



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:08 AM UTC

PDB ID : 4YB7 / pdb_00004yb7
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

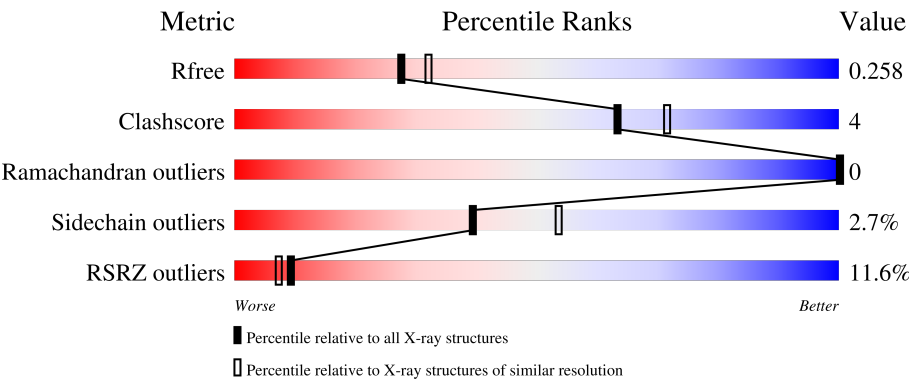
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	300	8% 91% 7% ..
1	B	300	10% 89% 8% ..
1	C	300	12% 86% 11% ..
1	D	300	11% 91% 6% ..
1	E	300	8% 91% 6% ..

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Mol	Chain	Length	Quality of chain
1	F	300	6% 90% 7% ..
1	G	300	13% 89% 7% ..
1	H	300	17% 89% 9% .
1	I	300	15% 88% 9% ..
1	J	300	6% 91% 7% ..
1	K	300	13% 88% 8% ..
1	L	300	18% 88% 8% ..

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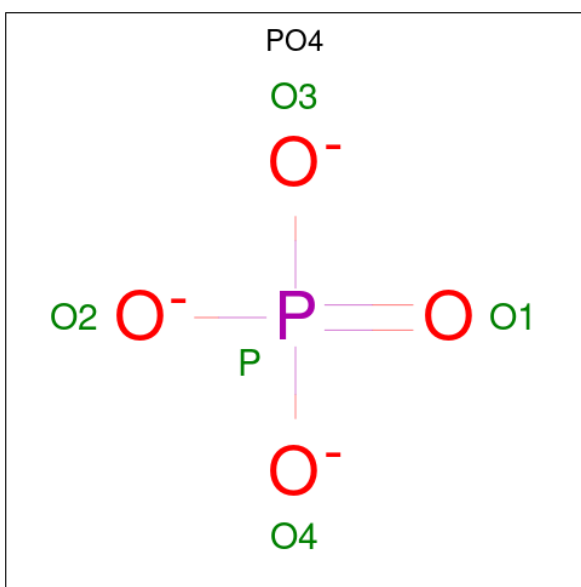
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Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP Q5HSJ4
A	0	GLY	-	expression tag	UNP Q5HSJ4
F	0	GLY	-	expression tag	UNP Q5HSJ4
G	0	GLY	-	expression tag	UNP Q5HSJ4
H	0	GLY	-	expression tag	UNP Q5HSJ4
J	0	GLY	-	expression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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

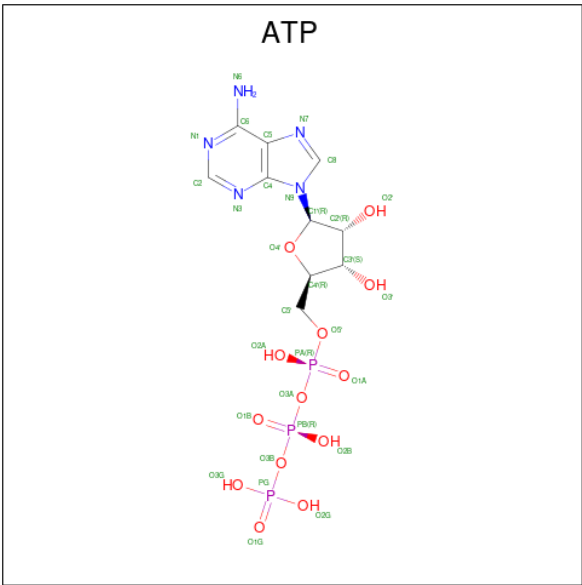
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	L	1	Total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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



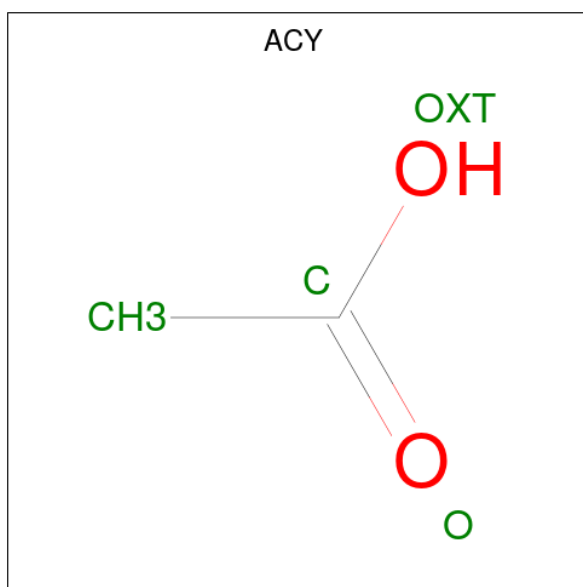
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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 (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 6 is water.

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

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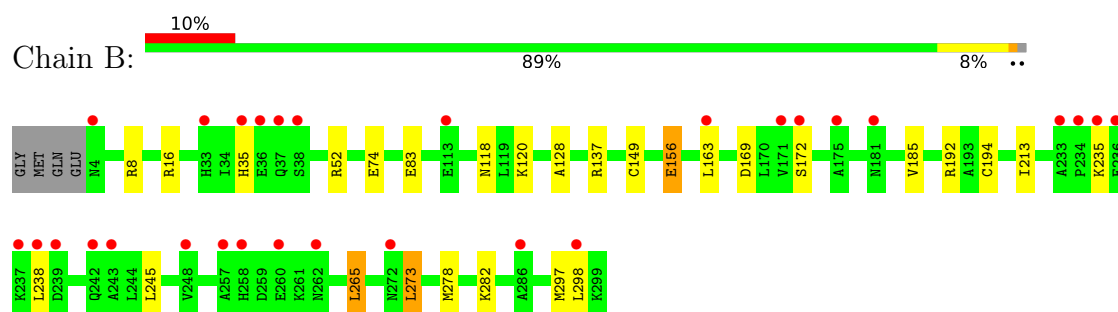
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	13	Total	O	0	0
			13	13		

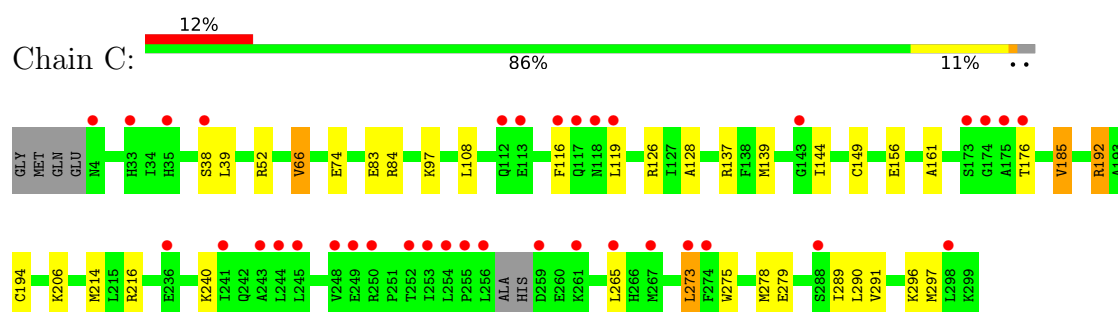
3 Residue-property plots [i](#)

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.

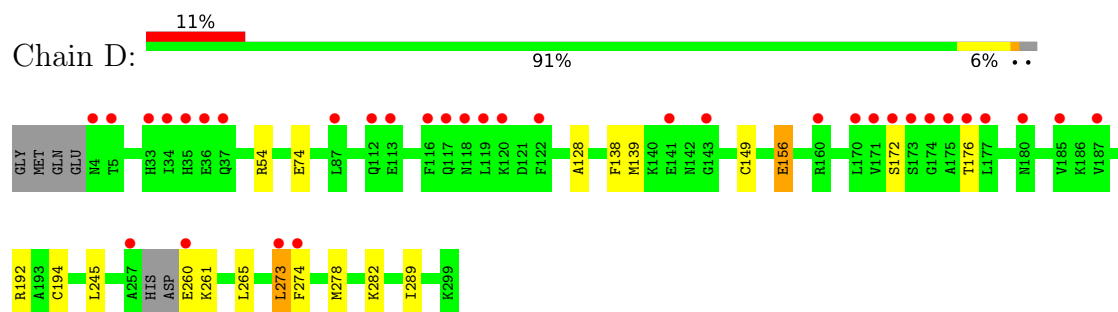
- Molecule 1: ATP phosphoribosyltransferase



- Molecule 1: ATP phosphoribosyltransferase

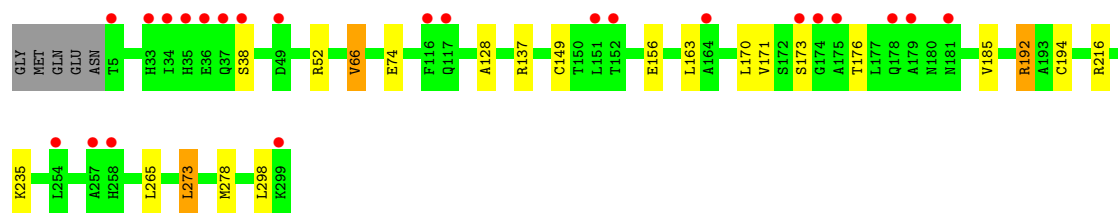


- Molecule 1: ATP phosphoribosyltransferase

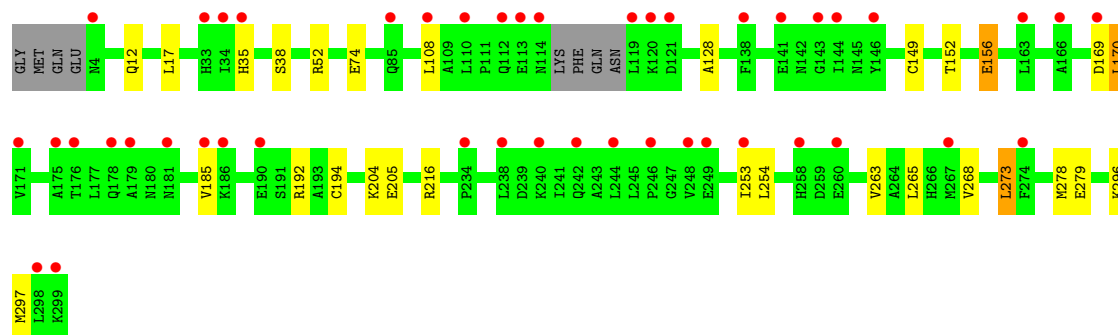
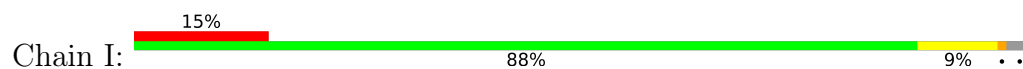


- Molecule 1: ATP phosphoribosyltransferase

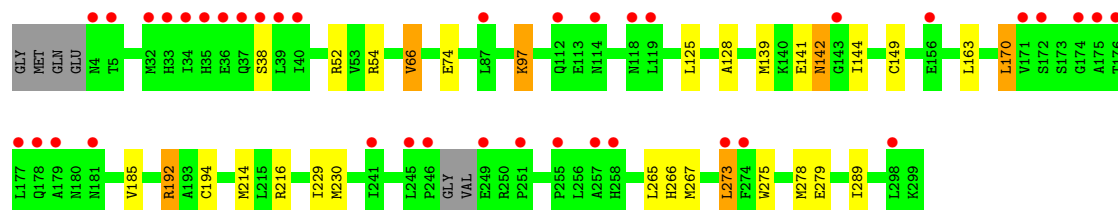
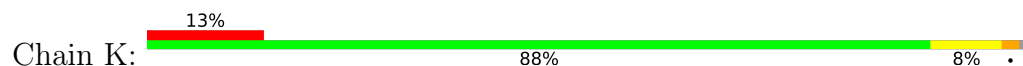




• Molecule 1: ATP phosphoribosyltransferase



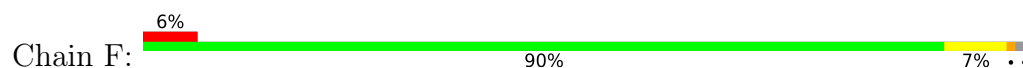
• Molecule 1: ATP phosphoribosyltransferase



• Molecule 1: ATP phosphoribosyltransferase

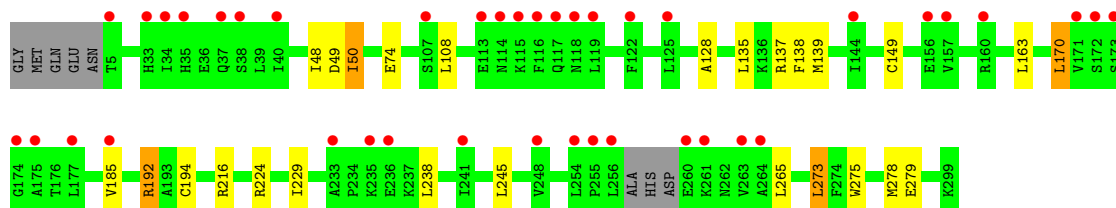
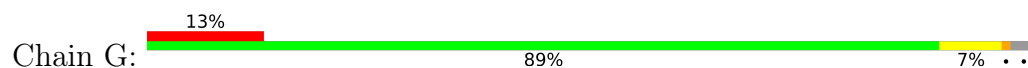


• Molecule 1: ATP phosphoribosyltransferase

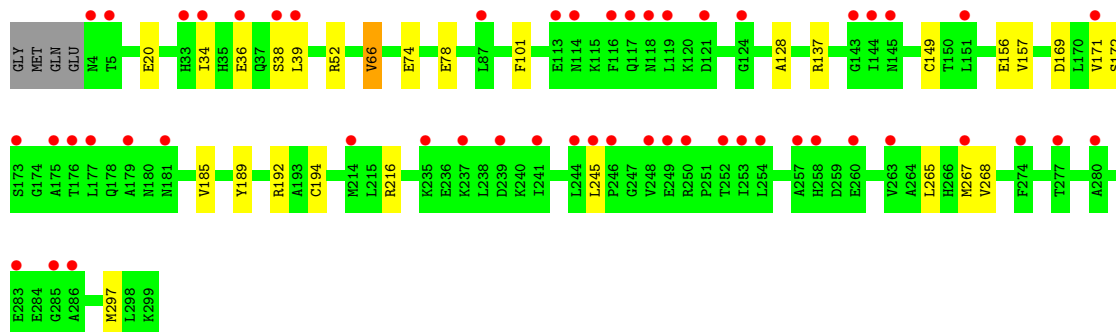
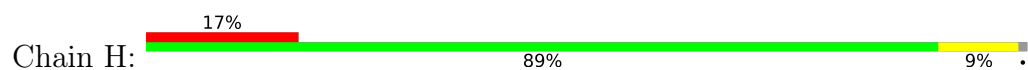




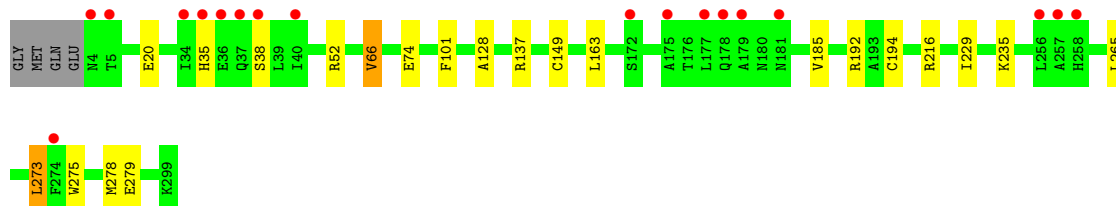
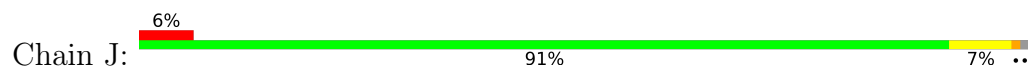
- Molecule 1: ATP phosphoribosyltransferase



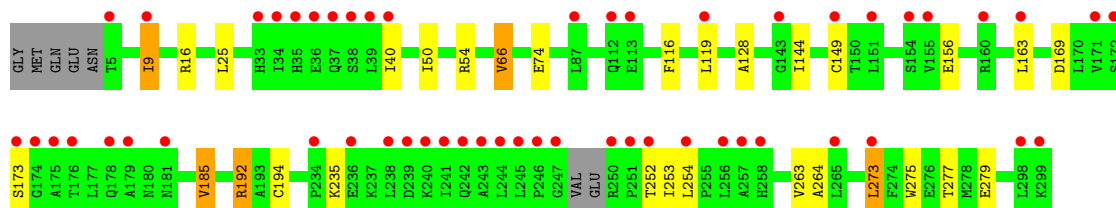
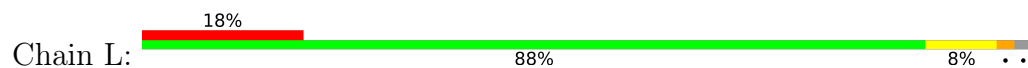
- Molecule 1: ATP phosphoribosyltransferase



- Molecule 1: ATP phosphoribosyltransferase



- Molecule 1: ATP phosphoribosyltransferase



4 Data and refinement statistics

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 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.20) 98.1 (50.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.90%)	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 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: ATP, PO4, ACY, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.68	0/2229	0.85	3/3020 (0.1%)
1	B	0.66	0/2257	0.82	4/3055 (0.1%)
1	C	0.64	0/2225	0.86	5/3011 (0.2%)
1	D	0.62	0/2195	0.81	2/2977 (0.1%)
1	E	0.58	0/2231	0.86	7/3026 (0.2%)
1	F	0.61	0/2216	0.80	3/2997 (0.1%)
1	G	0.60	0/2174	0.85	6/2950 (0.2%)
1	H	0.57	1/2190 (0.0%)	0.84	8/2974 (0.3%)
1	I	0.62	0/2197	0.80	2/2976 (0.1%)
1	J	0.60	0/2247	0.81	4/3042 (0.1%)
1	K	0.60	0/2194	0.83	5/2975 (0.2%)
1	L	0.60	0/2174	0.83	3/2952 (0.1%)
All	All	0.61	1/26529 (0.0%)	0.83	52/35955 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	34	ILE	C-N	-5.56	1.26	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	192	ARG	NE-CZ-NH2	8.94	127.25	119.20
1	F	192	ARG	NE-CZ-NH2	8.93	127.23	119.20
1	C	192	ARG	NE-CZ-NH2	8.90	127.21	119.20
1	L	192	ARG	NE-CZ-NH2	8.73	127.06	119.20
1	E	192	ARG	NE-CZ-NH2	8.71	127.04	119.20
1	K	192	ARG	NE-CZ-NH2	8.69	127.02	119.20
1	G	224	ARG	NE-CZ-NH2	8.28	126.65	119.20
1	A	225	GLU	N-CA-C	8.15	119.94	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	224	ARG	NE-CZ-NH1	-7.97	113.53	121.50
1	C	192	ARG	NE-CZ-NH1	-7.70	113.80	121.50
1	F	192	ARG	NE-CZ-NH1	-7.68	113.82	121.50
1	B	192	ARG	NE-CZ-NH2	7.58	126.02	119.20
1	H	34	ILE	O-C-N	-7.58	114.62	123.03
1	C	137	ARG	NE-CZ-NH2	7.55	125.99	119.20
1	G	192	ARG	NE-CZ-NH1	-7.54	113.96	121.50
1	E	137	ARG	NE-CZ-NH2	7.48	125.94	119.20
1	E	192	ARG	NE-CZ-NH1	-7.47	114.03	121.50
1	H	137	ARG	NE-CZ-NH2	7.45	125.90	119.20
1	J	137	ARG	NE-CZ-NH2	7.45	125.90	119.20
1	L	192	ARG	NE-CZ-NH1	-7.42	114.08	121.50
1	K	192	ARG	NE-CZ-NH1	-7.42	114.08	121.50
1	G	137	ARG	NE-CZ-NH2	7.25	125.73	119.20
1	B	137	ARG	NE-CZ-NH2	7.16	125.64	119.20
1	A	192	ARG	NE-CZ-NH2	-6.99	112.91	119.20
1	H	39	LEU	N-CA-C	6.97	118.96	111.36
1	I	192	ARG	NE-CZ-NH2	-6.86	113.03	119.20
1	B	192	ARG	NE-CZ-NH1	-6.81	114.69	121.50
1	J	192	ARG	NE-CZ-NH2	-6.74	113.13	119.20
1	H	192	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	E	216	ARG	NE-CZ-NH1	-6.61	114.89	121.50
1	E	216	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	D	192	ARG	NE-CZ-NH2	-6.44	113.40	119.20
1	K	142	ASN	N-CA-C	-6.25	100.33	110.20
1	K	54	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	E	173	SER	N-CA-C	-5.98	101.92	110.59
1	F	126	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	C	137	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	B	137	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	C	126	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	H	137	ARG	NE-CZ-NH1	-5.80	115.69	121.50
1	E	137	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	A	192	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	H	192	ARG	NE-CZ-NH1	5.69	127.19	121.50
1	J	192	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	I	192	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	G	137	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	J	137	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	L	173	SER	N-CA-C	-5.44	103.52	110.53
1	D	192	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	K	97	LYS	CB-CG-CD	5.38	123.68	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	36	GLU	N-CA-C	-5.18	105.76	111.71
1	H	157	VAL	N-CA-C	5.06	115.78	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2202	0	2219	16	0
1	B	2228	0	2247	24	0
1	C	2198	0	2200	29	0
1	D	2168	0	2142	27	0
1	E	2203	0	2185	12	1
1	F	2191	0	2190	15	1
1	G	2149	0	2110	25	0
1	H	2162	0	2109	18	0
1	I	2169	0	2159	22	0
1	J	2218	0	2210	22	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1	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	212	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 (212) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K: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:HD2	1:D:139:MET:HE3	1.19	1.04
1:C:296:LYS:HD3	1:K:278:MET:HE2	1.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:PHE:CD2	1:D:139:MET:HE3	1.93	1.03
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	0.89
1:B:245:LEU:CD2	1:B:273:LEU:HD11	2.04	0.87
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:138:PHE:HD1	1:G:139:MET:HE2	1.45	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: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:I:74:GLU:HG3	1:I:194:CYS:SG	2.28	0.73
1:H:38:SER:O	1:H:52:ARG:NE	2.20	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:D:138:PHE:CE2	1:D:139:MET:HE1	2.24	0.72
1:G:74:GLU:HG3	1:G:194:CYS:SG	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:GLU:OE2	1:H:216:ARG:HD2	1.89	0.71
1:D:138:PHE:HE2	1:D:139:MET:HE1	1.56	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:G:138:PHE:CD1	1:G:139:MET:HE2	2.25	0.70
1:D:138:PHE:CD2	1:D:139:MET:HE2	2.25	0.69
1:C:279:GLU:OE2	1:I:216:ARG:HD2	1.93	0.68
1:G:108:LEU:HD11	1:G:139:MET:HE1	1.76	0.68
1:I:253:ILE:CG2	1:I:263:VAL:HG21	2.23	0.68
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
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: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: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:C:108:LEU:HD11	1:C:139:MET:HE1	1.83	0.60
1:G:163:LEU:CD2	1:H:66:VAL:HG11	2.32	0.60
1:G:50:ILE:N	1:G:50:ILE:HD12	2.17	0.59
1:D:139:MET:HE2	1:D:139:MET:HA	1.83	0.59
1:D:260:GLU:OE1	1:D:260:GLU:N	2.35	0.59
1:I:254:LEU:O	1:I:263:VAL:HG23	2.02	0.59
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:135:LEU:HD11	1:G:139:MET:HE3	1.87	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:K:170:LEU:HD23	4:K:302:ATP:C2	2.40	0.56
1:G:216:ARG:HD2	1:J:279:GLU:OE2	2.04	0.56
1:H:245:LEU:CB	1:H:267:MET:HE1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:12:GLN:NE2	1:I:17:LEU:H	2.05	0.54
1:A:66:VAL:CG1	1:F:163:LEU:CD2	2.85	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:C:216:ARG:HG2	1:K:275:TRP:CD2	2.43	0.54
1:I:108:LEU:O	1:I:185:VAL:HG12	2.08	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:J:163:LEU:HD22	1:L:66:VAL:CG1	2.36	0.53
1:B:156:GLU:HG2	1:C:39:LEU:CD1	2.39	0.53
1:A:119:LEU:HB2	6:A:425:HOH:O	2.09	0.53
1:G:135:LEU:CD1	1:G:139:MET:HE3	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: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:N	1:G:50:ILE:CD1	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:HG2	1:B:52:ARG:HH11	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:I:279:GLU:OE2	1:K:216:ARG:HD2	2.14	0.48
1:J:128:ALA:HA	1:J:149:CYS:O	2.14	0.48
1:C:119:LEU:HD23	1:C:144:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:49:ASP:C	1:G:50:ILE:HD12	2.39	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:HG23	1:L:40:ILE:O	2.14	0.47
1:B:163:LEU:CD2	1:C:66:VAL:HG11	2.44	0.47
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:J:163:LEU:HD23	1:L:66:VAL:CG1	2.45	0.47
1:L:9:ILE:HD13	1:L:25:LEU:HD11	1.96	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: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:273:LEU:HD23	1:D:278:MET:SD	2.57	0.44
1:A:128:ALA:HA	1:A:149:CYS:O	2.16	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:C:156:GLU:OE1	1:C:176:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:GLU:CD	1:E:176:THR:CG2	2.88	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:275:TRP:CD1	6:G:426:HOH:O	2.72	0.43
1:G:273:LEU:HD23	1:G:278:MET:SD	2.59	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
1:E:273:LEU:HD23	1:E:278:MET:SD	2.59	0.42
1:C:296:LYS:HD3	1:K:278:MET:CE	2.27	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:E:156:GLU:CD	1:E:176:THR:HG21	2.33	0.42
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:273:LEU:HD23	1:A:278:MET:SD	2.60	0.41
1:K:97:LYS:HB2	1:K:214:MET:HE1	2.02	0.41
1:B:297:MET:HA	1:D:289:ILE:O	2.20	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: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:K:229:ILE:HD11	1:K:273:LEU:HD13	2.03	0.41
1:G:48:ILE:HG22	1:G:50:ILE:CD1	2.50	0.41
1:L:9:ILE:HG23	1:L:9:ILE:O	2.21	0.41
1:L:116:PHE:CE2	1:L:185:VAL:HG13	2.55	0.41
1:I:170:LEU:HD23	4:I:303:ATP:C2	2.55	0.41
1:F:116:PHE:CE2	1:F:185:VAL:HG13	2.56	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:HD12	1:B:238:LEU:HA	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:C:97:LYS:HB2	1:C:214:MET:HE1	2.03	0.40
1:A:54:ARG:NH1	1:F:54:ARG:NH2	2.69	0.40
1:I:156:GLU:H	1:I:156:GLU:CD	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

5.3.1 Protein backbone

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 ⓘ

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%)	220 (97%)	7 (3%)	35	48
1	B	234/263 (89%)	228 (97%)	6 (3%)	40	55
1	C	228/263 (87%)	221 (97%)	7 (3%)	35	48
1	D	219/263 (83%)	216 (99%)	3 (1%)	59	75
1	E	229/263 (87%)	222 (97%)	7 (3%)	35	48
1	F	228/263 (87%)	222 (97%)	6 (3%)	40	55
1	G	218/263 (83%)	212 (97%)	6 (3%)	38	52
1	H	215/263 (82%)	212 (99%)	3 (1%)	59	75
1	I	223/263 (85%)	216 (97%)	7 (3%)	35	48
1	J	230/263 (88%)	225 (98%)	5 (2%)	45	61
1	K	218/263 (83%)	209 (96%)	9 (4%)	27	37
1	L	215/263 (82%)	209 (97%)	6 (3%)	38	52
All	All	2684/3156 (85%)	2612 (97%)	72 (3%)	39	53

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	HIS
1	B	156	GLU
1	B	185	VAL
1	B	213	ILE
1	B	265	LEU
1	B	273	LEU
1	C	66	VAL
1	C	83	GLU
1	C	185	VAL
1	C	192	ARG
1	C	240	LYS
1	C	265	LEU
1	C	273	LEU
1	D	156	GLU

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Mol	Chain	Res	Type
1	D	265	LEU
1	D	273	LEU
1	E	66	VAL
1	E	170	LEU
1	E	171	VAL
1	E	185	VAL
1	E	192	ARG
1	E	265	LEU
1	E	273	LEU
1	I	35	HIS
1	I	156	GLU
1	I	170	LEU
1	I	204	LYS
1	I	205	GLU
1	I	265	LEU
1	I	273	LEU
1	K	66	VAL
1	K	125	LEU
1	K	144	ILE
1	K	170	LEU
1	K	185	VAL
1	K	192	ARG
1	K	265	LEU
1	K	267	MET
1	K	273	LEU
1	A	66	VAL
1	A	137	ARG
1	A	140	LYS
1	A	170	LEU
1	A	185	VAL
1	A	265	LEU
1	A	273	LEU
1	F	170	LEU
1	F	177	LEU
1	F	185	VAL
1	F	192	ARG
1	F	265	LEU
1	F	273	LEU
1	G	50	ILE
1	G	170	LEU
1	G	185	VAL
1	G	192	ARG

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Mol	Chain	Res	Type
1	G	265	LEU
1	G	273	LEU
1	H	66	VAL
1	H	185	VAL
1	H	265	LEU
1	J	35	HIS
1	J	66	VAL
1	J	185	VAL
1	J	265	LEU
1	J	273	LEU
1	L	9	ILE
1	L	66	VAL
1	L	185	VAL
1	L	192	ARG
1	L	252	THR
1	L	273	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	HIS
1	B	35	HIS
1	B	114	ASN
1	B	133	GLN
1	B	180	ASN
1	C	33	HIS
1	C	114	ASN
1	C	180	ASN
1	D	35	HIS
1	D	114	ASN
1	D	180	ASN
1	E	114	ASN
1	I	12	GLN
1	I	145	ASN
1	I	242	GLN
1	K	85	GLN
1	K	145	ASN
1	K	148	ASN
1	K	242	GLN
1	A	80	ASN
1	A	114	ASN
1	A	145	ASN

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Mol	Chain	Res	Type
1	A	180	ASN
1	F	117	GLN
1	F	118	ASN
1	G	145	ASN
1	G	242	GLN
1	H	114	ASN
1	J	114	ASN
1	J	133	GLN
1	J	145	ASN
1	J	148	ASN
1	L	33	HIS
1	L	114	ASN
1	L	145	ASN
1	L	242	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 oligosaccharides 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	A	302	2	32,33,33	1.49	5 (15%)	48,52,52	1.85	9 (18%)
3	PO4	C	303	-	4,4,4	0.91	0	6,6,6	0.38	0
4	ATP	L	302	2	32,33,33	1.54	5 (15%)	48,52,52	2.12	13 (27%)
3	PO4	J	302	-	4,4,4	0.87	0	6,6,6	0.52	0
4	ATP	D	302	2	32,33,33	1.49	4 (12%)	48,52,52	1.89	11 (22%)
4	ATP	I	303	2	32,33,33	1.40	6 (18%)	48,52,52	1.97	12 (25%)
4	ATP	G	302	2	32,33,33	1.51	4 (12%)	48,52,52	2.02	12 (25%)
4	ATP	J	303	2	32,33,33	1.29	4 (12%)	48,52,52	1.88	13 (27%)
4	ATP	E	303	2	32,33,33	1.45	5 (15%)	48,52,52	1.85	10 (20%)
3	PO4	E	302	-	4,4,4	0.80	0	6,6,6	0.62	0
4	ATP	B	303	2	32,33,33	1.48	6 (18%)	48,52,52	1.84	11 (22%)
5	ACY	J	304	-	3,3,3	0.85	0	3,3,3	0.71	0
3	PO4	B	302	-	4,4,4	0.87	0	6,6,6	0.57	0
4	ATP	C	304	2	32,33,33	1.49	4 (12%)	48,52,52	2.07	12 (25%)
4	ATP	K	302	2	32,33,33	1.46	4 (12%)	48,52,52	1.93	9 (18%)
3	PO4	C	302	-	4,4,4	1.01	0	6,6,6	0.52	0
4	ATP	H	302	2	32,33,33	1.55	7 (21%)	48,52,52	1.72	10 (20%)
4	ATP	F	302	2	32,33,33	1.53	6 (18%)	48,52,52	1.94	12 (25%)
3	PO4	I	302	-	4,4,4	0.90	0	6,6,6	0.47	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	C	304	2	-	5/22/38/38	0/3/3/3
4	ATP	A	302	2	-	6/22/38/38	0/3/3/3
4	ATP	D	302	2	-	3/22/38/38	0/3/3/3
4	ATP	J	303	2	-	2/22/38/38	0/3/3/3
4	ATP	L	302	2	-	8/22/38/38	0/3/3/3
4	ATP	E	303	2	-	9/22/38/38	0/3/3/3
4	ATP	K	302	2	-	6/22/38/38	0/3/3/3
4	ATP	I	303	2	-	5/22/38/38	0/3/3/3
4	ATP	G	302	2	-	2/22/38/38	0/3/3/3
4	ATP	B	303	2	-	4/22/38/38	0/3/3/3
4	ATP	H	302	2	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	F	302	2	-	4/22/38/38	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	302	ATP	C5-C4	5.02	1.48	1.39
4	E	303	ATP	C5-C4	4.88	1.47	1.39
4	L	302	ATP	C5-C4	4.86	1.47	1.39
4	H	302	ATP	C5-C4	4.83	1.47	1.39
4	D	302	ATP	C5-C4	4.81	1.47	1.39
4	B	303	ATP	C5-C4	4.78	1.47	1.39
4	G	302	ATP	C5-C4	4.76	1.47	1.39
4	F	302	ATP	C5-C4	4.69	1.47	1.39
4	A	302	ATP	C5-C4	4.67	1.47	1.39
4	I	303	ATP	C5-C4	4.60	1.47	1.39
4	C	304	ATP	C5-C4	4.52	1.47	1.39
4	J	303	ATP	C5-C4	4.51	1.47	1.39
4	C	304	ATP	C5-C6	3.69	1.51	1.41
4	G	302	ATP	PB-O3B	3.47	1.63	1.59
4	K	302	ATP	C5-C6	3.42	1.50	1.41
4	D	302	ATP	PA-O3A	3.22	1.63	1.59
4	G	302	ATP	C5-C6	3.18	1.49	1.41
4	L	302	ATP	C5-C6	3.14	1.49	1.41
4	F	302	ATP	C5-C6	3.13	1.49	1.41
4	L	302	ATP	PB-O3B	3.11	1.62	1.59
4	D	302	ATP	C5-C6	3.03	1.49	1.41
4	B	303	ATP	PB-O3B	3.00	1.62	1.59
4	B	303	ATP	C5-C6	2.96	1.49	1.41
4	H	302	ATP	PA-O3A	2.93	1.62	1.59
4	C	304	ATP	C8-N7	2.87	1.37	1.31
4	J	303	ATP	C5-C6	2.83	1.48	1.41
4	H	302	ATP	C5-C6	2.82	1.48	1.41
4	L	302	ATP	C8-N7	2.77	1.37	1.31
4	E	303	ATP	PB-O3B	2.77	1.62	1.59
4	E	303	ATP	C8-N7	2.71	1.36	1.31
4	A	302	ATP	C5-C6	2.70	1.48	1.41
4	H	302	ATP	PB-O3B	2.70	1.62	1.59
4	K	302	ATP	C8-N7	2.68	1.36	1.31
4	B	303	ATP	C8-N7	2.67	1.36	1.31
4	A	302	ATP	C8-N7	2.67	1.36	1.31
4	A	302	ATP	PA-O3A	2.61	1.62	1.59
4	F	302	ATP	C8-N7	2.59	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	303	ATP	C5-C6	2.57	1.48	1.41
4	I	303	ATP	C5-C6	2.55	1.48	1.41
4	F	302	ATP	PB-O3B	2.54	1.62	1.59
4	J	303	ATP	C8-N7	2.54	1.36	1.31
4	G	302	ATP	C8-N7	2.51	1.36	1.31
4	I	303	ATP	PB-O3B	2.44	1.62	1.59
4	F	302	ATP	PA-O3A	2.44	1.62	1.59
4	E	303	ATP	C5-N7	-2.42	1.34	1.39
4	D	302	ATP	C8-N7	2.41	1.36	1.31
4	H	302	ATP	C5-N7	-2.40	1.34	1.39
4	H	302	ATP	C8-N7	2.39	1.36	1.31
4	I	303	ATP	C5-N7	-2.38	1.34	1.39
4	A	302	ATP	PB-O3B	2.30	1.62	1.59
4	I	303	ATP	C8-N7	2.28	1.36	1.31
4	L	302	ATP	C5-N7	-2.24	1.35	1.39
4	B	303	ATP	C5-N7	-2.18	1.35	1.39
4	K	302	ATP	PA-O3A	2.12	1.61	1.59
4	H	302	ATP	PB-O3A	2.10	1.61	1.59
4	C	304	ATP	PB-O3B	2.09	1.61	1.59
4	I	303	ATP	PA-O3A	2.09	1.61	1.59
4	B	303	ATP	PA-O3A	2.04	1.61	1.59
4	J	303	ATP	C4-N9	-2.03	1.33	1.37
4	F	302	ATP	C5-N7	-2.01	1.35	1.39

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	ATP	C5-C4-N3	-7.37	116.57	126.72
4	C	304	ATP	C5-C4-N3	-6.95	117.14	126.72
4	G	302	ATP	C5-C4-N3	-6.84	117.29	126.72
4	K	302	ATP	C5-C4-N3	-6.48	117.80	126.72
4	I	303	ATP	C5-C4-N3	-6.43	117.87	126.72
4	F	302	ATP	C5-C4-N3	-6.29	118.06	126.72
4	E	303	ATP	C5-C4-N3	-6.05	118.38	126.72
4	A	302	ATP	C5-C4-N3	-6.02	118.42	126.72
4	B	303	ATP	C5-C4-N3	-5.83	118.69	126.72
4	J	303	ATP	C5-C4-N3	-5.71	118.85	126.72
4	L	302	ATP	N3-C4-N9	5.68	136.82	127.17
4	H	302	ATP	C5-C4-N3	-5.54	119.09	126.72
4	D	302	ATP	C5-C4-N3	-5.48	119.17	126.72
4	I	303	ATP	N3-C4-N9	5.37	136.31	127.17
4	G	302	ATP	N3-C4-N9	5.37	136.30	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	303	ATP	N3-C4-N9	5.06	135.77	127.17
4	K	302	ATP	N3-C4-N9	4.97	135.63	127.17
4	F	302	ATP	N3-C4-N9	4.87	135.46	127.17
4	A	302	ATP	N3-C4-N9	4.82	135.37	127.17
4	L	302	ATP	C2-N3-C4	4.78	123.52	111.83
4	C	304	ATP	N3-C4-N9	4.71	135.17	127.17
4	C	304	ATP	C2-N3-C4	4.67	123.25	111.83
4	G	302	ATP	C2-N3-C4	4.55	122.94	111.83
4	H	302	ATP	N3-C4-N9	4.54	134.89	127.17
4	K	302	ATP	C2-N3-C4	4.54	122.92	111.83
4	J	303	ATP	N3-C4-N9	4.43	134.70	127.17
4	D	302	ATP	N3-C2-N1	-4.32	122.04	128.58
4	I	303	ATP	C2-N3-C4	4.32	122.38	111.83
4	F	302	ATP	C2-N3-C4	4.30	122.34	111.83
4	D	302	ATP	N3-C4-N9	4.30	134.48	127.17
4	C	304	ATP	C4-C5-N7	-4.25	105.72	110.58
4	B	303	ATP	N3-C4-N9	4.21	134.33	127.17
4	H	302	ATP	N3-C2-N1	-4.15	122.30	128.58
4	D	302	ATP	C2-N3-C4	4.12	121.90	111.83
4	A	302	ATP	C2-N3-C4	4.12	121.89	111.83
4	J	303	ATP	C2-N3-C4	4.09	121.83	111.83
4	B	303	ATP	C2-N3-C4	4.08	121.80	111.83
4	I	303	ATP	N3-C2-N1	-4.04	122.46	128.58
4	L	302	ATP	N3-C2-N1	-4.04	122.47	128.58
4	K	302	ATP	N3-C2-N1	-4.04	122.47	128.58
4	H	302	ATP	C2-N3-C4	3.99	121.57	111.83
4	B	303	ATP	N3-C2-N1	-3.94	122.62	128.58
4	F	302	ATP	N3-C2-N1	-3.92	122.65	128.58
4	E	303	ATP	C2-N3-C4	3.89	121.32	111.83
4	G	302	ATP	N3-C2-N1	-3.84	122.76	128.58
4	B	303	ATP	C4-C5-N7	-3.82	106.21	110.58
4	L	302	ATP	C4-C5-N7	-3.82	106.22	110.58
4	G	302	ATP	C4-C5-N7	-3.79	106.25	110.58
4	K	302	ATP	C4-C5-N7	-3.77	106.27	110.58
4	J	303	ATP	N3-C2-N1	-3.76	122.89	128.58
4	C	304	ATP	N3-C2-N1	-3.73	122.94	128.58
4	A	302	ATP	N3-C2-N1	-3.69	123.00	128.58
4	J	303	ATP	C4-C5-N7	-3.50	106.58	110.58
4	E	303	ATP	N3-C2-N1	-3.41	123.42	128.58
4	L	302	ATP	C5-N7-C8	3.29	108.61	103.45
4	G	302	ATP	C5-N7-C8	3.19	108.46	103.45
4	D	302	ATP	C4-C5-N7	-3.19	106.94	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	303	ATP	C4-N9-C8	3.14	109.04	105.74
4	F	302	ATP	O2B-PB-O3B	3.14	115.75	107.27
4	C	304	ATP	C5-N7-C8	3.07	108.28	103.45
4	D	302	ATP	O3A-PA-O1A	-3.07	101.46	110.70
4	A	302	ATP	C4-C5-N7	-2.98	107.17	110.58
4	B	303	ATP	C5-N7-C8	2.90	108.02	103.45
4	F	302	ATP	C4-C5-N7	-2.89	107.28	110.58
4	J	303	ATP	C5-N7-C8	2.85	107.93	103.45
4	K	302	ATP	C5-N7-C8	2.83	107.90	103.45
4	G	302	ATP	C4-N9-C8	2.82	108.70	105.74
4	J	303	ATP	N9-C8-N7	-2.78	109.99	113.94
4	H	302	ATP	C4-C5-N7	-2.78	107.41	110.58
4	K	302	ATP	C6-C5-N7	2.68	137.25	132.09
4	F	302	ATP	O2A-PA-O1A	2.65	124.78	112.44
4	D	302	ATP	C6-C5-N7	2.65	137.19	132.09
4	G	302	ATP	N9-C8-N7	-2.65	110.18	113.94
4	E	303	ATP	O4'-C1'-N9	2.64	113.16	108.09
4	C	304	ATP	O3G-PG-O3B	2.64	113.48	104.64
4	B	303	ATP	C6-C5-N7	2.59	137.08	132.09
4	K	302	ATP	C4-N9-C8	2.58	108.45	105.74
4	J	303	ATP	O2A-PA-O1A	2.54	124.26	112.44
4	J	303	ATP	O3G-PG-O2G	2.53	117.30	107.80
4	E	303	ATP	C4-C5-N7	-2.50	107.72	110.58
4	A	302	ATP	C4-N9-C8	2.50	108.36	105.74
4	G	302	ATP	O2B-PB-O3B	2.48	113.99	107.27
4	G	302	ATP	C6-C5-N7	2.48	136.87	132.09
4	I	303	ATP	C4-C5-N7	-2.47	107.76	110.58
4	J	303	ATP	C6-C5-N7	2.47	136.84	132.09
4	E	303	ATP	C4-N9-C8	2.46	108.32	105.74
4	D	302	ATP	C4-N9-C8	2.45	108.31	105.74
4	I	303	ATP	C3'-C2'-C1'	2.44	106.08	101.46
4	B	303	ATP	C4-N9-C8	2.40	108.26	105.74
4	B	303	ATP	N9-C8-N7	-2.40	110.53	113.94
4	C	304	ATP	C6-C5-N7	2.38	136.69	132.09
4	H	302	ATP	C4-N9-C8	2.38	108.24	105.74
4	F	302	ATP	O3B-PG-O1G	-2.37	98.58	111.04
4	L	302	ATP	C2'-C3'-C4'	-2.37	98.04	102.61
4	D	302	ATP	C2-N1-C6	2.36	122.61	118.73
4	E	303	ATP	O3G-PG-O2G	2.35	116.60	107.80
4	A	302	ATP	C5-N7-C8	2.32	107.10	103.45
4	F	302	ATP	O4'-C1'-N9	2.32	112.54	108.09
4	C	304	ATP	N9-C8-N7	-2.32	110.65	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	ATP	O2A-PA-O1A	2.31	123.18	112.44
4	C	304	ATP	O4'-C1'-N9	2.30	112.51	108.09
4	C	304	ATP	O2B-PB-O3B	2.29	113.46	107.27
4	L	302	ATP	N9-C8-N7	-2.28	110.70	113.94
4	E	303	ATP	O2A-PA-O1A	2.26	122.94	112.44
4	H	302	ATP	O3B-PG-O1G	-2.25	99.18	111.04
4	C	304	ATP	C3'-C2'-C1'	2.24	105.71	101.46
4	I	303	ATP	O2G-PG-O3B	2.23	112.13	104.64
4	L	302	ATP	O4'-C1'-N9	2.23	112.36	108.09
4	J	303	ATP	O2B-PB-O1B	2.21	122.75	112.44
4	I	303	ATP	C4-N9-C8	2.21	108.06	105.74
4	K	302	ATP	N9-C8-N7	-2.21	110.81	113.94
4	E	303	ATP	C5-N7-C8	2.19	106.89	103.45
4	H	302	ATP	C2-N1-C6	2.18	122.31	118.73
4	B	303	ATP	O2B-PB-O3B	2.18	113.16	107.27
4	F	302	ATP	C4-N9-C8	2.18	108.02	105.74
4	D	302	ATP	C5-N7-C8	2.14	106.81	103.45
4	L	302	ATP	C6-C5-N7	2.13	136.19	132.09
4	A	302	ATP	O2A-PA-O3A	-2.11	101.56	107.27
4	H	302	ATP	C6-C5-N7	2.11	136.15	132.09
4	F	302	ATP	C5-N7-C8	2.10	106.75	103.45
4	I	303	ATP	O2A-PA-O1A	2.09	122.18	112.44
4	I	303	ATP	O3B-PG-O1G	-2.09	100.06	111.04
4	A	302	ATP	C3'-C2'-C1'	2.08	105.40	101.46
4	F	302	ATP	O2G-PG-O3B	2.06	111.53	104.64
4	H	302	ATP	C5-N7-C8	2.06	106.68	103.45
4	G	302	ATP	O2A-PA-O1A	2.05	121.96	112.44
4	J	303	ATP	C3'-C2'-C1'	2.05	105.33	101.46
4	G	302	ATP	C3'-C2'-C1'	2.04	105.32	101.46
4	L	302	ATP	O2B-PB-O1B	2.04	121.91	112.44
4	I	303	ATP	O3G-PG-O2G	2.03	115.43	107.80
4	L	302	ATP	C4-N9-C8	2.03	107.87	105.74
4	D	302	ATP	O2B-PB-O3B	2.03	112.75	107.27
4	L	302	ATP	O3G-PG-O2G	2.02	115.39	107.80
4	I	303	ATP	C5-N7-C8	2.02	106.63	103.45

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	303	ATP	C5'-O5'-PA-O1A
4	K	302	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	K	302	ATP	O4'-C4'-C5'-O5'
4	K	302	ATP	C3'-C4'-C5'-O5'
4	H	302	ATP	C5'-O5'-PA-O3A
4	L	302	ATP	PB-O3B-PG-O3G
4	L	302	ATP	C5'-O5'-PA-O2A
4	L	302	ATP	C5'-O5'-PA-O3A
4	G	302	ATP	PB-O3B-PG-O1G
4	D	302	ATP	C2'-C1'-N9-C8
4	I	303	ATP	PB-O3A-PA-O1A
4	E	303	ATP	C5'-O5'-PA-O2A
4	E	303	ATP	C5'-O5'-PA-O3A
4	L	302	ATP	C5'-O5'-PA-O1A
4	E	303	ATP	PG-O3B-PB-O1B
4	L	302	ATP	O4'-C4'-C5'-O5'
4	K	302	ATP	PG-O3B-PB-O2B
4	A	302	ATP	PB-O3A-PA-O1A
4	F	302	ATP	PG-O3B-PB-O1B
4	H	302	ATP	PG-O3B-PB-O1B
4	B	303	ATP	C2'-C1'-N9-C8
4	A	302	ATP	O4'-C1'-N9-C8
4	J	303	ATP	O4'-C1'-N9-C8
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	H	302	ATP	C2'-C1'-N9-C8
4	E	303	ATP	O4'-C4'-C5'-O5'
4	F	302	ATP	O4'-C1'-N9-C8
4	B	303	ATP	PG-O3B-PB-O2B
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	E	303	ATP	PG-O3B-PB-O2B
4	E	303	ATP	PA-O3A-PB-O1B
4	E	303	ATP	PB-O3A-PA-O2A
4	I	303	ATP	PG-O3B-PB-O2B
4	I	303	ATP	PB-O3A-PA-O2A
4	A	302	ATP	PA-O3A-PB-O1B
4	F	302	ATP	PG-O3B-PB-O2B
4	H	302	ATP	PG-O3B-PB-O2B
4	C	304	ATP	O4'-C1'-N9-C8
4	I	303	ATP	O4'-C1'-N9-C8
4	G	302	ATP	O4'-C1'-N9-C8

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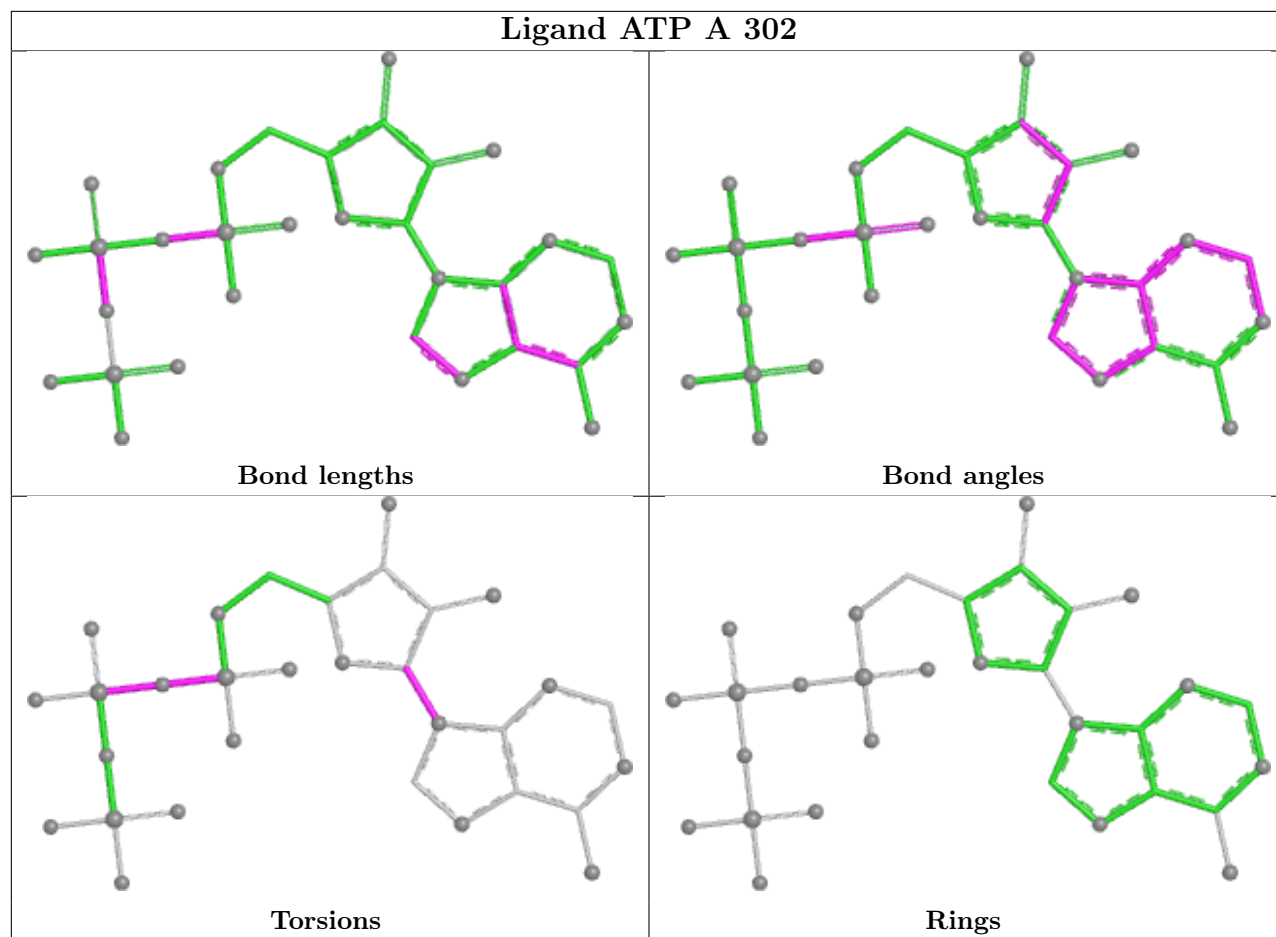
Mol	Chain	Res	Type	Atoms
4	A	302	ATP	C2'-C1'-N9-C8
4	J	303	ATP	C2'-C1'-N9-C8
4	L	302	ATP	PB-O3B-PG-O1G
4	D	302	ATP	O4'-C1'-N9-C8
4	E	303	ATP	O4'-C1'-N9-C8
4	C	304	ATP	PB-O3A-PA-O2A
4	D	302	ATP	PA-O3A-PB-O2B
4	I	303	ATP	PA-O3A-PB-O2B
4	K	302	ATP	PA-O3A-PB-O2B
4	K	302	ATP	PB-O3A-PA-O1A
4	A	302	ATP	PA-O3A-PB-O2B
4	A	302	ATP	PB-O3A-PA-O2A
4	F	302	ATP	PB-O3A-PA-O1A
4	H	302	ATP	PB-O3A-PA-O2A
4	L	302	ATP	PG-O3B-PB-O1B

There are no ring outliers.

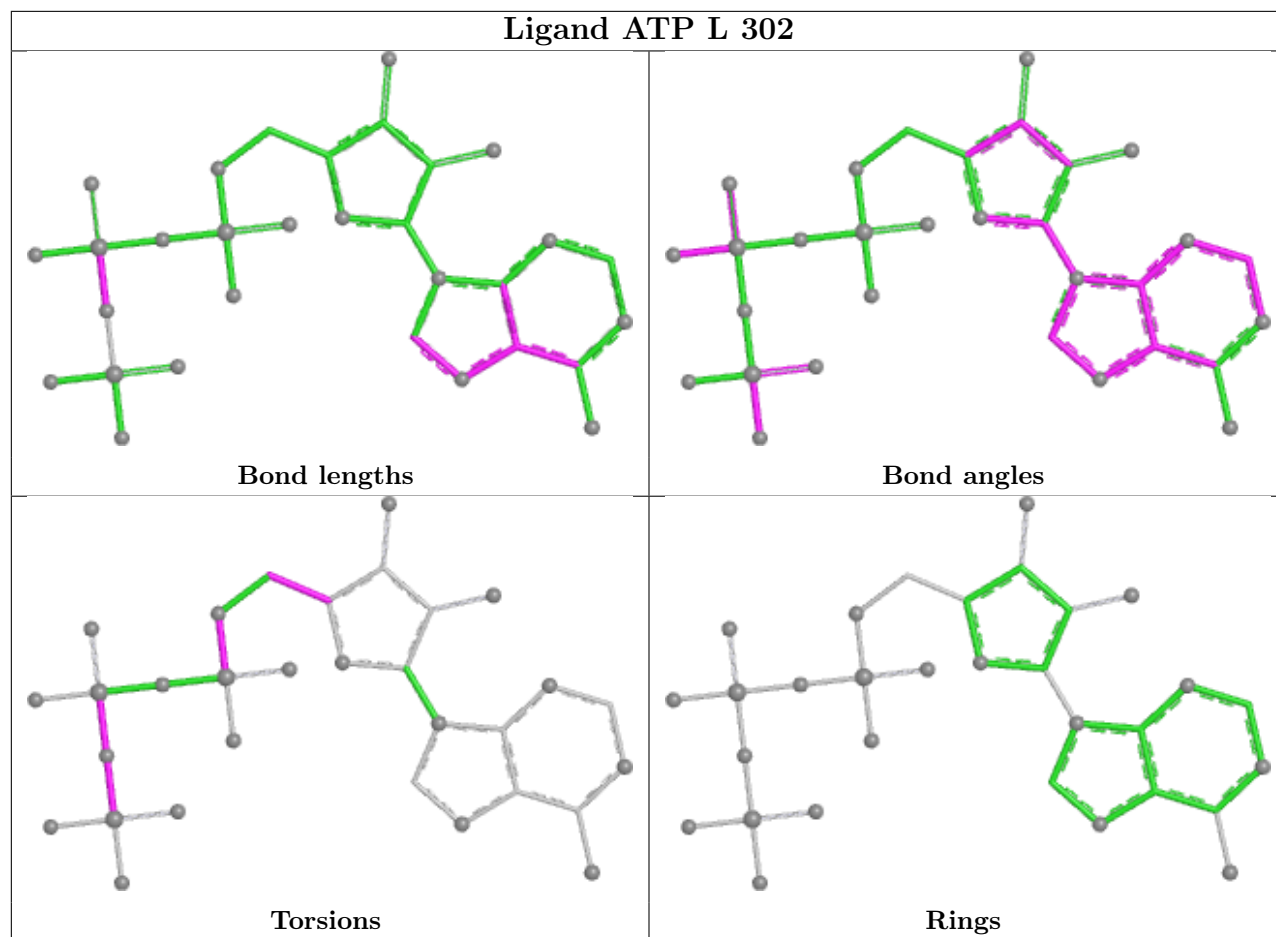
8 monomers are involved in 13 short contacts:

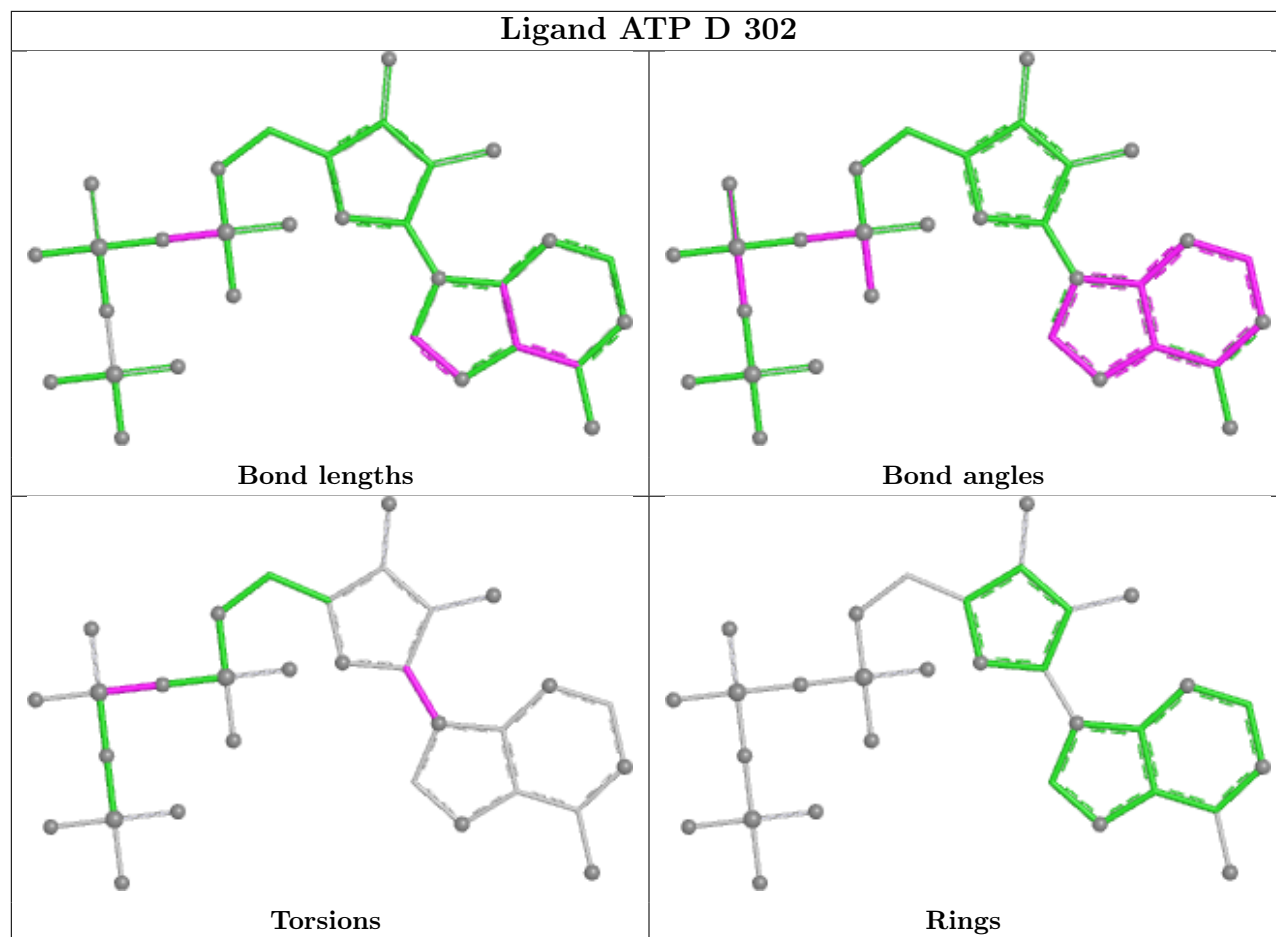
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	ATP	2	0
4	L	302	ATP	2	0
4	D	302	ATP	2	0
4	I	303	ATP	1	0
4	G	302	ATP	1	0
4	J	303	ATP	2	0
4	B	303	ATP	2	0
4	K	302	ATP	1	0

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.

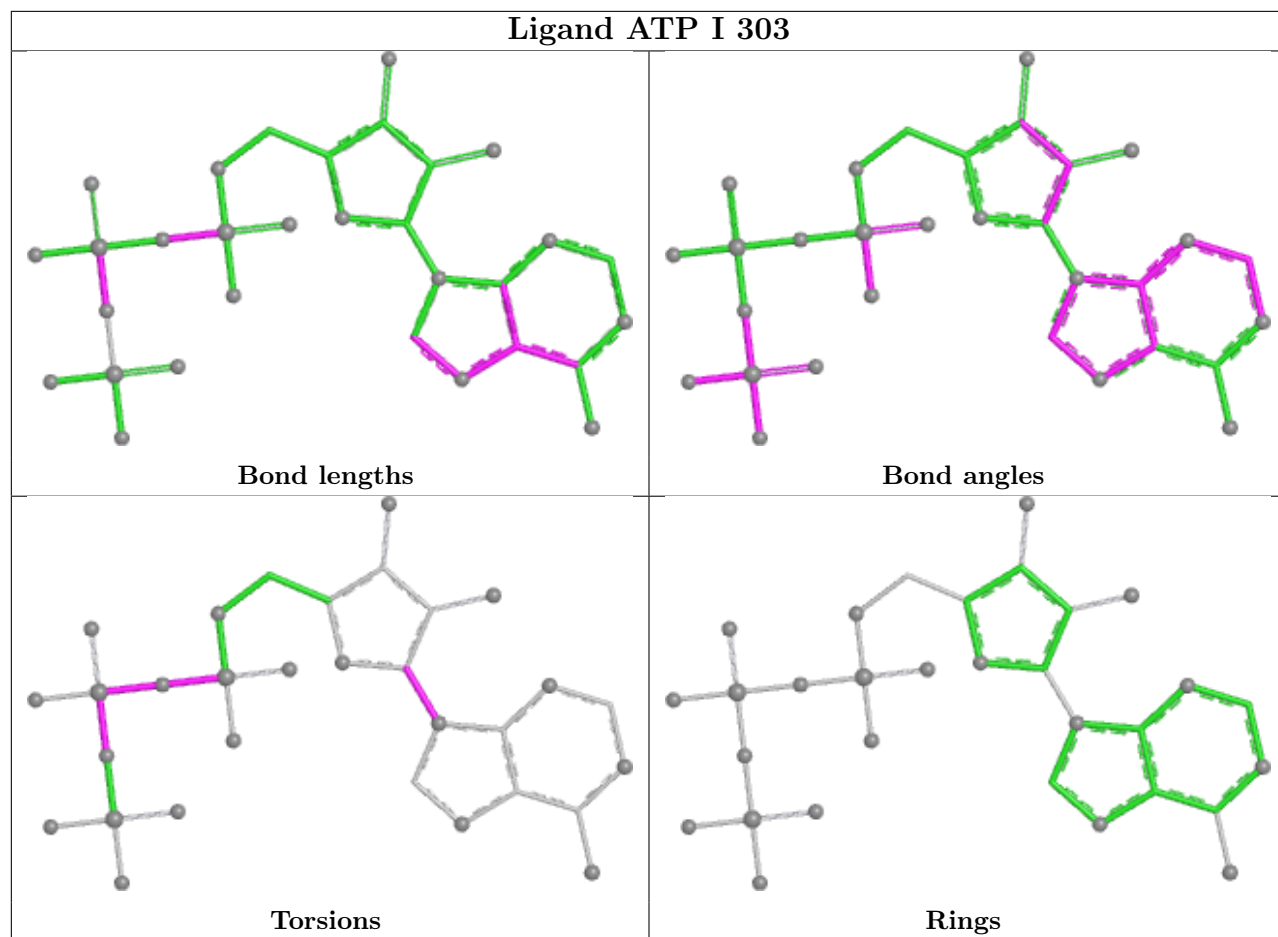


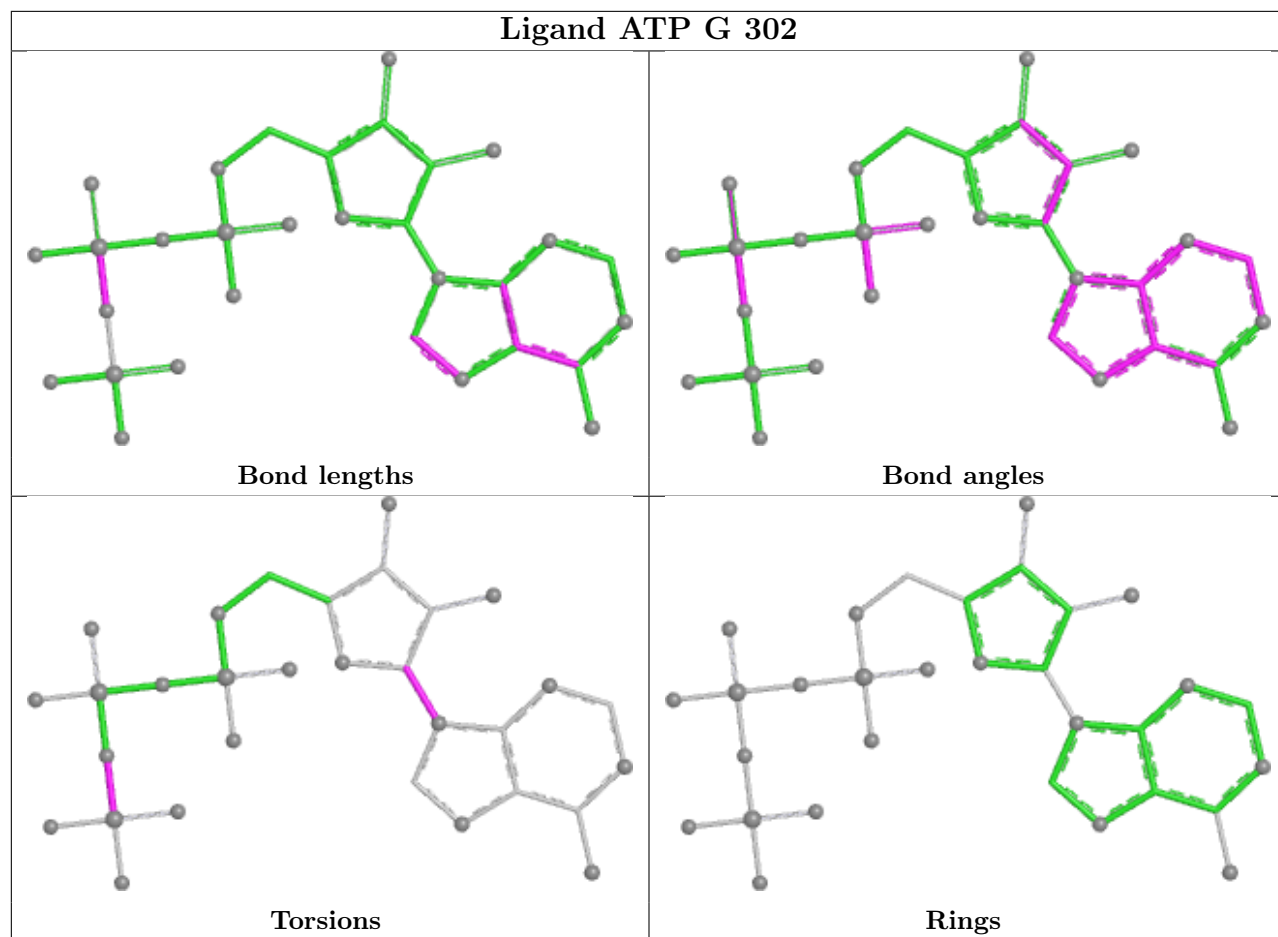
Ligand ATP L 302



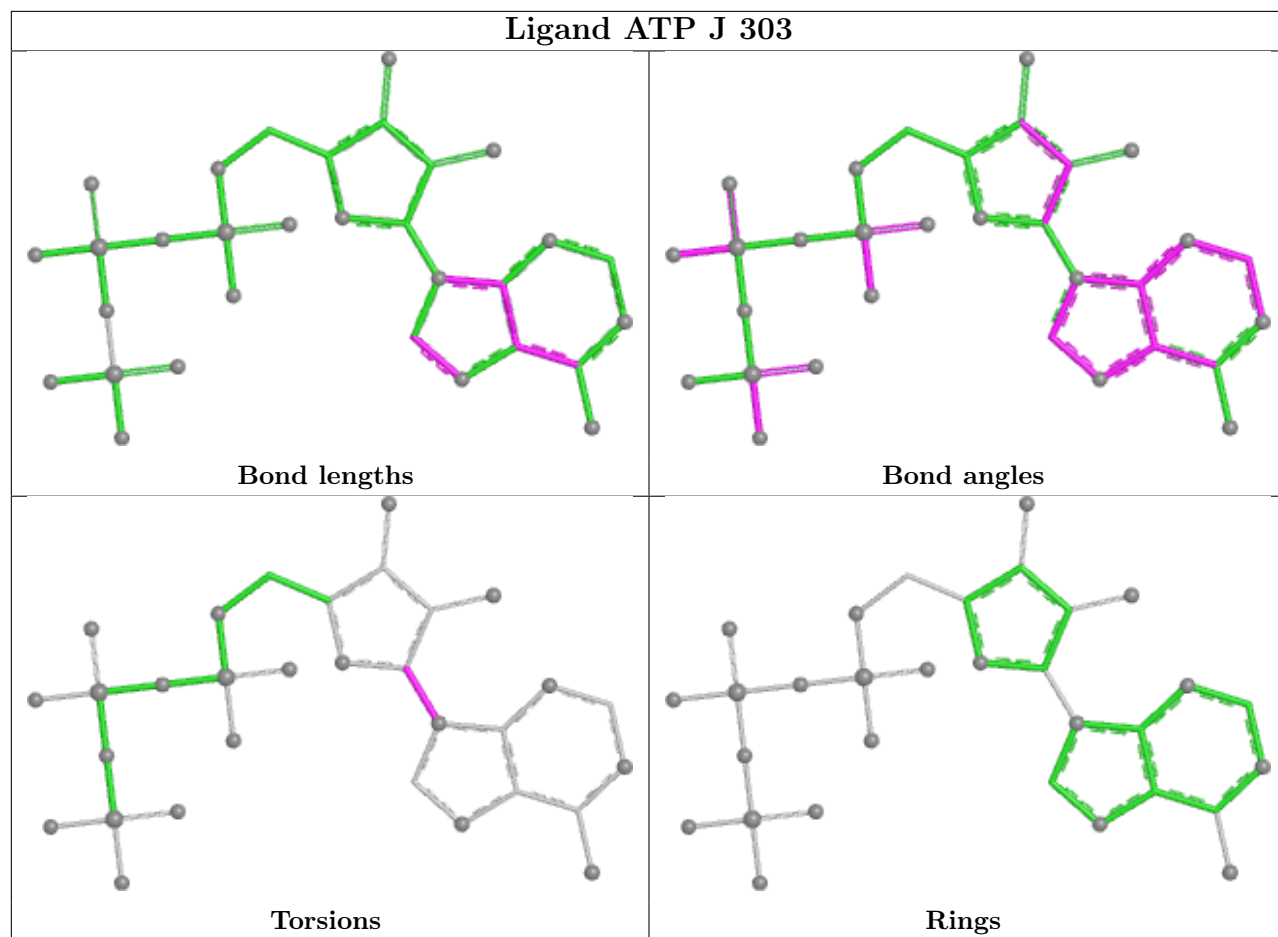


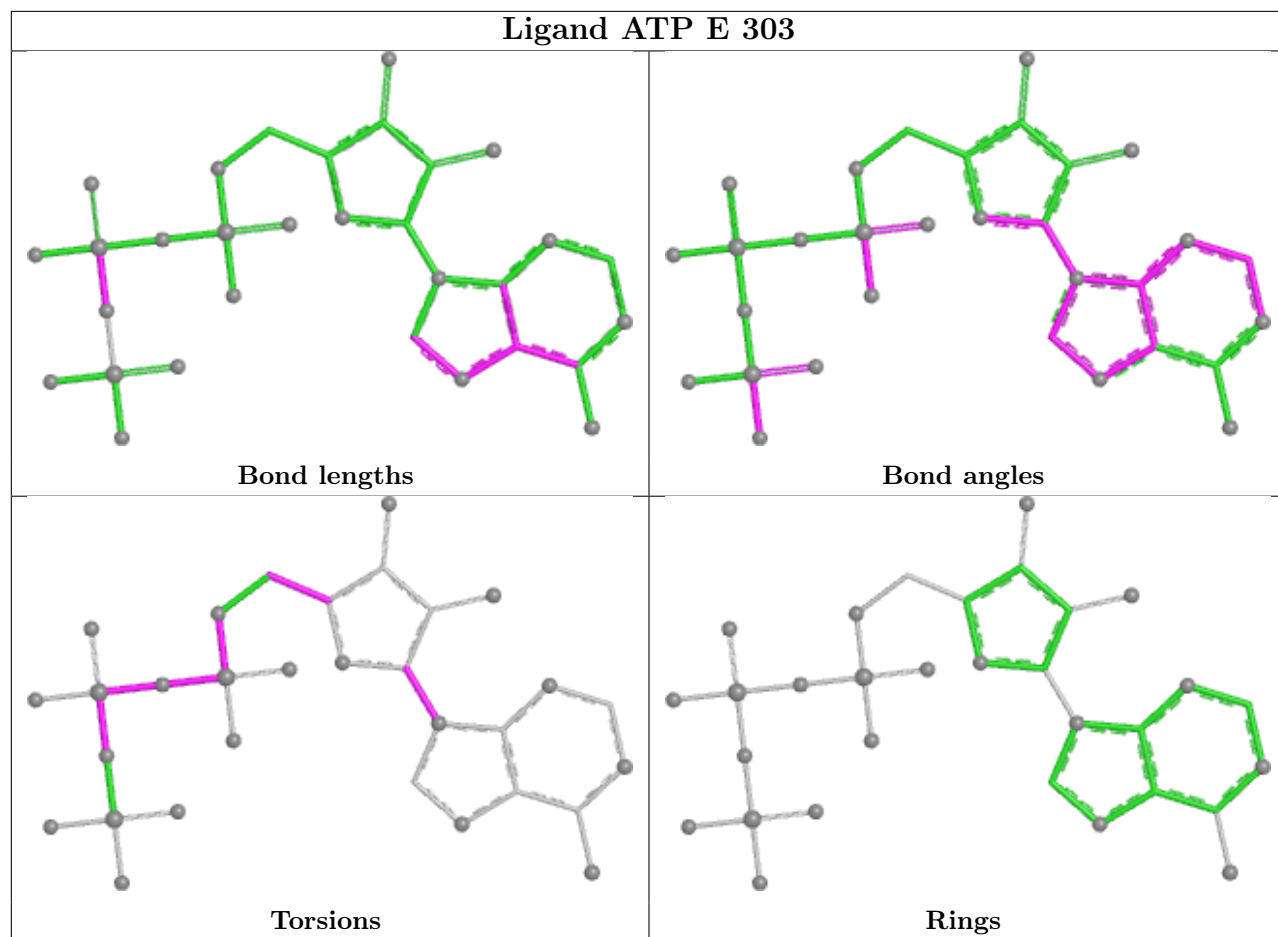
Ligand ATP I 303

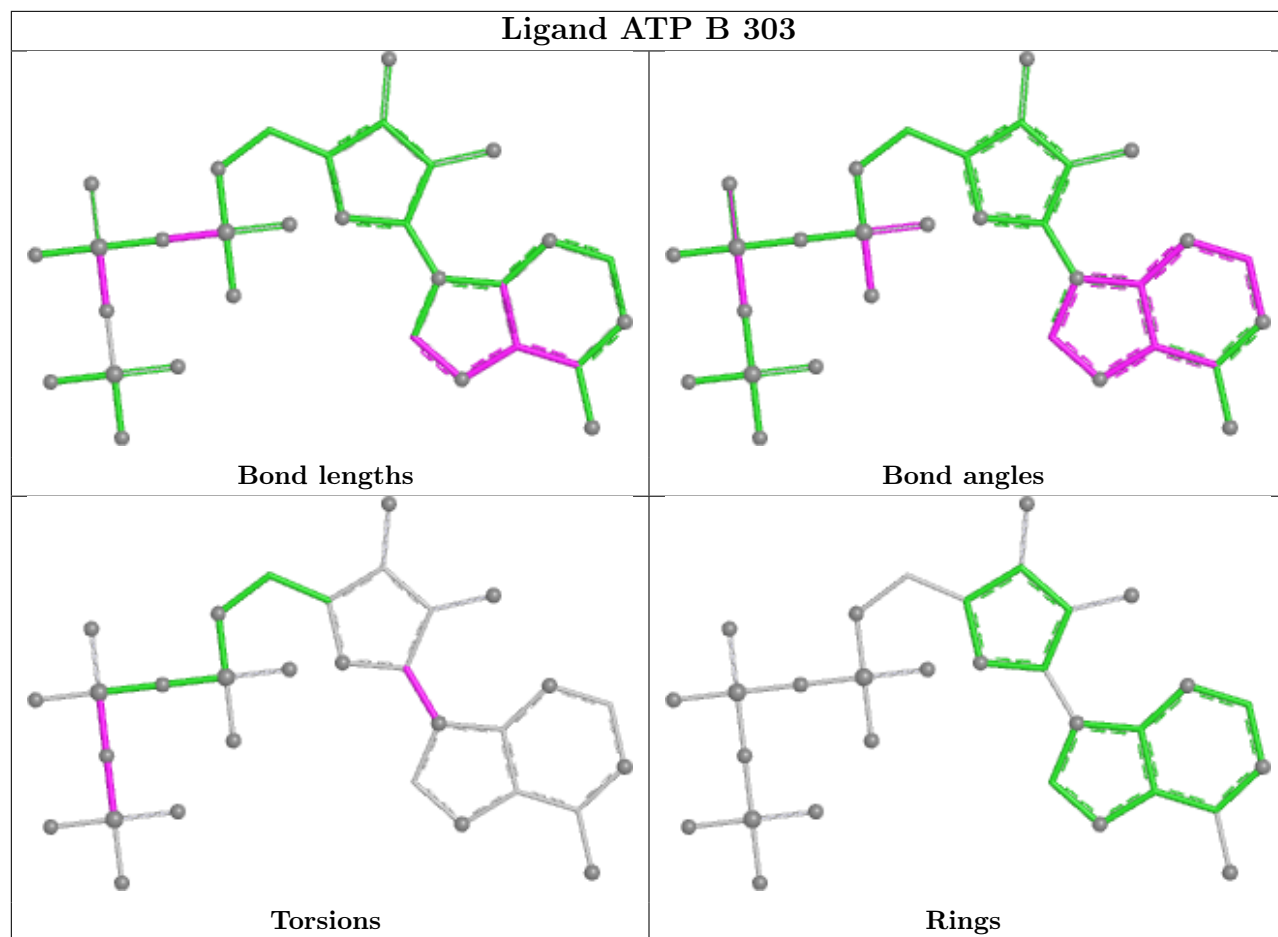


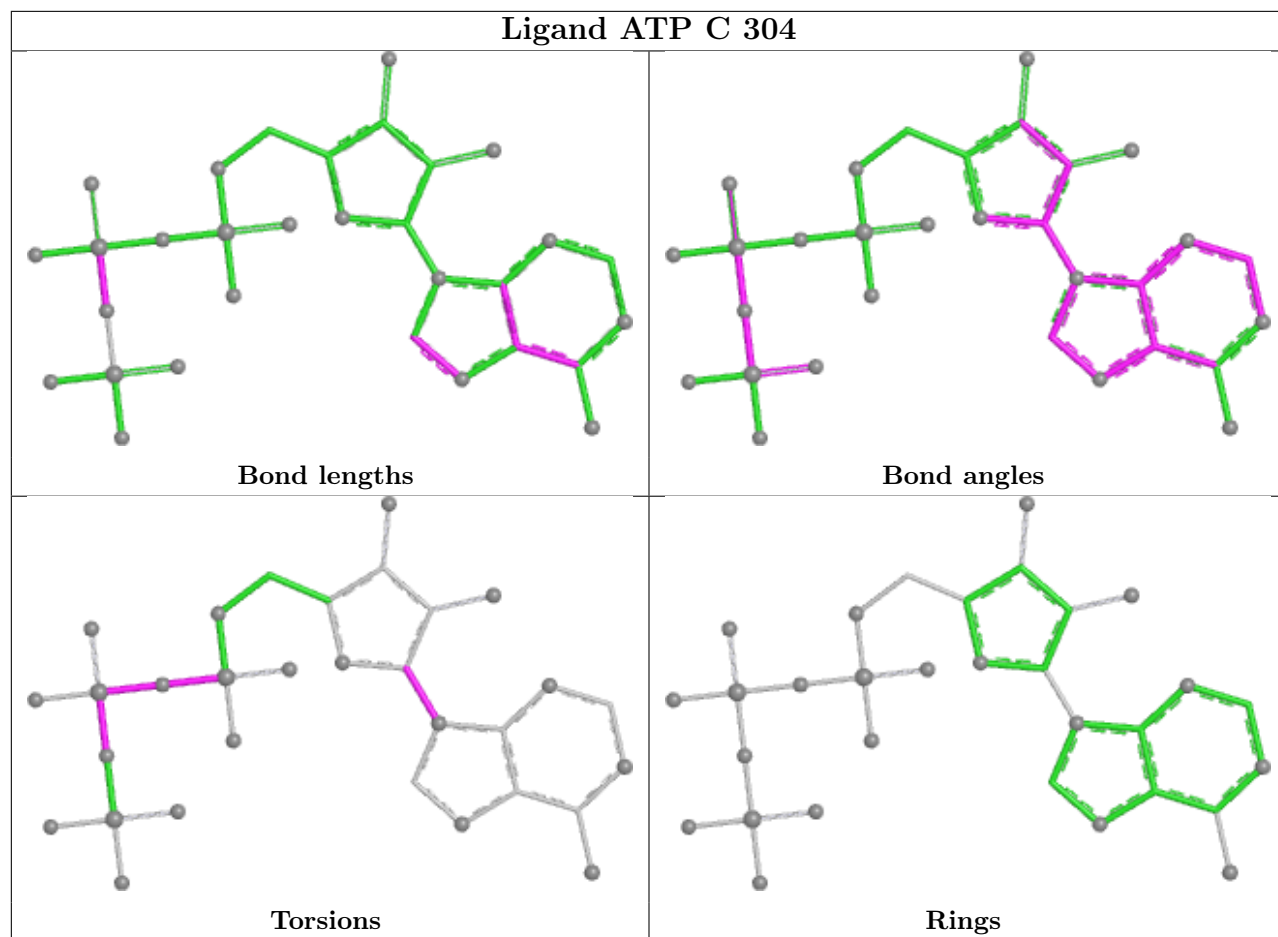


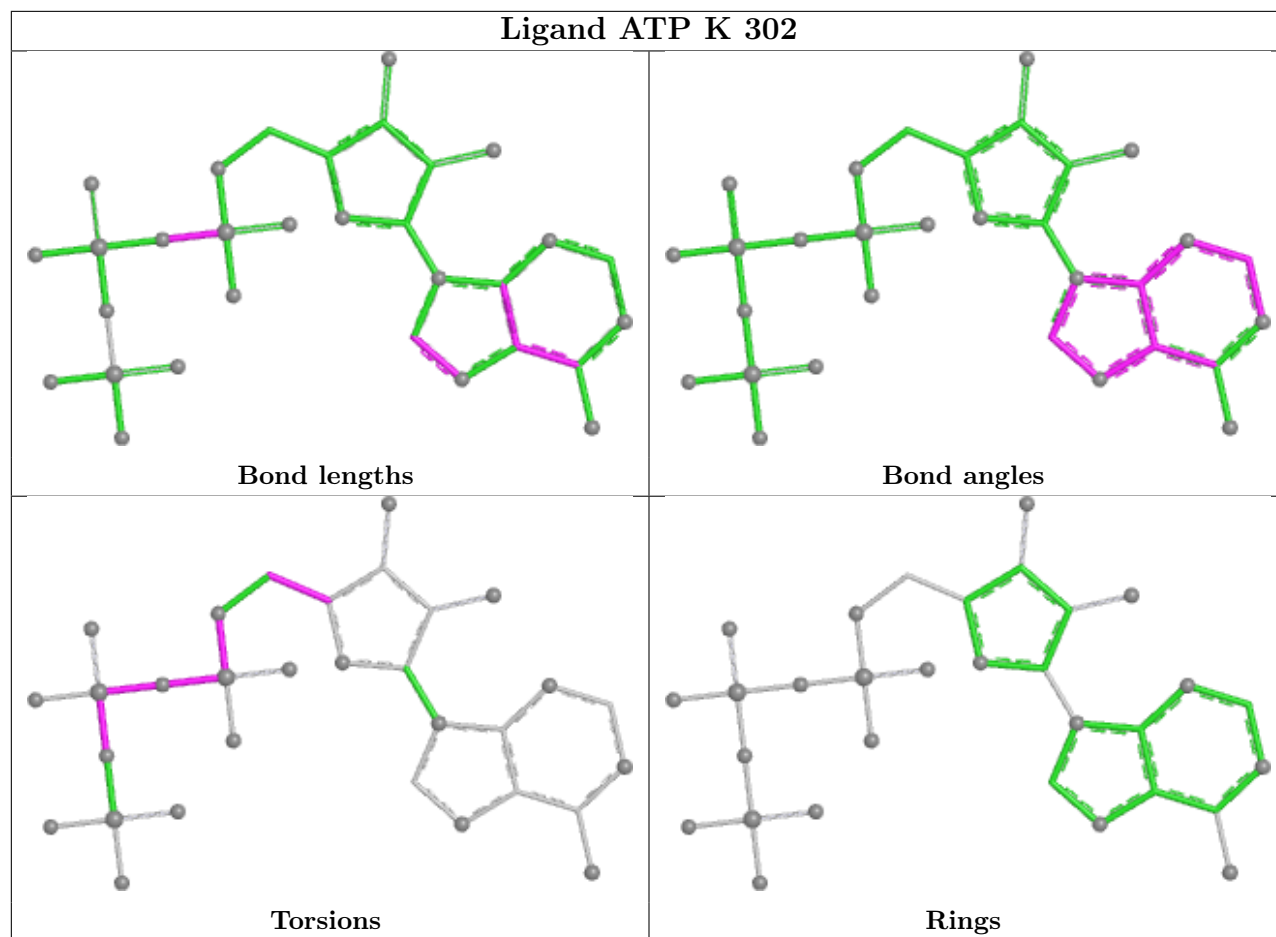
Ligand ATP J 303

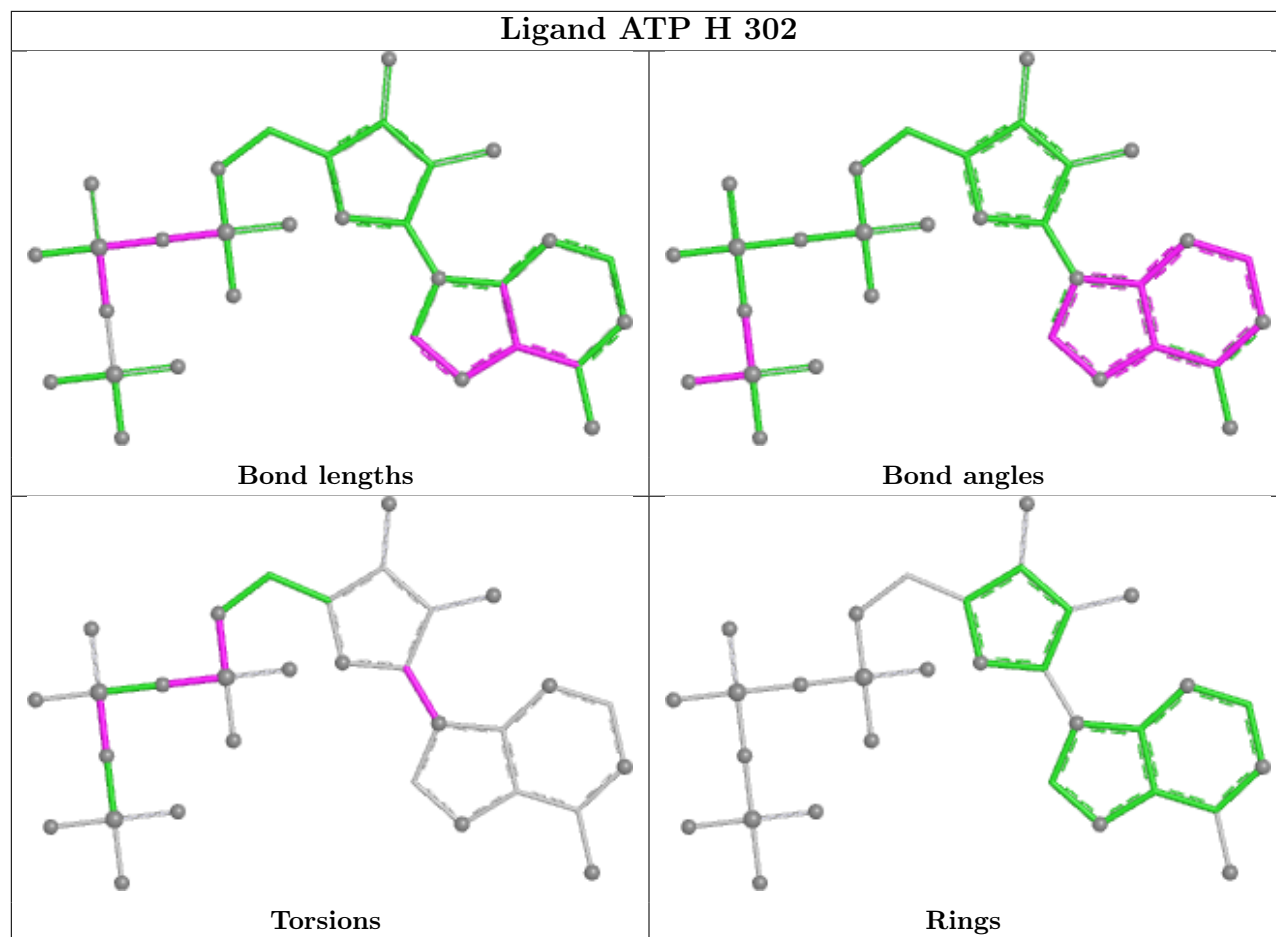


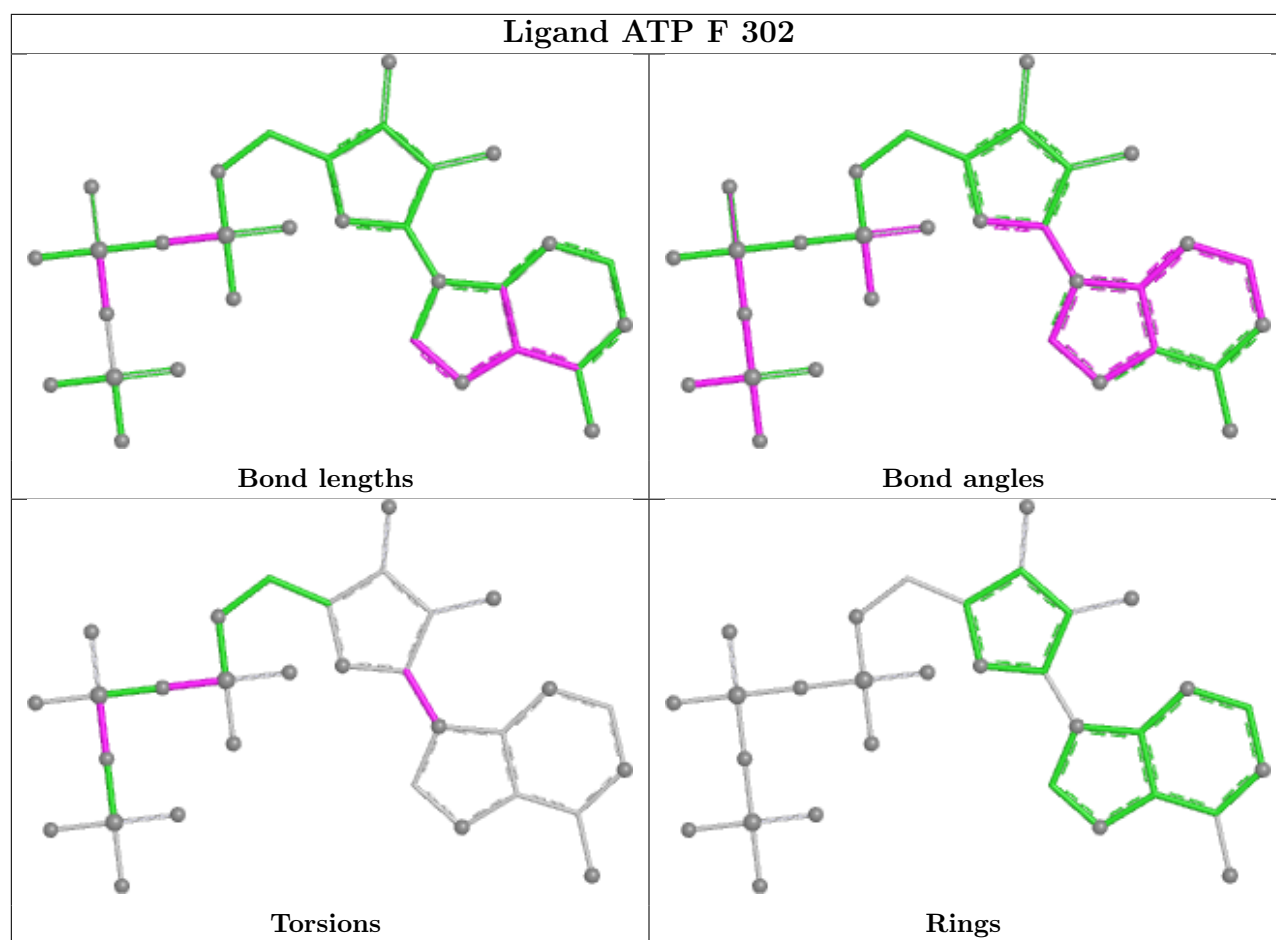












5.7 Other polymers [i](#)

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, 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	296/300 (98%)	0.45	24 (8%) 18 15	18, 35, 64, 92	0
1	B	296/300 (98%)	0.53	29 (9%) 13 10	18, 38, 72, 92	0
1	C	294/300 (98%)	0.64	36 (12%) 8 6	14, 39, 77, 94	1 (0%)
1	D	294/300 (98%)	0.78	34 (11%) 9 7	23, 43, 79, 99	0
1	E	295/300 (98%)	0.78	23 (7%) 19 16	23, 49, 78, 100	0
1	F	293/300 (97%)	0.56	19 (6%) 25 22	14, 42, 69, 85	1 (0%)
1	G	292/300 (97%)	0.82	40 (13%) 6 5	23, 44, 77, 99	0
1	H	295/300 (98%)	1.16	52 (17%) 4 3	33, 55, 85, 102	0
1	I	292/300 (97%)	0.91	45 (15%) 5 4	23, 48, 82, 92	0
1	J	296/300 (98%)	0.54	18 (6%) 27 24	23, 42, 69, 82	0
1	K	294/300 (98%)	1.06	38 (12%) 7 5	18, 52, 81, 102	1 (0%)
1	L	293/300 (97%)	1.15	53 (18%) 3 2	21, 52, 82, 91	1 (0%)
All	All	3530/3600 (98%)	0.78	411 (11%) 9 7	14, 45, 78, 102	4 (0%)

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	GLU	5.9
1	E	35	HIS	5.4
1	K	175	ALA	5.2
1	D	118	ASN	5.2
1	D	175	ALA	5.1
1	L	181	ASN	5.1
1	A	259	ASP	4.9
1	G	173	SER	4.8
1	L	173	SER	4.8
1	C	175	ALA	4.8
1	D	171	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	38	SER	4.7
1	D	173	SER	4.6
1	E	175	ALA	4.5
1	J	257	ALA	4.5
1	H	175	ALA	4.5
1	G	5	THR	4.4
1	L	247	GLY	4.4
1	K	172	SER	4.4
1	C	259	ASP	4.4
1	L	243	ALA	4.3
1	E	173	SER	4.3
1	H	4	ASN	4.3
1	L	171	VAL	4.3
1	D	4	ASN	4.3
1	H	244	LEU	4.2
1	A	260	GLU	4.2
1	L	35	HIS	4.1
1	B	239	ASP	4.1
1	J	5	THR	4.1
1	A	257	ALA	4.1
1	H	248	VAL	4.1
1	I	4	ASN	4.1
1	I	179	ALA	4.0
1	C	174	GLY	4.0
1	H	34	ILE	4.0
1	L	172	SER	4.0
1	K	171	VAL	4.0
1	D	119	LEU	4.0
1	L	246	PRO	3.9
1	L	238	LEU	3.9
1	D	185	VAL	3.9
1	I	121	ASP	3.9
1	C	119	LEU	3.9
1	A	36	GLU	3.8
1	L	5	THR	3.8
1	C	116	PHE	3.8
1	A	175	ALA	3.8
1	L	175	ALA	3.8
1	I	119	LEU	3.8
1	L	36	GLU	3.7
1	H	36	GLU	3.7
1	F	116	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	185	VAL	3.7
1	F	175	ALA	3.7
1	L	119	LEU	3.7
1	A	38	SER	3.7
1	H	119	LEU	3.6
1	H	173	SER	3.6
1	F	260	GLU	3.6
1	E	34	ILE	3.6
1	B	260	GLU	3.6
1	C	256	LEU	3.6
1	E	257	ALA	3.6
1	C	254	LEU	3.5
1	K	5	THR	3.5
1	I	248	VAL	3.5
1	C	117	GLN	3.5
1	I	144	ILE	3.5
1	K	35	HIS	3.5
1	D	274	PHE	3.5
1	I	114	ASN	3.5
1	B	36	GLU	3.5
1	F	248	VAL	3.5
1	D	257	ALA	3.5
1	K	38	SER	3.5
1	D	35	HIS	3.5
1	L	34	ILE	3.5
1	I	175	ALA	3.4
1	L	179	ALA	3.4
1	G	260	GLU	3.4
1	B	238	LEU	3.4
1	H	118	ASN	3.4
1	G	37	GLN	3.4
1	H	274	PHE	3.4
1	K	179	ALA	3.4
1	G	175	ALA	3.4
1	K	249	GLU	3.4
1	D	143	GLY	3.4
1	G	119	LEU	3.4
1	C	248	VAL	3.4
1	H	179	ALA	3.4
1	H	143	GLY	3.4
1	G	40	ILE	3.3
1	G	122	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	258	HIS	3.3
1	I	186	LYS	3.3
1	D	174	GLY	3.3
1	C	4	ASN	3.3
1	H	121	ASP	3.3
1	L	273	LEU	3.3
1	H	280	ALA	3.3
1	K	4	ASN	3.3
1	H	116	PHE	3.3
1	H	176	THR	3.3
1	L	236	GLU	3.3
1	L	252	THR	3.3
1	L	245	LEU	3.2
1	K	251	PRO	3.2
1	G	144	ILE	3.2
1	L	39	LEU	3.2
1	L	241	ILE	3.2
1	H	277	THR	3.2
1	L	240	LYS	3.2
1	B	234	PRO	3.2
1	E	36	GLU	3.2
1	I	176	THR	3.2
1	H	249	GLU	3.1
1	C	143	GLY	3.1
1	A	4	ASN	3.1
1	H	239	ASP	3.1
1	J	258	HIS	3.1
1	L	33	HIS	3.1
1	K	87	LEU	3.1
1	B	243	ALA	3.1
1	I	169	ASP	3.1
1	K	245	LEU	3.1
1	F	256	LEU	3.1
1	A	261	LYS	3.1
1	A	35	HIS	3.0
1	G	35	HIS	3.0
1	L	258	HIS	3.0
1	L	38	SER	3.0
1	G	160	ARG	3.0
1	K	181	ASN	3.0
1	H	245	LEU	3.0
1	F	35	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	5	THR	3.0
1	G	172	SER	3.0
1	D	116	PHE	3.0
1	G	116	PHE	3.0
1	K	257	ALA	3.0
1	J	4	ASN	3.0
1	H	246	PRO	3.0
1	C	298	LEU	2.9
1	D	273	LEU	2.9
1	B	4	ASN	2.9
1	H	285	GLY	2.9
1	L	113	GLU	2.9
1	I	298	LEU	2.9
1	K	112	GLN	2.9
1	G	114	ASN	2.9
1	G	117	GLN	2.9
1	A	181	ASN	2.9
1	D	37	GLN	2.9
1	G	177	LEU	2.9
1	D	141	GLU	2.9
1	L	239	ASP	2.9
1	E	33	HIS	2.8
1	D	122	PHE	2.8
1	L	174	GLY	2.8
1	L	256	LEU	2.8
1	H	260	GLU	2.8
1	C	35	HIS	2.8
1	J	181	ASN	2.8
1	G	236	GLU	2.8
1	A	115	LYS	2.8
1	A	240	LYS	2.8
1	H	263	VAL	2.8
1	L	160	ARG	2.8
1	H	124	GLY	2.8
1	I	246	PRO	2.8
1	D	36	GLU	2.8
1	K	156	GLU	2.8
1	D	87	LEU	2.8
1	B	237	LYS	2.8
1	G	115	LYS	2.8
1	K	176	THR	2.7
1	G	118	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	37	GLN	2.7
1	B	38	SER	2.7
1	B	235	LYS	2.7
1	B	37	GLN	2.7
1	L	112	GLN	2.7
1	A	88	GLY	2.7
1	C	255	PRO	2.7
1	C	250	ARG	2.7
1	L	244	LEU	2.7
1	B	33	HIS	2.7
1	J	35	HIS	2.7
1	J	256	LEU	2.7
1	B	35	HIS	2.7
1	L	257	ALA	2.7
1	I	113	GLU	2.7
1	D	172	SER	2.7
1	K	177	LEU	2.7
1	K	273	LEU	2.7
1	C	261	LYS	2.6
1	F	299	LYS	2.6
1	D	260	GLU	2.6
1	B	171	VAL	2.6
1	H	114	ASN	2.6
1	L	298	LEU	2.6
1	K	274	PHE	2.6
1	G	171	VAL	2.6
1	G	174	GLY	2.6
1	G	38	SER	2.6
1	C	245	LEU	2.6
1	L	87	LEU	2.6
1	I	120	LYS	2.6
1	I	249	GLU	2.6
1	K	36	GLU	2.6
1	H	171	VAL	2.6
1	G	34	ILE	2.6
1	H	253	ILE	2.6
1	I	178	GLN	2.6
1	C	249	GLU	2.6
1	C	118	ASN	2.6
1	H	145	ASN	2.6
1	E	174	GLY	2.6
1	D	33	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	258	HIS	2.6
1	A	245	LEU	2.5
1	L	151	LEU	2.5
1	J	175	ALA	2.5
1	C	274	PHE	2.5
1	E	258	HIS	2.5
1	I	299	LYS	2.5
1	H	235	LYS	2.5
1	E	37	GLN	2.5
1	I	260	GLU	2.5
1	H	250	ARG	2.5
1	A	173	SER	2.5
1	I	163	LEU	2.5
1	H	177	LEU	2.5
1	K	143	GLY	2.5
1	K	246	PRO	2.5
1	H	33	HIS	2.5
1	D	5	THR	2.5
1	D	112	GLN	2.5
1	E	178	GLN	2.5
1	J	34	ILE	2.5
1	L	250	ARG	2.5
1	L	254	LEU	2.5
1	E	179	ALA	2.5
1	H	117	GLN	2.5
1	G	113	GLU	2.4
1	J	172	SER	2.4
1	K	34	ILE	2.4
1	B	258	HIS	2.4
1	C	252	THR	2.4
1	C	173	SER	2.4
1	K	241	ILE	2.4
1	K	32	MET	2.4
1	F	298	LEU	2.4
1	I	35	HIS	2.4
1	B	242	GLN	2.4
1	K	114	ASN	2.4
1	E	164	ALA	2.4
1	K	174	GLY	2.4
1	D	176	THR	2.4
1	L	176	THR	2.4
1	B	172	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	38	SER	2.4
1	D	187	VAL	2.4
1	A	238	LEU	2.4
1	L	265	LEU	2.4
1	D	117	GLN	2.4
1	I	146	TYR	2.4
1	K	37	GLN	2.4
1	L	178	GLN	2.4
1	E	181	ASN	2.4
1	I	240	LYS	2.4
1	H	5	THR	2.4
1	J	40	ILE	2.4
1	I	244	LEU	2.4
1	J	37	GLN	2.4
1	G	107	SER	2.3
1	D	34	ILE	2.3
1	G	157	VAL	2.3
1	G	125	LEU	2.3
1	J	177	LEU	2.3
1	A	262	ASN	2.3
1	L	154	SER	2.3
1	G	33	HIS	2.3
1	J	178	GLN	2.3
1	E	254	LEU	2.3
1	I	108	LEU	2.3
1	K	298	LEU	2.3
1	C	112	GLN	2.3
1	L	242	GLN	2.3
1	A	256	LEU	2.3
1	I	181	ASN	2.3
1	F	4	ASN	2.3
1	K	255	PRO	2.3
1	F	174	GLY	2.3
1	C	267	MET	2.3
1	G	233	ALA	2.3
1	G	264	ALA	2.3
1	J	179	ALA	2.3
1	J	36	GLU	2.3
1	G	261	LYS	2.3
1	H	144	ILE	2.3
1	G	256	LEU	2.2
1	J	274	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	234	PRO	2.2
1	I	267	MET	2.2
1	B	233	ALA	2.2
1	E	152	THR	2.2
1	L	299	LYS	2.2
1	L	40	ILE	2.2
1	I	171	VAL	2.2
1	L	163	LEU	2.2
1	I	234	PRO	2.2
1	A	246	PRO	2.2
1	D	113	GLU	2.2
1	I	33	HIS	2.2
1	I	258	HIS	2.2
1	B	286	ALA	2.2
1	D	120	LYS	2.2
1	E	299	LYS	2.2
1	G	254	LEU	2.2
1	H	254	LEU	2.2
1	A	248	VAL	2.2
1	L	155	VAL	2.2
1	I	274	PHE	2.2
1	D	180	ASN	2.2
1	F	118	ASN	2.2
1	G	255	PRO	2.2
1	C	236	GLU	2.2
1	I	112	GLN	2.2
1	K	33	HIS	2.2
1	F	117	GLN	2.2
1	B	163	LEU	2.2
1	I	110	LEU	2.2
1	K	40	ILE	2.2
1	B	181	ASN	2.2
1	H	267	MET	2.2
1	E	117	GLN	2.2
1	C	176	THR	2.2
1	C	243	ALA	2.2
1	C	288	SER	2.2
1	B	298	LEU	2.1
1	E	151	LEU	2.1
1	G	241	ILE	2.1
1	H	151	LEU	2.1
1	A	239	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	214	MET	2.1
1	G	248	VAL	2.1
1	F	113	GLU	2.1
1	G	235	LYS	2.1
1	H	283	GLU	2.1
1	F	5	THR	2.1
1	H	252	THR	2.1
1	H	257	ALA	2.1
1	C	241	ILE	2.1
1	C	244	LEU	2.1
1	F	254	LEU	2.1
1	H	87	LEU	2.1
1	I	141	GLU	2.1
1	G	263	VAL	2.1
1	I	143	GLY	2.1
1	B	257	ALA	2.1
1	E	38	SER	2.1
1	F	267	MET	2.1
1	C	113	GLU	2.1
1	C	265	LEU	2.1
1	C	273	LEU	2.1
1	I	190	GLU	2.1
1	I	34	ILE	2.1
1	I	253	ILE	2.1
1	K	119	LEU	2.1
1	A	273	LEU	2.1
1	K	118	ASN	2.1
1	H	181	ASN	2.1
1	C	33	HIS	2.1
1	E	116	PHE	2.1
1	I	138	PHE	2.1
1	L	149	CYS	2.1
1	B	175	ALA	2.1
1	I	166	ALA	2.1
1	A	179	ALA	2.1
1	H	286	ALA	2.1
1	D	177	LEU	2.1
1	I	85	GLN	2.1
1	H	39	LEU	2.1
1	H	241	ILE	2.1
1	L	9	ILE	2.1
1	F	251	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	185	VAL	2.1
1	F	176	THR	2.0
1	G	156	GLU	2.0
1	I	242	GLN	2.0
1	K	178	GLN	2.0
1	H	258	HIS	2.0
1	B	272	ASN	2.0
1	F	169	ASP	2.0
1	C	253	ILE	2.0
1	B	248	VAL	2.0
1	L	143	GLY	2.0
1	H	237	LYS	2.0
1	B	113	GLU	2.0
1	C	38	SER	2.0
1	H	113	GLU	2.0
1	B	262	ASN	2.0
1	D	170	LEU	2.0
1	E	49	ASP	2.0
1	I	238	LEU	2.0
1	K	39	LEU	2.0
1	D	160	ARG	2.0
1	L	251	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACY	J	304	4/4	0.27	0.25	56,60,62,65	0

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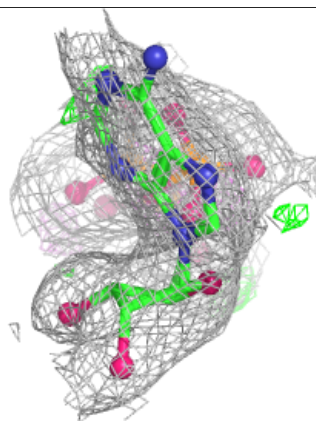
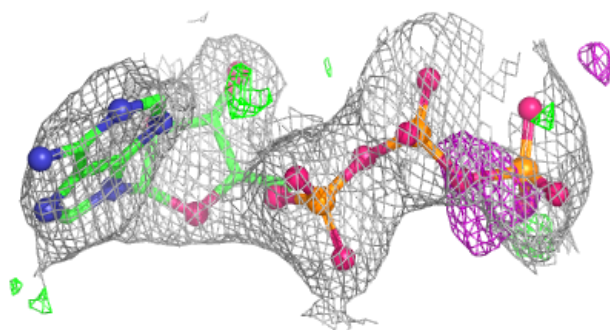
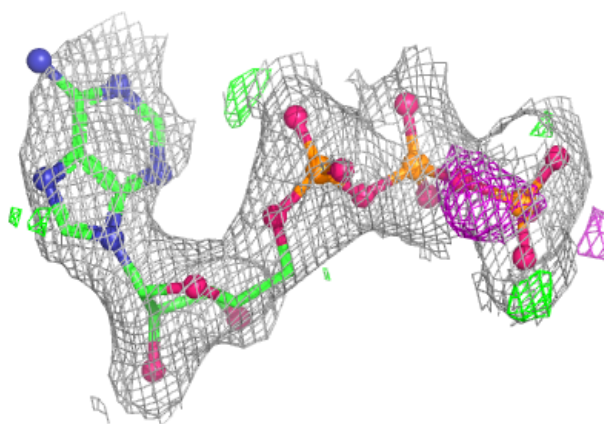
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	E	302	5/5	0.35	0.17	103,108,109,114	0
3	PO4	J	302	5/5	0.53	0.19	128,130,132,136	0
3	PO4	I	302	5/5	0.59	0.14	93,96,97,98	0
3	PO4	C	303	5/5	0.60	0.11	98,101,108,110	0
3	PO4	B	302	5/5	0.62	0.15	92,95,99,99	0
3	PO4	C	302	5/5	0.63	0.13	92,104,106,111	0
2	MG	K	301	1/1	0.73	0.16	70,70,70,70	0
2	MG	L	301	1/1	0.81	0.15	62,62,62,62	0
4	ATP	L	302	31/31	0.86	0.12	38,55,69,70	0
4	ATP	K	302	31/31	0.87	0.12	39,59,71,76	0
4	ATP	H	302	31/31	0.88	0.10	45,56,68,72	0
4	ATP	G	302	31/31	0.89	0.10	37,52,62,68	0
4	ATP	E	303	31/31	0.89	0.10	44,54,70,74	0
4	ATP	I	303	31/31	0.90	0.10	37,48,68,77	0
2	MG	E	301	1/1	0.90	0.07	59,59,59,59	0
4	ATP	D	302	31/31	0.92	0.10	42,56,70,71	0
4	ATP	A	302	31/31	0.92	0.10	27,45,61,62	0
4	ATP	F	302	31/31	0.93	0.09	28,42,58,59	0
2	MG	I	301	1/1	0.93	0.05	43,43,43,43	0
4	ATP	B	303	31/31	0.93	0.09	36,43,53,55	0
4	ATP	C	304	31/31	0.93	0.09	28,40,54,56	0
2	MG	G	301	1/1	0.93	0.06	51,51,51,51	0
4	ATP	J	303	31/31	0.94	0.09	30,44,60,66	0
2	MG	D	301	1/1	0.95	0.09	49,49,49,49	0
2	MG	H	301	1/1	0.95	0.05	55,55,55,55	0
2	MG	J	301	1/1	0.96	0.04	42,42,42,42	0
2	MG	B	301	1/1	0.96	0.08	39,39,39,39	0
2	MG	F	301	1/1	0.96	0.06	39,39,39,39	0
2	MG	C	301	1/1	0.97	0.06	45,45,45,45	0
2	MG	A	301	1/1	0.97	0.11	44,44,44,44	0

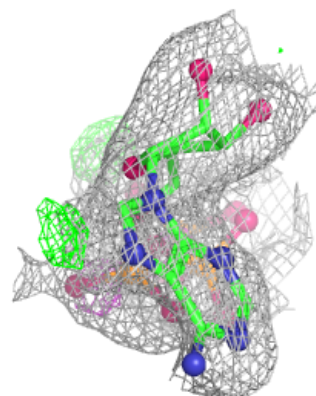
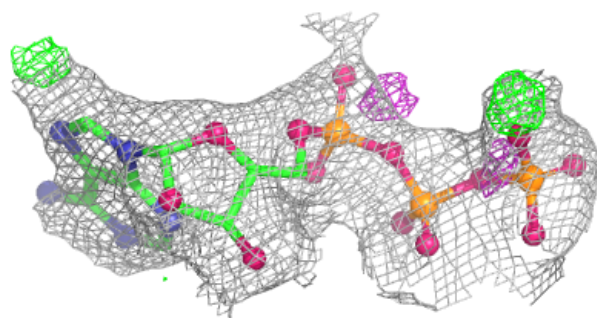
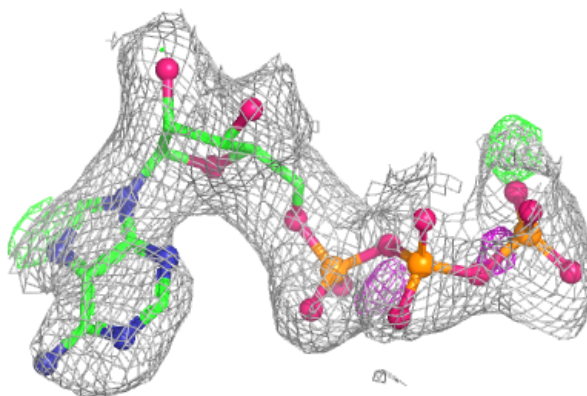
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

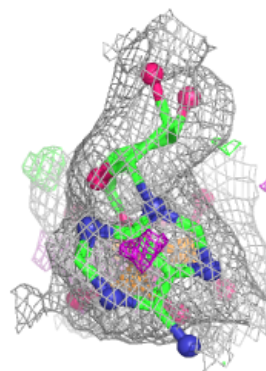
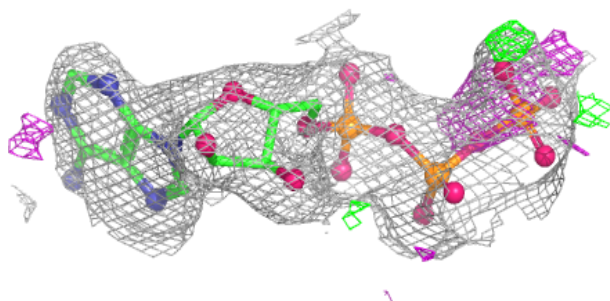
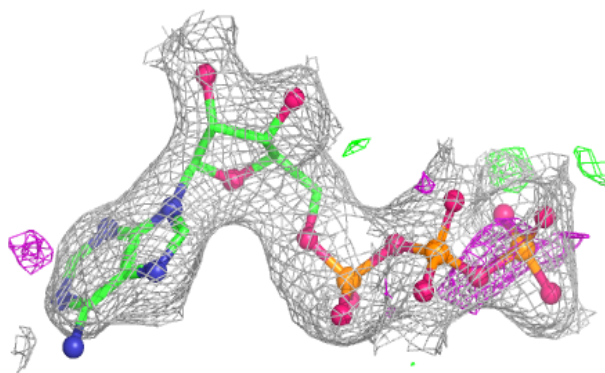
**Electron density around ATP K 302:**

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

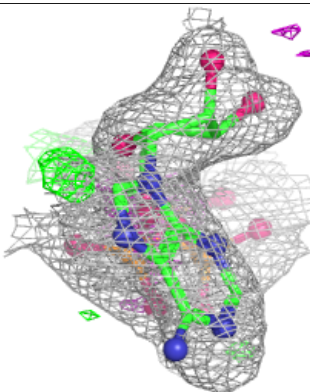
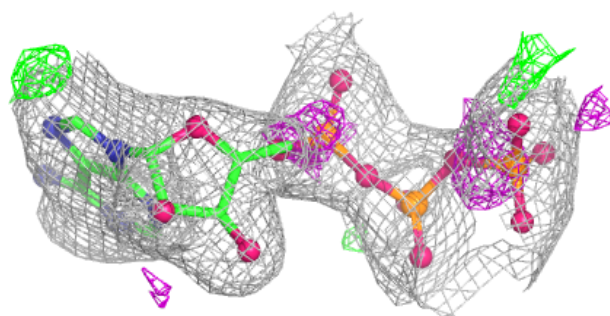
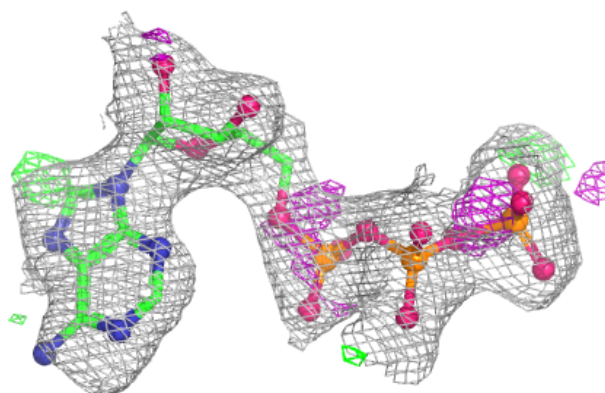


Electron density around ATP H 302:

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

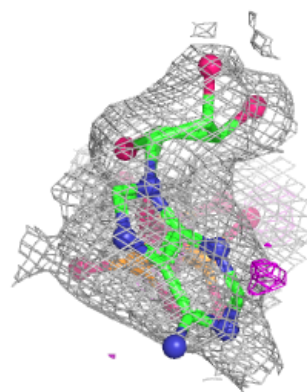
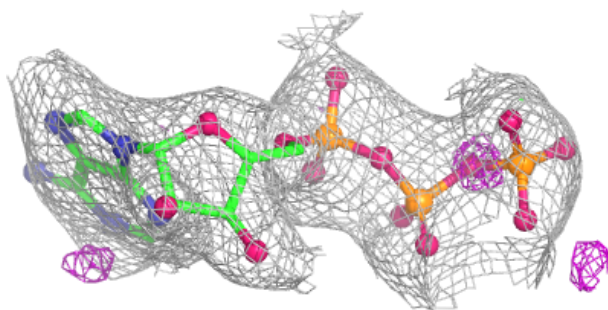
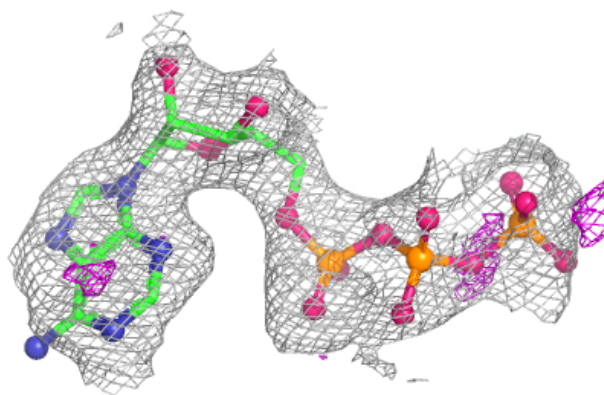
**Electron density around ATP G 302:**

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

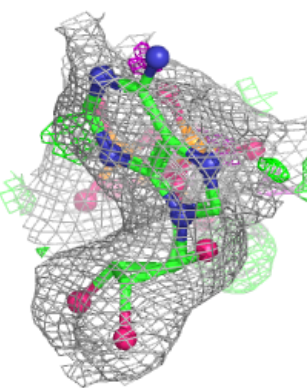
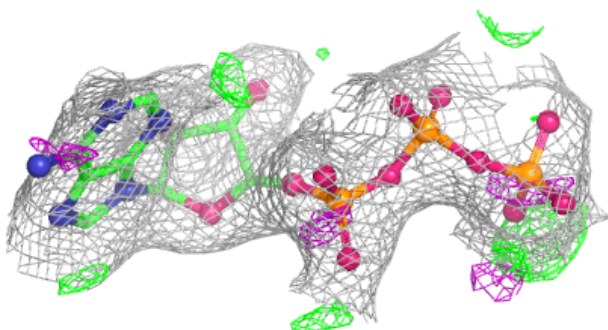
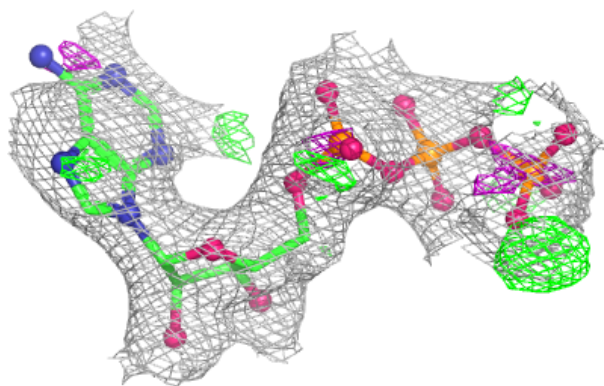


Electron density around ATP E 303:

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

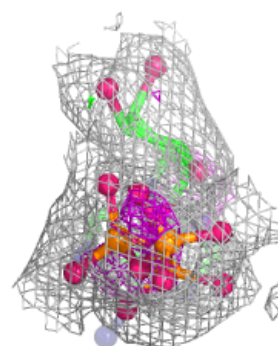
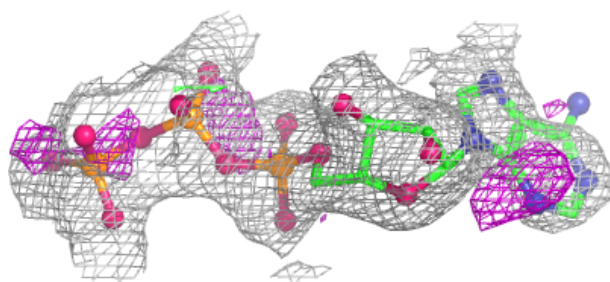
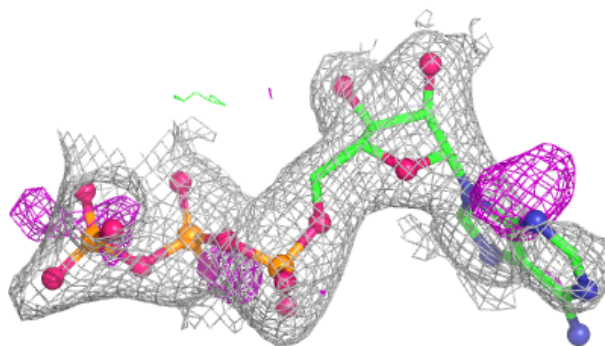
**Electron density around ATP I 303:**

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

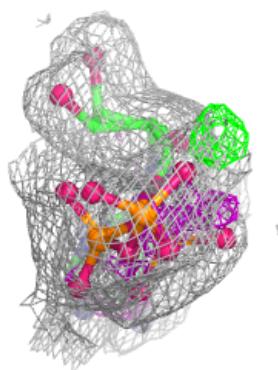
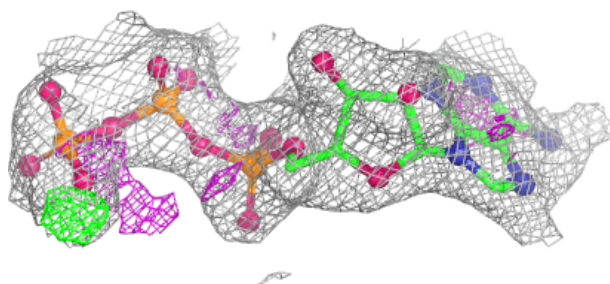
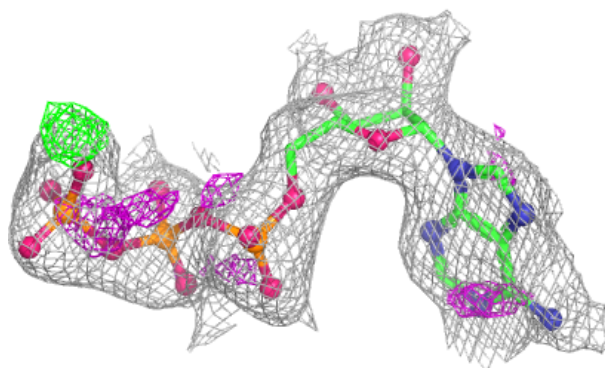


Electron density around ATP D 302:

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

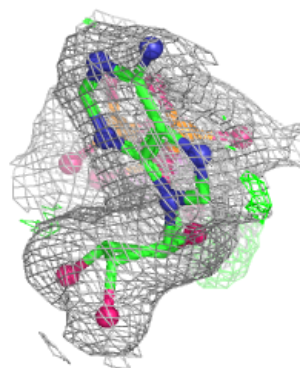
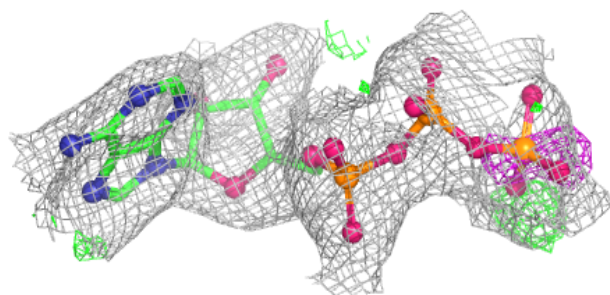
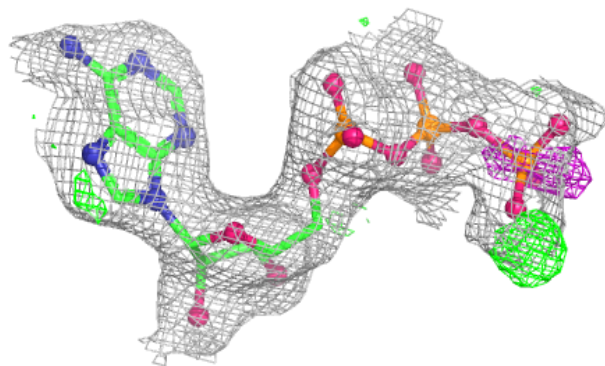
**Electron density around ATP A 302:**

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

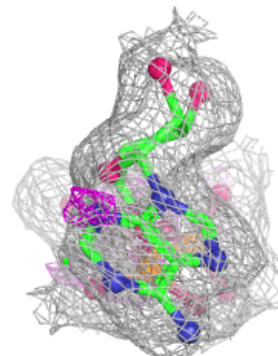
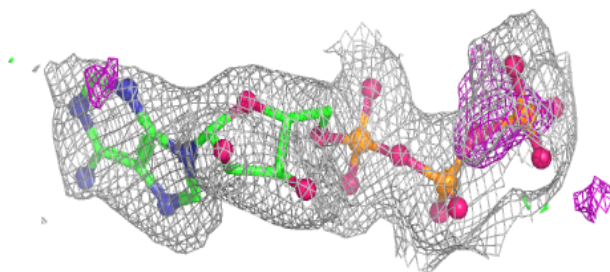
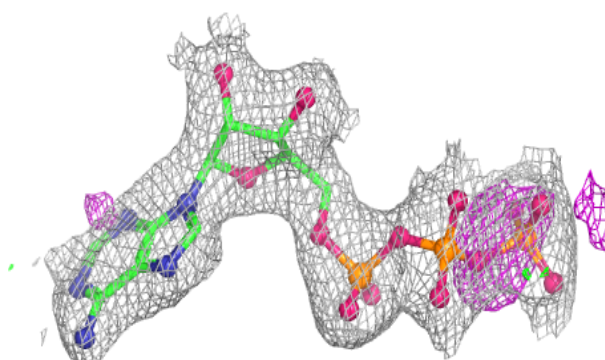


Electron density around ATP F 302:

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

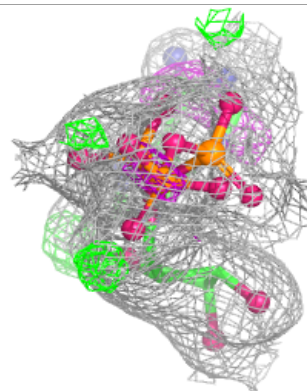
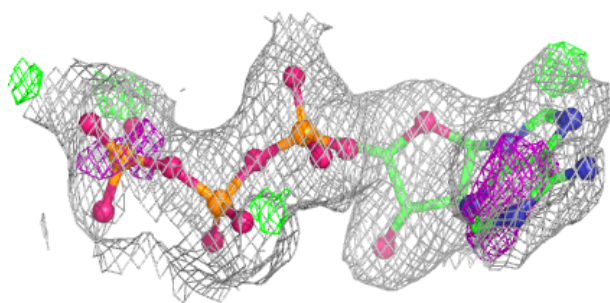
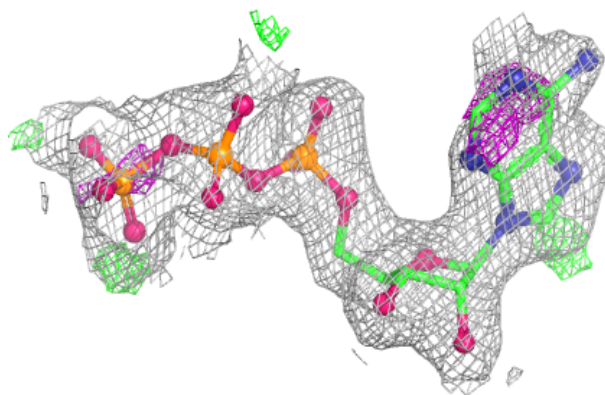
**Electron density around ATP B 303:**

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

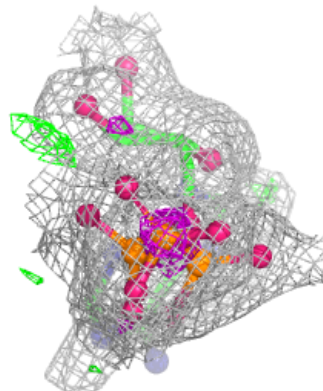
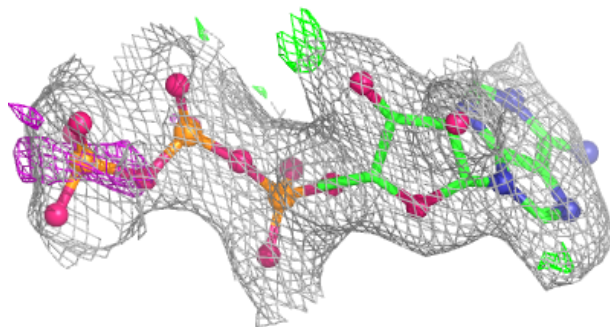
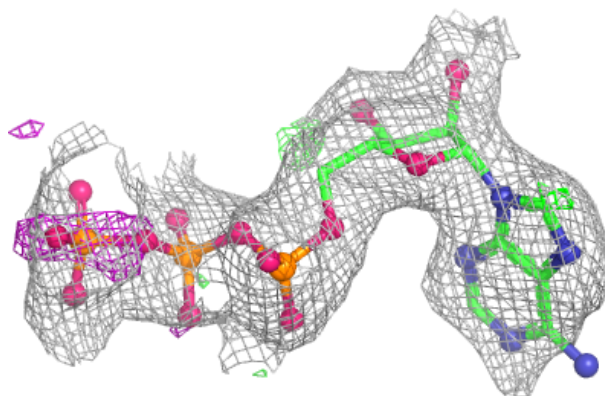


Electron density around ATP C 304:

$2mF_o-DF_c$ (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.