



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2023 – 09:34 pm GMT

PDB ID : 7PLJ  
Title : Structure of Polyphosphate kinase 2 from *Deinococcus radiodurans*, in complex with ATP and polyphosphates.  
Authors : Silva, S.T.N.; Romao, C.V.  
Deposited on : 2021-08-31  
Resolution : 1.64 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.32.1  
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) : 2.32.1

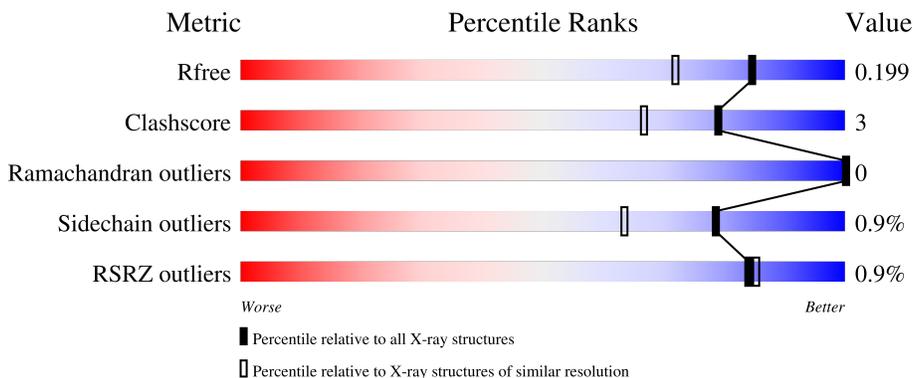
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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  $\geq 3$ , 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	266	 2% 93% 6%
1	B	266	 % 93% 7%
1	C	266	 % 94% 6%
1	D	266	 94% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	B	303	-	-	X	-
6	GOL	C	306	-	X	-	-

## 2 Entry composition [i](#)

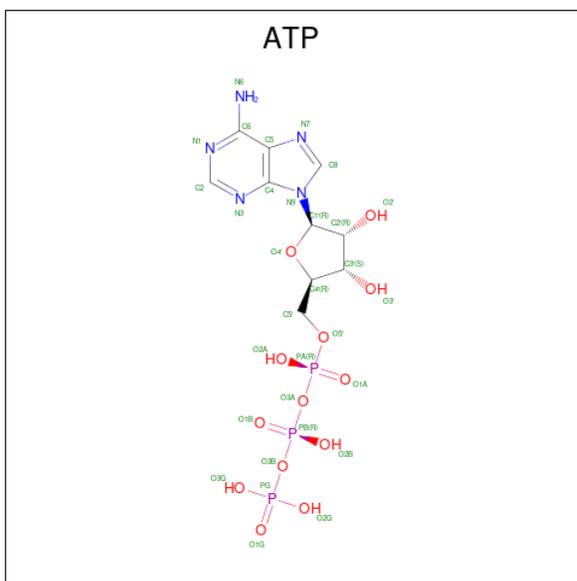
There are 11 unique types of molecules in this entry. The entry contains 10455 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PPK2 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	Total 2158	C 1368	N 382	O 405	S 3	0	0	0
1	B	266	Total 2181	C 1382	N 388	O 408	S 3	1	3	0
1	C	266	Total 2186	C 1386	N 388	O 409	S 3	1	4	0
1	D	266	Total 2178	C 1380	N 387	O 408	S 3	0	3	0

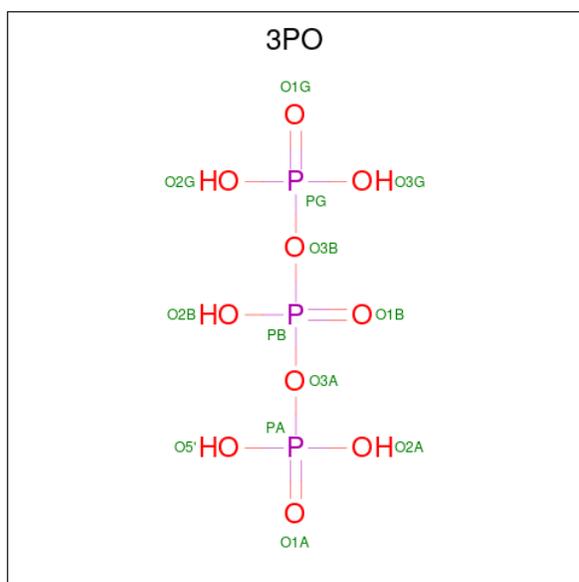
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

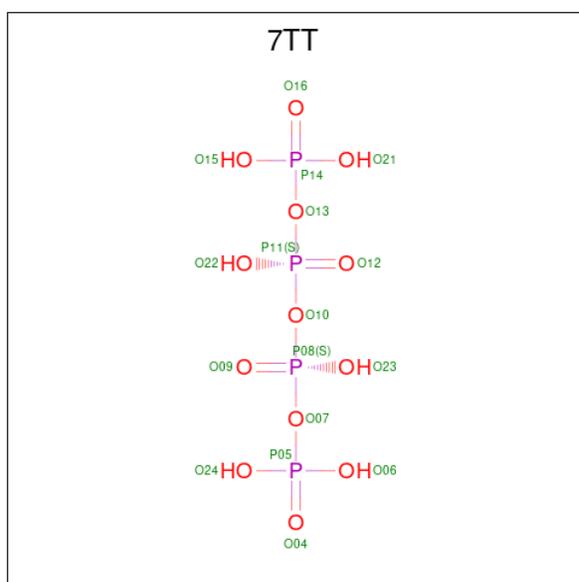
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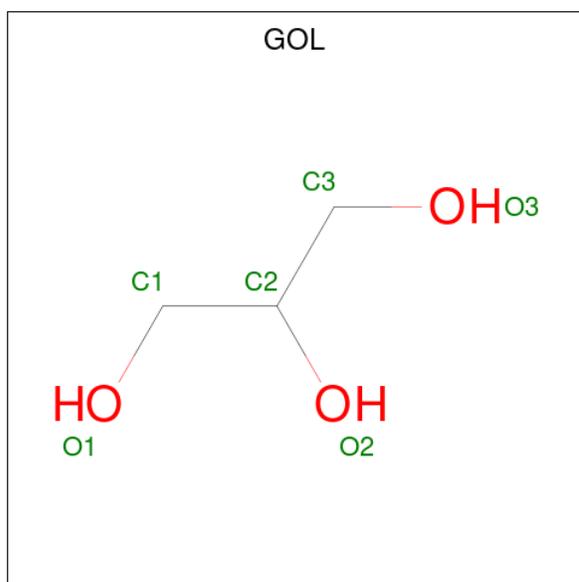
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			13	10	3		

- Molecule 5 is Tetraphosphate (three-letter code: 7TT) (formula:  $H_6O_{13}P_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			17	13	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

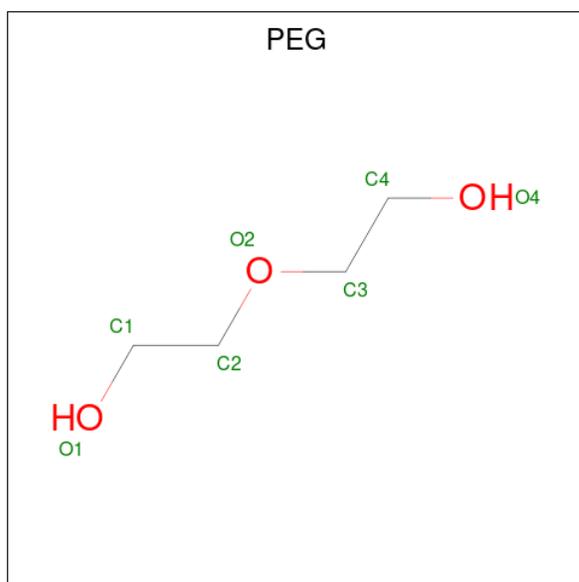


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

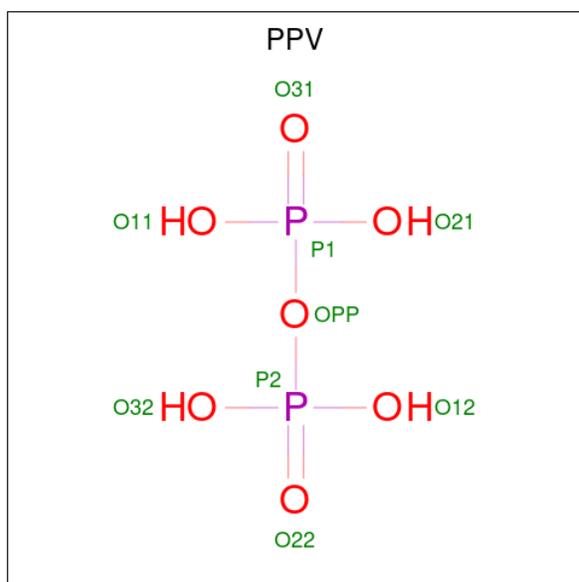
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



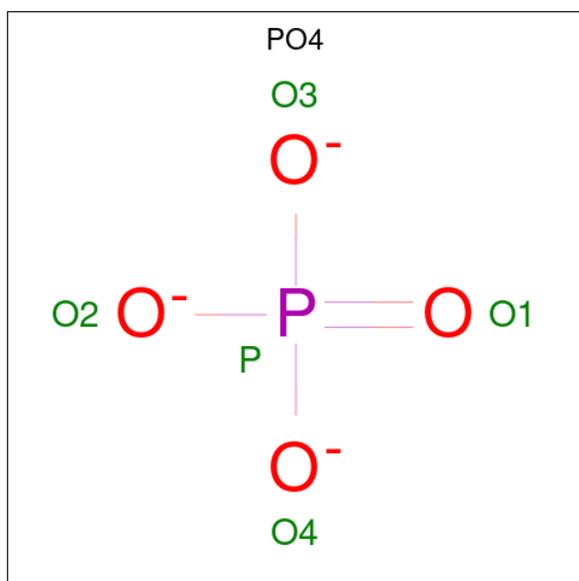
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 7 4 3	0	0
8	C	1	Total C O 7 4 3	0	0
8	C	1	Total C O 14 8 6	0	1
8	D	1	Total C O 14 8 6	0	1
8	D	1	Total C O 14 8 6	0	1

- Molecule 9 is PYROPHOSPHATE (three-letter code: PPV) (formula:  $H_4O_7P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	P	0	0
			9	7	2		
9	C	1	Total	O	P	0	0
			9	7	2		
9	C	1	Total	O	P	0	0
			9	7	2		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	O	P	0	0
			5	4	1		

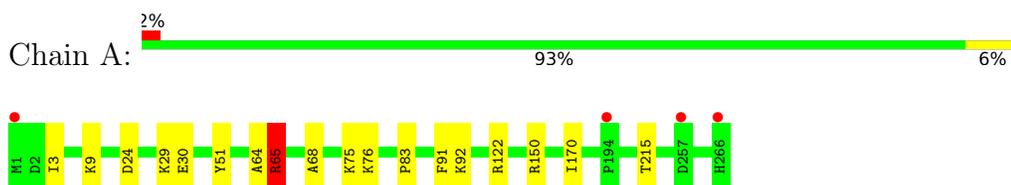
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	325	Total	O	0	7
			333	333		
11	B	304	Total	O	0	10
			316	316		
11	C	302	Total	O	0	7
			309	309		
11	D	325	Total	O	0	9
			334	334		

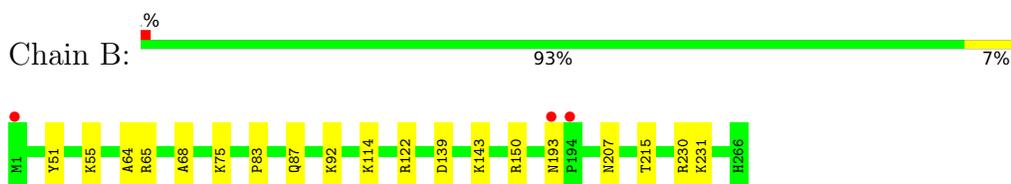
### 3 Residue-property plots [i](#)

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.

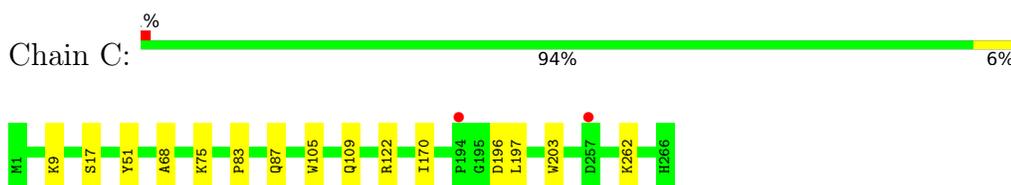
- Molecule 1: PPK2 domain-containing protein



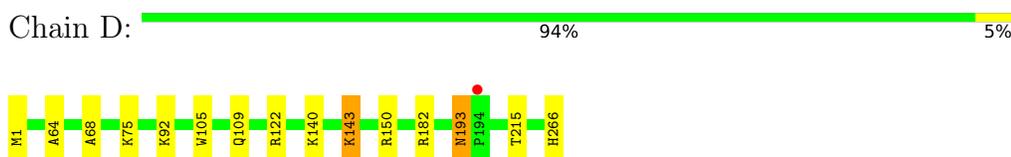
- Molecule 1: PPK2 domain-containing protein



- Molecule 1: PPK2 domain-containing protein



- Molecule 1: PPK2 domain-containing protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.85Å 137.14Å 85.02Å 90.00° 116.89° 90.00°	Depositor
Resolution (Å)	40.04 – 1.64 93.69 – 1.64	Depositor EDS
% Data completeness (in resolution range)	75.7 (40.04-1.64) 75.7 (93.69-1.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.63Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.169 , 0.202 0.168 , 0.199	Depositor DCC
$R_{free}$ test set	6828 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 3PO, PPV, 7TT, ATP, PEG, GOL, PO4

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	0.61	0/2209	0.71	1/2990 (0.0%)
1	B	0.55	0/2235	0.67	0/3023
1	C	0.60	0/2243	0.71	0/3035
1	D	0.60	0/2235	0.70	0/3024
All	All	0.59	0/8922	0.70	1/12072 (0.0%)

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	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	65	ARG	Sidechain
1	B	122	ARG	Sidechain
1	C	122	ARG	Sidechain
1	D	122	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2158	0	2125	13	0
1	B	2181	0	2154	19	0
1	C	2186	0	2160	10	0
1	D	2178	0	2150	11	0
2	A	62	0	24	0	0
2	B	62	0	24	0	0
2	C	62	0	24	0	0
2	D	62	0	24	0	0
3	A	27	0	12	0	0
3	D	27	0	12	0	0
4	A	13	0	0	0	0
5	A	17	0	0	1	0
6	A	6	0	8	1	0
6	B	12	0	15	5	0
6	C	6	0	7	1	0
6	D	12	0	16	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	7	0	10	0	0
8	C	21	0	30	4	0
8	D	28	0	40	2	0
9	B	9	0	0	0	0
9	C	18	0	0	1	0
10	D	5	0	0	0	0
11	A	333	0	0	3	0
11	B	316	0	0	4	0
11	C	309	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	334	0	0	2	0
All	All	10455	0	8835	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 50 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:C:17:SER:HA	8:C:307[B]:PEG:H31	1.63	0.80
1:A:92:LYS:NZ	1:B:51:TYR:OH	2.21	0.74
1:C:203:TRP:HE1	8:C:307[B]:PEG:H12	1.55	0.72
1:B:231:LYS:H	6:B:303:GOL:H11	1.60	0.66
1:D:105:TRP:O	1:D:109[B]:GLN:HG3	1.99	0.61

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	264/266 (99%)	258 (98%)	6 (2%)	0	100	100
1	B	267/266 (100%)	261 (98%)	6 (2%)	0	100	100
1	C	268/266 (101%)	262 (98%)	6 (2%)	0	100	100
1	D	267/266 (100%)	262 (98%)	5 (2%)	0	100	100
All	All	1066/1064 (100%)	1043 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	228/228 (100%)	225 (99%)	3 (1%)	69	47
1	B	231/228 (101%)	231 (100%)	0	100	100
1	C	232/228 (102%)	230 (99%)	2 (1%)	78	63
1	D	231/228 (101%)	228 (99%)	3 (1%)	69	47
All	All	922/912 (101%)	914 (99%)	8 (1%)	78	63

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	193	ASN
1	D	143	LYS
1	C	262	LYS
1	C	9	LYS
1	D	1	MET

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

Mol	Chain	Res	Type
1	A	109	GLN
1	B	207	ASN
1	D	193	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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	3PO	A	304	-	8,12,12	1.23	1 (12%)	15,20,20	1.35	2 (13%)
2	ATP	C	301	7	26,33,33	0.74	1 (3%)	31,52,52	1.02	2 (6%)
8	PEG	C	305	-	6,6,6	0.29	0	5,5,5	0.22	0
2	ATP	A	301	7	26,33,33	0.71	0	31,52,52	0.96	2 (6%)
8	PEG	D	307[A]	-	6,6,6	0.11	0	5,5,5	0.22	0
6	GOL	C	306	-	5,5,5	1.62	1 (20%)	5,5,5	1.07	1 (20%)
6	GOL	B	306	-	5,5,5	1.19	0	5,5,5	0.80	0
6	GOL	B	303	-	5,5,5	1.06	0	5,5,5	1.29	1 (20%)
8	PEG	D	305[B]	-	6,6,6	0.17	0	5,5,5	0.11	0
2	ATP	B	301	7	26,33,33	0.66	0	31,52,52	0.93	2 (6%)
8	PEG	B	304	-	6,6,6	0.24	0	5,5,5	0.17	0
6	GOL	A	306	-	5,5,5	1.19	1 (20%)	5,5,5	0.75	0
2	ATP	A	302	7	26,33,33	0.78	0	31,52,52	0.90	1 (3%)
3	ADP	D	304	-	24,29,29	1.09	3 (12%)	29,45,45	1.33	4 (13%)
8	PEG	C	307[A]	-	6,6,6	0.21	0	5,5,5	0.10	0
9	PPV	C	303	-	6,8,8	0.79	0	13,13,13	1.10	1 (7%)
3	ADP	A	303	-	24,29,29	1.14	2 (8%)	29,45,45	1.46	4 (13%)
9	PPV	B	305	-	6,8,8	0.59	0	13,13,13	1.15	1 (7%)
5	7TT	A	305	-	10,16,16	1.86	2 (20%)	17,27,27	1.10	3 (17%)
2	ATP	D	302	7	26,33,33	0.72	0	31,52,52	0.98	2 (6%)
8	PEG	D	305[A]	-	6,6,6	0.16	0	5,5,5	0.06	0
6	GOL	D	306	-	5,5,5	0.86	0	5,5,5	1.27	1 (20%)
2	ATP	C	302	7	26,33,33	0.62	0	31,52,52	0.94	0
2	ATP	B	302	7	26,33,33	0.76	0	31,52,52	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PEG	D	307[B]	-	6,6,6	0.21	0	5,5,5	0.12	0
6	GOL	D	303	-	5,5,5	1.11	0	5,5,5	1.10	1 (20%)
8	PEG	C	307[B]	-	6,6,6	0.14	0	5,5,5	0.17	0
10	PO4	D	308	-	4,4,4	0.71	0	6,6,6	0.83	0
2	ATP	D	301	7	26,33,33	0.72	0	31,52,52	1.00	2 (6%)
9	PPV	C	304	-	6,8,8	0.73	0	13,13,13	1.29	1 (7%)

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	3PO	A	304	-	-	0/12/12/12	-
2	ATP	C	301	7	-	2/18/38/38	0/3/3/3
8	PEG	C	305	-	-	2/4/4/4	-
2	ATP	A	301	7	-	5/18/38/38	0/3/3/3
8	PEG	D	307[A]	-	-	2/4/4/4	-
6	GOL	C	306	-	-	4/4/4/4	-
6	GOL	B	306	-	-	0/4/4/4	-
6	GOL	B	303	-	-	2/4/4/4	-
8	PEG	D	305[B]	-	-	2/4/4/4	-
2	ATP	B	301	7	-	5/18/38/38	0/3/3/3
8	PEG	B	304	-	-	2/4/4/4	-
6	GOL	A	306	-	-	0/4/4/4	-
2	ATP	A	302	7	-	8/18/38/38	0/3/3/3
3	ADP	D	304	-	-	1/12/32/32	0/3/3/3
8	PEG	C	307[A]	-	-	2/4/4/4	-
9	PPV	C	303	-	-	1/6/6/6	-
3	ADP	A	303	-	-	2/12/32/32	0/3/3/3
9	PPV	B	305	-	-	3/6/6/6	-
5	7TT	A	305	-	-	1/18/18/18	-
2	ATP	D	302	7	-	6/18/38/38	0/3/3/3
8	PEG	D	305[A]	-	-	1/4/4/4	-
6	GOL	D	306	-	-	4/4/4/4	-
2	ATP	C	302	7	-	4/18/38/38	0/3/3/3
2	ATP	B	302	7	-	8/18/38/38	0/3/3/3
8	PEG	D	307[B]	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	303	-	-	0/4/4/4	-
8	PEG	C	307[B]	-	-	3/4/4/4	-
2	ATP	D	301	7	-	5/18/38/38	0/3/3/3
9	PPV	C	304	-	-	3/6/6/6	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	305	7TT	P14-O16	4.52	1.65	1.50
6	C	306	GOL	O2-C2	-3.30	1.33	1.43
5	A	305	7TT	P05-O04	3.18	1.60	1.50
3	D	304	ADP	C5-C4	2.91	1.48	1.40
3	A	303	ADP	C5-C4	2.83	1.48	1.40

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	ADP	N3-C2-N1	-4.00	122.42	128.68
4	A	304	3PO	PB-O3B-PG	-3.51	120.77	132.83
3	A	303	ADP	C2-N1-C6	3.27	124.35	118.75
3	D	304	ADP	N3-C2-N1	-3.09	123.84	128.68
4	A	304	3PO	PB-O3A-PA	-2.89	122.92	132.83

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	ATP	C5'-O5'-PA-O2A
2	B	302	ATP	PB-O3B-PG-O3G
2	B	302	ATP	C5'-O5'-PA-O2A
2	C	302	ATP	PB-O3B-PG-O2G
2	C	302	ATP	PB-O3B-PG-O3G

There are no ring outliers.

8 monomers are involved in 15 short contacts:

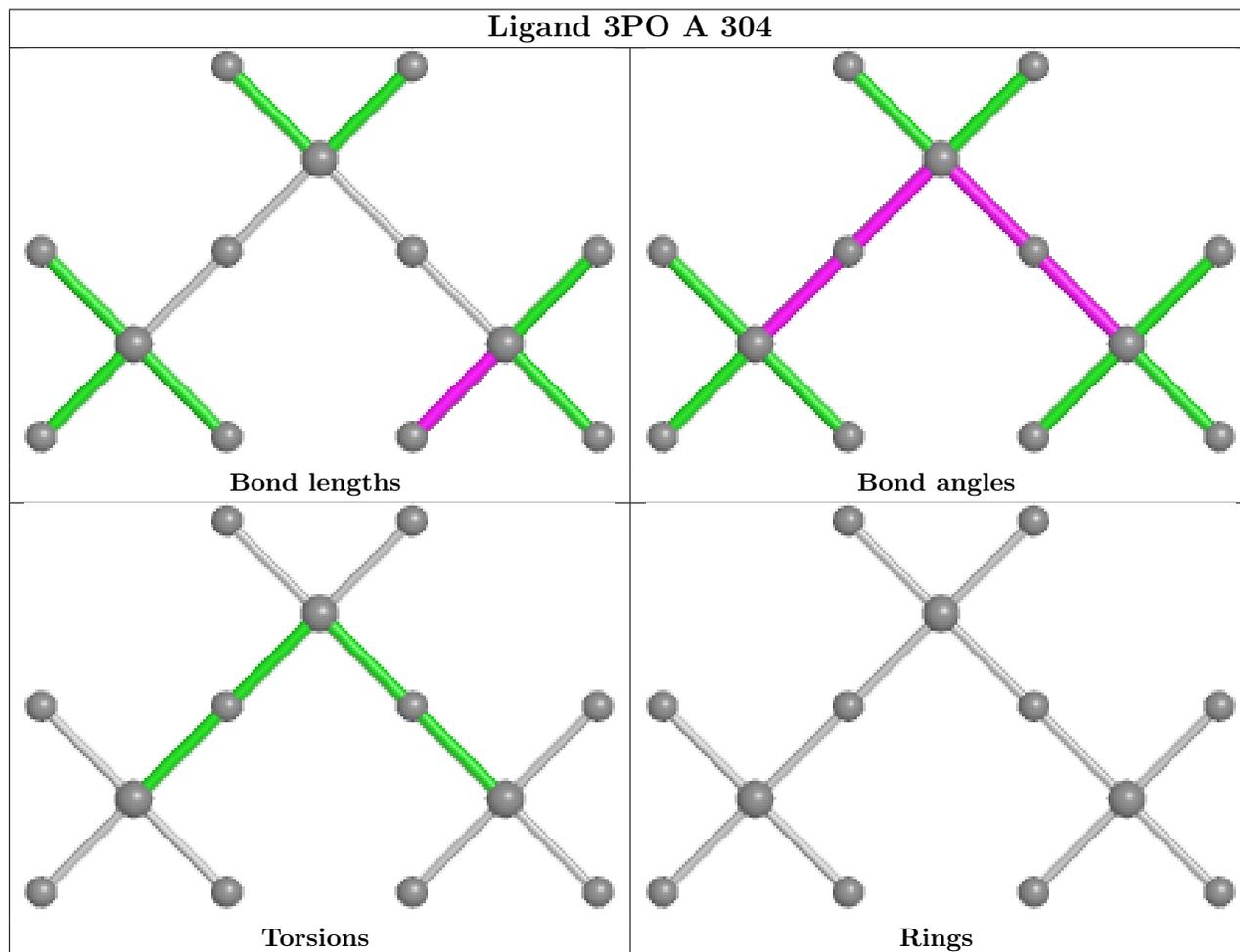
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	307[A]	PEG	2	0
6	C	306	GOL	1	0
6	B	303	GOL	5	0

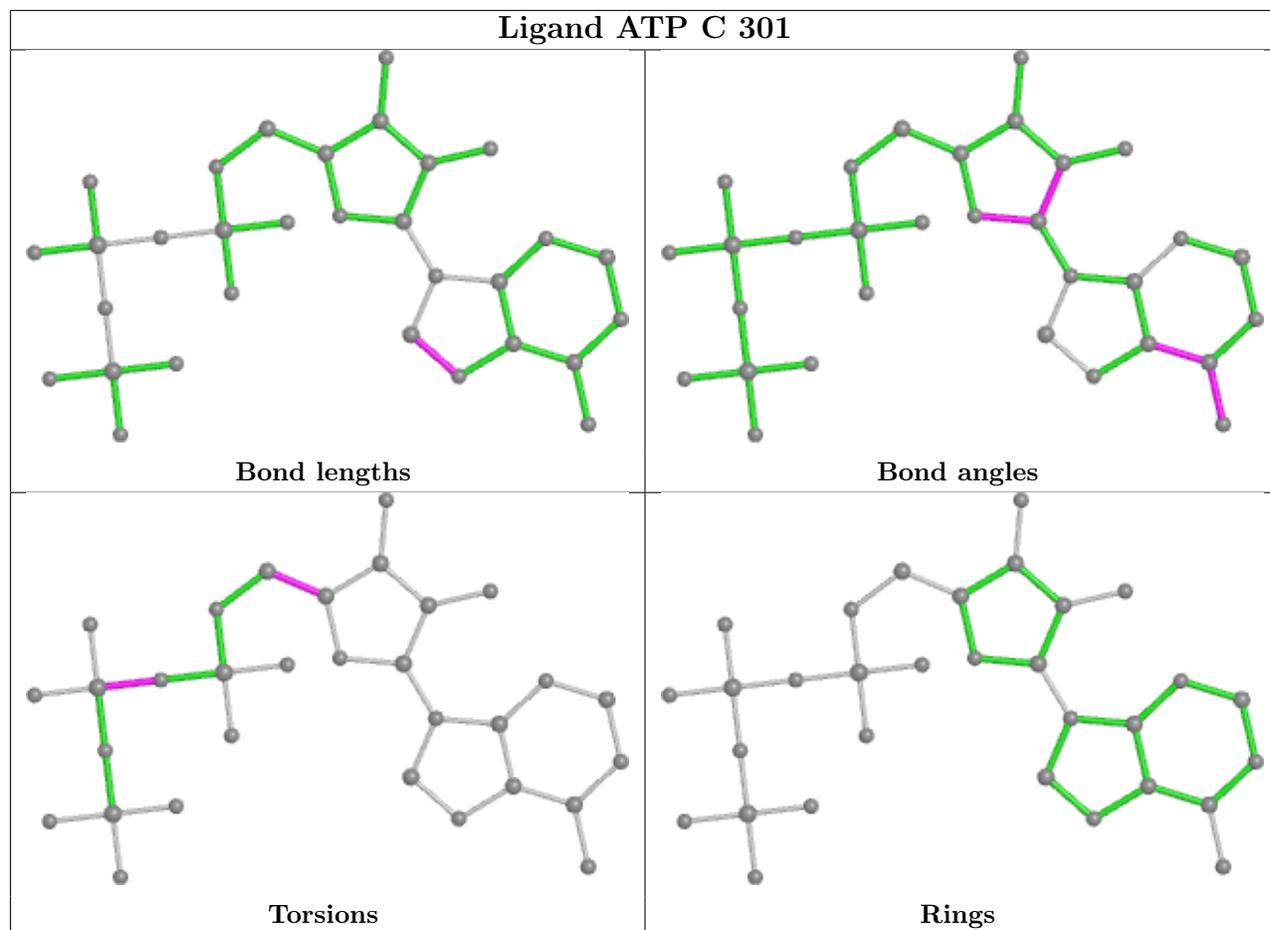
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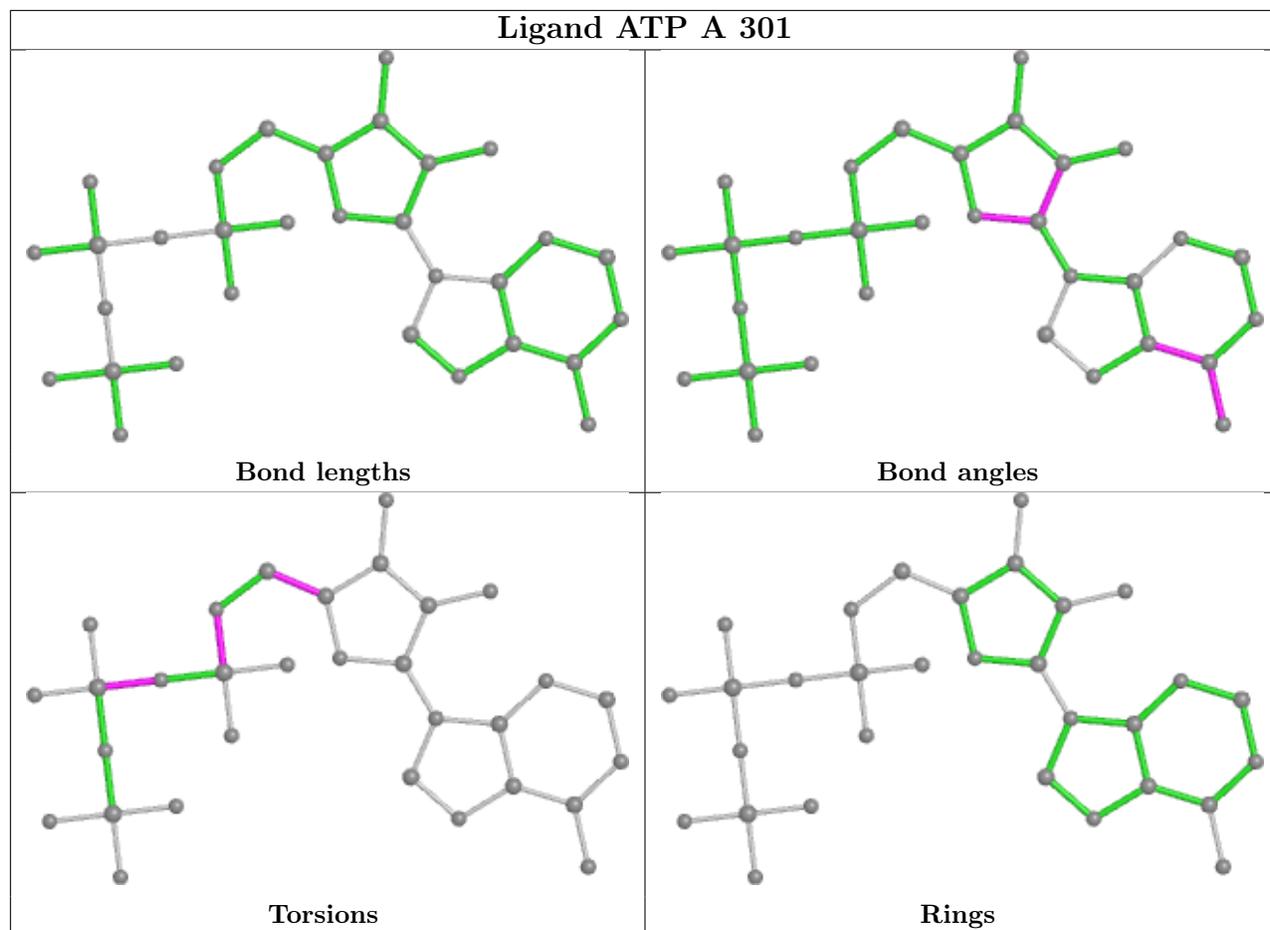
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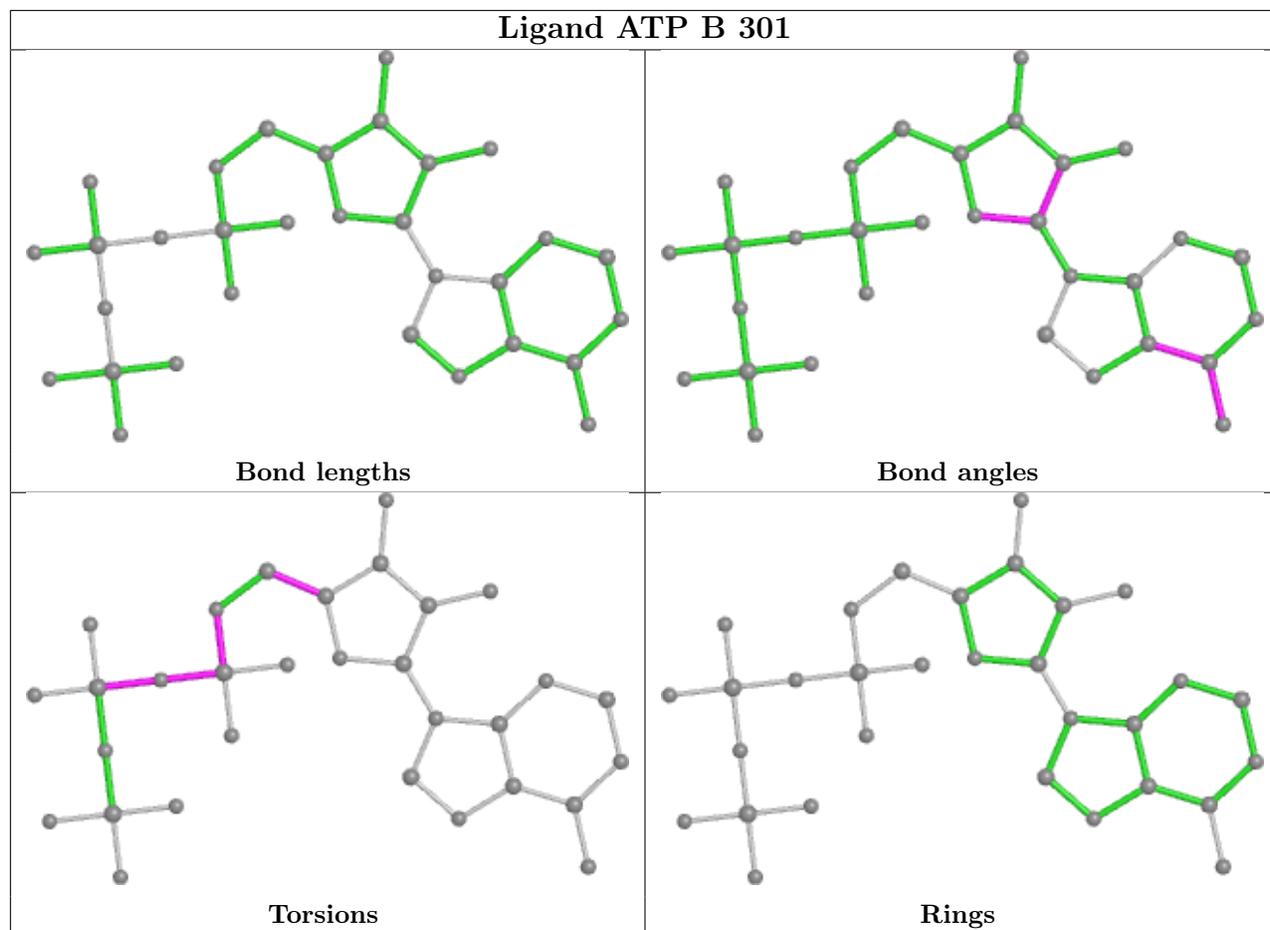
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	306	GOL	1	0
8	C	307[A]	PEG	2	0
9	C	303	PPV	1	0
5	A	305	7TT	1	0
8	C	307[B]	PEG	2	0

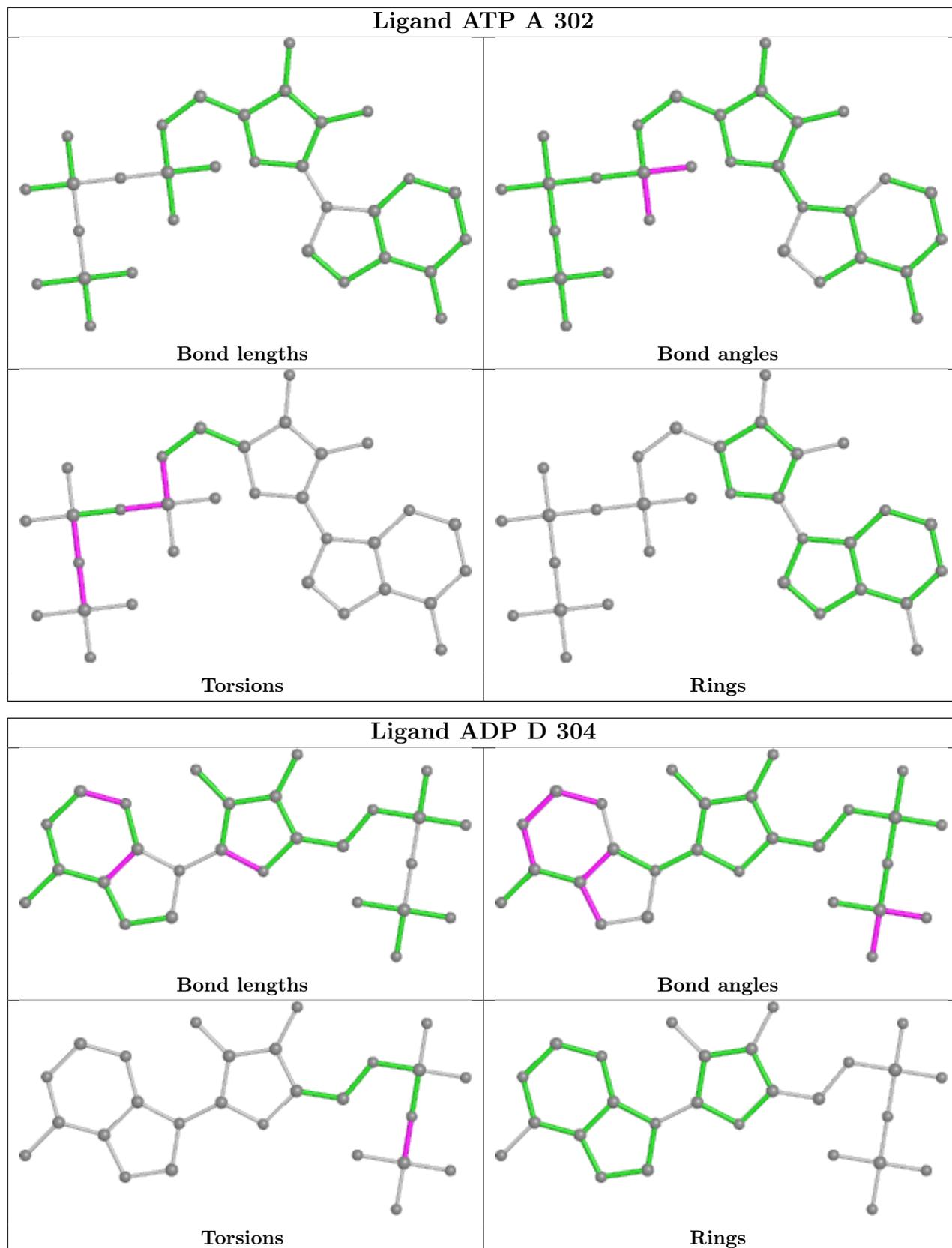
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

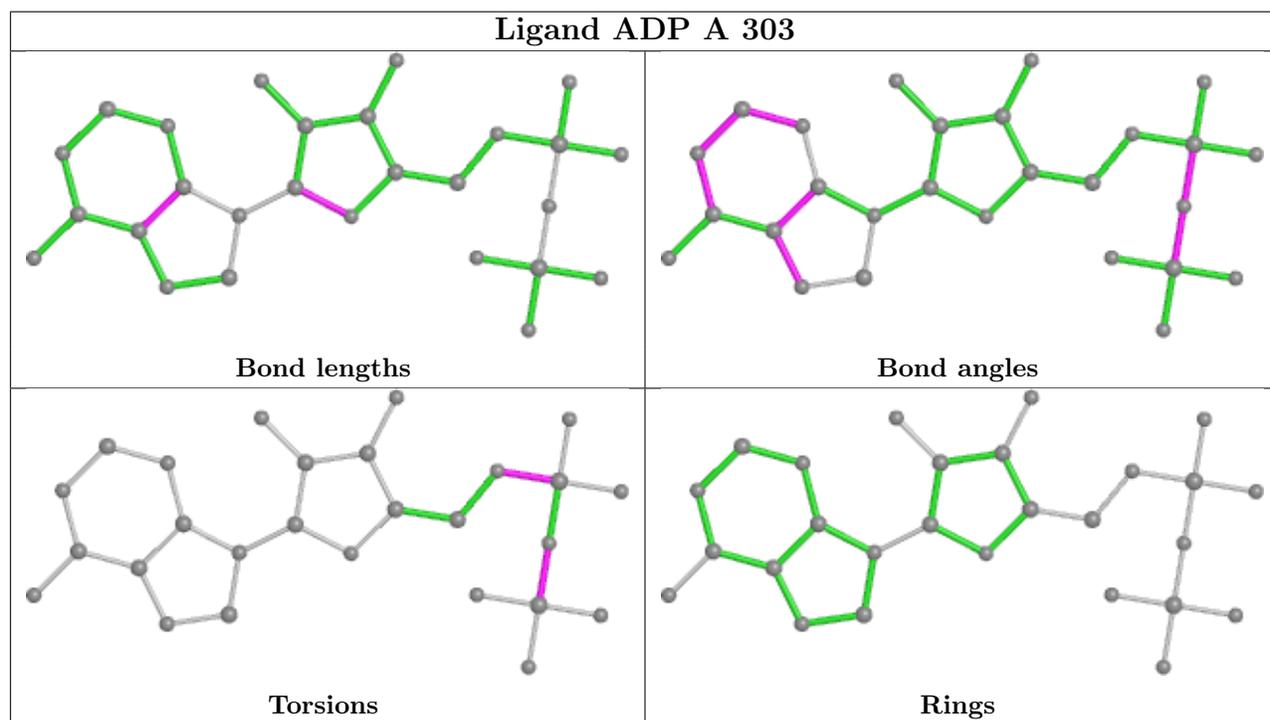
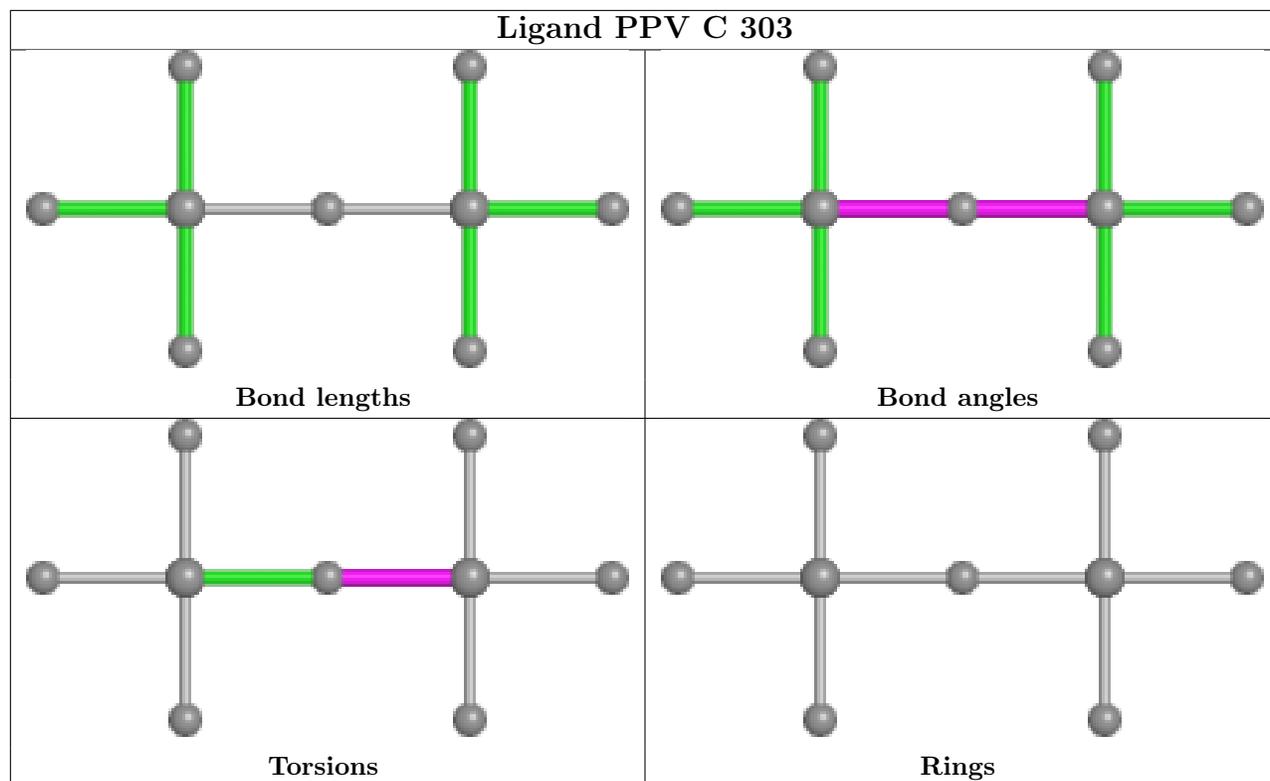


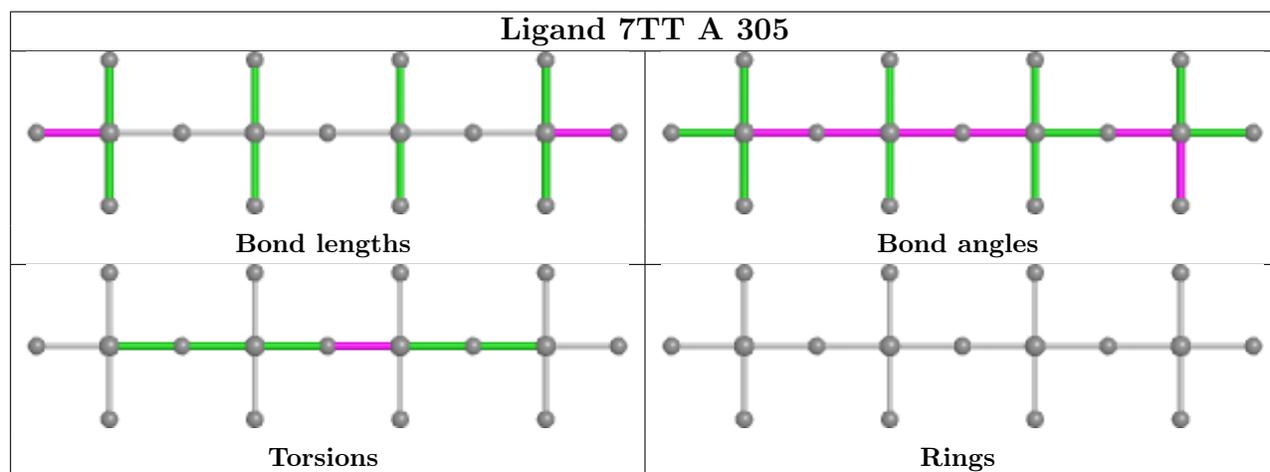
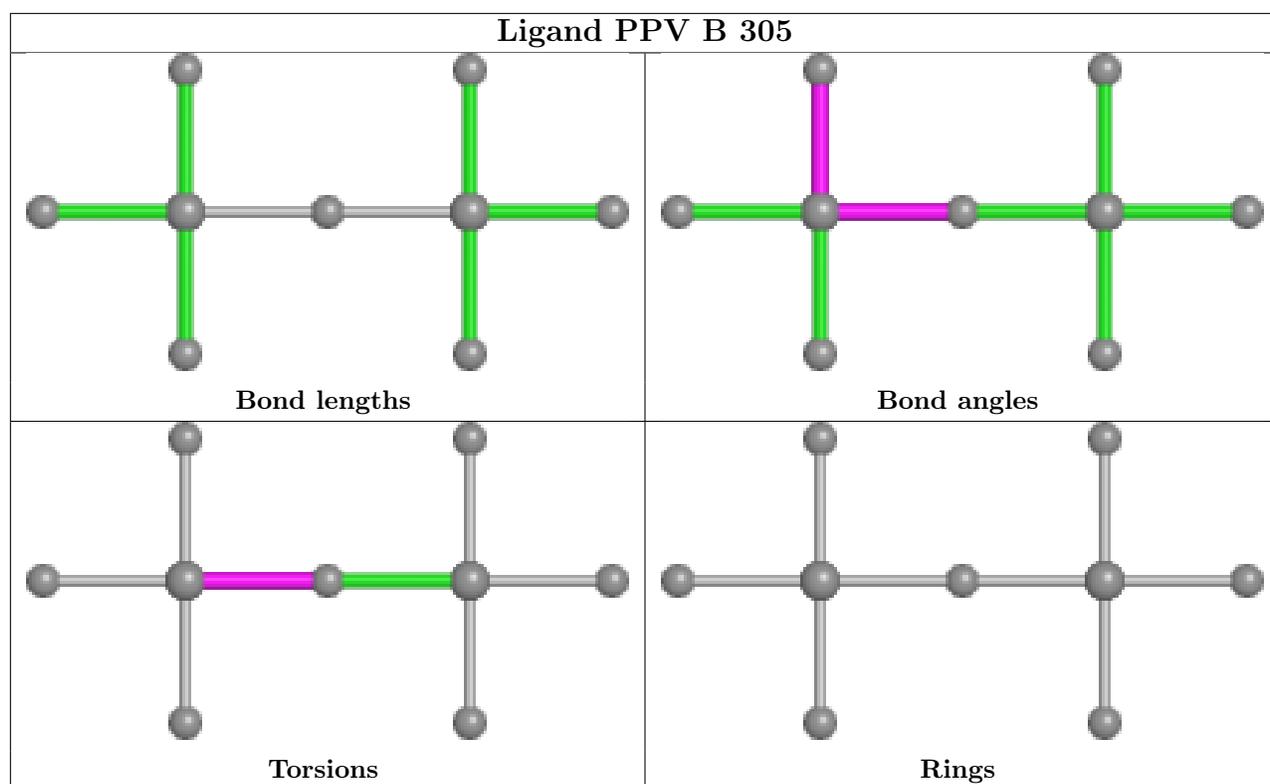


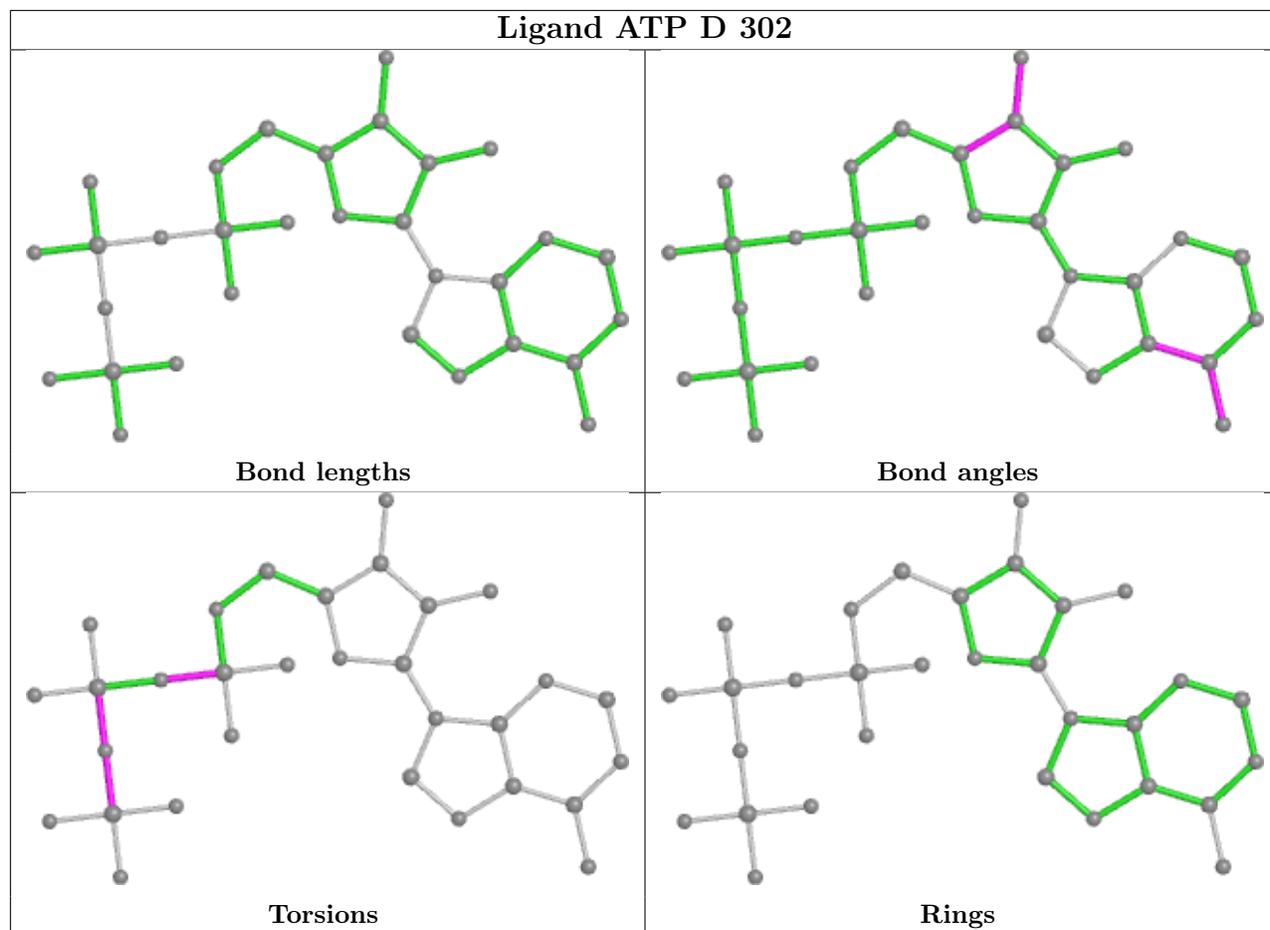


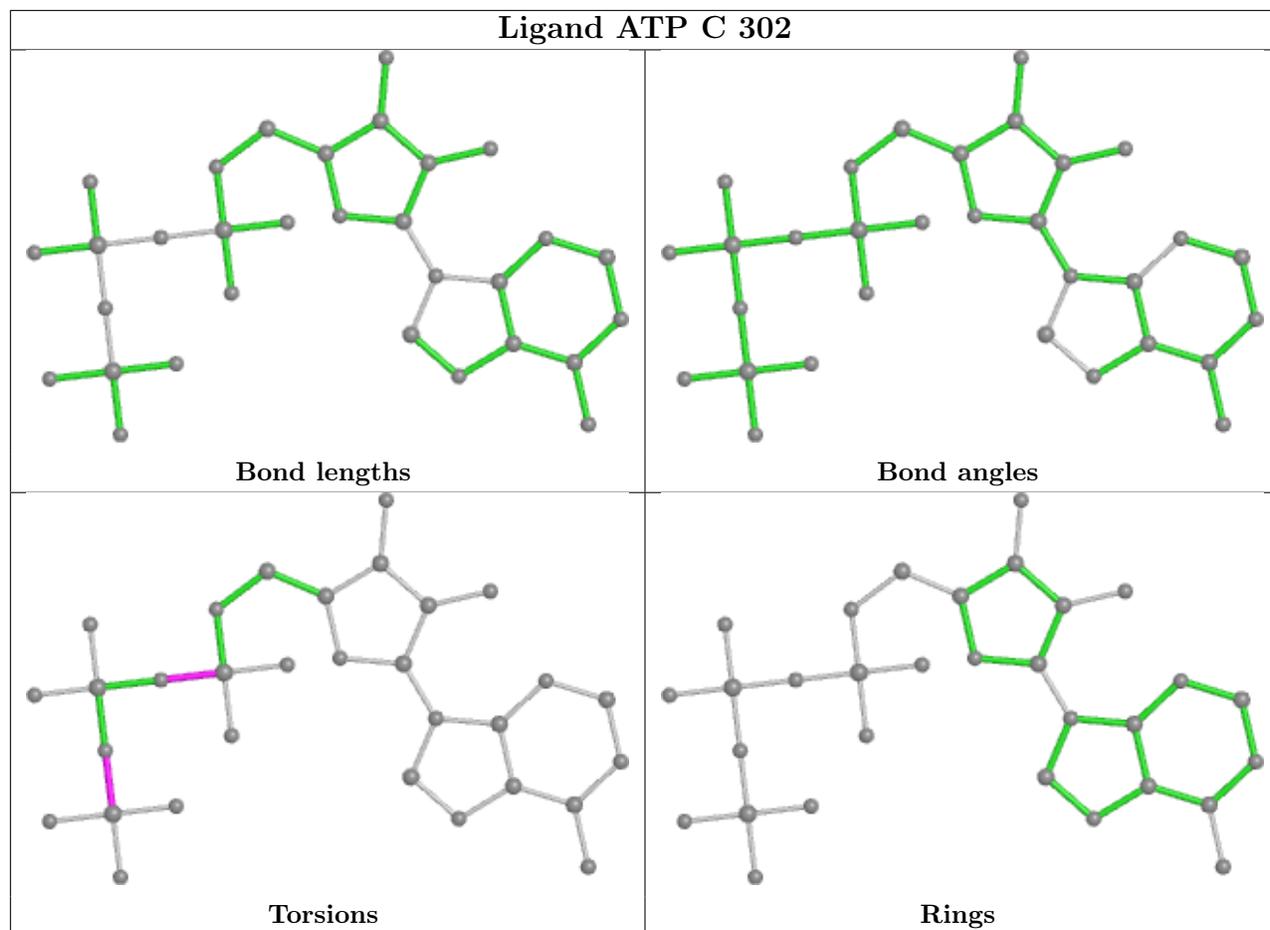


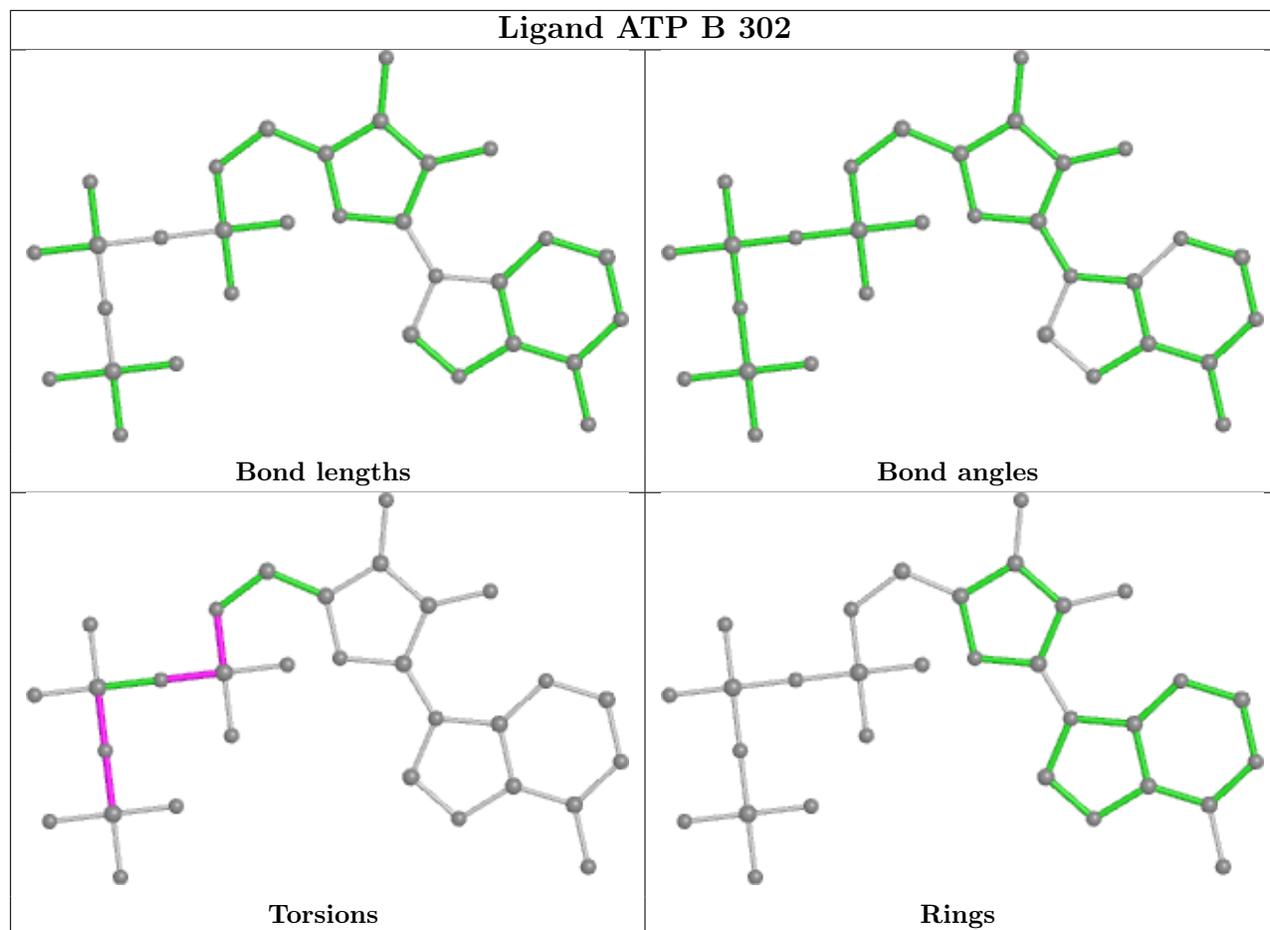


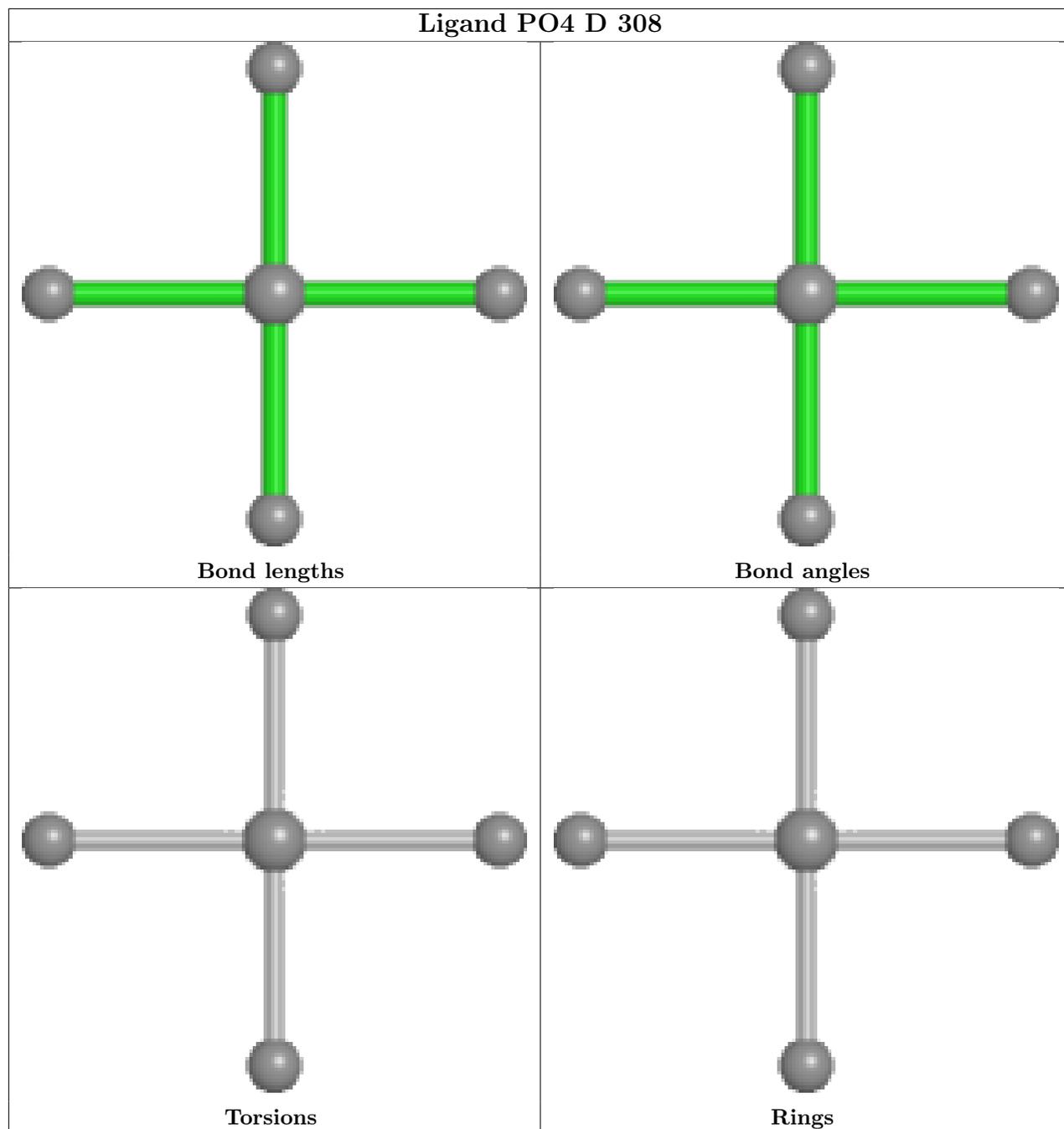


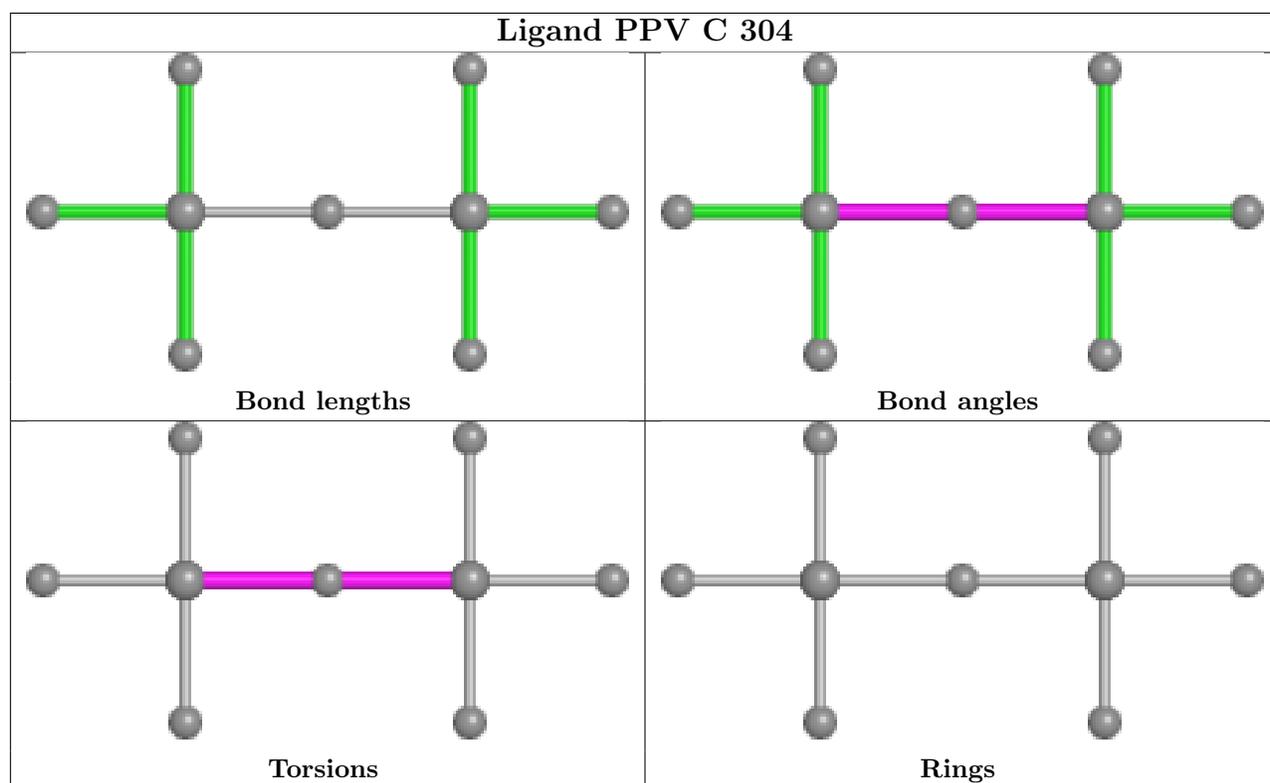
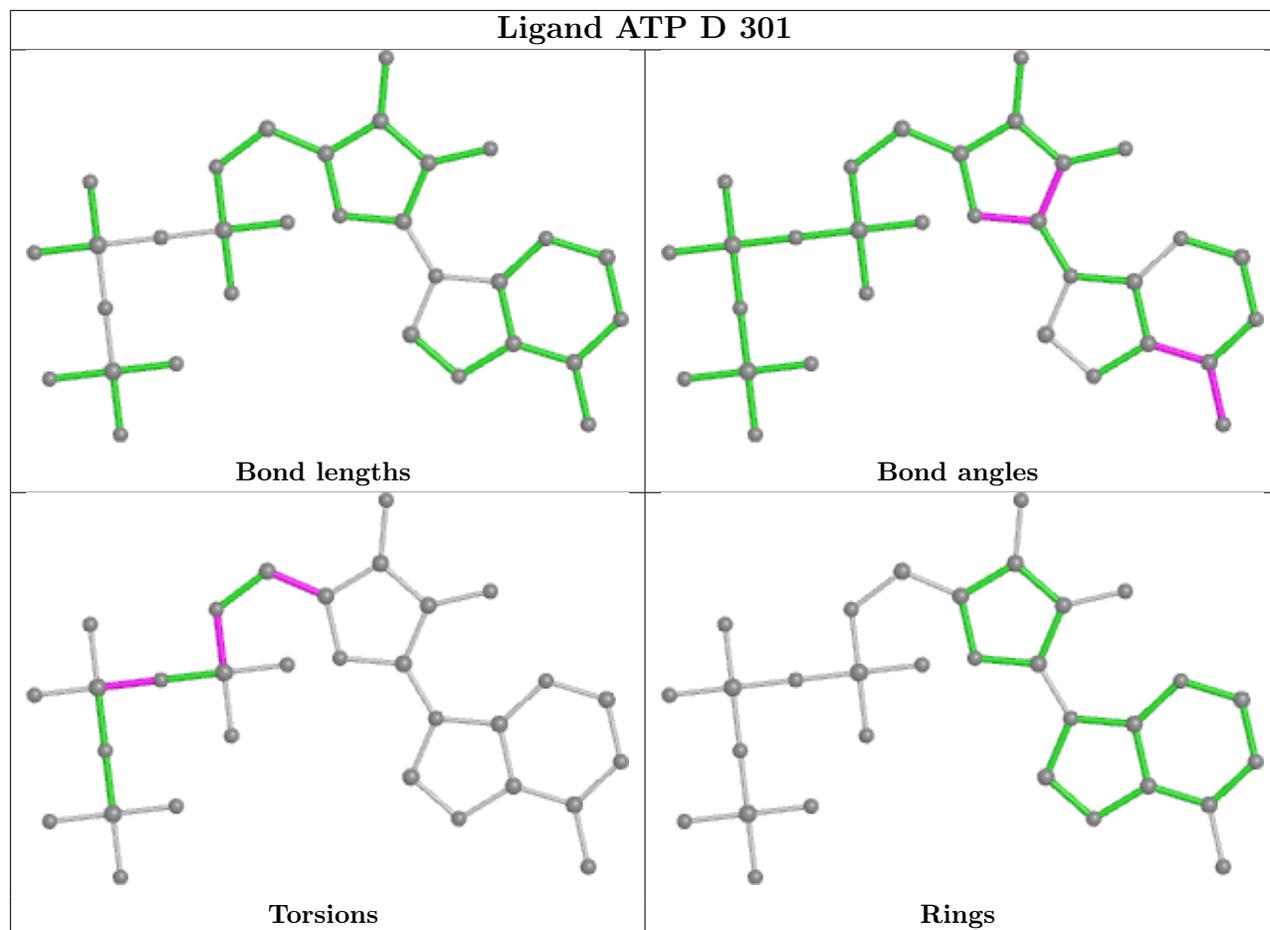












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	266/266 (100%)	-0.40	4 (1%) 73 74	11, 18, 36, 67	2 (0%)
1	B	266/266 (100%)	-0.40	3 (1%) 80 81	11, 19, 36, 65	3 (1%)
1	C	266/266 (100%)	-0.41	2 (0%) 86 87	11, 19, 35, 85	4 (1%)
1	D	266/266 (100%)	-0.44	1 (0%) 92 92	10, 18, 31, 49	3 (1%)
All	All	1064/1064 (100%)	-0.41	10 (0%) 84 85	10, 18, 35, 85	12 (1%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	ASP	5.1
1	B	194	PRO	4.9
1	A	257	ASP	3.7
1	D	194	PRO	3.6
1	A	194	PRO	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 [i](#)

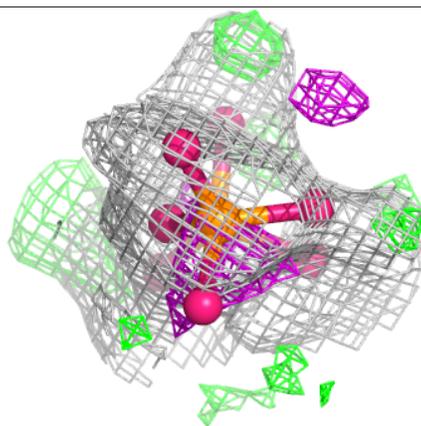
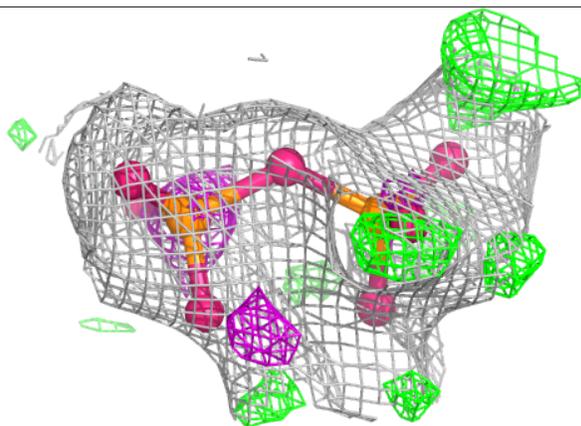
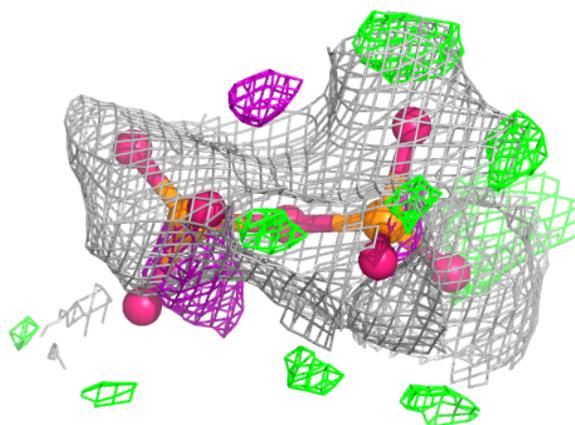
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	PEG	C	305	7/7	0.57	0.18	34,36,38,41	0
8	PEG	D	307[A]	7/7	0.57	0.28	27,28,30,31	7
8	PEG	D	307[B]	7/7	0.57	0.28	28,29,31,33	7
9	PPV	B	305	9/9	0.64	0.27	51,57,70,79	0
8	PEG	D	305[B]	7/7	0.78	0.15	30,32,35,36	7
8	PEG	D	305[A]	7/7	0.78	0.15	31,32,33,35	7
6	GOL	B	306	6/6	0.79	0.10	39,40,43,44	0
6	GOL	D	306	6/6	0.79	0.23	21,29,36,38	2
8	PEG	C	307[B]	7/7	0.83	0.29	27,30,32,33	7
8	PEG	C	307[A]	7/7	0.83	0.29	24,30,32,34	7
8	PEG	B	304	7/7	0.84	0.19	36,40,47,49	0
3	ADP	D	304	27/27	0.86	0.18	25,43,62,72	1
6	GOL	C	306	6/6	0.86	0.25	19,21,28,30	6
3	ADP	A	303	27/27	0.87	0.14	21,33,40,47	2
5	7TT	A	305	17/17	0.88	0.16	18,29,41,42	17
10	PO4	D	308	5/5	0.88	0.11	17,17,27,30	5
9	PPV	C	303	9/9	0.89	0.15	26,29,40,44	7
6	GOL	B	303	6/6	0.93	0.20	19,25,35,40	0
6	GOL	A	306	6/6	0.94	0.11	14,18,20,24	2
4	3PO	A	304	13/13	0.94	0.10	17,24,32,34	4
6	GOL	D	303	6/6	0.94	0.14	15,27,29,31	0
9	PPV	C	304	9/9	0.95	0.17	26,39,44,49	1
2	ATP	C	302	31/31	0.98	0.07	9,16,20,22	0
2	ATP	D	301	31/31	0.98	0.07	12,15,19,22	0
2	ATP	B	301	31/31	0.98	0.07	14,18,21,25	0
2	ATP	B	302	31/31	0.99	0.07	14,20,25,29	0
2	ATP	C	301	31/31	0.99	0.06	11,14,19,23	0
2	ATP	A	302	31/31	0.99	0.08	10,18,22,24	0
2	ATP	A	301	31/31	0.99	0.06	11,14,18,21	0
2	ATP	D	302	31/31	0.99	0.07	12,20,25,30	0
7	MG	B	307	1/1	0.99	0.04	16,16,16,16	0
7	MG	A	307	1/1	1.00	0.05	12,12,12,12	0
7	MG	C	308	1/1	1.00	0.07	14,14,14,14	0
7	MG	D	309	1/1	1.00	0.05	13,13,13,13	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.

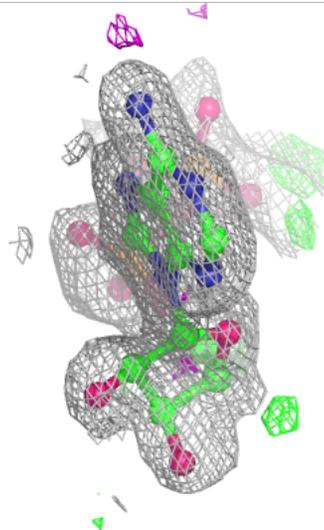
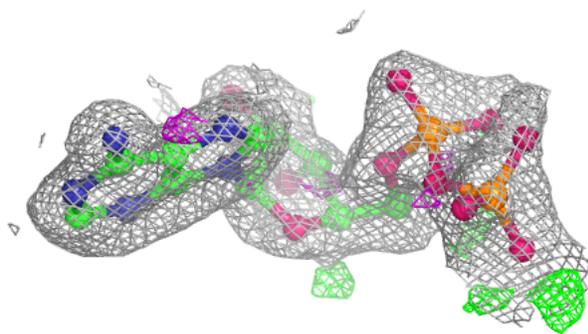
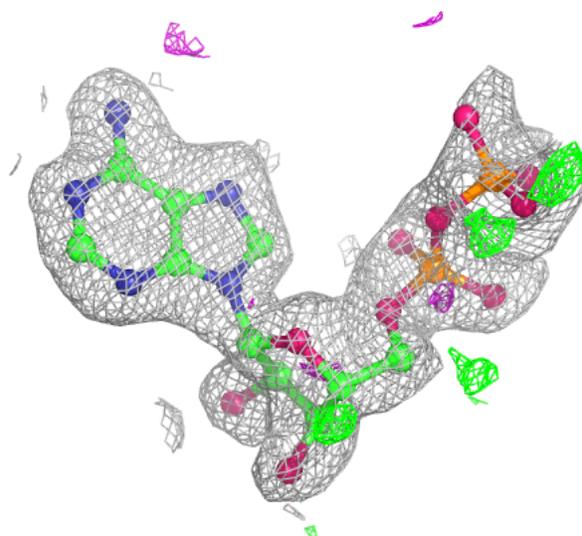
**Electron density around PPV B 305:**

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



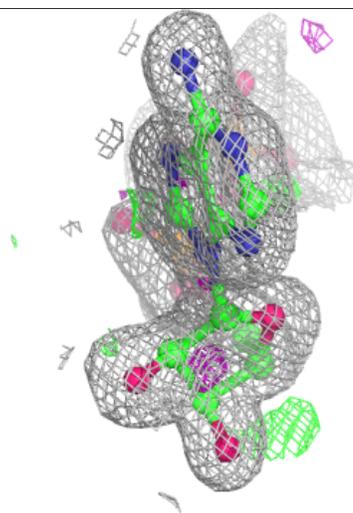
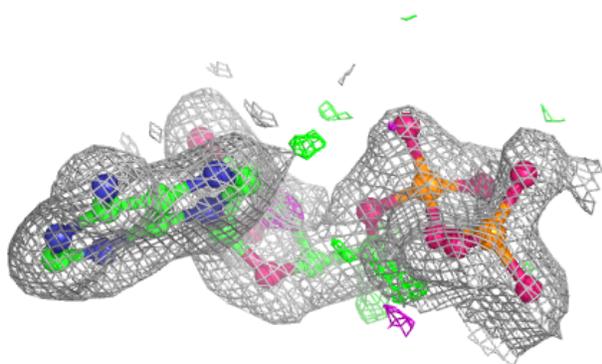
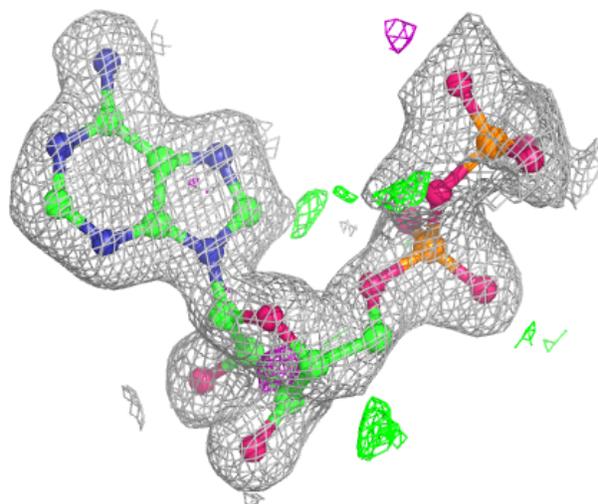
**Electron density around ADP D 304:**

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



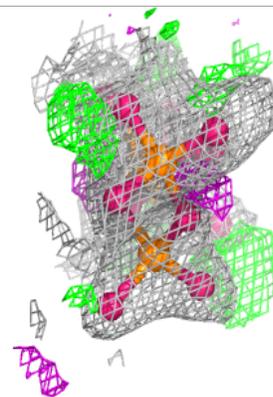
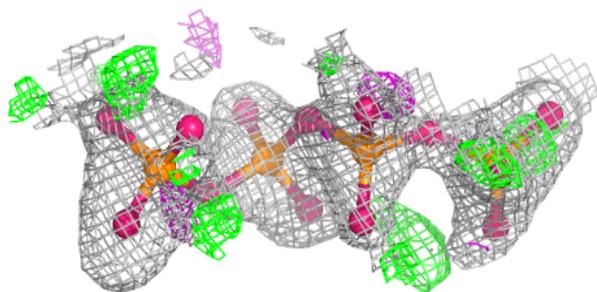
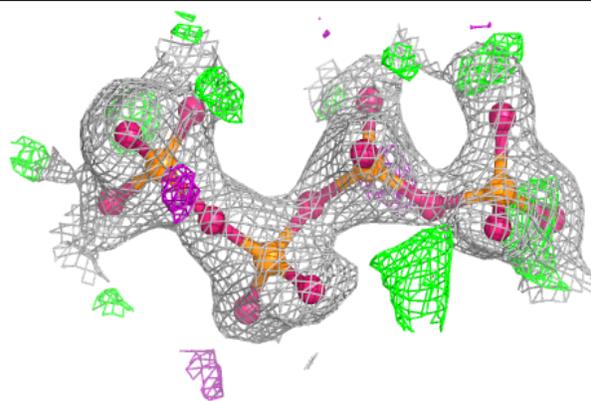
**Electron density around ADP A 303:**

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and green (positive)



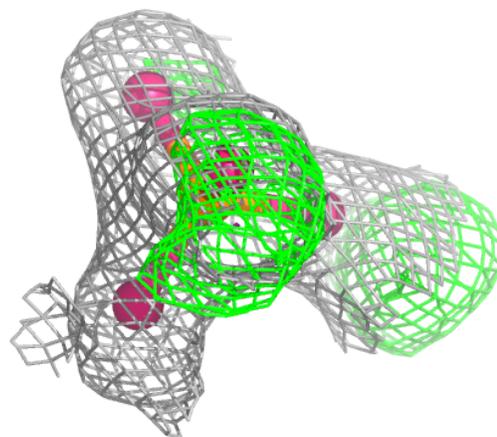
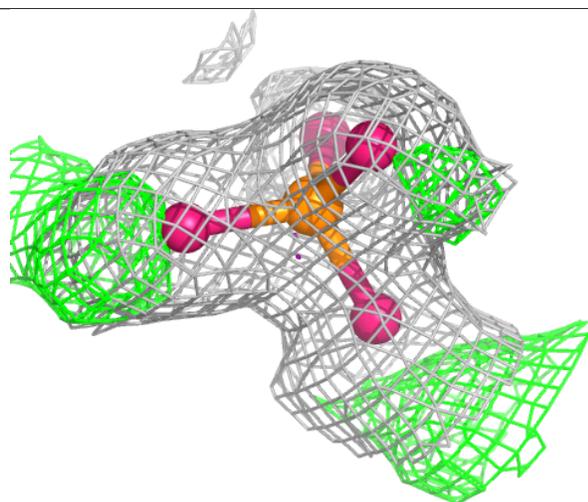
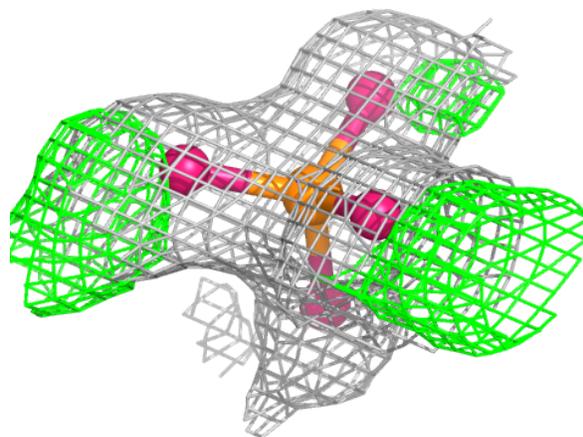
**Electron density around 7TT A 305:**

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and green (positive)



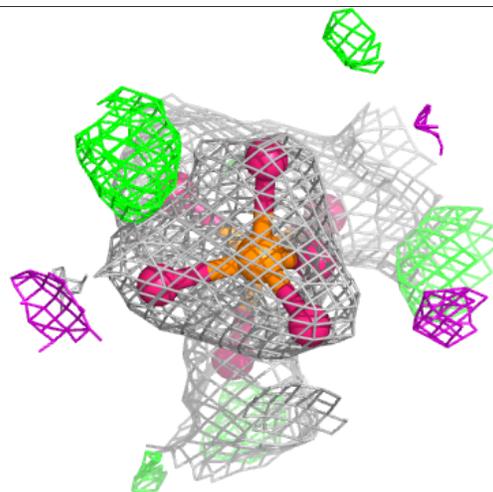
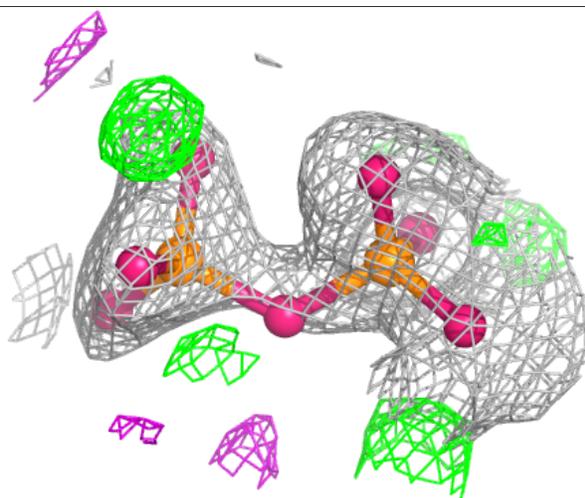
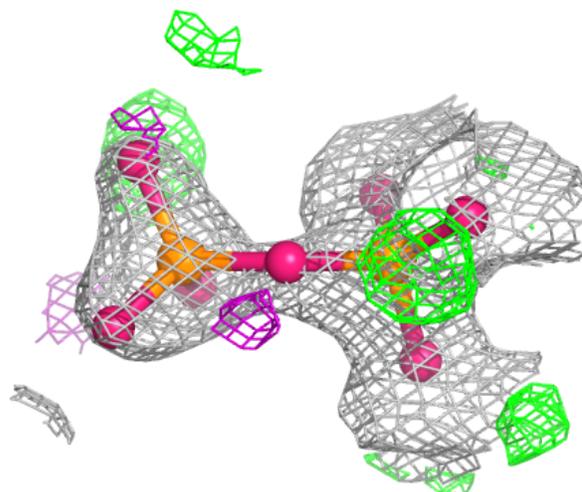
**Electron density around PO4 D 308:**

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



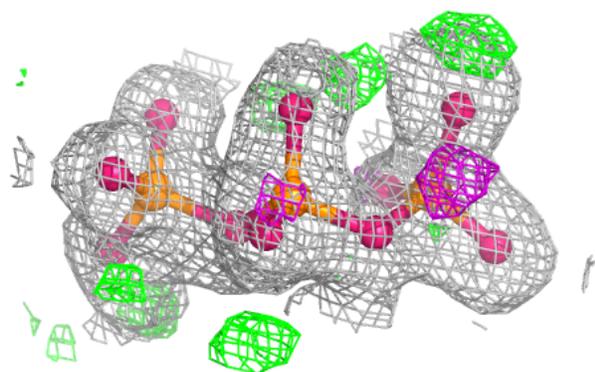
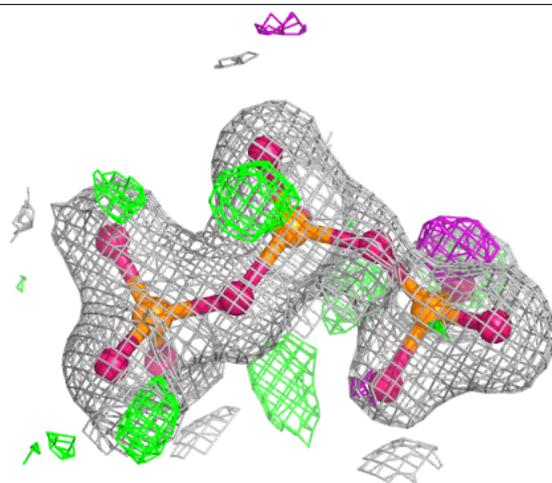
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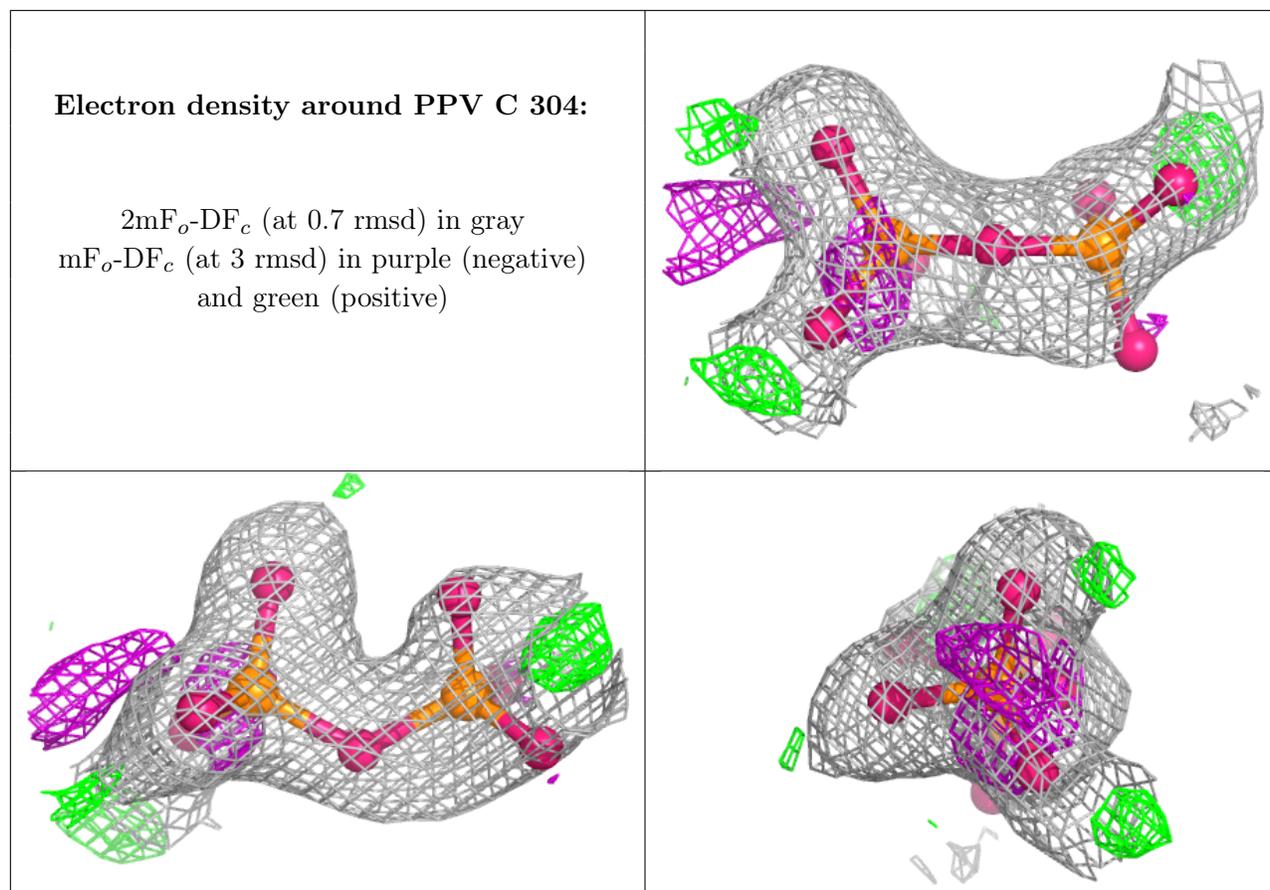
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and green (positive)



**Electron density around 3PO A 304:**

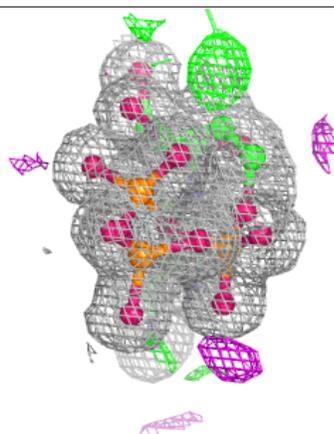
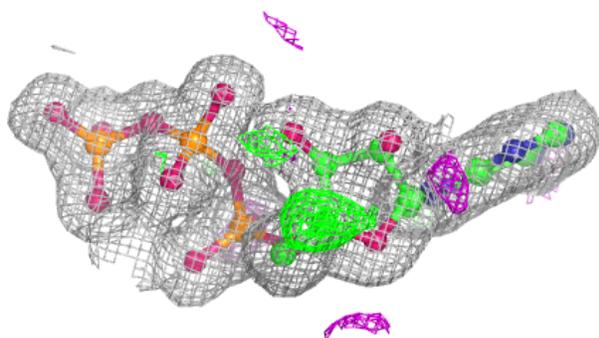
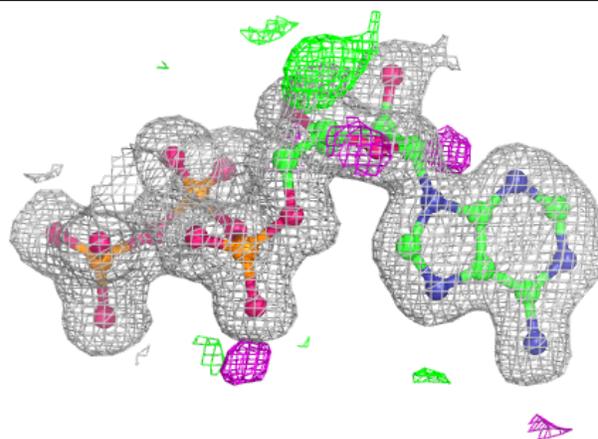
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



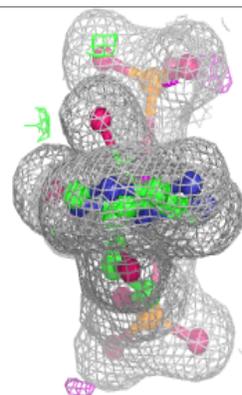
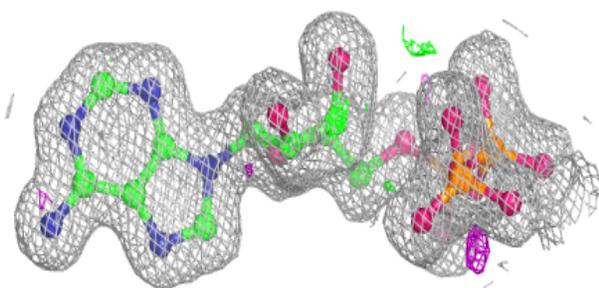
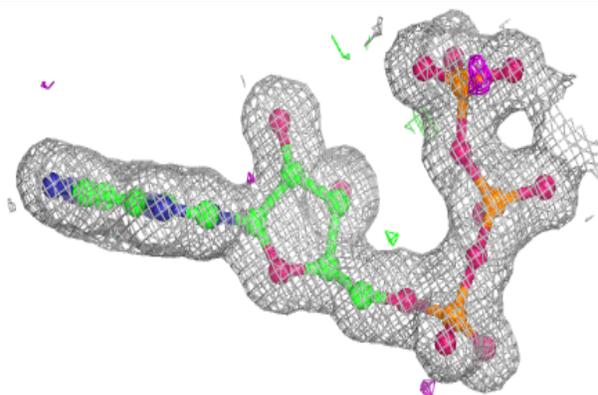


**Electron density around ATP C 302:**

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

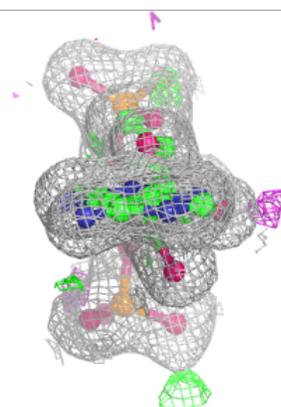
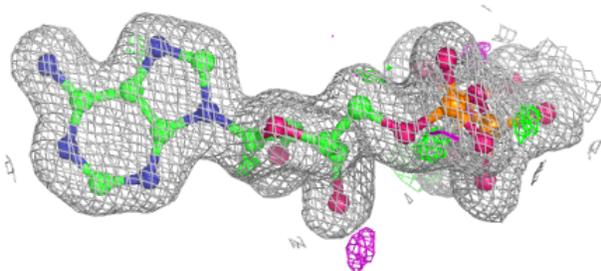
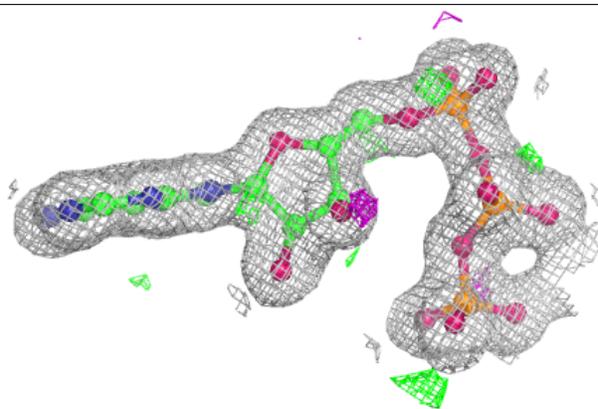
**Electron density around ATP D 301:**

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

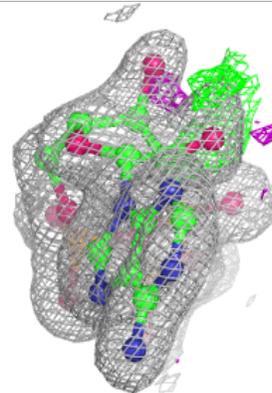
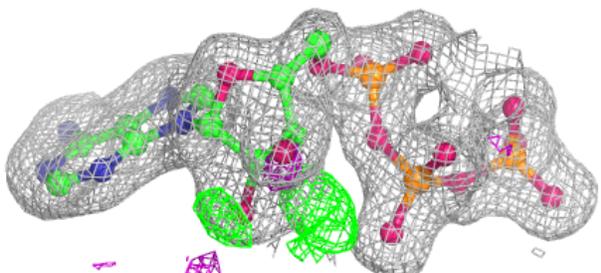
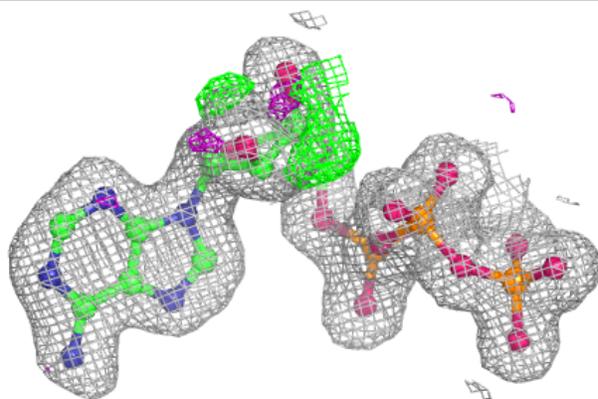


**Electron density around ATP B 301:**

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

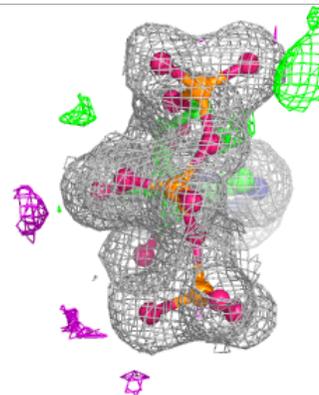
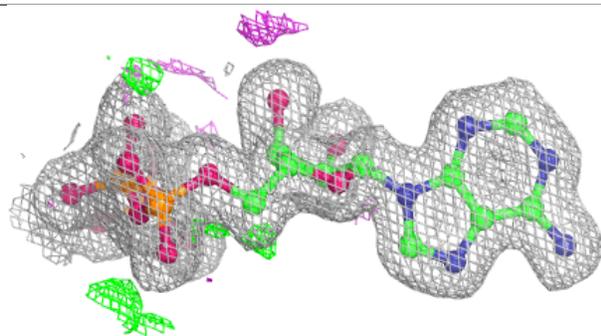
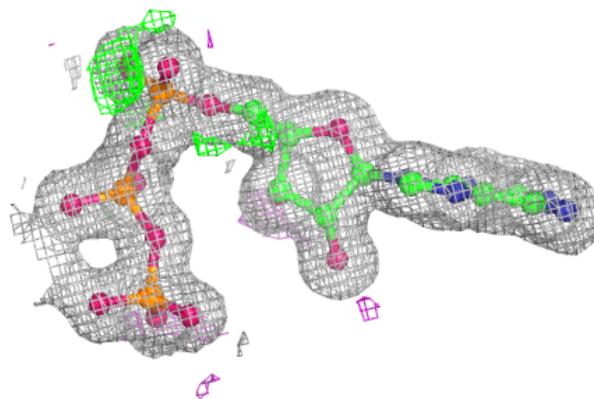
**Electron density around ATP B 302:**

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

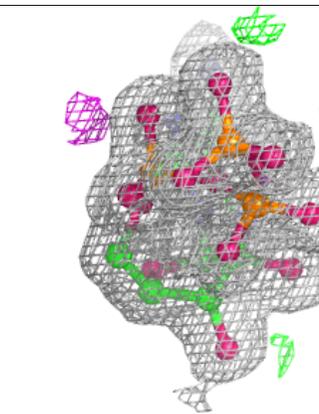
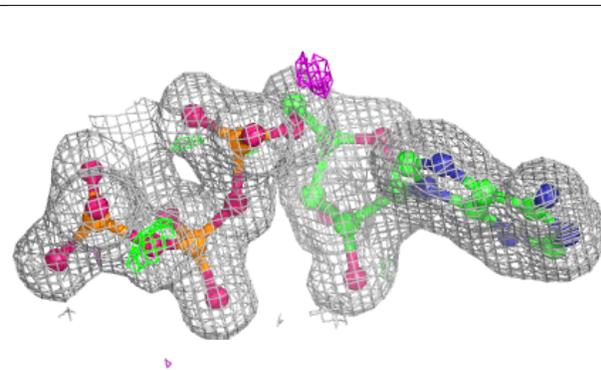
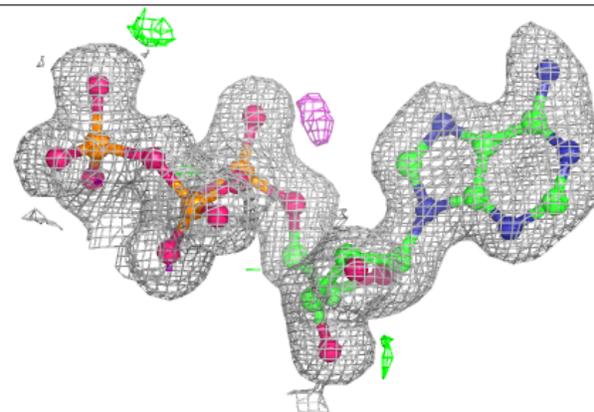


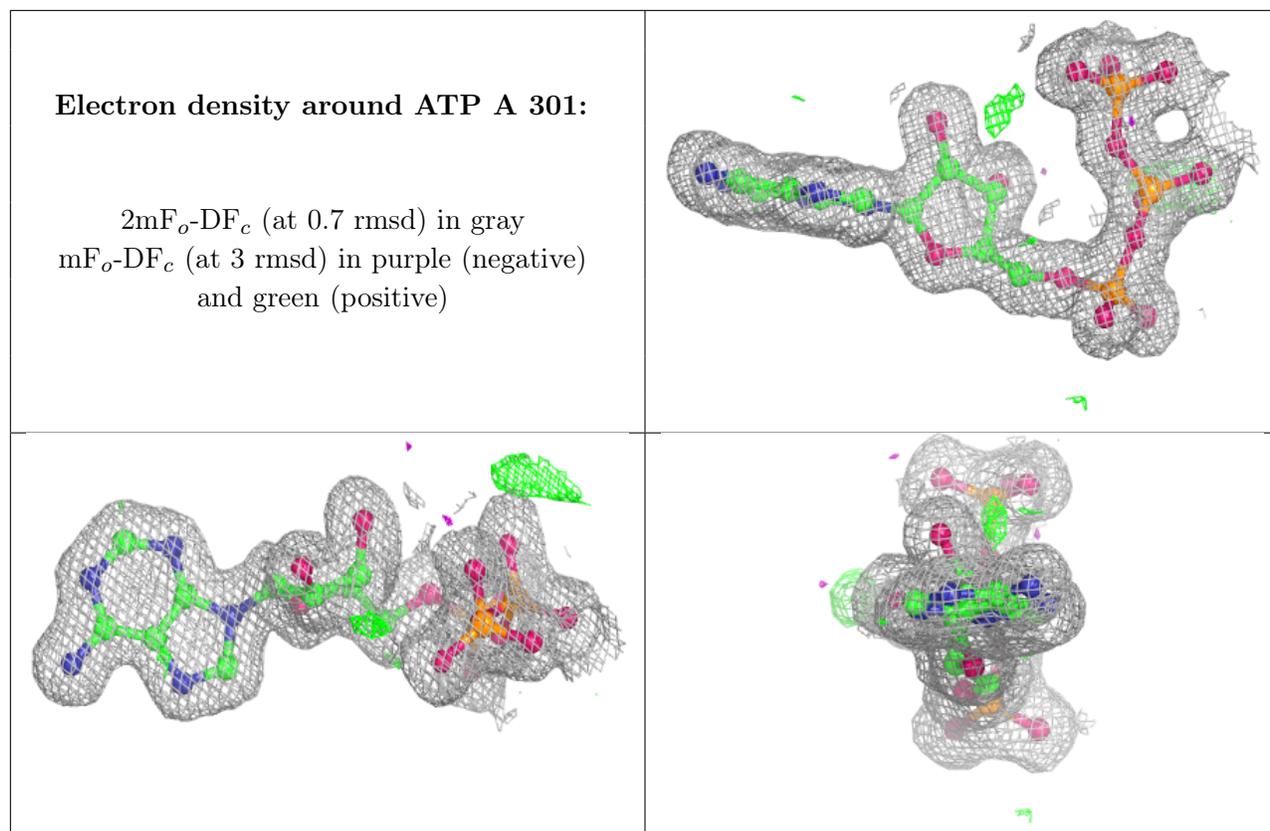
**Electron density around ATP C 301:**

$2mF_o-DF_c$  (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:**

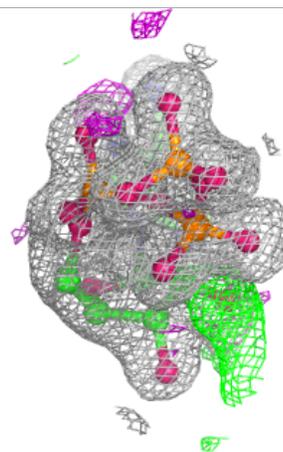
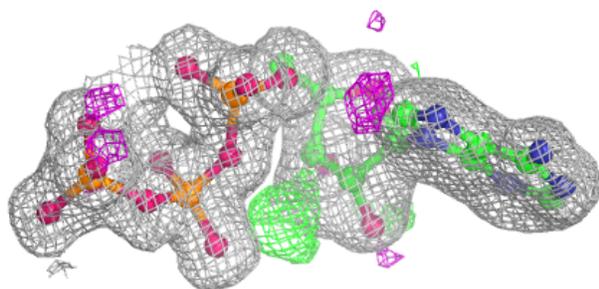
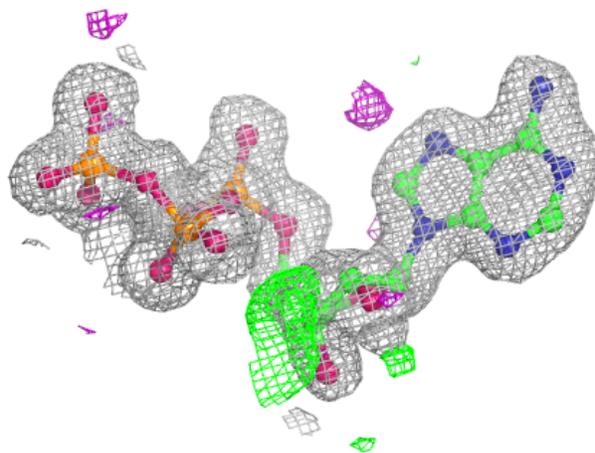
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





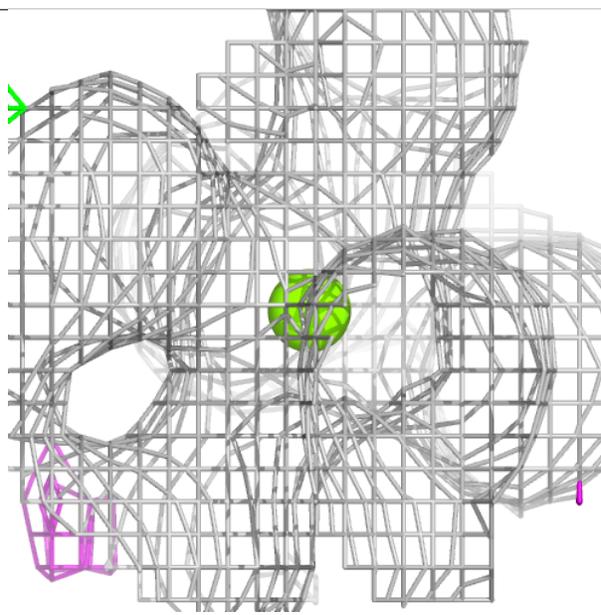
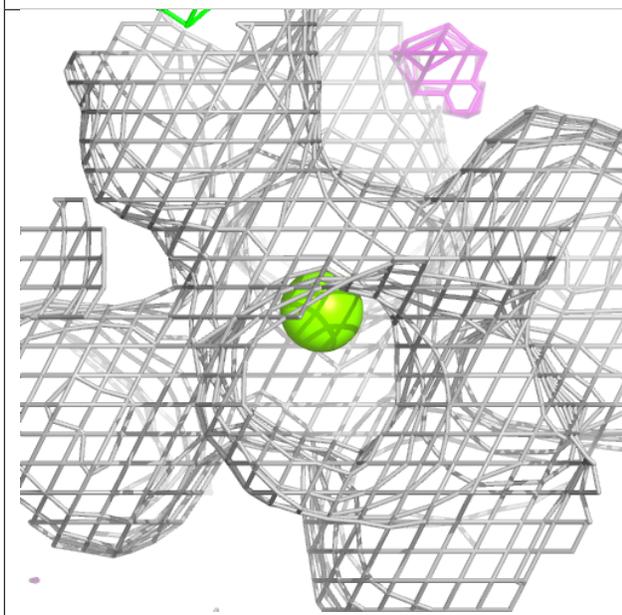
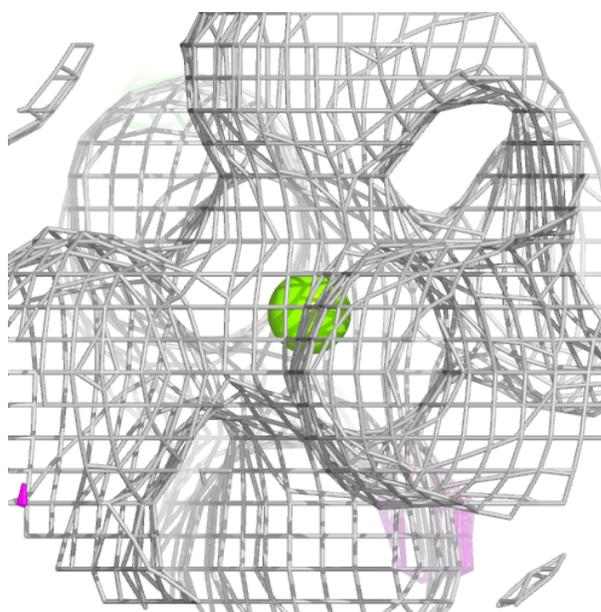
**Electron density around ATP D 302:**

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



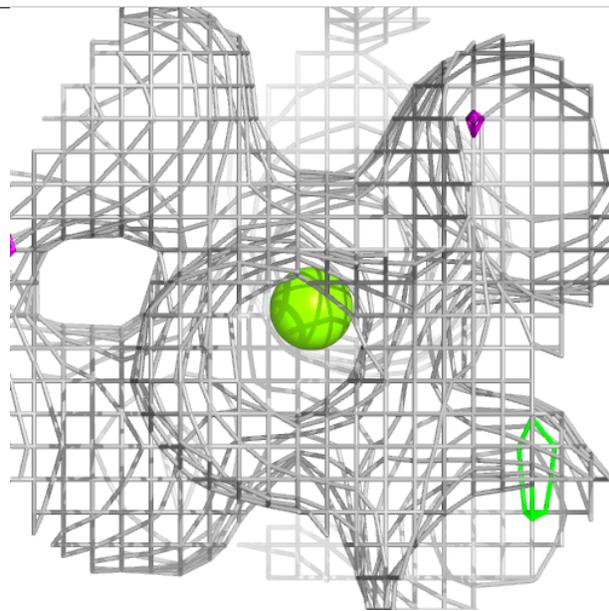
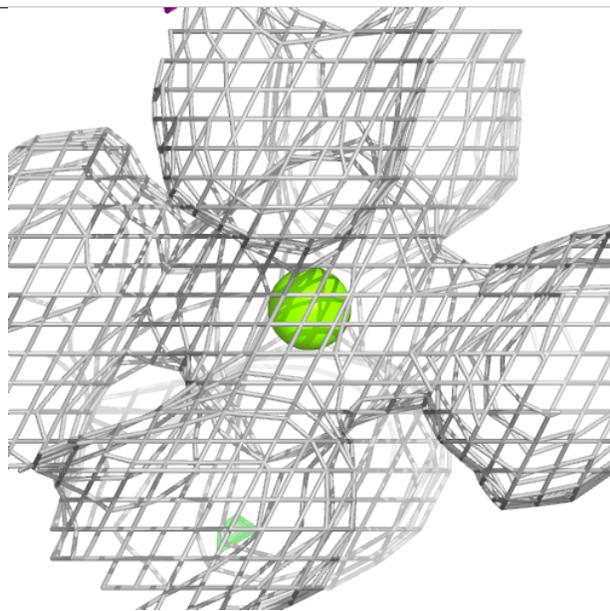
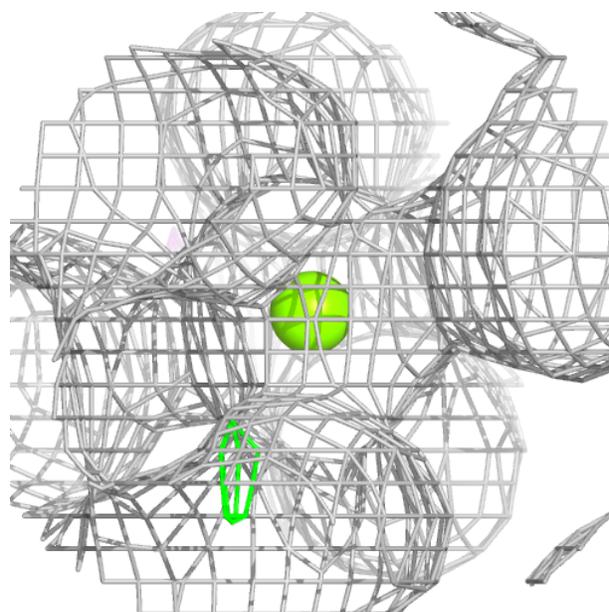
**Electron density around MG B 307:**

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



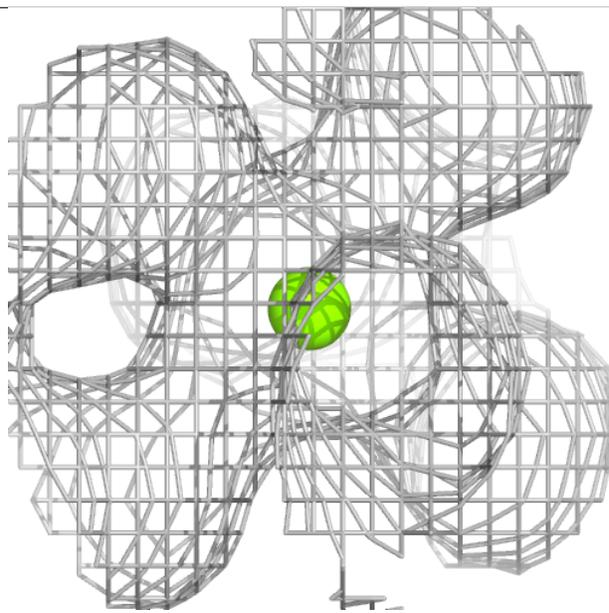
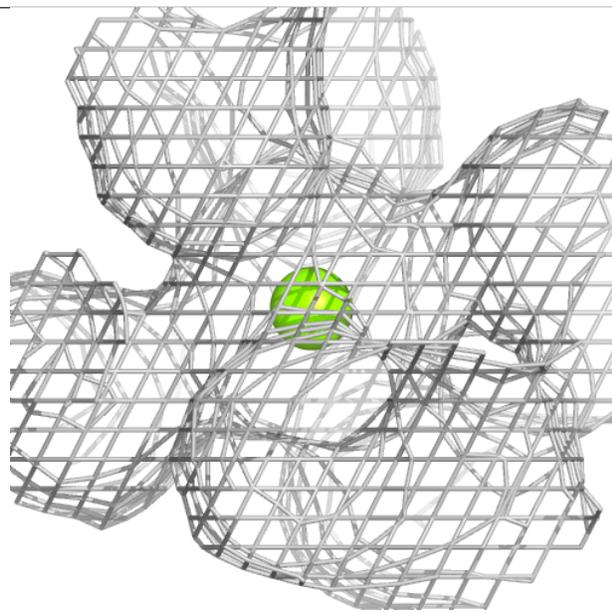
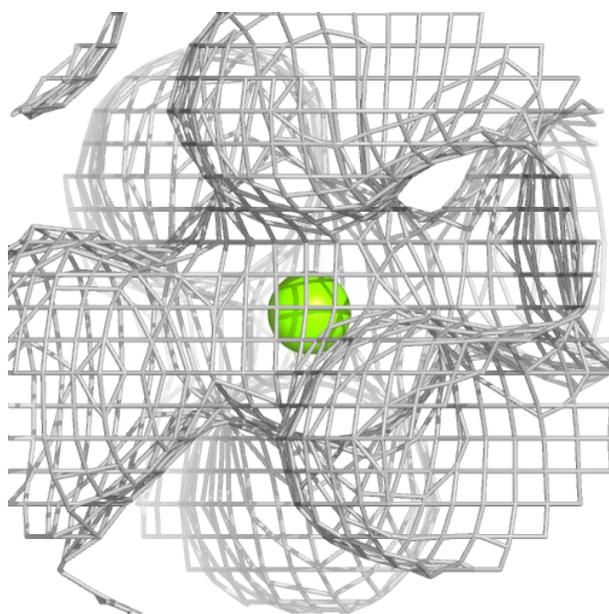
**Electron density around MG A 307:**

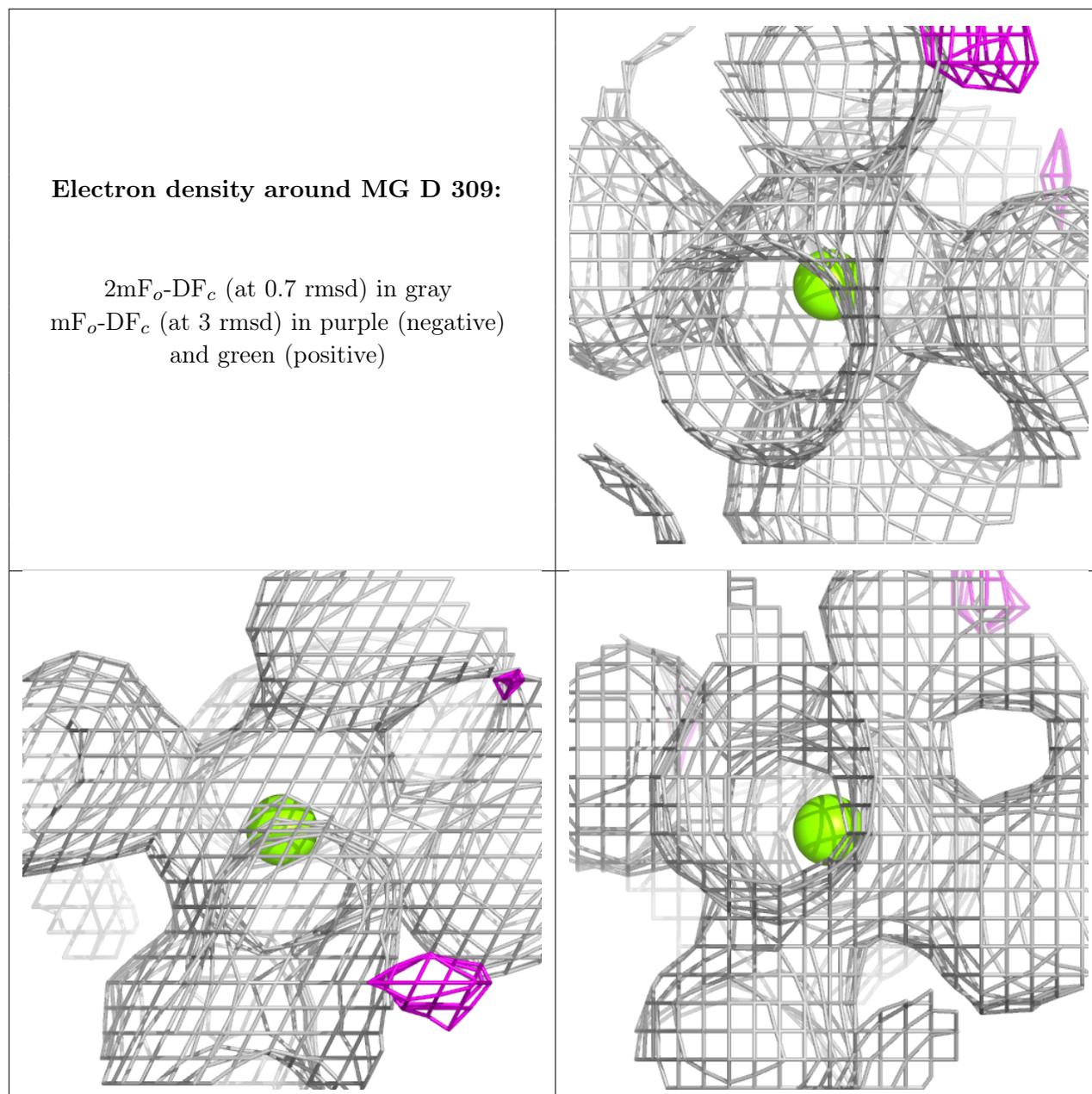
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG C 308:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.