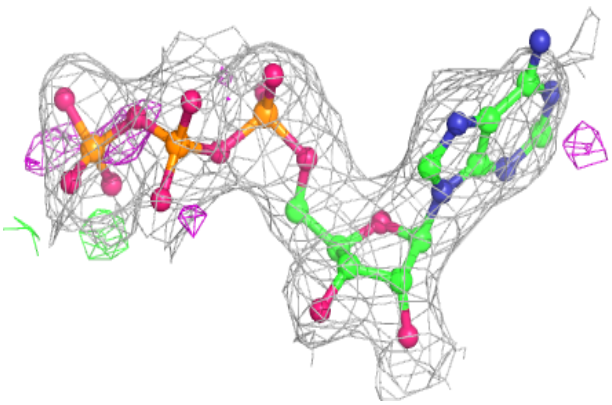


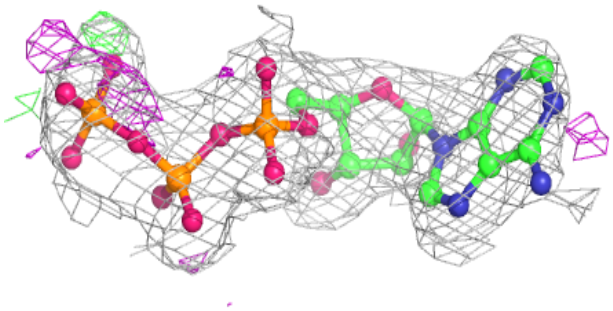


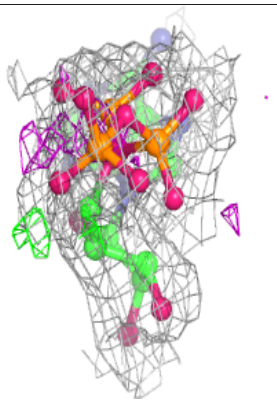


Electron density around ATP H 302:

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

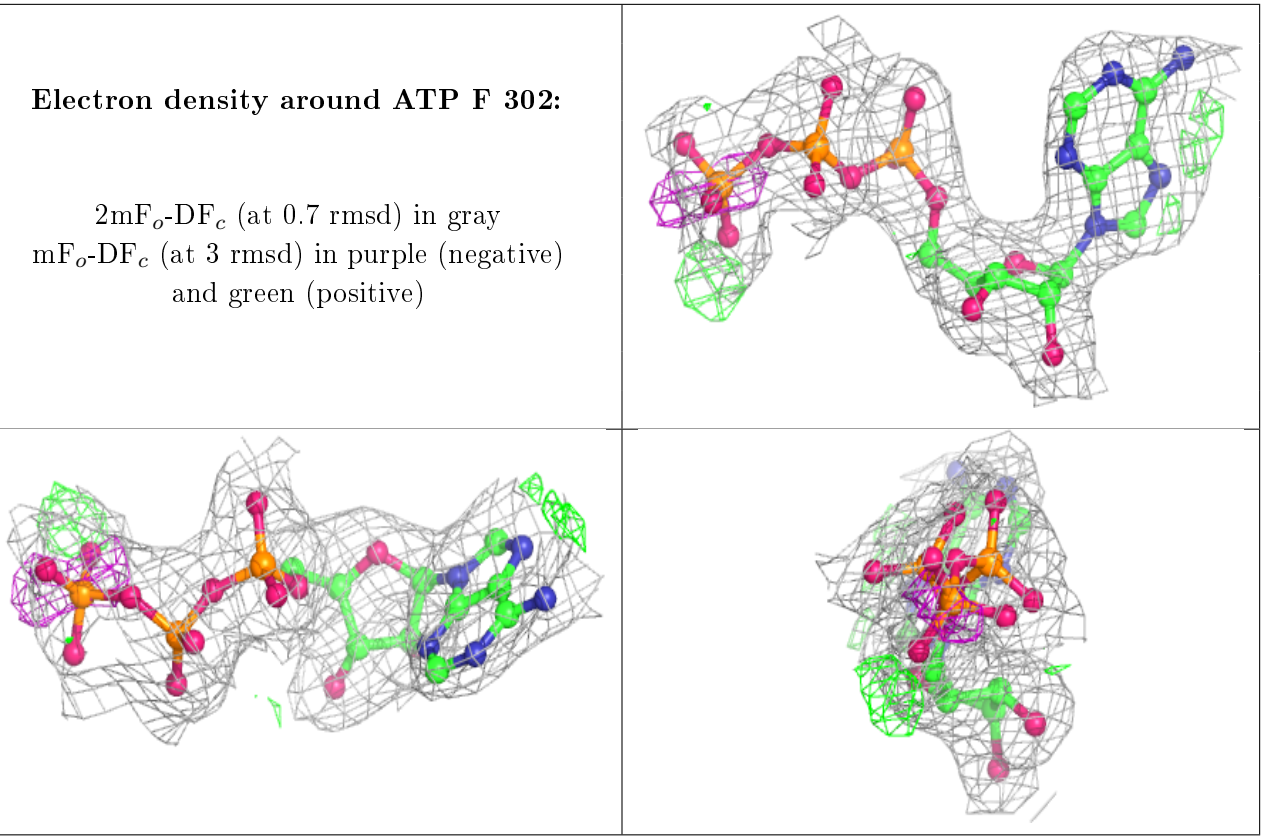






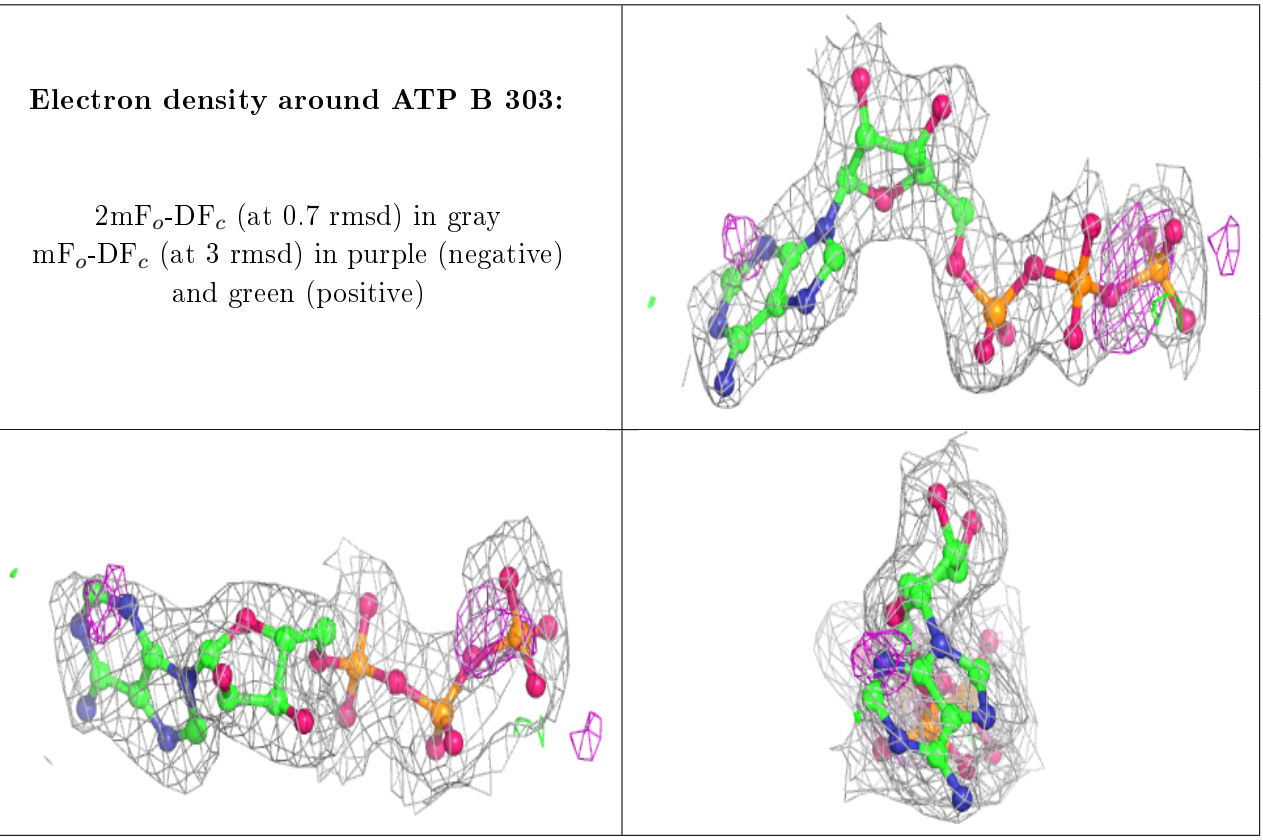
Electron density around ATP F 302:

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



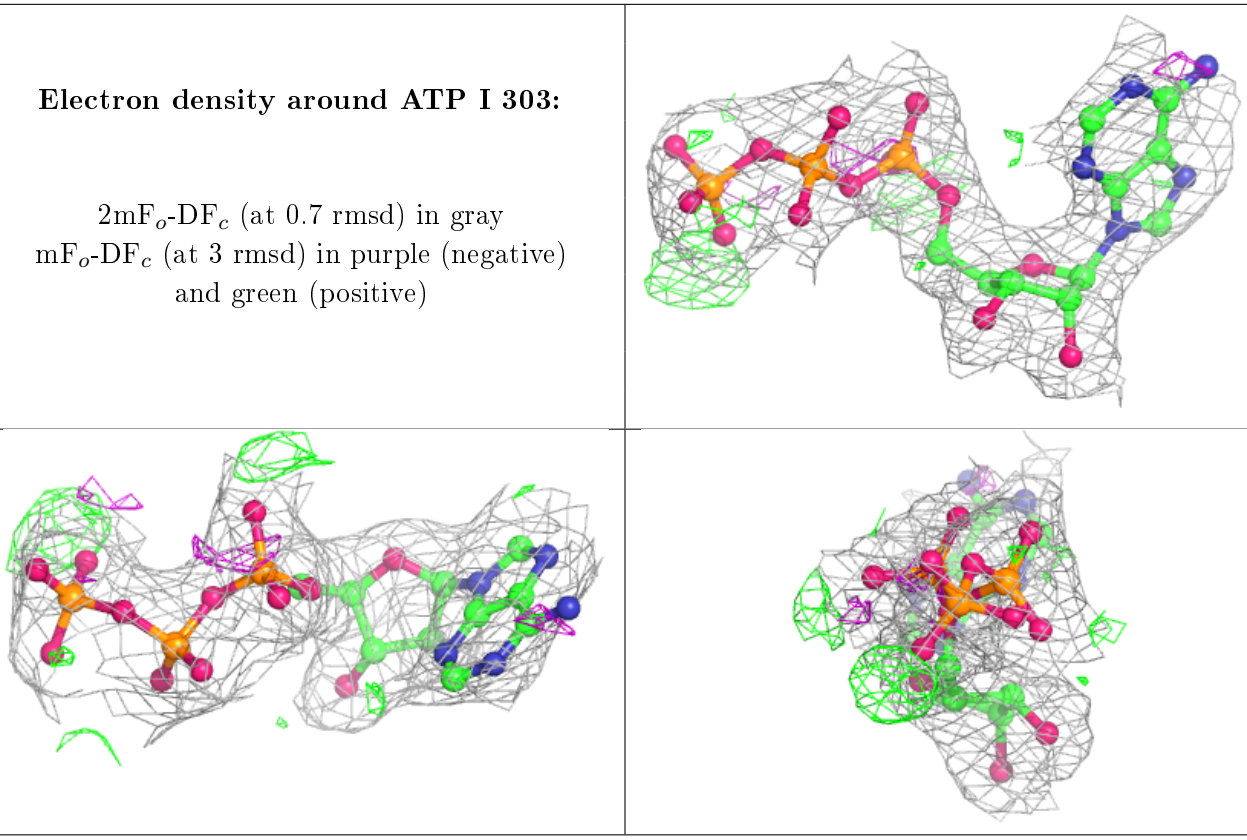
Electron density around ATP B 303:

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



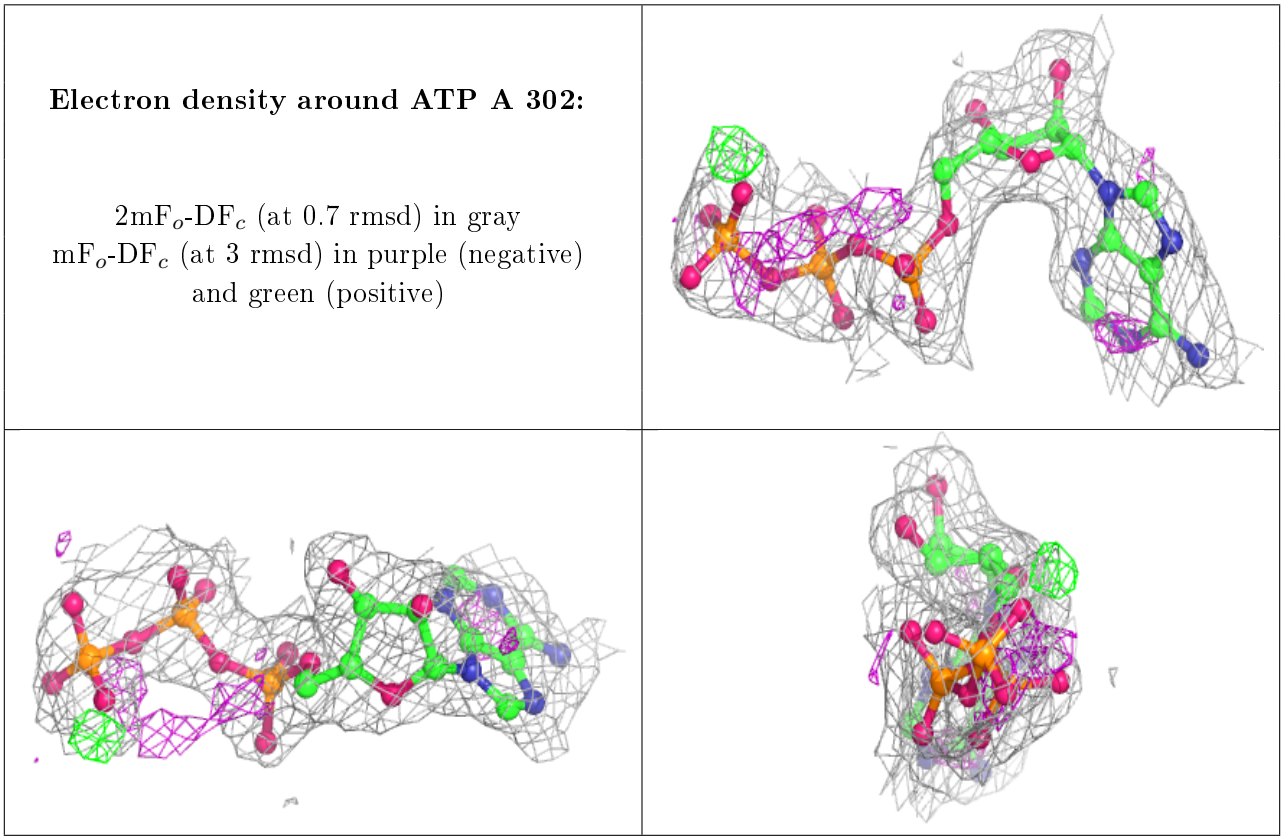
Electron density around ATP I 303:

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



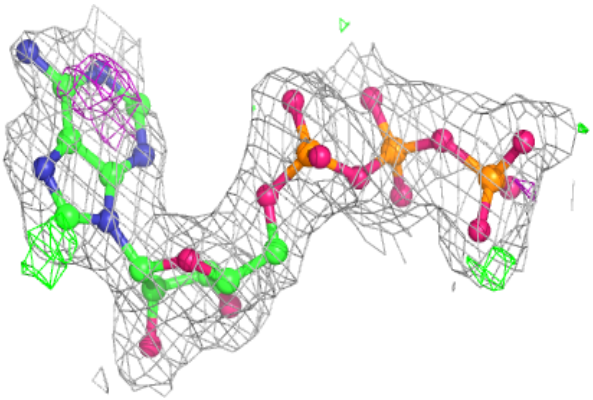
Electron density around ATP A 302:

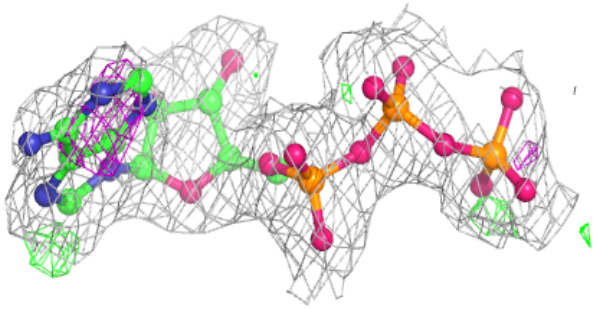
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

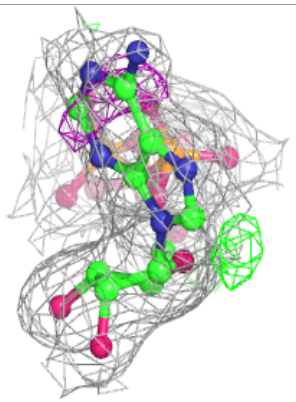


Electron density around ATP C 304:

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

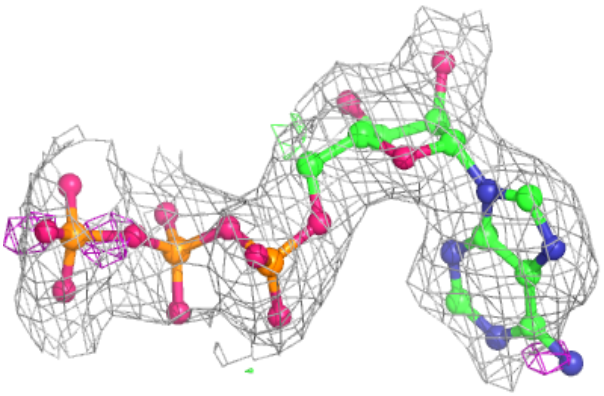


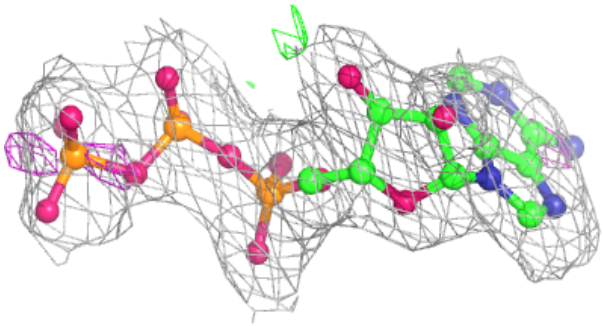


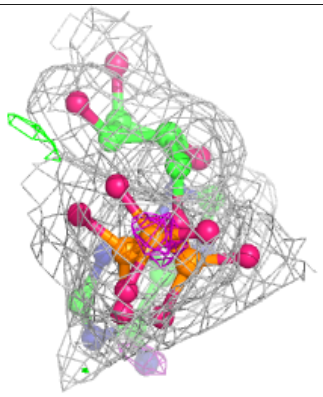


Electron density around ATP J 303:

$2mF_o$-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.