



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 03:50 PM BST

PDB ID : 3CIS
Title : The Crystal Structure of Rv2623 from Mycobacterium tuberculosis
Authors : Bilder, P.; Drumm, J.; Mi, K.; Chan, J.; Almo, S.C.
Deposited on : 2008-03-11
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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

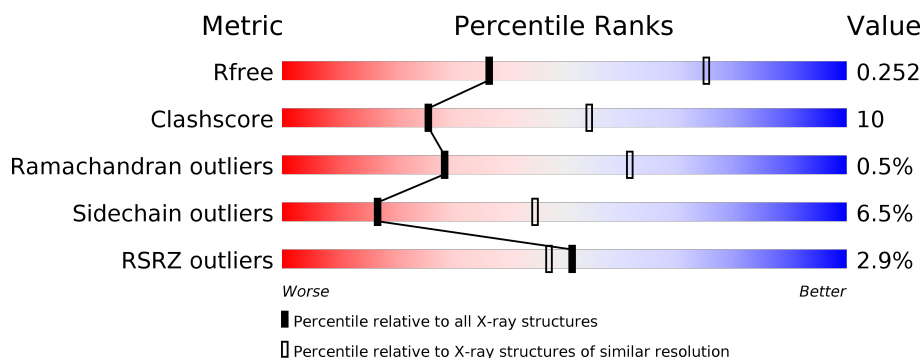
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	B	309	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	C	309	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 6%</div> </div> </div>
1	D	309	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	E	309	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 6%</div> </div> </div>
1	F	309	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>• 10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	309	<div><div>%</div><div><div></div><div>74%</div><div>17%</div><div>6%</div></div></div>
1	H	309	<div><div>5%</div><div><div></div><div>68%</div><div>20%</div><div>9%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18138 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2169	1363	397	402	7			
1	B	290	Total	C	N	O	S	0	0	0
			2174	1366	398	403	7			
1	C	290	Total	C	N	O	S	0	0	0
			2177	1368	398	404	7			
1	D	289	Total	C	N	O	S	0	0	0
			2168	1363	397	401	7			
1	E	291	Total	C	N	O	S	0	0	0
			2187	1372	400	408	7			
1	F	277	Total	C	N	O	S	0	0	0
			2081	1305	384	385	7			
1	G	292	Total	C	N	O	S	0	0	0
			2190	1374	401	408	7			
1	H	282	Total	C	N	O	S	0	0	0
			2121	1331	390	393	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP O06189
A	-10	ARG	-	expression tag	UNP O06189
A	-9	GLY	-	expression tag	UNP O06189
A	-8	SER	-	expression tag	UNP O06189
A	-7	HIS	-	expression tag	UNP O06189
A	-6	HIS	-	expression tag	UNP O06189
A	-5	HIS	-	expression tag	UNP O06189
A	-4	HIS	-	expression tag	UNP O06189
A	-3	HIS	-	expression tag	UNP O06189
A	-2	HIS	-	expression tag	UNP O06189
A	-1	GLY	-	expression tag	UNP O06189
A	0	SER	-	expression tag	UNP O06189
B	-11	MET	-	expression tag	UNP O06189

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ARG	-	expression tag	UNP O06189
B	-9	GLY	-	expression tag	UNP O06189
B	-8	SER	-	expression tag	UNP O06189
B	-7	HIS	-	expression tag	UNP O06189
B	-6	HIS	-	expression tag	UNP O06189
B	-5	HIS	-	expression tag	UNP O06189
B	-4	HIS	-	expression tag	UNP O06189
B	-3	HIS	-	expression tag	UNP O06189
B	-2	HIS	-	expression tag	UNP O06189
B	-1	GLY	-	expression tag	UNP O06189
B	0	SER	-	expression tag	UNP O06189
C	-11	MET	-	expression tag	UNP O06189
C	-10	ARG	-	expression tag	UNP O06189
C	-9	GLY	-	expression tag	UNP O06189
C	-8	SER	-	expression tag	UNP O06189
C	-7	HIS	-	expression tag	UNP O06189
C	-6	HIS	-	expression tag	UNP O06189
C	-5	HIS	-	expression tag	UNP O06189
C	-4	HIS	-	expression tag	UNP O06189
C	-3	HIS	-	expression tag	UNP O06189
C	-2	HIS	-	expression tag	UNP O06189
C	-1	GLY	-	expression tag	UNP O06189
C	0	SER	-	expression tag	UNP O06189
D	-11	MET	-	expression tag	UNP O06189
D	-10	ARG	-	expression tag	UNP O06189
D	-9	GLY	-	expression tag	UNP O06189
D	-8	SER	-	expression tag	UNP O06189
D	-7	HIS	-	expression tag	UNP O06189
D	-6	HIS	-	expression tag	UNP O06189
D	-5	HIS	-	expression tag	UNP O06189
D	-4	HIS	-	expression tag	UNP O06189
D	-3	HIS	-	expression tag	UNP O06189
D	-2	HIS	-	expression tag	UNP O06189
D	-1	GLY	-	expression tag	UNP O06189
D	0	SER	-	expression tag	UNP O06189
E	-11	MET	-	expression tag	UNP O06189
E	-10	ARG	-	expression tag	UNP O06189
E	-9	GLY	-	expression tag	UNP O06189
E	-8	SER	-	expression tag	UNP O06189
E	-7	HIS	-	expression tag	UNP O06189
E	-6	HIS	-	expression tag	UNP O06189
E	-5	HIS	-	expression tag	UNP O06189

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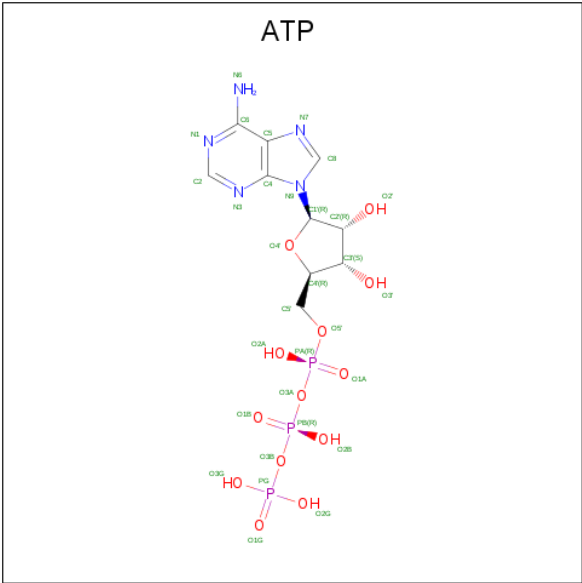
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP O06189
E	-3	HIS	-	expression tag	UNP O06189
E	-2	HIS	-	expression tag	UNP O06189
E	-1	GLY	-	expression tag	UNP O06189
E	0	SER	-	expression tag	UNP O06189
F	-11	MET	-	expression tag	UNP O06189
F	-10	ARG	-	expression tag	UNP O06189
F	-9	GLY	-	expression tag	UNP O06189
F	-8	SER	-	expression tag	UNP O06189
F	-7	HIS	-	expression tag	UNP O06189
F	-6	HIS	-	expression tag	UNP O06189
F	-5	HIS	-	expression tag	UNP O06189
F	-4	HIS	-	expression tag	UNP O06189
F	-3	HIS	-	expression tag	UNP O06189
F	-2	HIS	-	expression tag	UNP O06189
F	-1	GLY	-	expression tag	UNP O06189
F	0	SER	-	expression tag	UNP O06189
G	-11	MET	-	expression tag	UNP O06189
G	-10	ARG	-	expression tag	UNP O06189
G	-9	GLY	-	expression tag	UNP O06189
G	-8	SER	-	expression tag	UNP O06189
G	-7	HIS	-	expression tag	UNP O06189
G	-6	HIS	-	expression tag	UNP O06189
G	-5	HIS	-	expression tag	UNP O06189
G	-4	HIS	-	expression tag	UNP O06189
G	-3	HIS	-	expression tag	UNP O06189
G	-2	HIS	-	expression tag	UNP O06189
G	-1	GLY	-	expression tag	UNP O06189
G	0	SER	-	expression tag	UNP O06189
H	-11	MET	-	expression tag	UNP O06189
H	-10	ARG	-	expression tag	UNP O06189
H	-9	GLY	-	expression tag	UNP O06189
H	-8	SER	-	expression tag	UNP O06189
H	-7	HIS	-	expression tag	UNP O06189
H	-6	HIS	-	expression tag	UNP O06189
H	-5	HIS	-	expression tag	UNP O06189
H	-4	HIS	-	expression tag	UNP O06189
H	-3	HIS	-	expression tag	UNP O06189
H	-2	HIS	-	expression tag	UNP O06189
H	-1	GLY	-	expression tag	UNP O06189
H	0	SER	-	expression tag	UNP O06189

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		
2	H	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	F	2	Total	Mg	0	0
			2	2		

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



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		
4	B	29	Total	O	0	0
			29	29		
4	C	56	Total	O	0	0
			56	56		
4	D	32	Total	O	0	0
			32	32		
4	E	55	Total	O	0	0
			55	55		
4	F	37	Total	O	0	0
			37	37		

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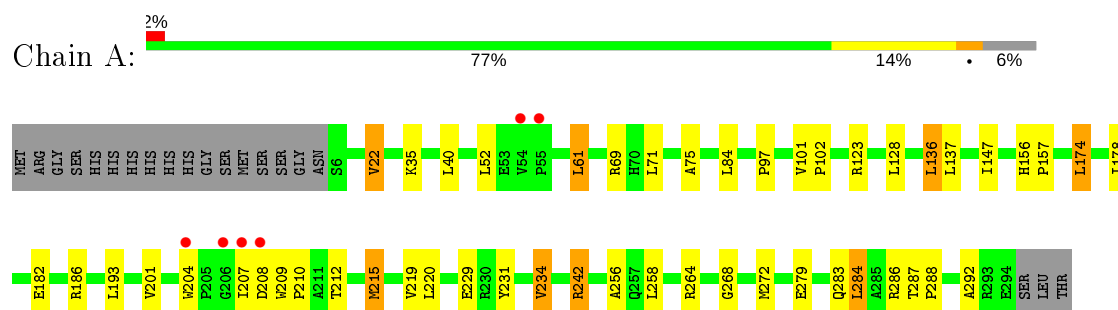
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	57	Total	O	0	0
			57	57		
4	H	37	Total	O	0	0
			37	37		

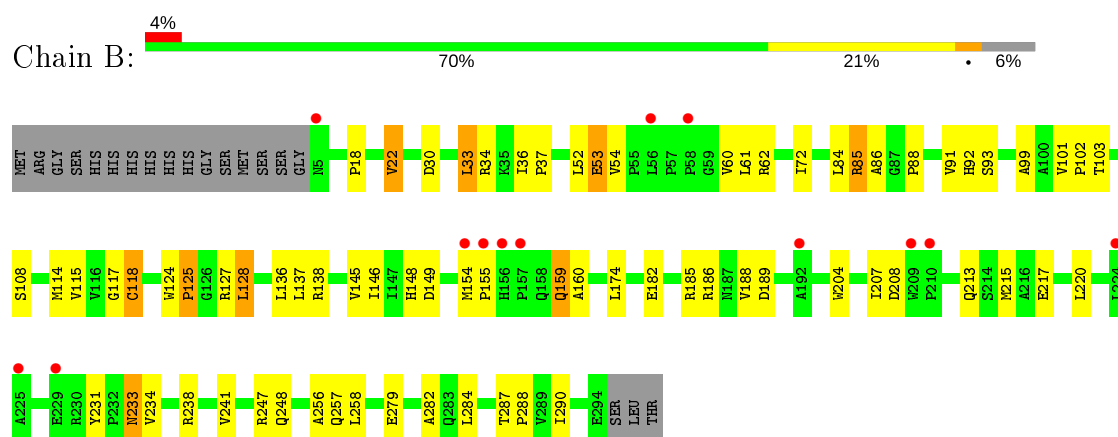
3 Residue-property plots [i](#)

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.

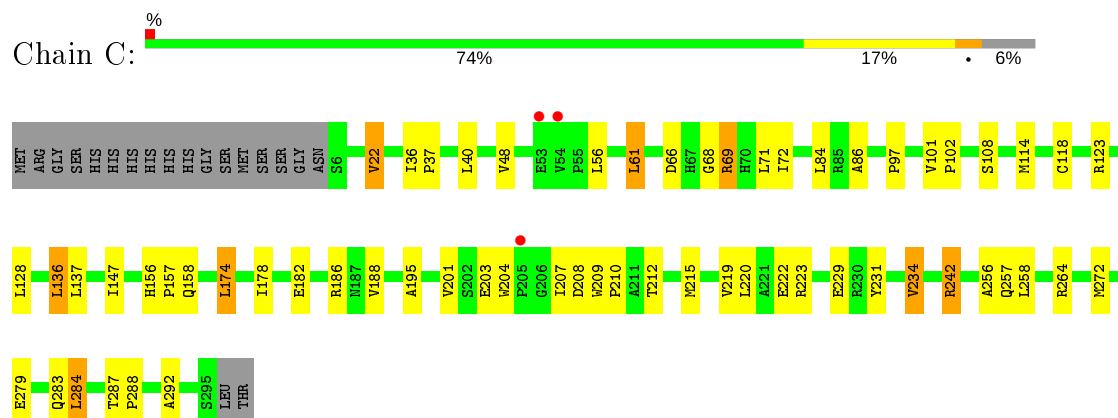
- Molecule 1: Uncharacterized protein



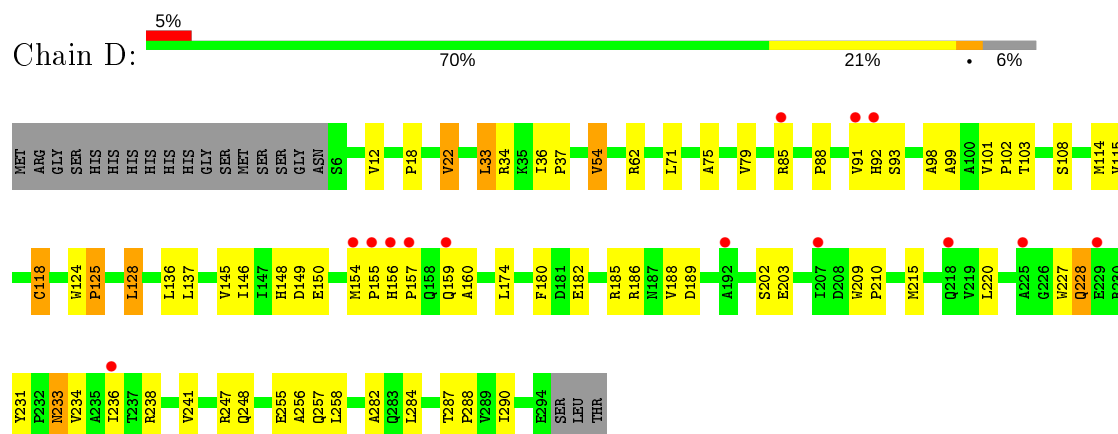
- Molecule 1: Uncharacterized protein



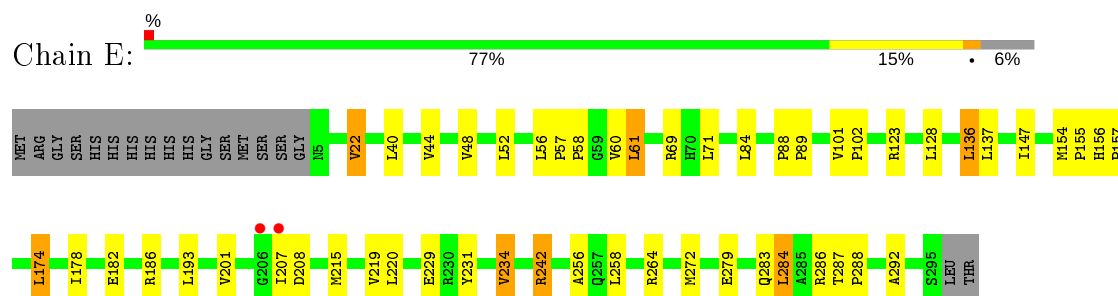
- Molecule 1: Uncharacterized protein



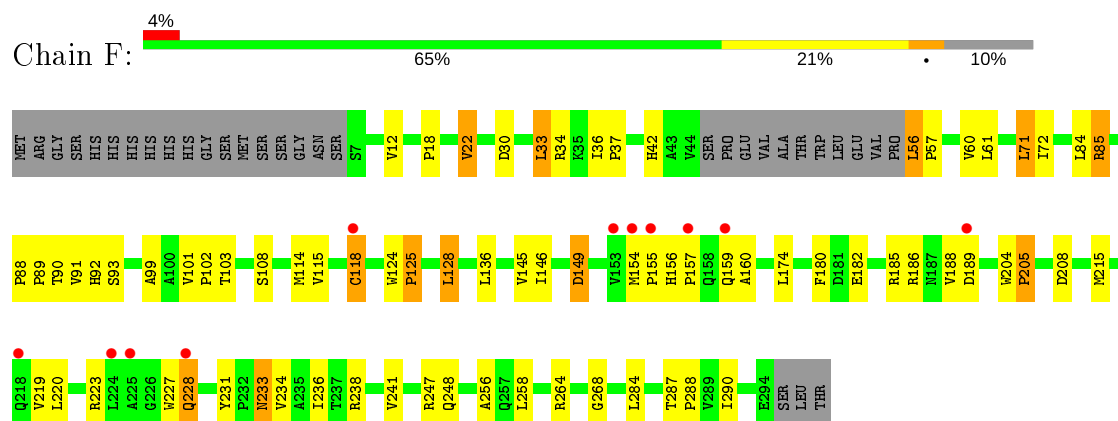
- Molecule 1: Uncharacterized protein



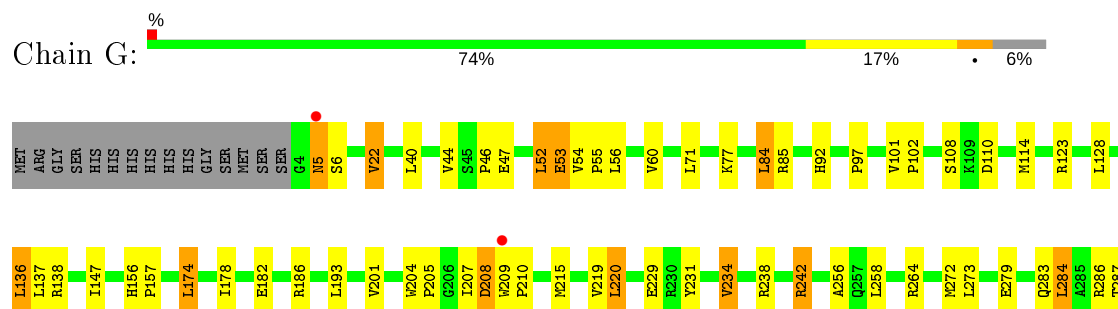
- Molecule 1: Uncharacterized protein

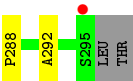


- Molecule 1: Uncharacterized protein

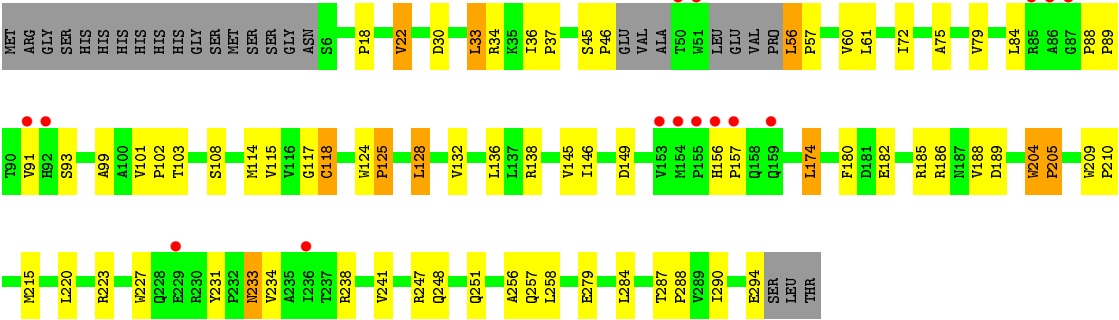


- Molecule 1: Uncharacterized protein





● Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	172.97Å 241.48Å 241.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 2.90 49.53 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.57-2.90) 97.4 (49.53-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.250 , 0.268 0.249 , 0.252	Depositor DCC
R_{free} test set	6123 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18138	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/2216	0.60	3/3035 (0.1%)
1	B	0.24	0/2221	0.60	3/3042 (0.1%)
1	C	0.26	0/2224	0.45	1/3046 (0.0%)
1	D	0.23	0/2215	0.44	2/3034 (0.1%)
1	E	0.26	0/2234	0.45	1/3059 (0.0%)
1	F	0.24	0/2123	0.44	2/2902 (0.1%)
1	G	0.31	0/2237	0.45	1/3063 (0.0%)
1	H	0.25	0/2165	0.44	2/2960 (0.1%)
All	All	0.26	0/17635	0.49	15/24141 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	ARG	NE-CZ-NH1	-16.33	112.14	120.30
1	A	242	ARG	NE-CZ-NH1	-15.48	112.56	120.30
1	B	238	ARG	NE-CZ-NH2	15.46	128.03	120.30
1	A	242	ARG	NE-CZ-NH2	15.07	127.83	120.30
1	B	238	ARG	CD-NE-CZ	7.76	134.46	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	47	GLU	Peptide

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	2169	0	2181	40	1
1	B	2174	0	2183	51	0
1	C	2177	0	2184	50	0
1	D	2168	0	2178	50	1
1	E	2187	0	2196	46	0
1	F	2081	0	2097	54	1
1	G	2190	0	2196	54	1
1	H	2121	0	2130	52	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	62	0	24	1	0
3	B	62	0	24	2	0
3	C	62	0	24	3	0
3	D	62	0	24	0	0
3	E	62	0	24	0	0
3	F	62	0	24	2	0
3	G	62	0	24	0	0
3	H	62	0	24	2	0
4	A	56	0	0	0	0
4	B	29	0	0	2	0
4	C	56	0	0	5	0
4	D	32	0	0	2	0
4	E	55	0	0	0	0
4	F	37	0	0	1	0
4	G	57	0	0	2	0
4	H	37	0	0	1	0
All	All	18138	0	17537	370	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 10.

The worst 5 of 370 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:B:247:ARG:NH2	1:E:229:GLU:O	2.00	0.95
1:F:228:GLN:HG2	1:F:236:ILE:HD12	1.51	0.91
1:B:85:ARG:HG2	1:B:86:ALA:H	1.34	0.89
1:C:229:GLU:O	1:H:247:ARG:NH2	2.08	0.86
1:D:241:VAL:HG11	1:D:248:GLN:HE21	1.41	0.85

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:247:ARG:NH2	1:G:229:GLU:O[3_556]	2.01	0.19
1:A:229:GLU:O	1:D:247:ARG:NH2[3_556]	2.16	0.04

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	287/309 (93%)	279 (97%)	8 (3%)	0	100	100
1	B	288/309 (93%)	276 (96%)	11 (4%)	1 (0%)	41	71
1	C	288/309 (93%)	277 (96%)	11 (4%)	0	100	100
1	D	287/309 (93%)	275 (96%)	10 (4%)	2 (1%)	22	54
1	E	289/309 (94%)	279 (96%)	10 (4%)	0	100	100
1	F	273/309 (88%)	263 (96%)	7 (3%)	3 (1%)	14	42
1	G	290/309 (94%)	280 (97%)	8 (3%)	2 (1%)	22	54
1	H	276/309 (89%)	266 (96%)	7 (2%)	3 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2278/2472 (92%)	2195 (96%)	72 (3%)	11 (0%)	29 61

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	205	PRO
1	H	205	PRO
1	G	6	SER
1	D	149	ASP
1	G	208	ASP

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	231/249 (93%)	217 (94%)	14 (6%)	18 48
1	B	231/249 (93%)	214 (93%)	17 (7%)	13 38
1	C	231/249 (93%)	216 (94%)	15 (6%)	17 45
1	D	230/249 (92%)	215 (94%)	15 (6%)	17 45
1	E	234/249 (94%)	221 (94%)	13 (6%)	21 52
1	F	221/249 (89%)	205 (93%)	16 (7%)	14 39
1	G	233/249 (94%)	217 (93%)	16 (7%)	15 41
1	H	226/249 (91%)	213 (94%)	13 (6%)	20 50
All	All	1837/1992 (92%)	1718 (94%)	119 (6%)	17 45

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	128	LEU
1	E	136	LEU
1	H	61	LEU
1	D	215	MET
1	D	284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	228	GLN
1	E	156	HIS
1	H	244	GLN
1	D	248	GLN
1	E	194	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	B	2101	2	26,33,33	1.34	3 (11%)	31,52,52	1.38	5 (16%)
3	ATP	H	2101	2	26,33,33	1.32	2 (7%)	31,52,52	1.55	4 (12%)
3	ATP	F	2101	2	26,33,33	1.42	2 (7%)	31,52,52	1.51	4 (12%)
3	ATP	H	2102	2	26,33,33	1.27	2 (7%)	31,52,52	1.54	4 (12%)
3	ATP	A	1101	2	26,33,33	1.36	2 (7%)	31,52,52	1.48	4 (12%)
3	ATP	G	1101	2	26,33,33	1.35	2 (7%)	31,52,52	1.47	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	E	1101	2	26,33,33	1.33	2 (7%)	31,52,52	1.50	5 (16%)
3	ATP	F	2102	2	26,33,33	1.30	2 (7%)	31,52,52	1.51	4 (12%)
3	ATP	E	1102	2	26,33,33	1.26	2 (7%)	31,52,52	1.35	4 (12%)
3	ATP	D	2102	2	26,33,33	1.24	2 (7%)	31,52,52	1.52	4 (12%)
3	ATP	B	2102	2	26,33,33	1.29	2 (7%)	31,52,52	1.56	5 (16%)
3	ATP	G	1102	2	26,33,33	1.28	2 (7%)	31,52,52	1.43	4 (12%)
3	ATP	C	1102	2	26,33,33	1.27	3 (11%)	31,52,52	1.47	4 (12%)
3	ATP	D	2101	2	26,33,33	1.38	3 (11%)	31,52,52	1.53	4 (12%)
3	ATP	A	1102	2	26,33,33	1.26	2 (7%)	31,52,52	1.46	3 (9%)
3	ATP	C	1101	2	26,33,33	1.34	2 (7%)	31,52,52	1.42	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	2101	2	-	4/18/38/38	0/3/3/3
3	ATP	H	2101	2	-	3/18/38/38	0/3/3/3
3	ATP	F	2101	2	-	3/18/38/38	0/3/3/3
3	ATP	H	2102	2	-	6/18/38/38	0/3/3/3
3	ATP	A	1101	2	-	3/18/38/38	0/3/3/3
3	ATP	G	1101	2	-	4/18/38/38	0/3/3/3
3	ATP	E	1101	2	-	2/18/38/38	0/3/3/3
3	ATP	F	2102	2	-	3/18/38/38	0/3/3/3
3	ATP	E	1102	2	-	8/18/38/38	0/3/3/3
3	ATP	D	2102	2	-	2/18/38/38	0/3/3/3
3	ATP	B	2102	2	-	4/18/38/38	0/3/3/3
3	ATP	G	1102	2	-	8/18/38/38	0/3/3/3
3	ATP	C	1102	2	-	7/18/38/38	0/3/3/3
3	ATP	D	2101	2	-	3/18/38/38	0/3/3/3
3	ATP	A	1102	2	-	5/18/38/38	0/3/3/3
3	ATP	C	1101	2	-	5/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1101	ATP	O4'-C1'	4.17	1.46	1.41
3	F	2101	ATP	O4'-C1'	4.13	1.46	1.41
3	A	1101	ATP	O4'-C1'	4.09	1.46	1.41
3	E	1101	ATP	PG-O1G	3.95	1.63	1.50
3	D	2101	ATP	PG-O1G	3.92	1.63	1.50

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2102	ATP	N3-C2-N1	-4.69	121.35	128.68
3	G	1101	ATP	N3-C2-N1	-4.65	121.40	128.68
3	H	2101	ATP	N3-C2-N1	-4.59	121.51	128.68
3	C	1102	ATP	N3-C2-N1	-4.58	121.52	128.68
3	C	1101	ATP	N3-C2-N1	-4.53	121.60	128.68

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2102	ATP	C5'-O5'-PA-O1A
3	E	1102	ATP	C5'-O5'-PA-O1A
3	B	2102	ATP	C5'-O5'-PA-O1A
3	A	1102	ATP	C5'-O5'-PA-O1A
3	C	1102	ATP	C5'-O5'-PA-O1A

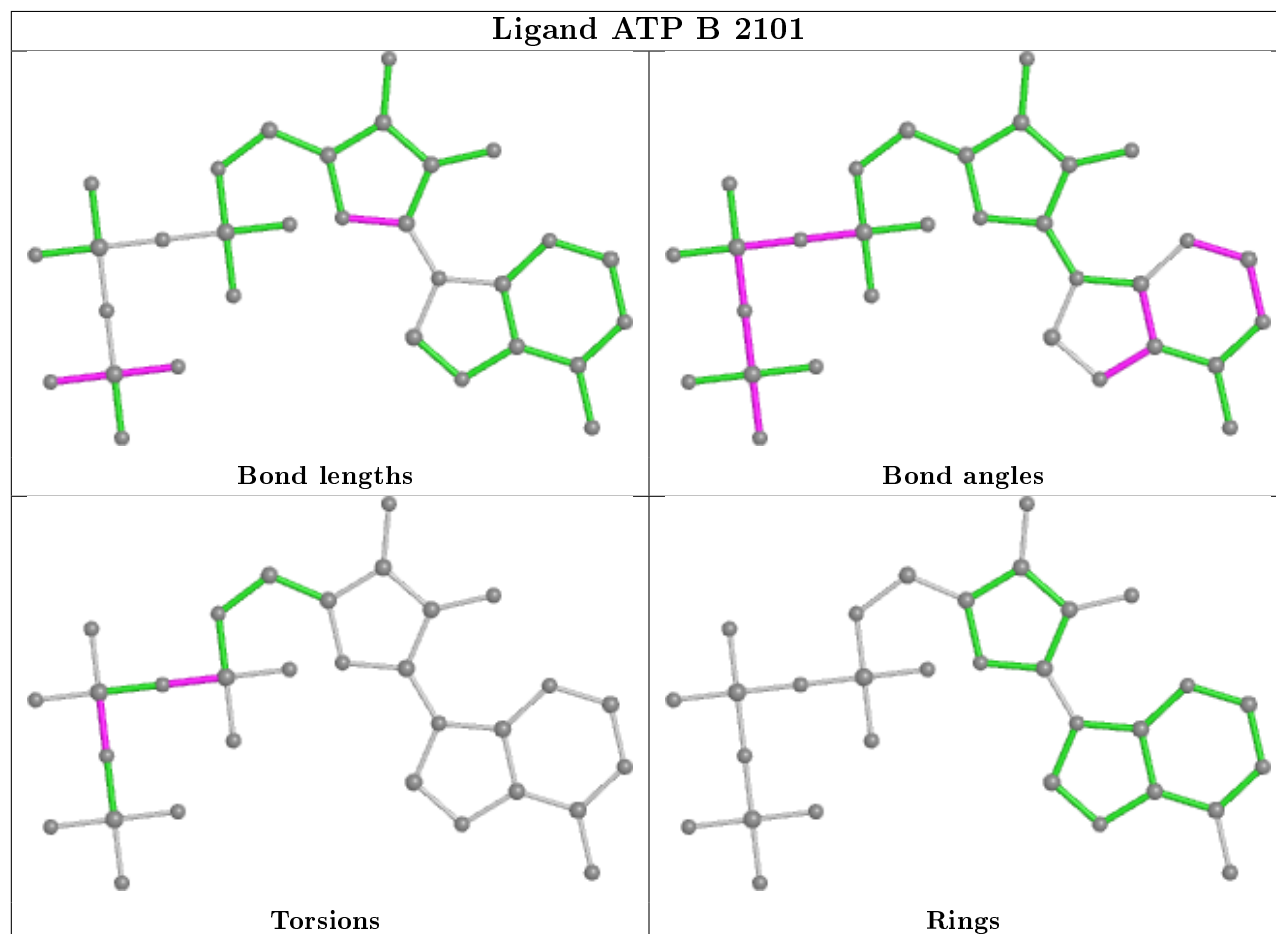
There are no ring outliers.

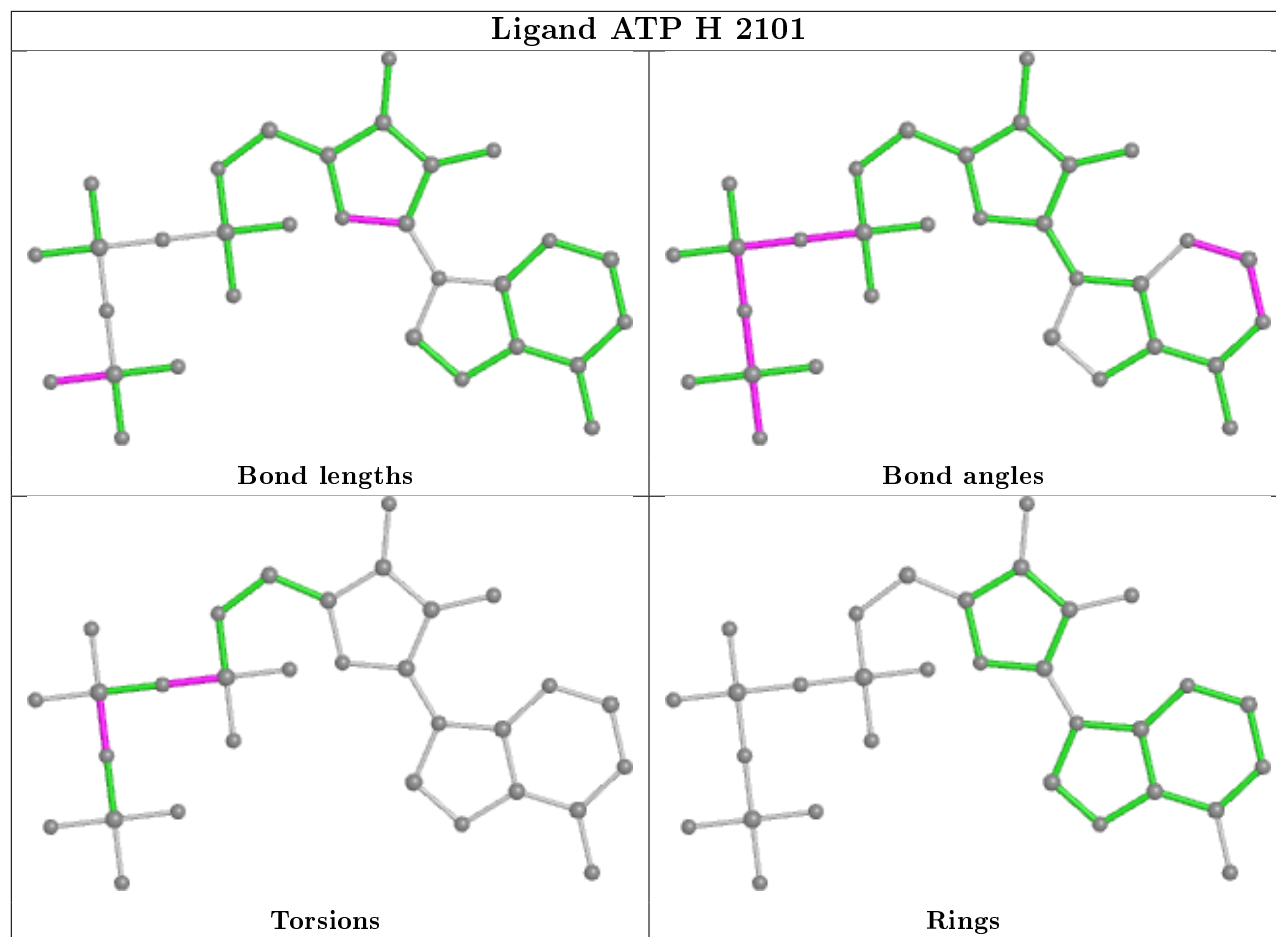
5 monomers are involved in 10 short contacts:

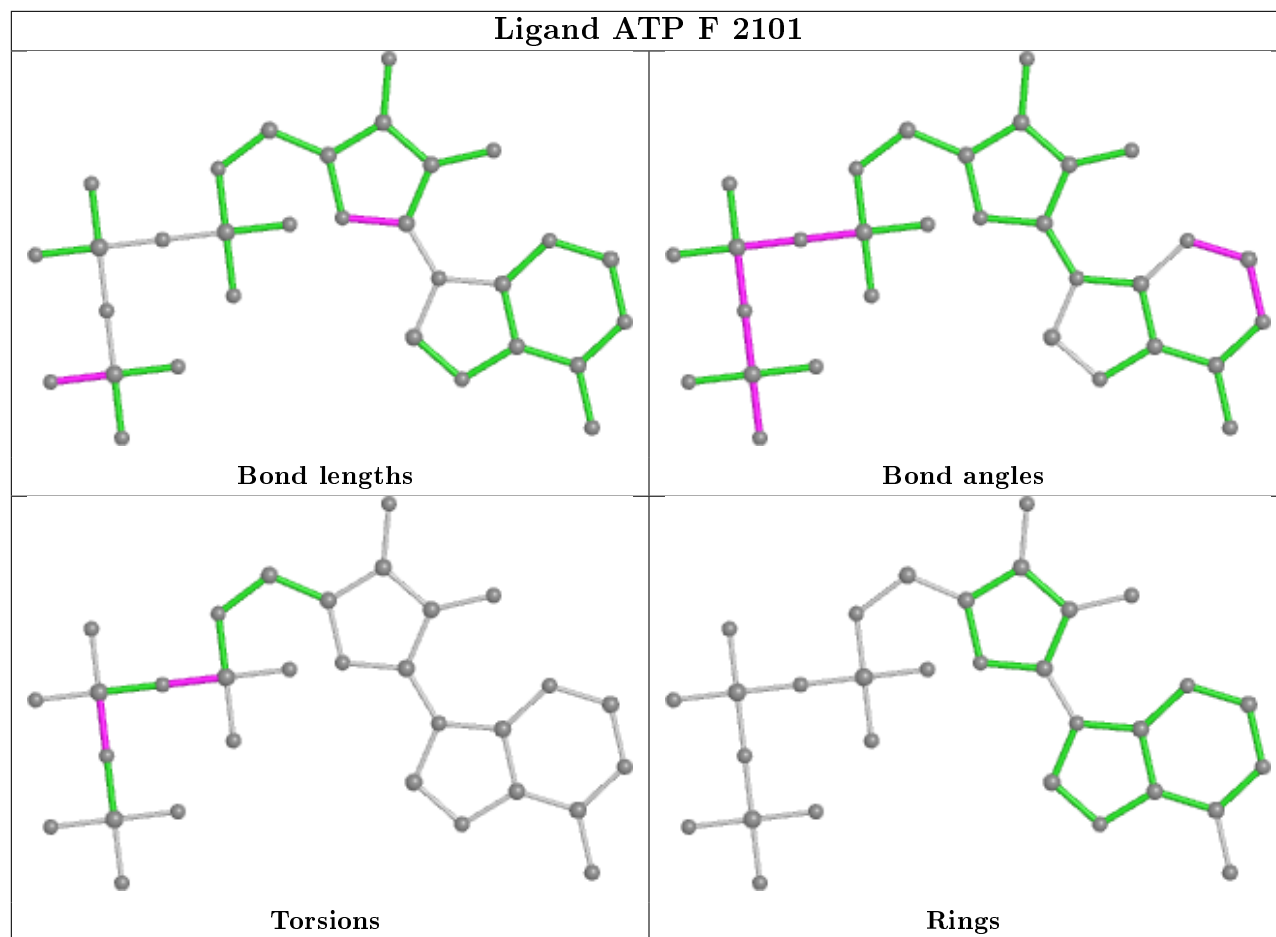
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2101	ATP	2	0
3	H	2101	ATP	2	0
3	F	2102	ATP	2	0
3	C	1102	ATP	3	0
3	A	1102	ATP	1	0

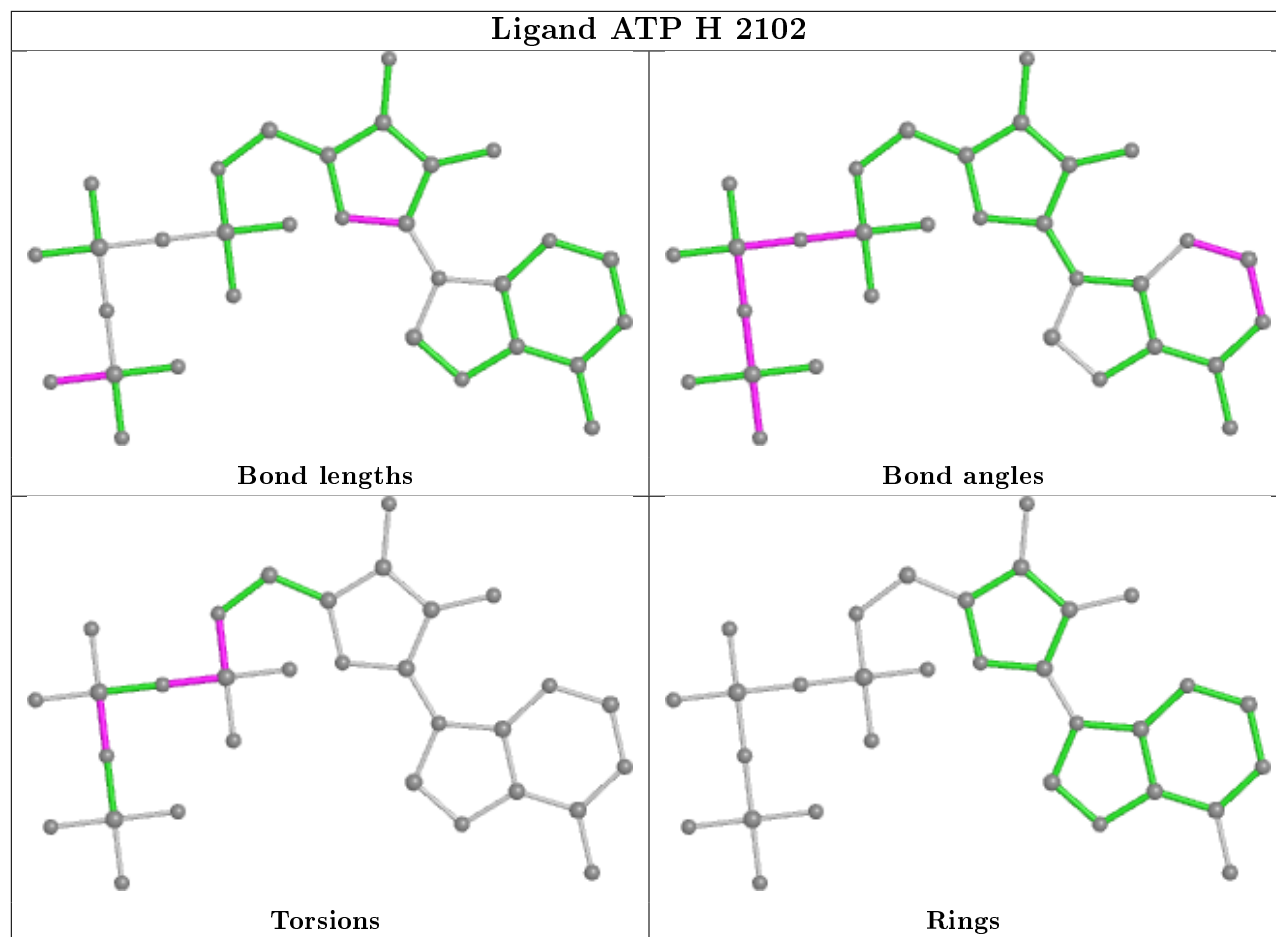
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

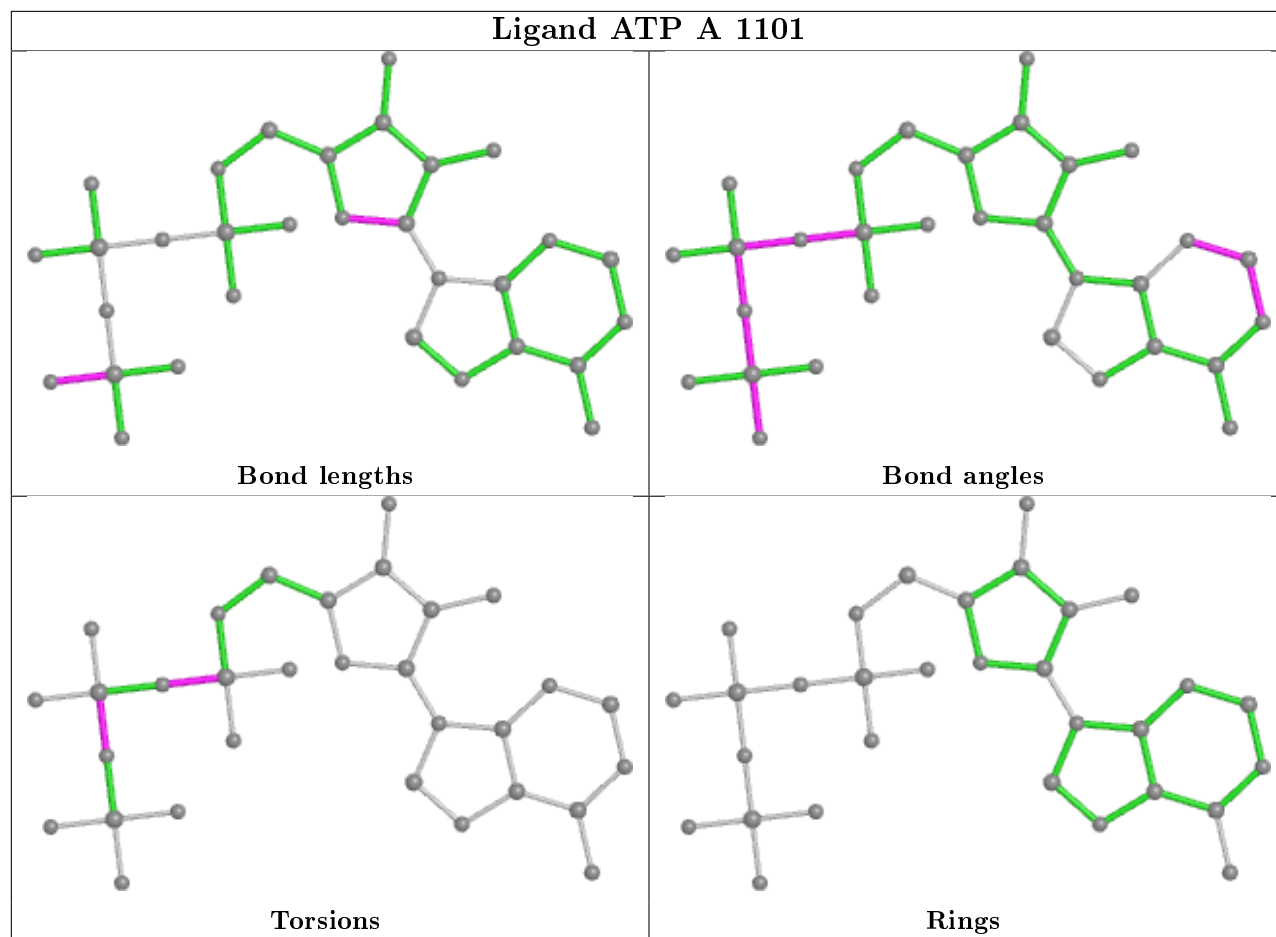
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

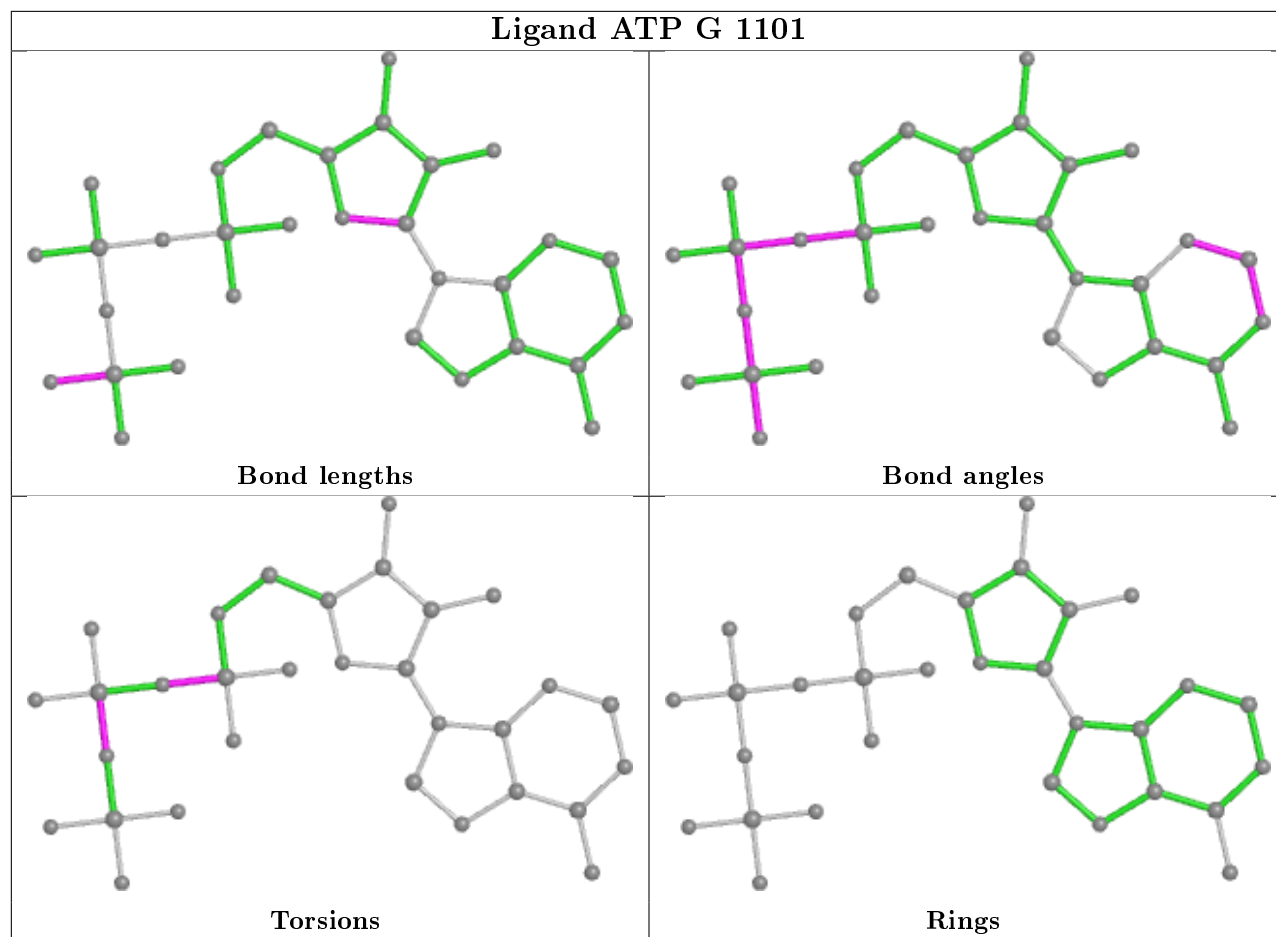


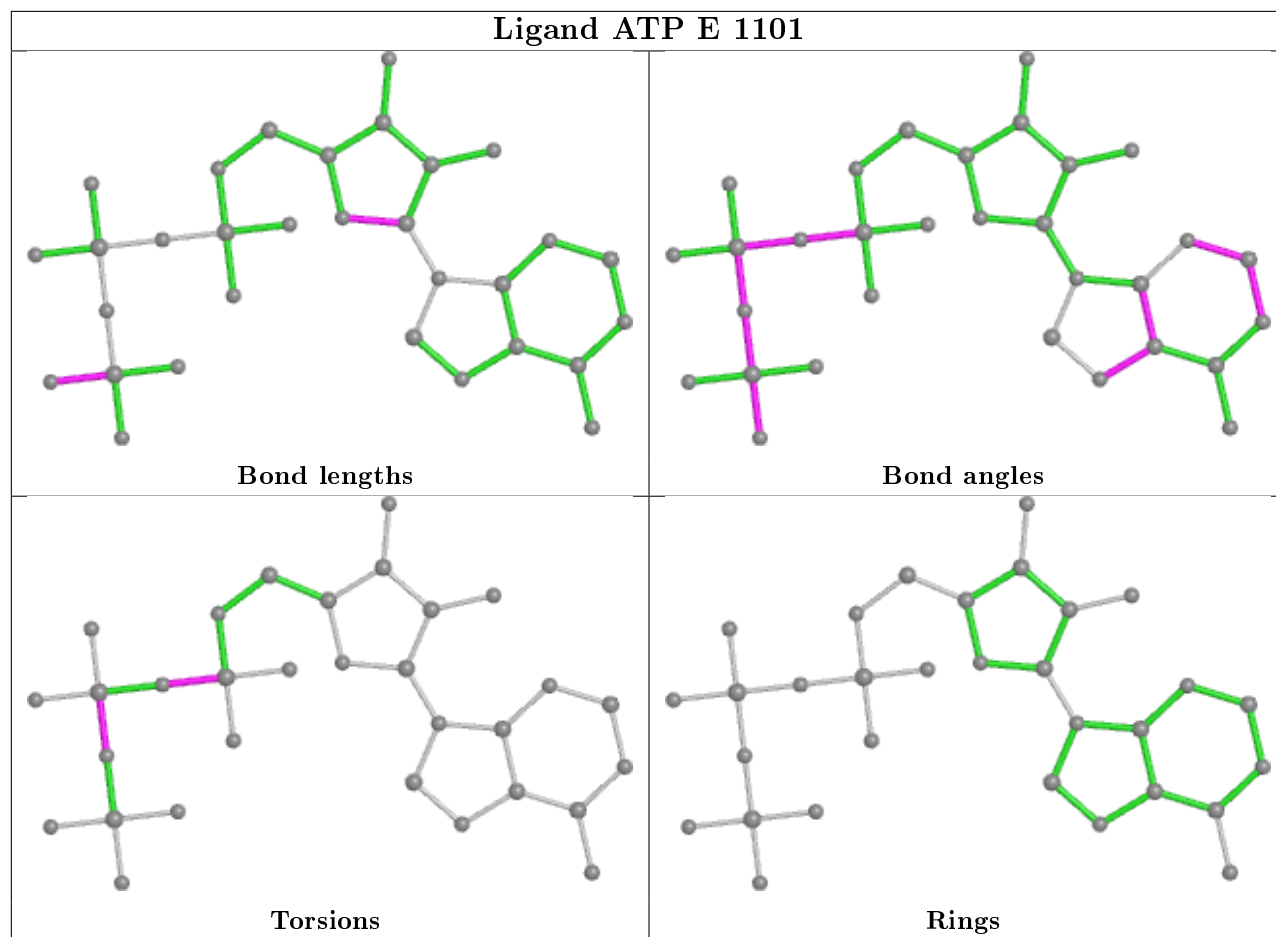


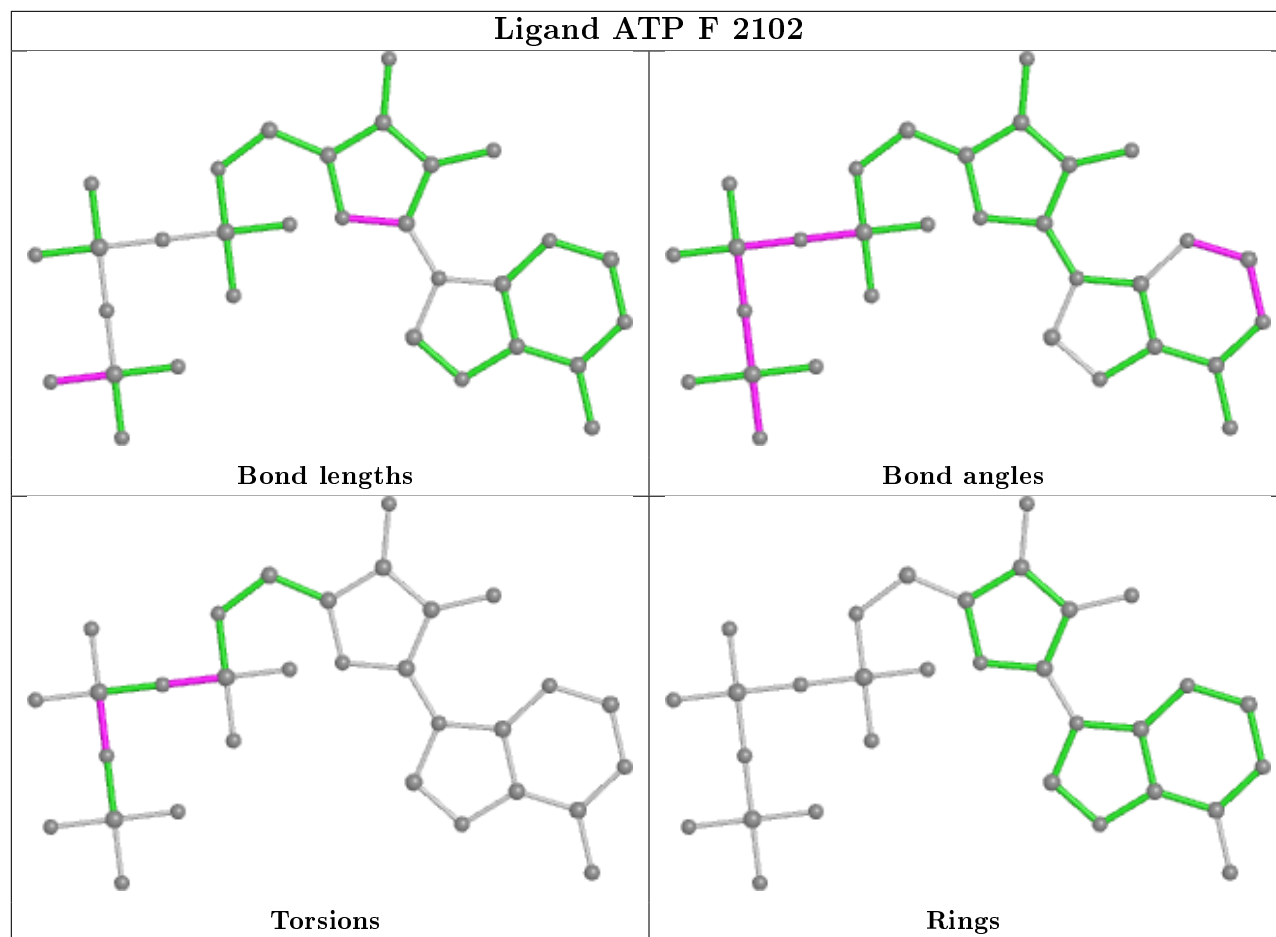


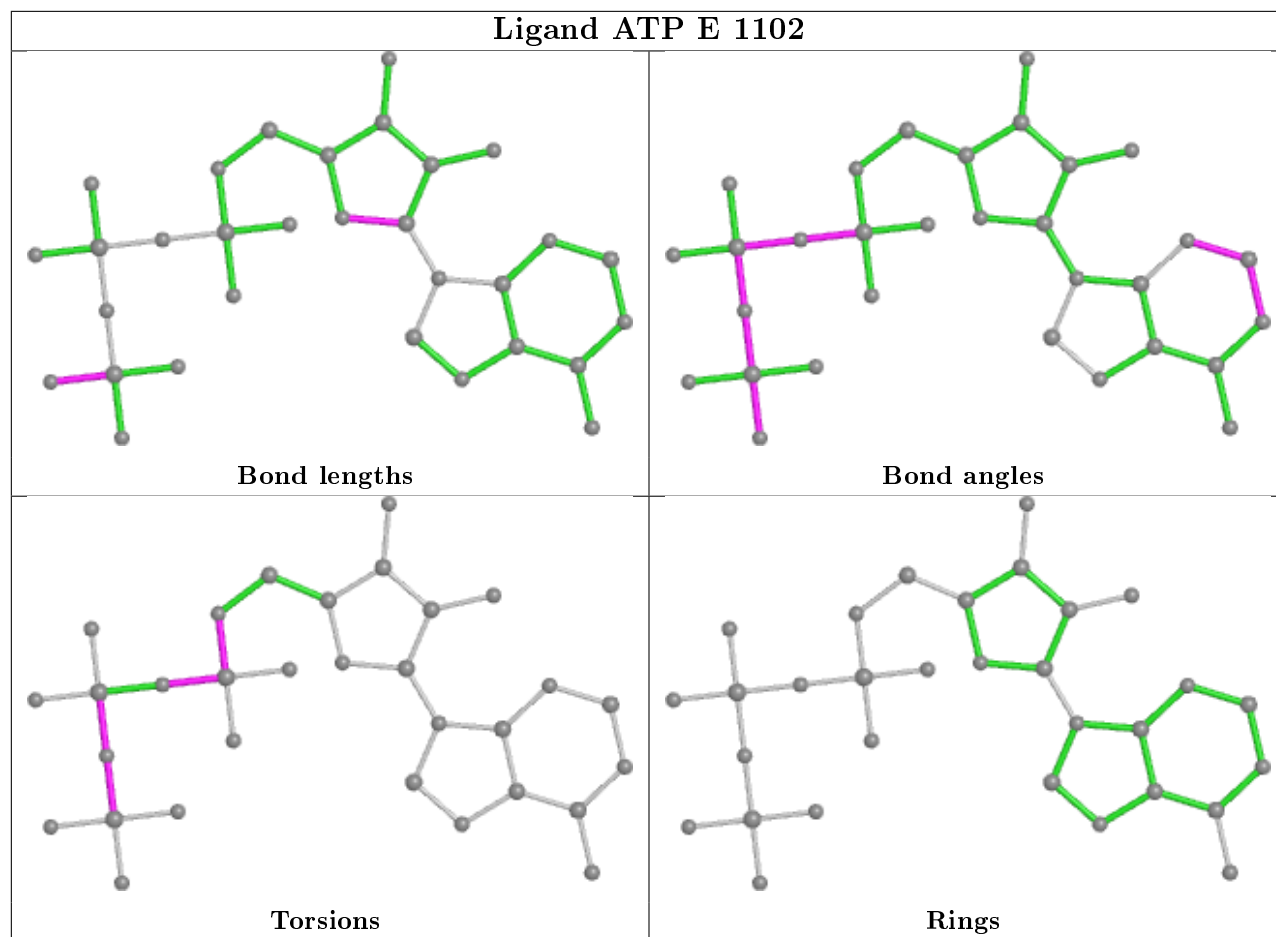


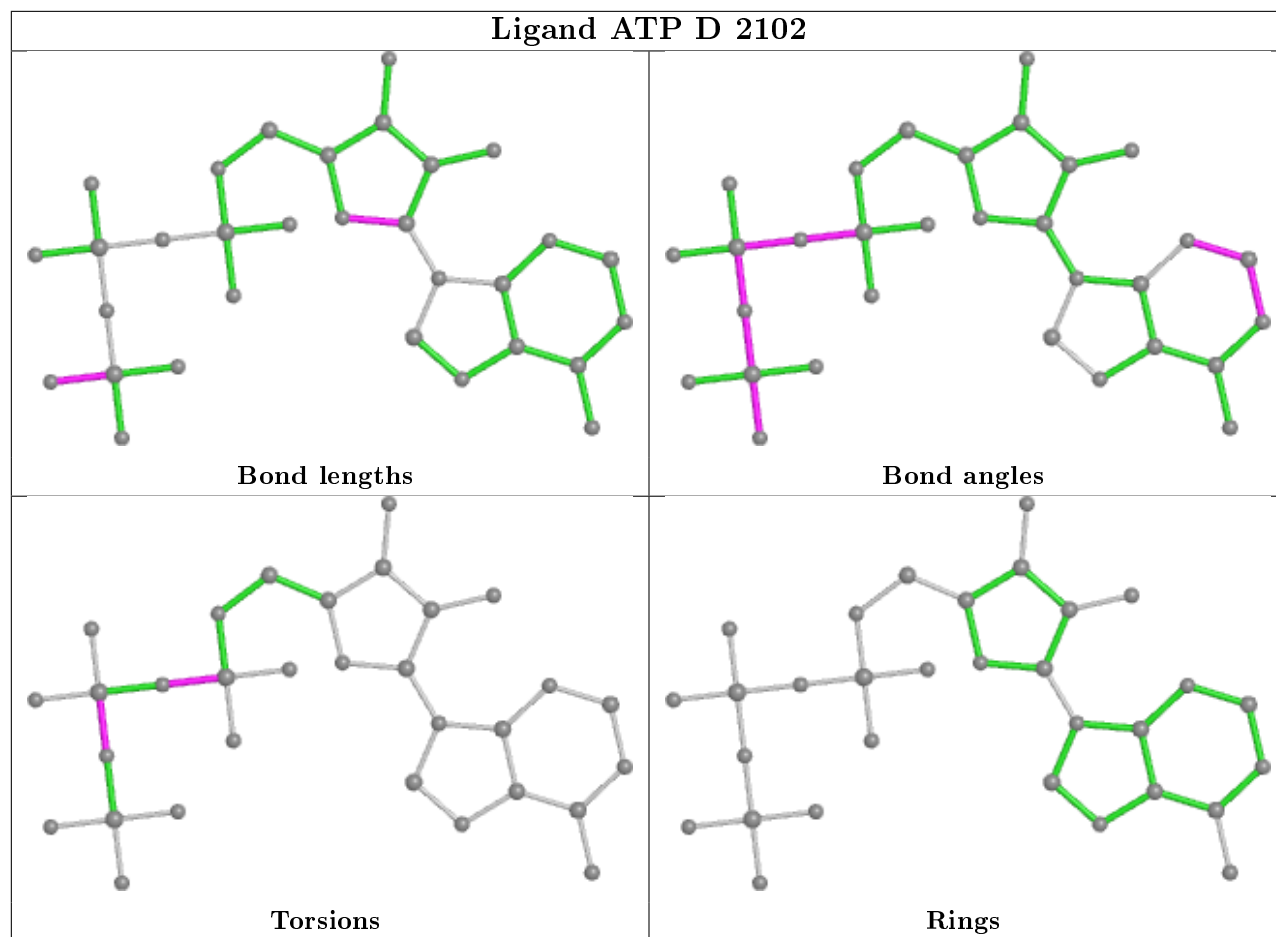


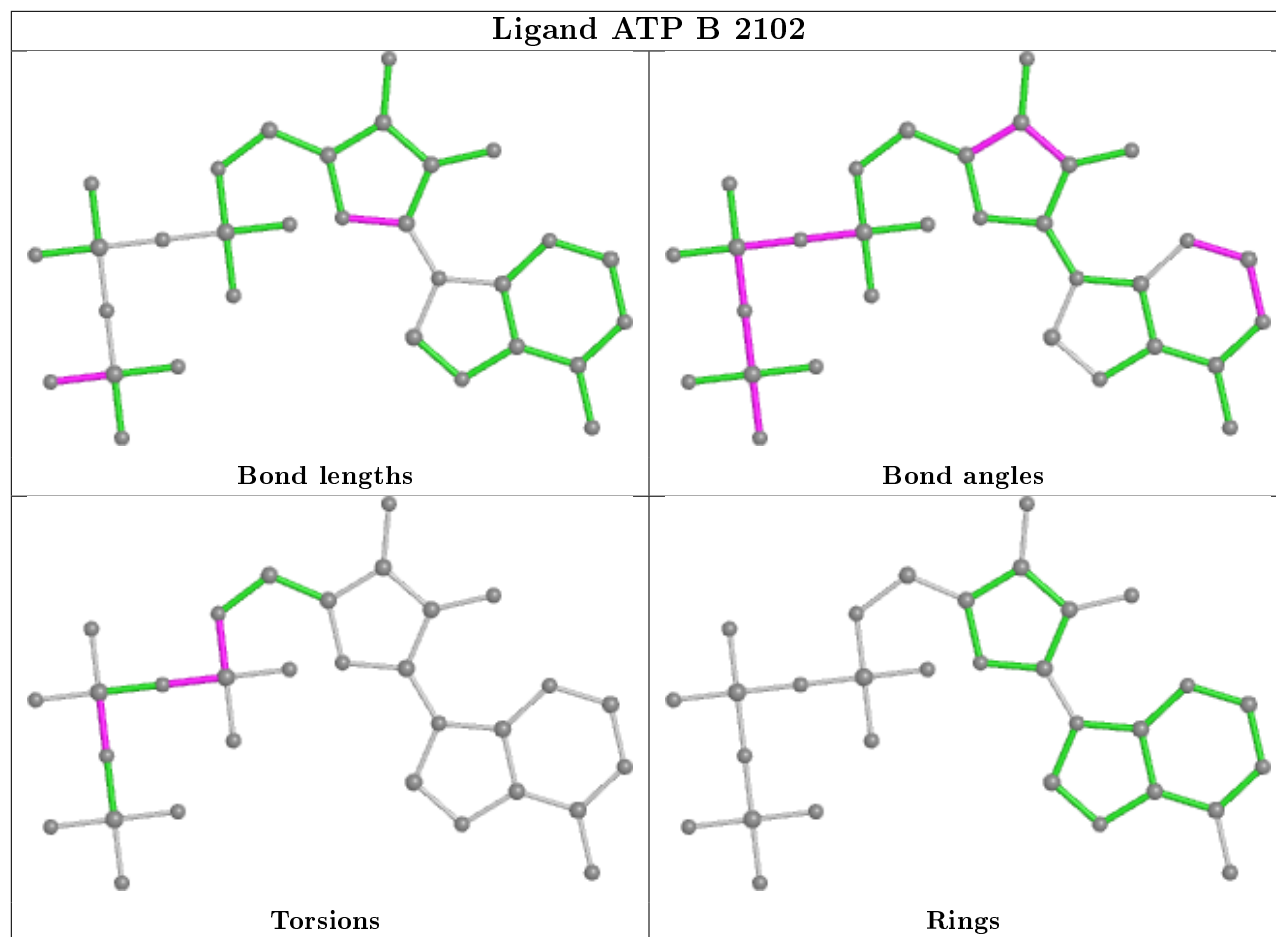


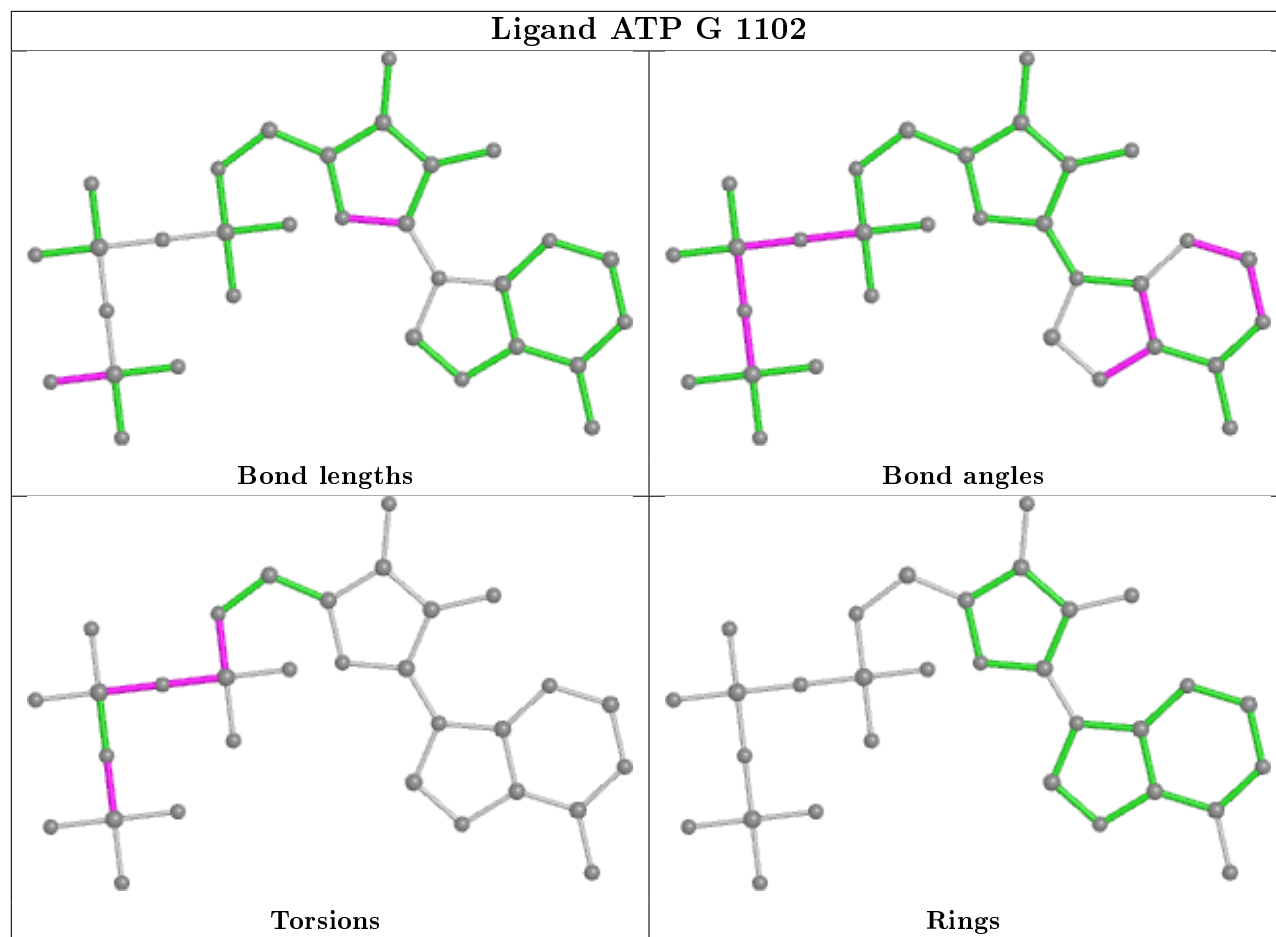


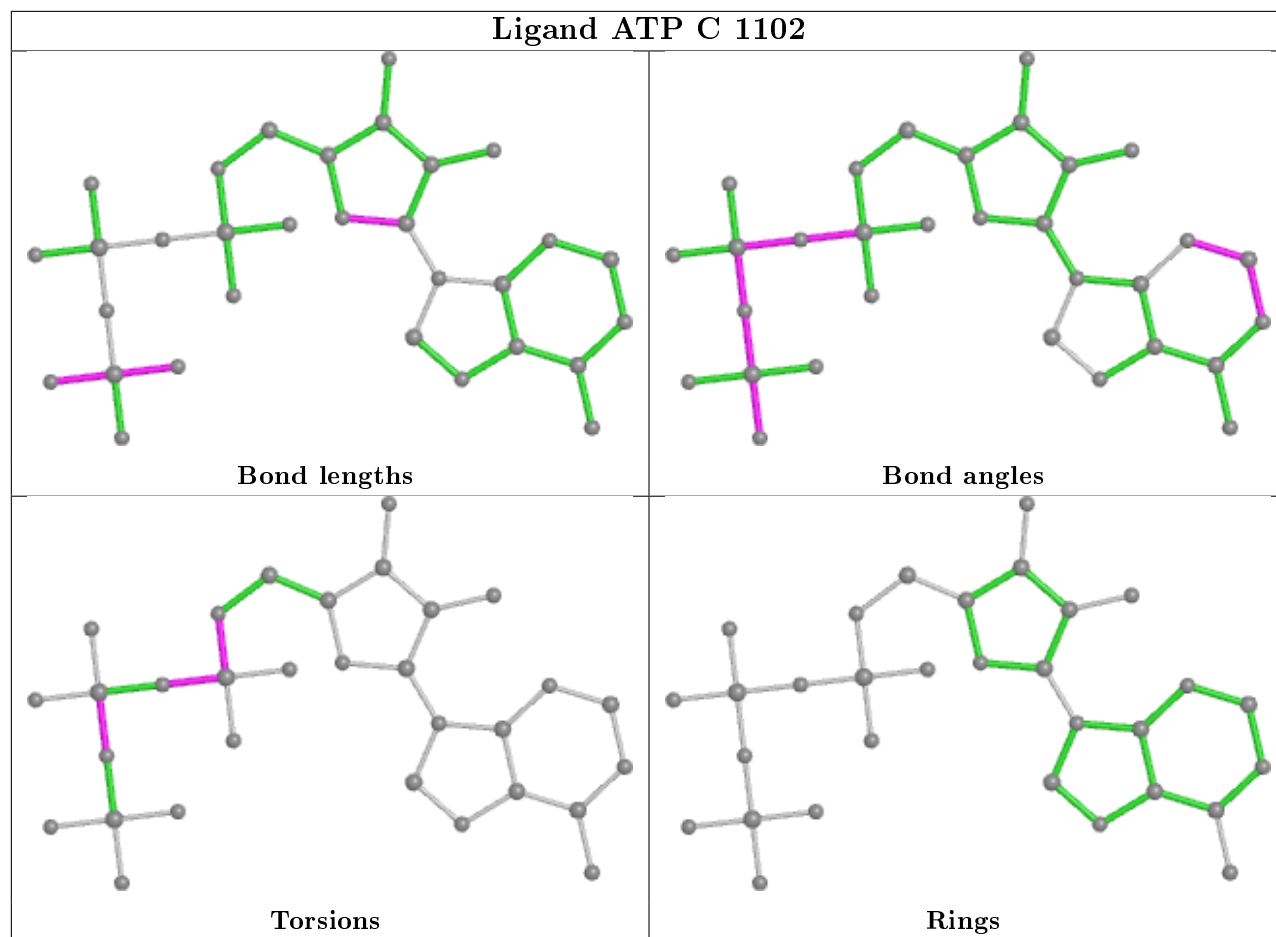


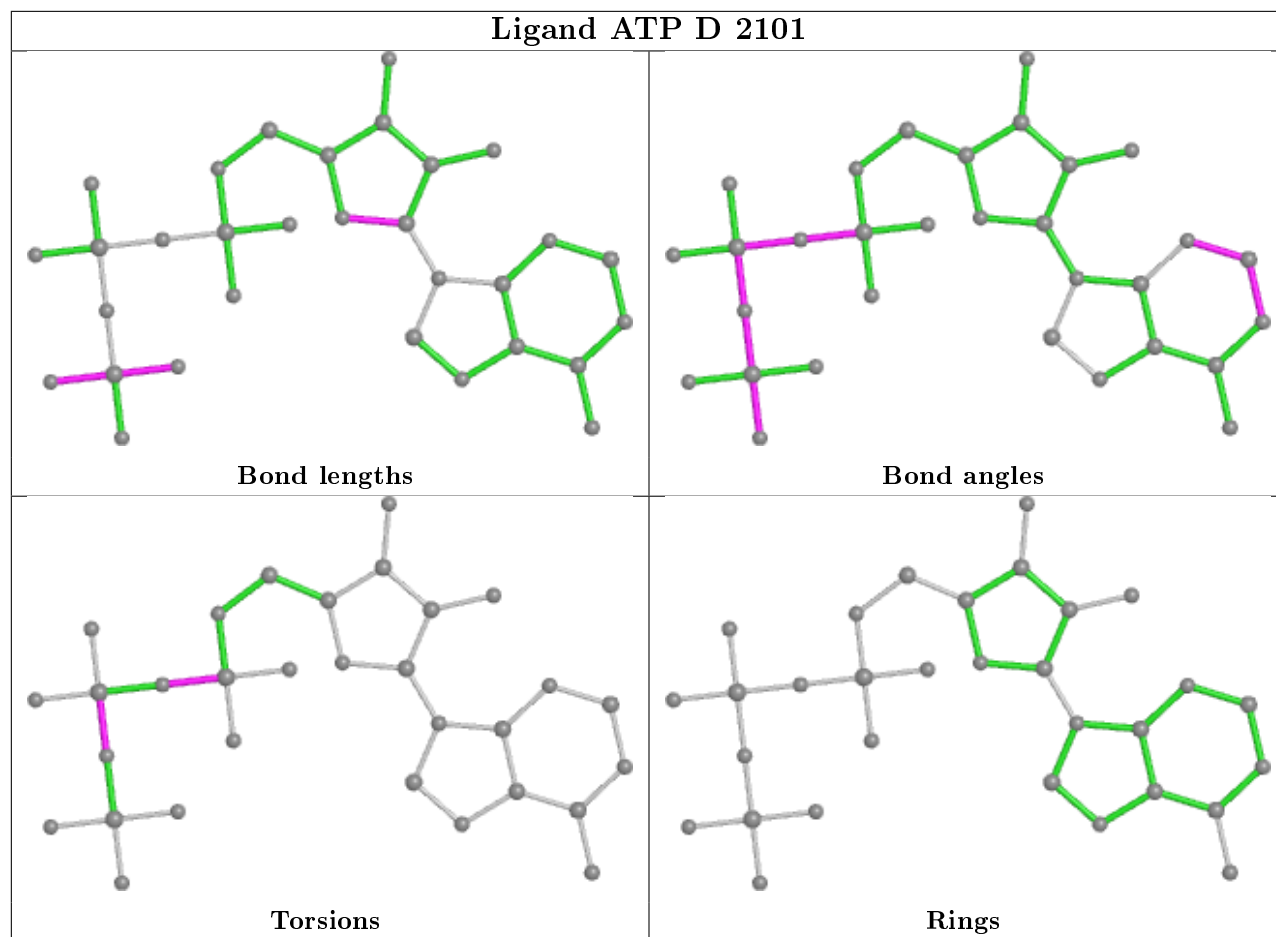


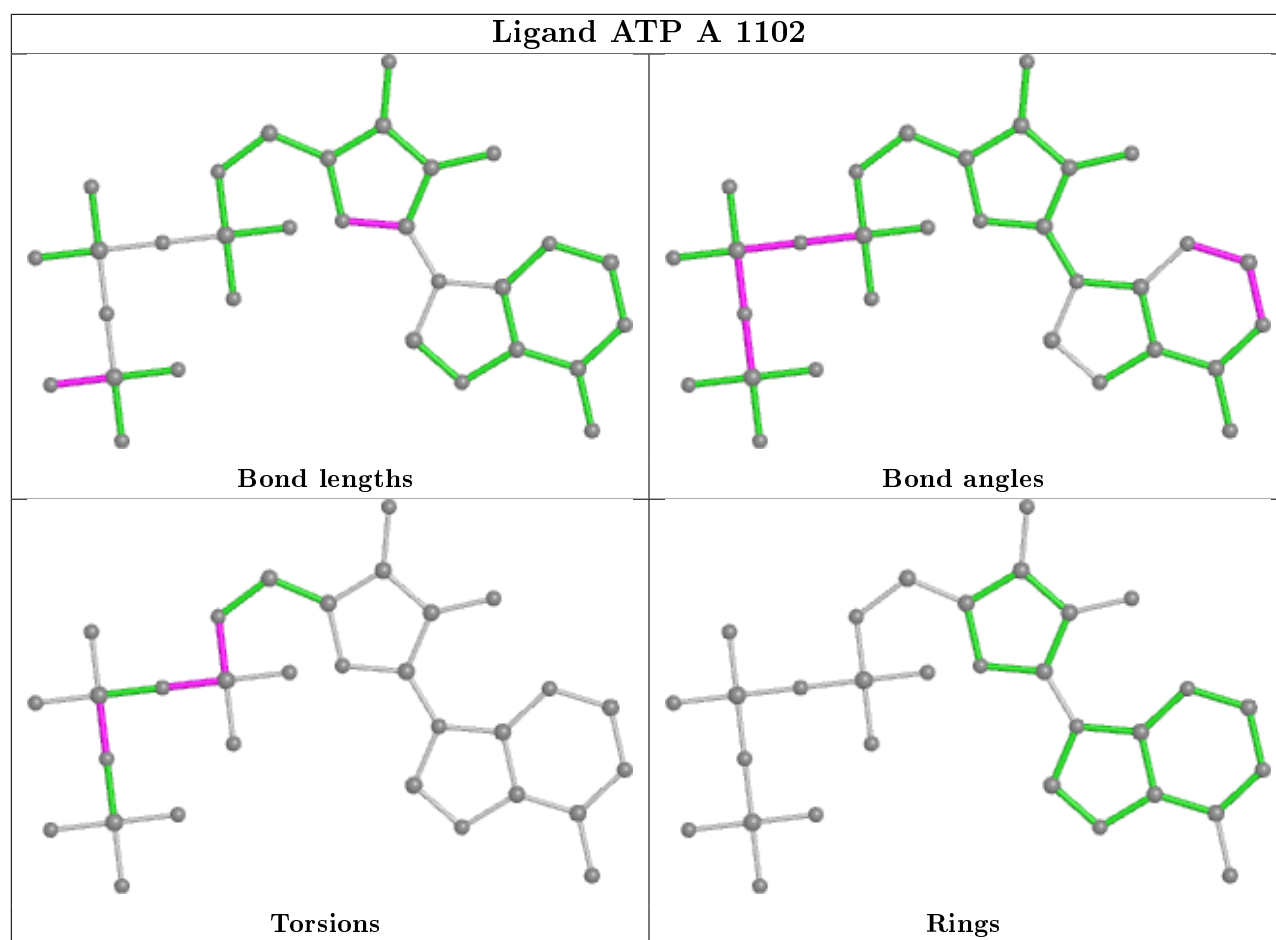


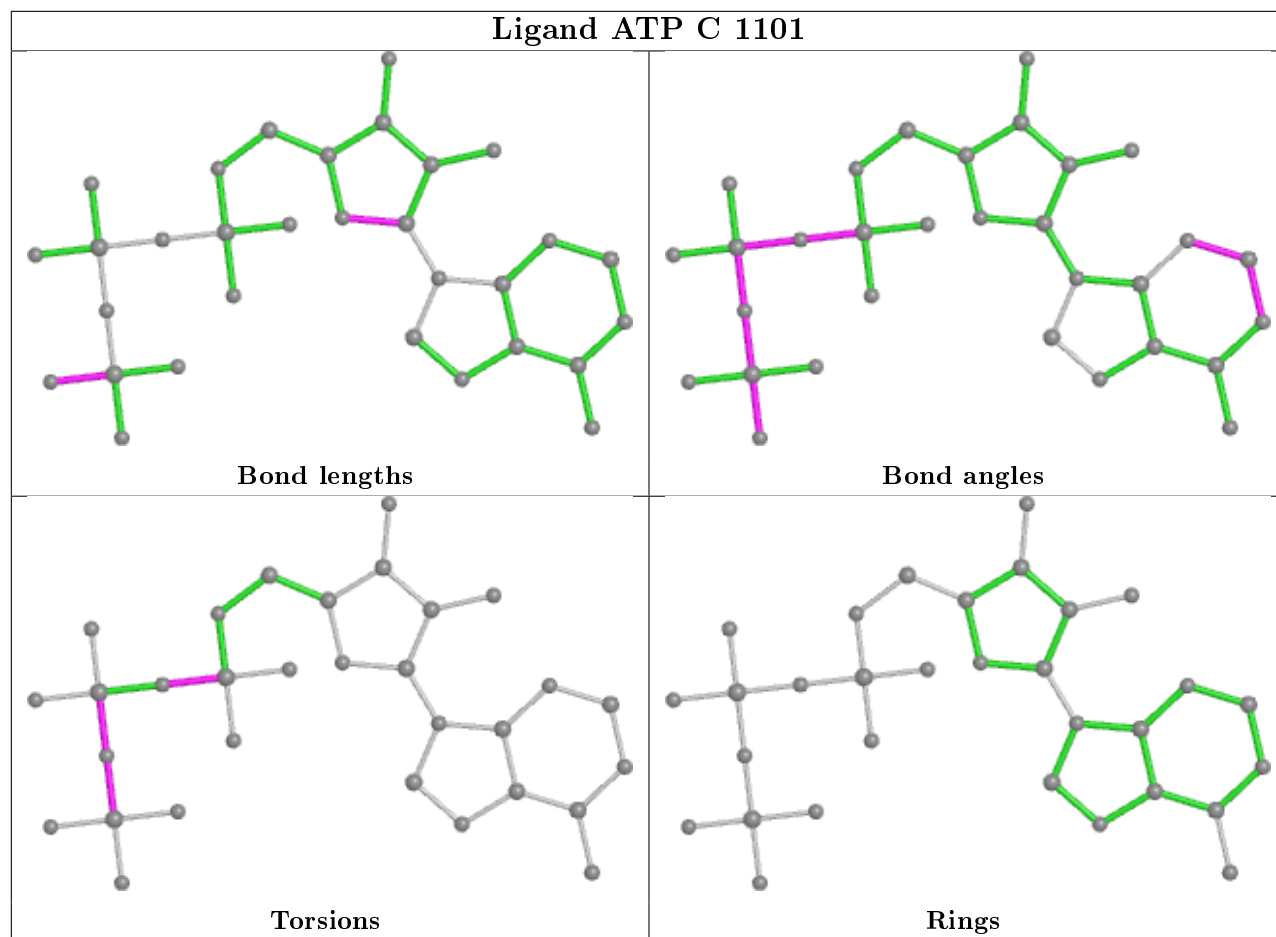












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/309 (93%)	-0.03	6 (2%) 63 61	21, 35, 71, 82	1 (0%)
1	B	290/309 (93%)	0.36	13 (4%) 33 29	27, 54, 82, 86	0
1	C	290/309 (93%)	-0.00	3 (1%) 82 82	21, 35, 70, 82	0
1	D	289/309 (93%)	0.31	14 (4%) 30 27	27, 54, 82, 86	0
1	E	291/309 (94%)	0.04	2 (0%) 87 87	21, 35, 70, 82	1 (0%)
1	F	277/309 (89%)	0.37	11 (3%) 38 33	27, 53, 82, 86	0
1	G	292/309 (94%)	0.00	3 (1%) 82 82	21, 35, 70, 82	0
1	H	282/309 (91%)	0.32	15 (5%) 26 22	27, 54, 83, 91	1 (0%)
All	All	2300/2472 (93%)	0.17	67 (2%) 51 47	21, 45, 79, 91	3 (0%)

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	PRO	4.9
1	A	54	VAL	3.8
1	D	156	HIS	3.7
1	H	157	PRO	3.5
1	B	156	HIS	3.4

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 ⓘ

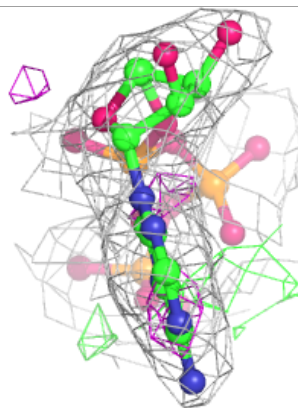
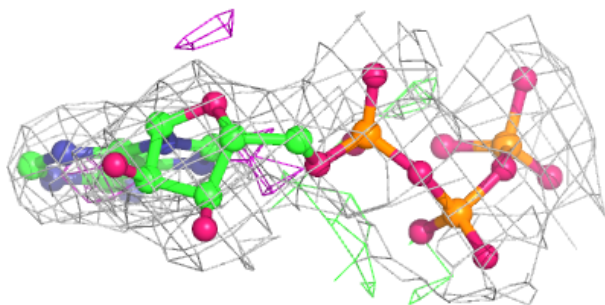
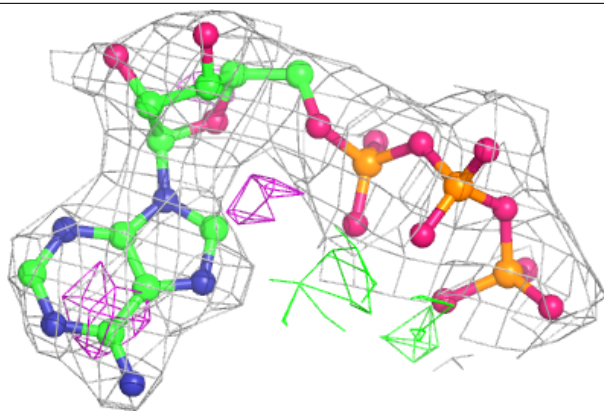
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	1001	1/1	0.72	0.15	24,24,24,24	0
2	MG	E	1001	1/1	0.82	0.24	21,21,21,21	0
2	MG	H	2001	1/1	0.84	0.22	31,31,31,31	0
2	MG	C	1002	1/1	0.86	0.15	31,31,31,31	0
2	MG	D	2001	1/1	0.87	0.17	32,32,32,32	0
2	MG	B	2002	1/1	0.87	0.28	40,40,40,40	0
2	MG	F	2002	1/1	0.87	0.42	37,37,37,37	0
2	MG	D	2002	1/1	0.88	0.32	36,36,36,36	0
2	MG	H	2002	1/1	0.91	0.30	30,30,30,30	0
2	MG	C	1001	1/1	0.92	0.25	24,24,24,24	0
2	MG	G	1001	1/1	0.93	0.28	24,24,24,24	0
2	MG	B	2001	1/1	0.94	0.21	41,41,41,41	0
3	ATP	E	1102	31/31	0.95	0.19	25,30,34,34	0
2	MG	F	2001	1/1	0.95	0.37	47,47,47,47	0
2	MG	A	1002	1/1	0.95	0.26	31,31,31,31	0
2	MG	E	1002	1/1	0.95	0.27	23,23,23,23	0
3	ATP	F	2102	31/31	0.96	0.17	27,32,35,35	0
3	ATP	A	1102	31/31	0.96	0.17	32,34,37,37	0
3	ATP	H	2102	31/31	0.96	0.16	26,31,34,34	0
3	ATP	B	2102	31/31	0.96	0.18	35,38,40,40	0
3	ATP	D	2102	31/31	0.96	0.17	32,35,37,37	0
3	ATP	D	2101	31/31	0.97	0.13	41,41,43,43	0
3	ATP	B	2101	31/31	0.97	0.14	44,45,46,46	0
3	ATP	C	1102	31/31	0.97	0.16	32,33,34,34	0
2	MG	G	1002	1/1	0.97	0.25	25,25,25,25	0
3	ATP	G	1102	31/31	0.97	0.16	27,29,32,32	0
3	ATP	F	2101	31/31	0.97	0.14	40,41,42,43	0
3	ATP	H	2101	31/31	0.97	0.13	40,41,42,42	0
3	ATP	E	1101	31/31	0.98	0.16	20,21,22,22	0
3	ATP	A	1101	31/31	0.98	0.15	19,21,24,25	0
3	ATP	C	1101	31/31	0.98	0.15	23,23,25,25	0
3	ATP	G	1101	31/31	0.98	0.15	18,20,22,22	0

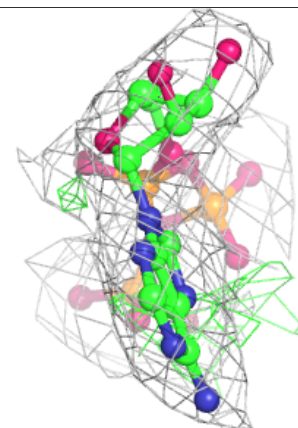
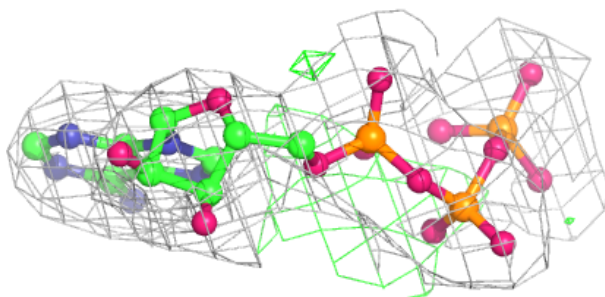
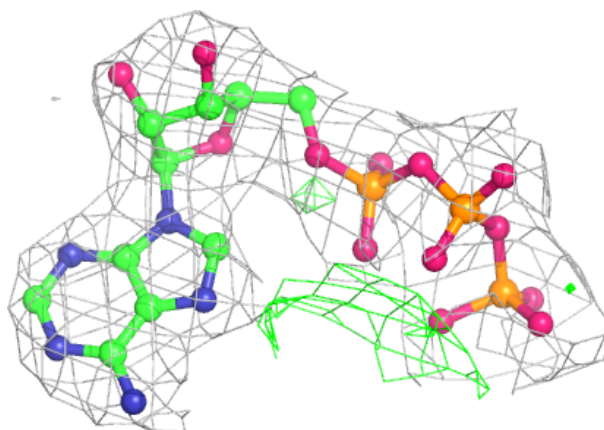
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP E 1102:

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

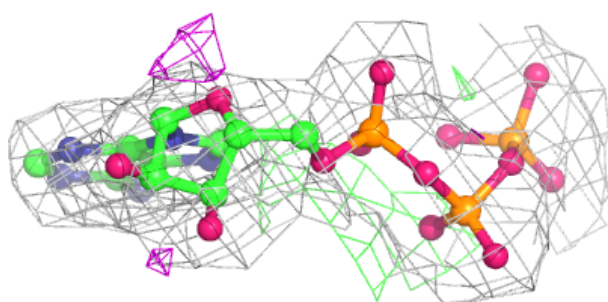
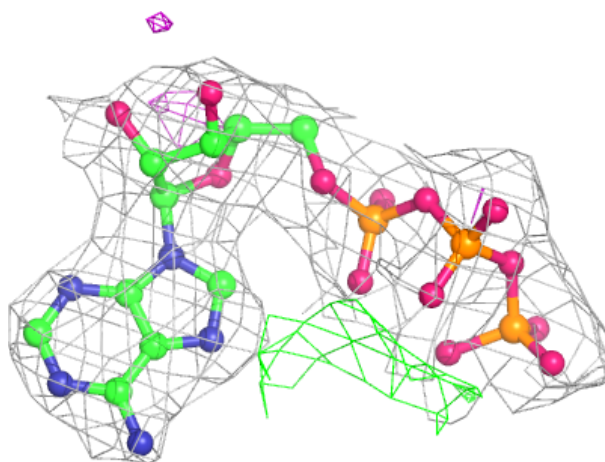
**Electron density around ATP F 2102:**

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



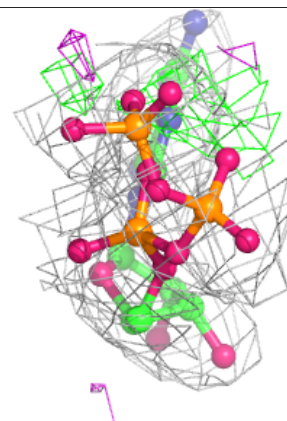
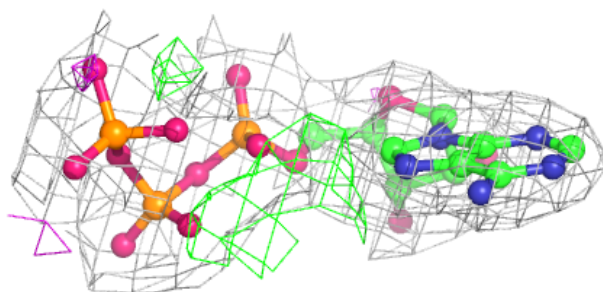
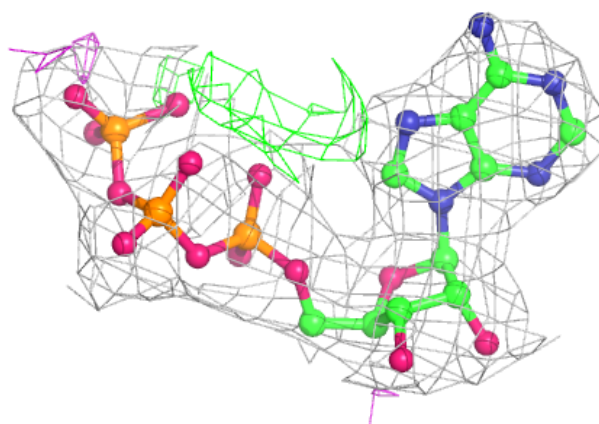
Electron density around ATP A 1102:

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

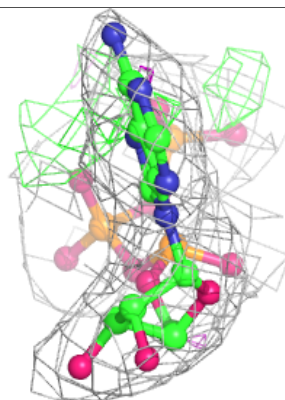
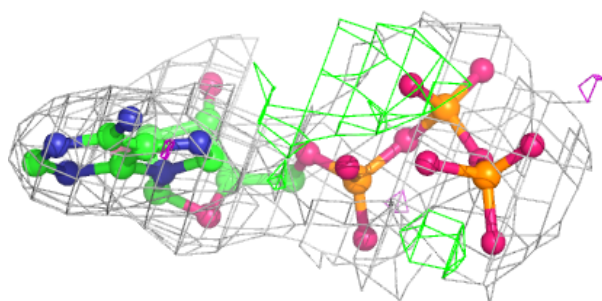
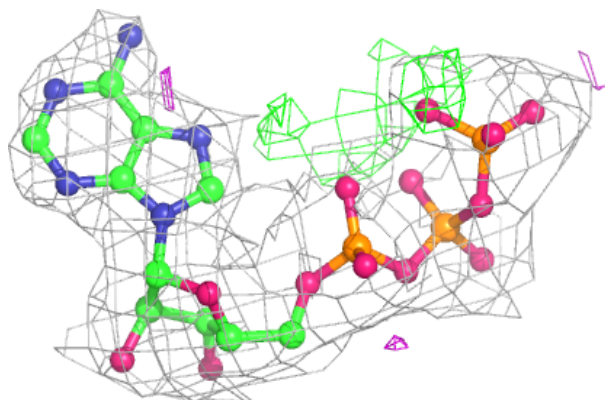


Electron density around ATP H 2102:

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

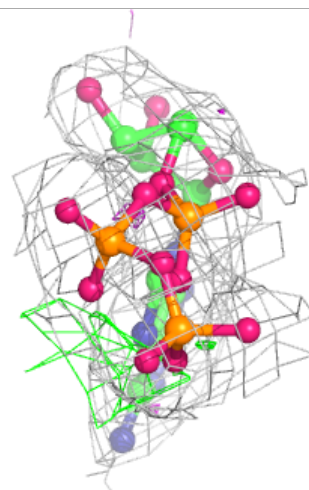
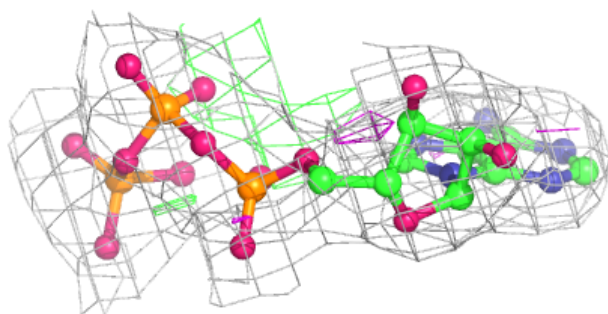
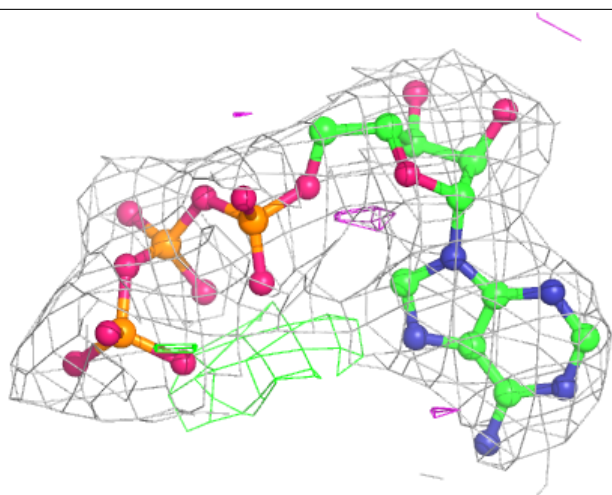
**Electron density around ATP B 2102:**

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



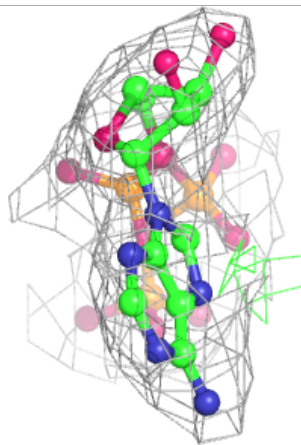
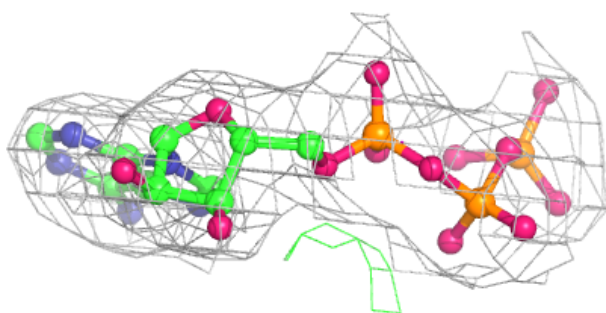
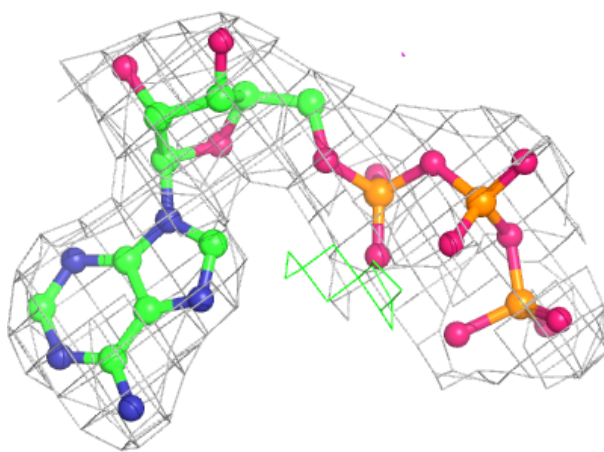
Electron density around ATP D 2102:

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



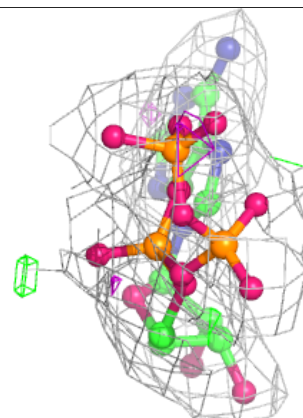
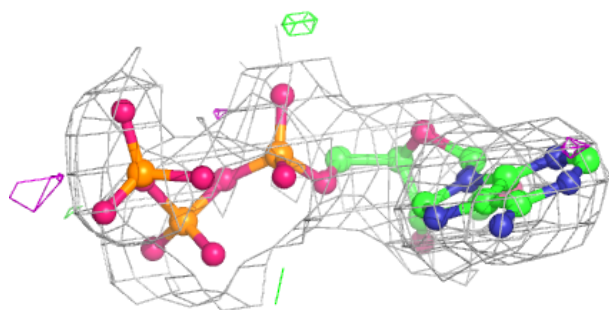
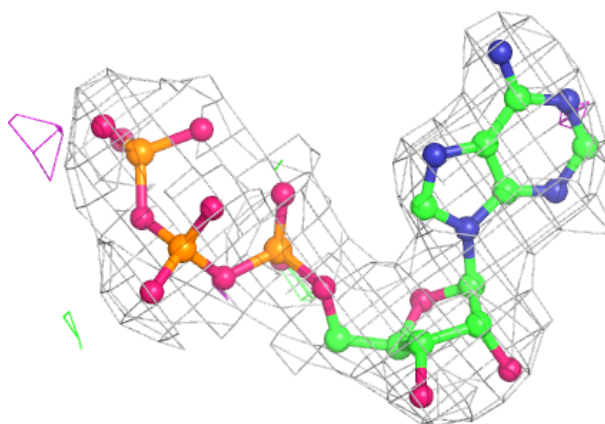
Electron density around ATP D 2101:

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

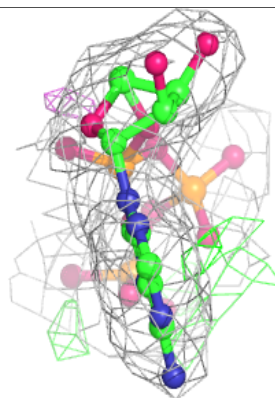
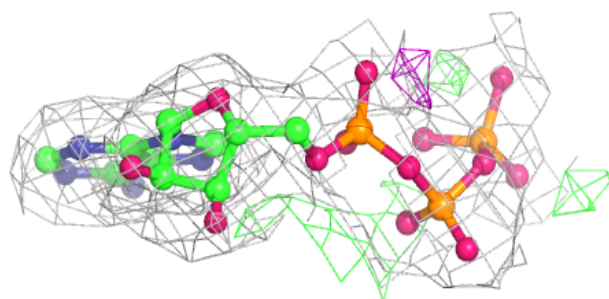
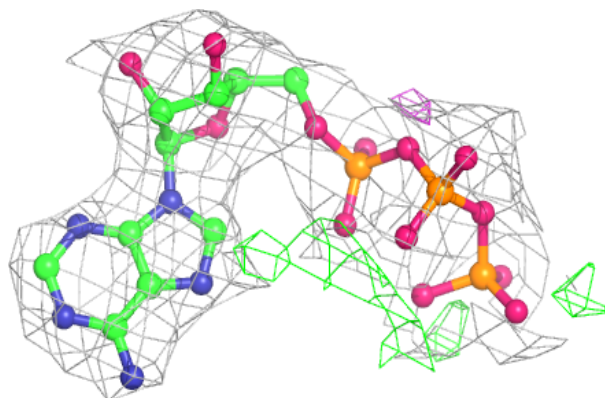


Electron density around ATP B 2101:

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

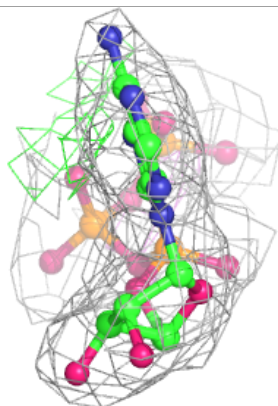
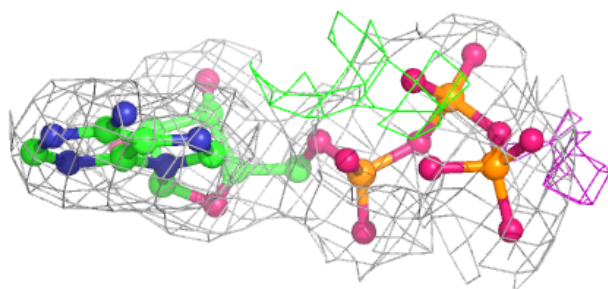
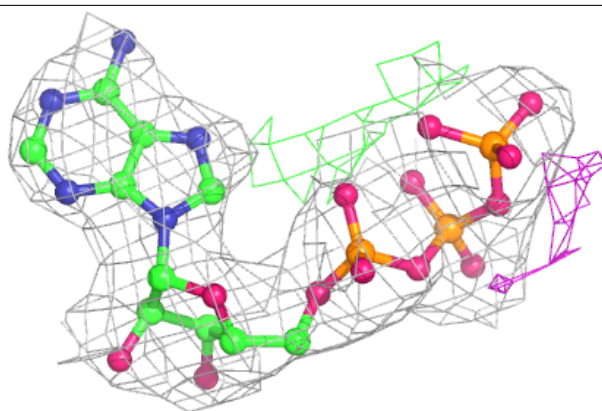
**Electron density around ATP C 1102:**

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

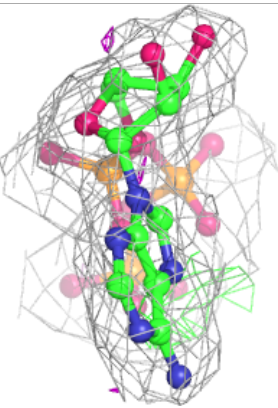
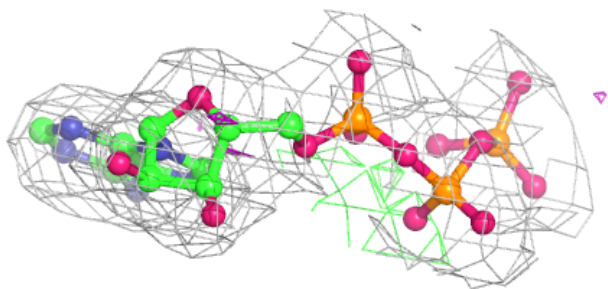
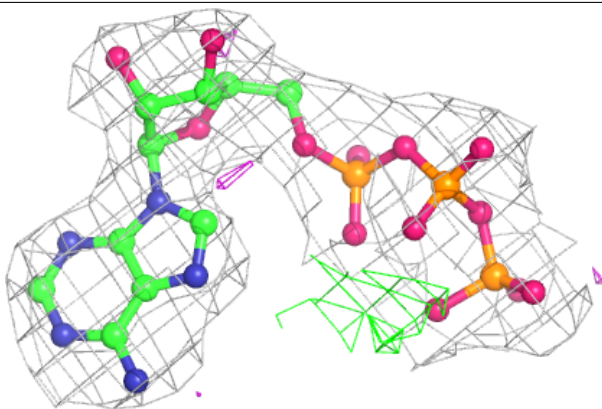


Electron density around ATP G 1102:

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

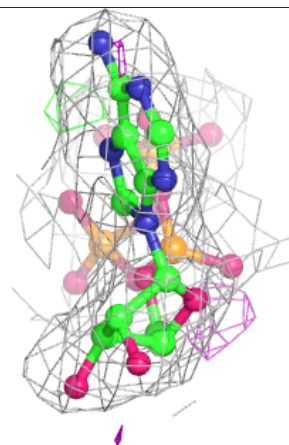
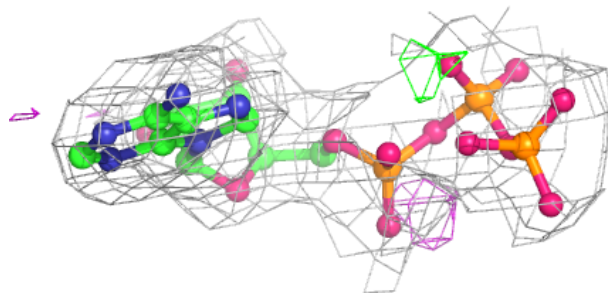
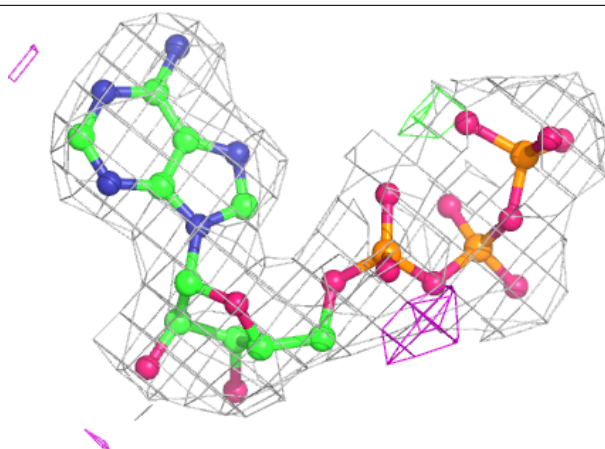
**Electron density around ATP F 2101:**

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



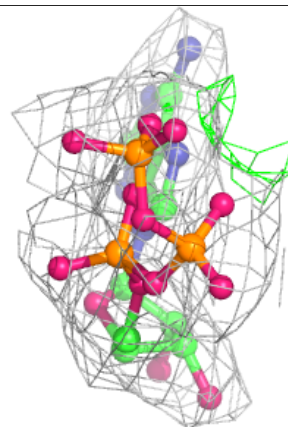
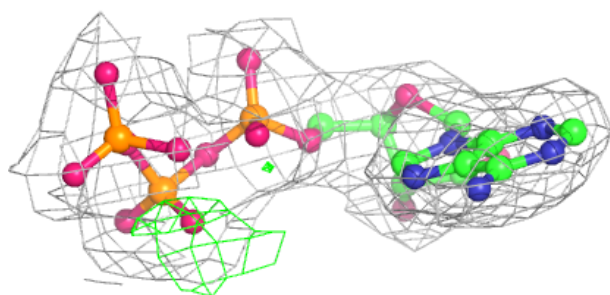
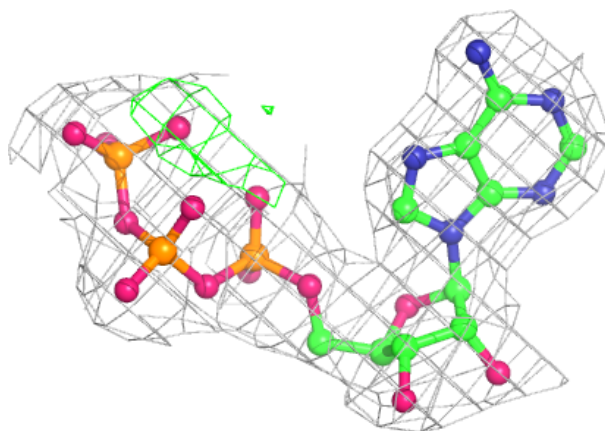
Electron density around ATP H 2101:

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



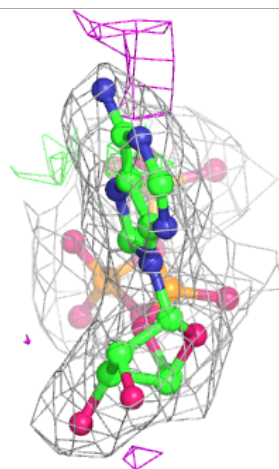
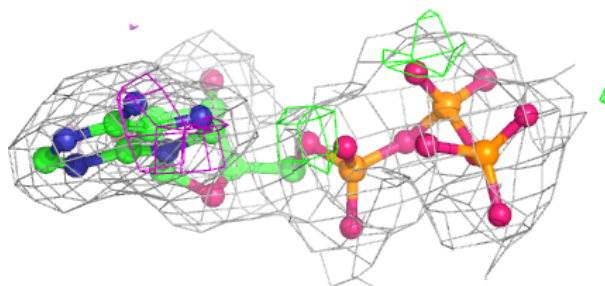
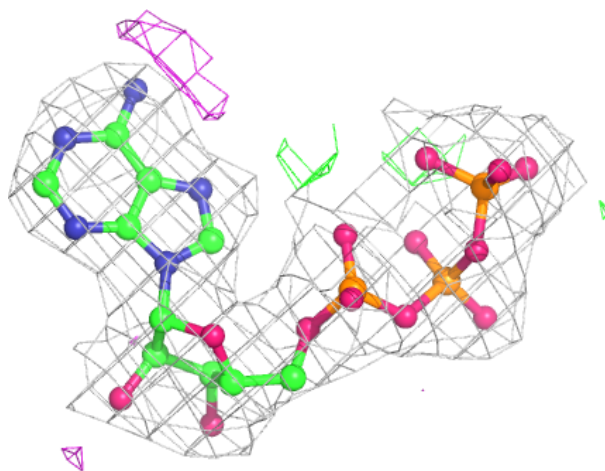
Electron density around ATP E 1101:

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



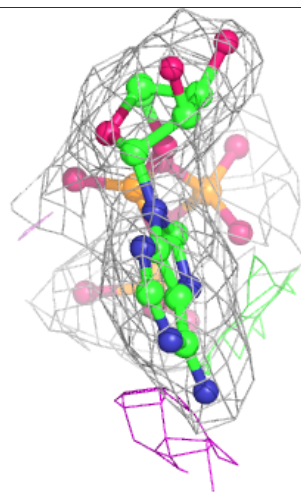
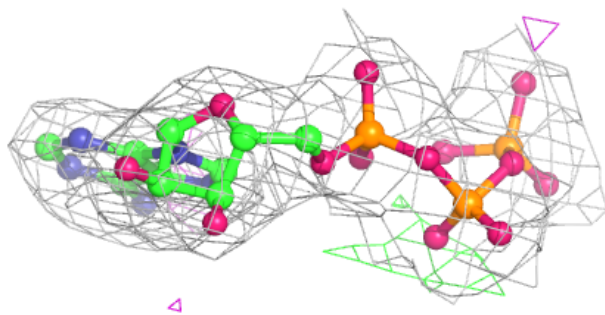
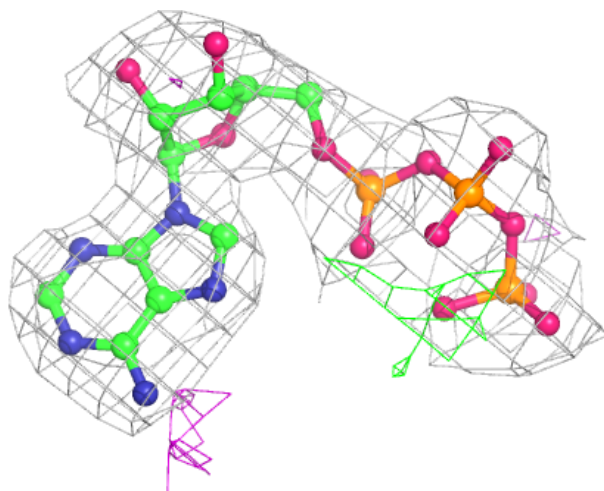
Electron density around ATP A 1101:

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



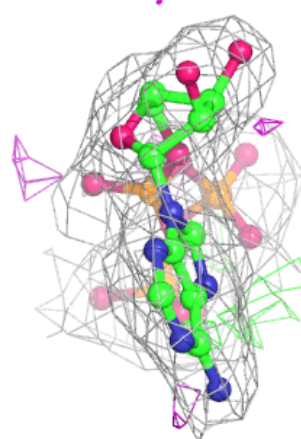
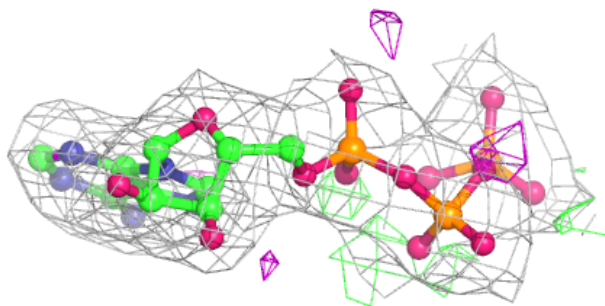
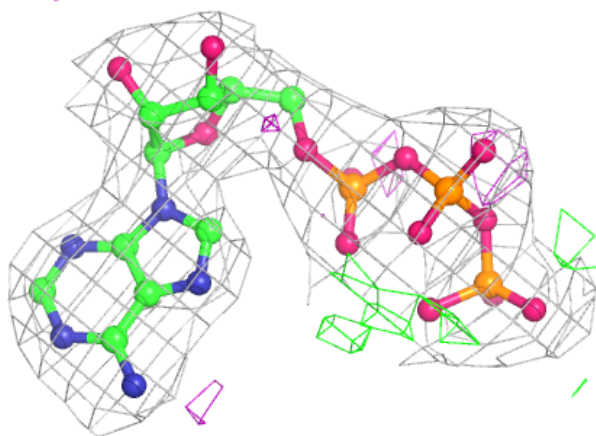
Electron density around ATP C 1101:

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



Electron density around ATP G 1101:

$2mF_o-DF_c$ (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.