



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2024 – 10:36 AM EDT

PDB ID : 8VHP  
Title : Crystal structure of E. coli class Ia ribonucleotide reductase alpha subunit W28A variant bound to CDP and two molecules of ATP  
Authors : Funk, M.A.; Zimanyi, C.M.; Drennan, C.L.  
Deposited on : 2024-01-02  
Resolution : 2.61 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.3

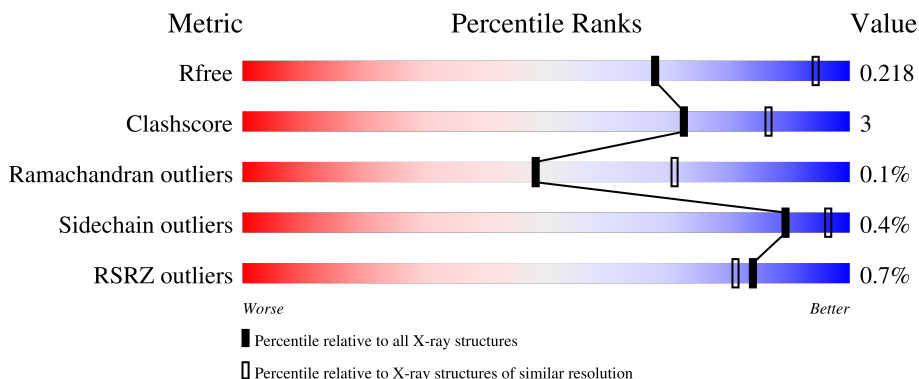
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	779	 86% 7% 6%
1	B	779	 87% 8% 6%
1	C	779	 87% 7% 6%
1	D	779	 84% 9% 7%
1	E	779	 85% 9% 6%

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Mol	Chain	Length	Quality of chain
1	F	779	 <p>% 87% 7% 6%</p>
1	G	779	 <p>% 86% 7% 6%</p>
1	H	779	 <p>% 86% 8% 6%</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 48995 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 Ribonucleoside-diphosphate reductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	731	5817	3693	999	1101	24	0	0	0
1	B	733	5829	3701	1001	1103	24	0	0	0
1	C	733	5849	3714	1004	1107	24	0	2	0
1	D	727	5789	3677	994	1094	24	0	0	0
1	E	733	5841	3710	1002	1105	24	0	1	0
1	F	732	5826	3699	1001	1102	24	0	0	0
1	G	729	5801	3685	996	1096	24	0	0	0
1	H	735	5861	3720	1007	1110	24	0	1	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P00452
A	-17	GLY	-	expression tag	UNP P00452
A	-16	SER	-	expression tag	UNP P00452
A	-15	SER	-	expression tag	UNP P00452
A	-14	HIS	-	expression tag	UNP P00452
A	-13	HIS	-	expression tag	UNP P00452
A	-12	HIS	-	expression tag	UNP P00452
A	-11	HIS	-	expression tag	UNP P00452
A	-10	HIS	-	expression tag	UNP P00452
A	-9	HIS	-	expression tag	UNP P00452
A	-8	SER	-	expression tag	UNP P00452
A	-7	SER	-	expression tag	UNP P00452
A	-6	GLY	-	expression tag	UNP P00452

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP P00452
A	-4	VAL	-	expression tag	UNP P00452
A	-3	PRO	-	expression tag	UNP P00452
A	-2	ARG	-	expression tag	UNP P00452
A	-1	GLY	-	expression tag	UNP P00452
A	0	SER	-	expression tag	UNP P00452
A	28	ALA	TRP	engineered mutation	UNP P00452
B	-18	MET	-	initiating methionine	UNP P00452
B	-17	GLY	-	expression tag	UNP P00452
B	-16	SER	-	expression tag	UNP P00452
B	-15	SER	-	expression tag	UNP P00452
B	-14	HIS	-	expression tag	UNP P00452
B	-13	HIS	-	expression tag	UNP P00452
B	-12	HIS	-	expression tag	UNP P00452
B	-11	HIS	-	expression tag	UNP P00452
B	-10	HIS	-	expression tag	UNP P00452
B	-9	HIS	-	expression tag	UNP P00452
B	-8	SER	-	expression tag	UNP P00452
B	-7	SER	-	expression tag	UNP P00452
B	-6	GLY	-	expression tag	UNP P00452
B	-5	LEU	-	expression tag	UNP P00452
B	-4	VAL	-	expression tag	UNP P00452
B	-3	PRO	-	expression tag	UNP P00452
B	-2	ARG	-	expression tag	UNP P00452
B	-1	GLY	-	expression tag	UNP P00452
B	0	SER	-	expression tag	UNP P00452
B	28	ALA	TRP	engineered mutation	UNP P00452
C	-18	MET	-	initiating methionine	UNP P00452
C	-17	GLY	-	expression tag	UNP P00452
C	-16	SER	-	expression tag	UNP P00452
C	-15	SER	-	expression tag	UNP P00452
C	-14	HIS	-	expression tag	UNP P00452
C	-13	HIS	-	expression tag	UNP P00452
C	-12	HIS	-	expression tag	UNP P00452
C	-11	HIS	-	expression tag	UNP P00452
C	-10	HIS	-	expression tag	UNP P00452
C	-9	HIS	-	expression tag	UNP P00452
C	-8	SER	-	expression tag	UNP P00452
C	-7	SER	-	expression tag	UNP P00452
C	-6	GLY	-	expression tag	UNP P00452
C	-5	LEU	-	expression tag	UNP P00452
C	-4	VAL	-	expression tag	UNP P00452

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	PRO	-	expression tag	UNP P00452
C	-2	ARG	-	expression tag	UNP P00452
C	-1	GLY	-	expression tag	UNP P00452
C	0	SER	-	expression tag	UNP P00452
C	28	ALA	TRP	engineered mutation	UNP P00452
D	-18	MET	-	initiating methionine	UNP P00452
D	-17	GLY	-	expression tag	UNP P00452
D	-16	SER	-	expression tag	UNP P00452
D	-15	SER	-	expression tag	UNP P00452
D	-14	HIS	-	expression tag	UNP P00452
D	-13	HIS	-	expression tag	UNP P00452
D	-12	HIS	-	expression tag	UNP P00452
D	-11	HIS	-	expression tag	UNP P00452
D	-10	HIS	-	expression tag	UNP P00452
D	-9	HIS	-	expression tag	UNP P00452
D	-8	SER	-	expression tag	UNP P00452
D	-7	SER	-	expression tag	UNP P00452
D	-6	GLY	-	expression tag	UNP P00452
D	-5	LEU	-	expression tag	UNP P00452
D	-4	VAL	-	expression tag	UNP P00452
D	-3	PRO	-	expression tag	UNP P00452
D	-2	ARG	-	expression tag	UNP P00452
D	-1	GLY	-	expression tag	UNP P00452
D	0	SER	-	expression tag	UNP P00452
D	28	ALA	TRP	engineered mutation	UNP P00452
E	-18	MET	-	initiating methionine	UNP P00452
E	-17	GLY	-	expression tag	UNP P00452
E	-16	SER	-	expression tag	UNP P00452
E	-15	SER	-	expression tag	UNP P00452
E	-14	HIS	-	expression tag	UNP P00452
E	-13	HIS	-	expression tag	UNP P00452
E	-12	HIS	-	expression tag	UNP P00452
E	-11	HIS	-	expression tag	UNP P00452
E	-10	HIS	-	expression tag	UNP P00452
E	-9	HIS	-	expression tag	UNP P00452
E	-8	SER	-	expression tag	UNP P00452
E	-7	SER	-	expression tag	UNP P00452
E	-6	GLY	-	expression tag	UNP P00452
E	-5	LEU	-	expression tag	UNP P00452
E	-4	VAL	-	expression tag	UNP P00452
E	-3	PRO	-	expression tag	UNP P00452
E	-2	ARG	-	expression tag	UNP P00452

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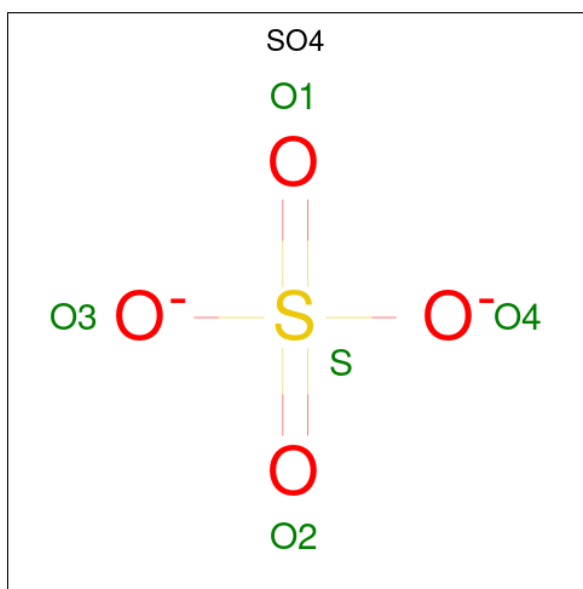
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP P00452
E	0	SER	-	expression tag	UNP P00452
E	28	ALA	TRP	engineered mutation	UNP P00452
F	-18	MET	-	initiating methionine	UNP P00452
F	-17	GLY	-	expression tag	UNP P00452
F	-16	SER	-	expression tag	UNP P00452
F	-15	SER	-	expression tag	UNP P00452
F	-14	HIS	-	expression tag	UNP P00452
F	-13	HIS	-	expression tag	UNP P00452
F	-12	HIS	-	expression tag	UNP P00452
F	-11	HIS	-	expression tag	UNP P00452
F	-10	HIS	-	expression tag	UNP P00452
F	-9	HIS	-	expression tag	UNP P00452
F	-8	SER	-	expression tag	UNP P00452
F	-7	SER	-	expression tag	UNP P00452
F	-6	GLY	-	expression tag	UNP P00452
F	-5	LEU	-	expression tag	UNP P00452
F	-4	VAL	-	expression tag	UNP P00452
F	-3	PRO	-	expression tag	UNP P00452
F	-2	ARG	-	expression tag	UNP P00452
F	-1	GLY	-	expression tag	UNP P00452
F	0	SER	-	expression tag	UNP P00452
F	28	ALA	TRP	engineered mutation	UNP P00452
G	-18	MET	-	initiating methionine	UNP P00452
G	-17	GLY	-	expression tag	UNP P00452
G	-16	SER	-	expression tag	UNP P00452
G	-15	SER	-	expression tag	UNP P00452
G	-14	HIS	-	expression tag	UNP P00452
G	-13	HIS	-	expression tag	UNP P00452
G	-12	HIS	-	expression tag	UNP P00452
G	-11	HIS	-	expression tag	UNP P00452
G	-10	HIS	-	expression tag	UNP P00452
G	-9	HIS	-	expression tag	UNP P00452
G	-8	SER	-	expression tag	UNP P00452
G	-7	SER	-	expression tag	UNP P00452
G	-6	GLY	-	expression tag	UNP P00452
G	-5	LEU	-	expression tag	UNP P00452
G	-4	VAL	-	expression tag	UNP P00452
G	-3	PRO	-	expression tag	UNP P00452
G	-2	ARG	-	expression tag	UNP P00452
G	-1	GLY	-	expression tag	UNP P00452
G	0	SER	-	expression tag	UNP P00452

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Chain	Residue	Modelled	Actual	Comment	Reference
G	28	ALA	TRP	engineered mutation	UNP P00452
H	-18	MET	-	initiating methionine	UNP P00452
H	-17	GLY	-	expression tag	UNP P00452
H	-16	SER	-	expression tag	UNP P00452
H	-15	SER	-	expression tag	UNP P00452
H	-14	HIS	-	expression tag	UNP P00452
H	-13	HIS	-	expression tag	UNP P00452
H	-12	HIS	-	expression tag	UNP P00452
H	-11	HIS	-	expression tag	UNP P00452
H	-10	HIS	-	expression tag	UNP P00452
H	-9	HIS	-	expression tag	UNP P00452
H	-8	SER	-	expression tag	UNP P00452
H	-7	SER	-	expression tag	UNP P00452
H	-6	GLY	-	expression tag	UNP P00452
H	-5	LEU	-	expression tag	UNP P00452
H	-4	VAL	-	expression tag	UNP P00452
H	-3	PRO	-	expression tag	UNP P00452
H	-2	ARG	-	expression tag	UNP P00452
H	-1	GLY	-	expression tag	UNP P00452
H	0	SER	-	expression tag	UNP P00452
H	28	ALA	TRP	engineered mutation	UNP P00452

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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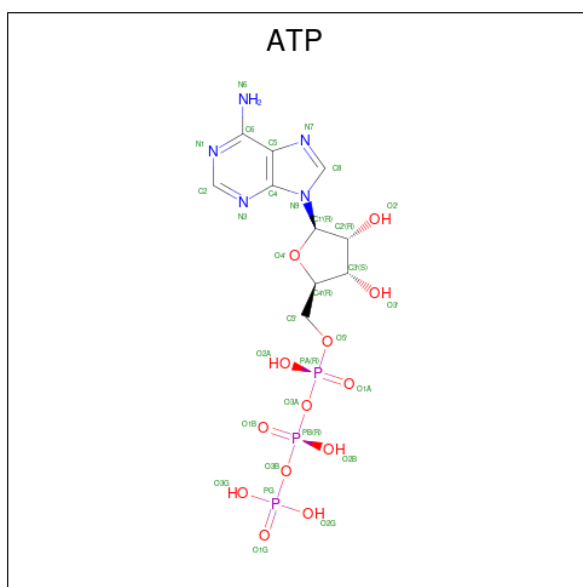
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	H	1	5	4	1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

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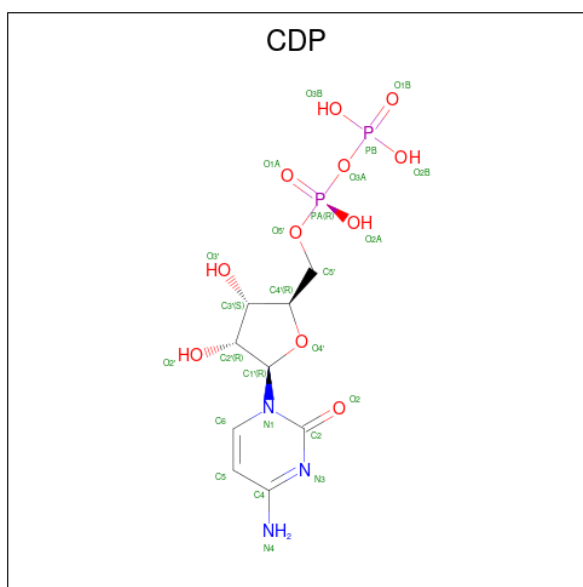
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G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

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

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

- Molecule 5 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>3</sub>O<sub>11</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	Total 25	C 9	N 3	O 11	P 2	0	0
5	B	1	Total 25	C 9	N 3	O 11	P 2	0	0
5	C	1	Total 25	C 9	N 3	O 11	P 2	0	0
5	D	1	Total 25	C 9	N 3	O 11	P 2	0	0
5	E	1	Total 25	C 9	N 3	O 11	P 2	0	0
5	F	1	Total 25	C 9	N 3	O 11	P 2	0	0
5	G	1	Total 25	C 9	N 3	O 11	P 2	0	0
5	H	1	Total 25	C 9	N 3	O 11	P 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	176	Total 176	O 176	0	0
6	B	138	Total 138	O 138	0	0
6	C	149	Total 149	O 149	0	0
6	D	160	Total 160	O 160	0	0

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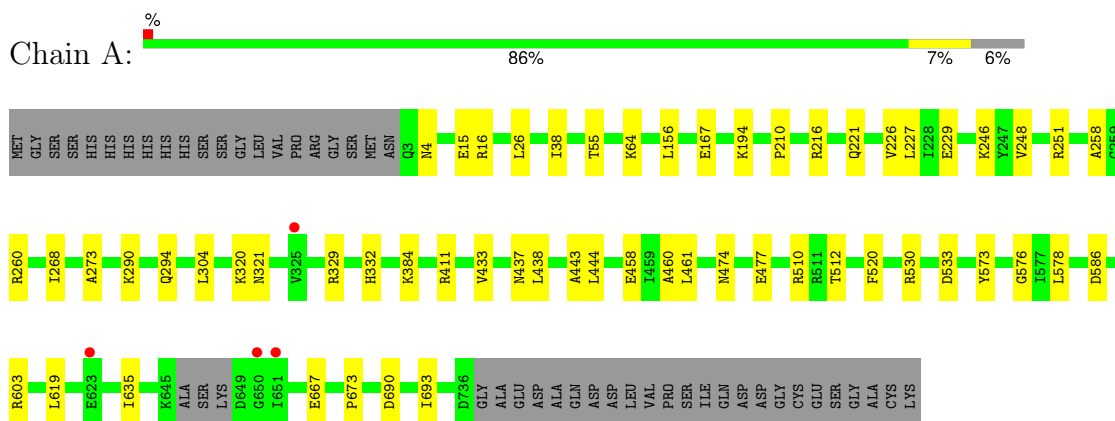
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	E	118	Total 118	O 118	0	0
6	F	139	Total 139	O 139	0	0
6	G	166	Total 166	O 166	0	0
6	H	176	Total 176	O 176	0	0

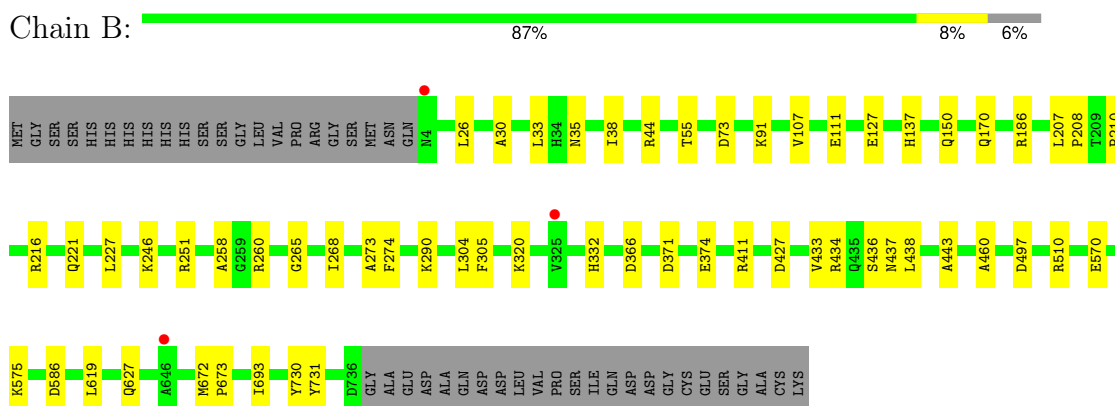
### 3 Residue-property plots [i](#)

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.

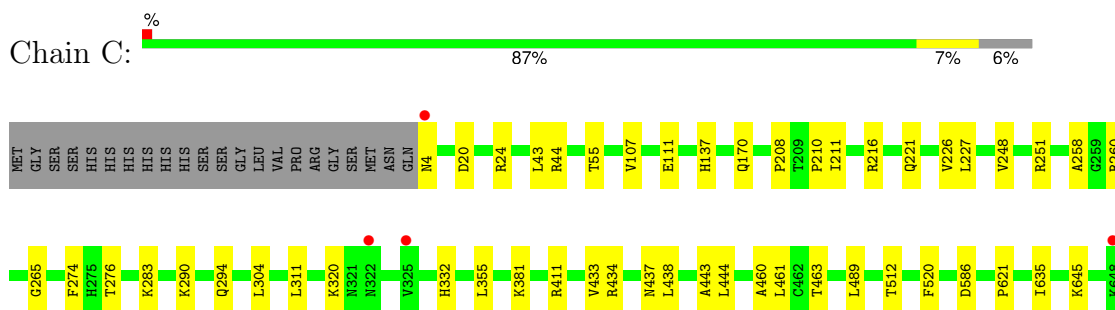
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

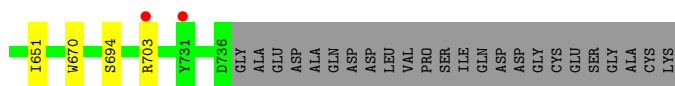


- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

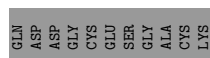
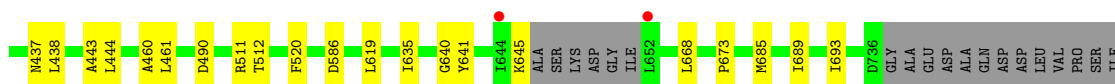
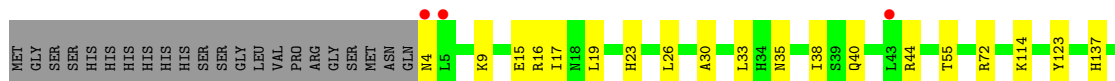
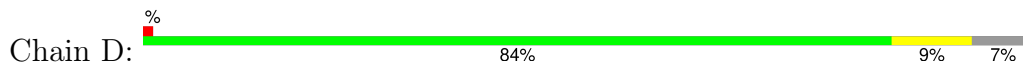


- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

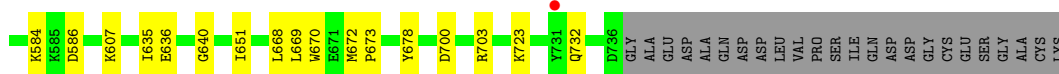
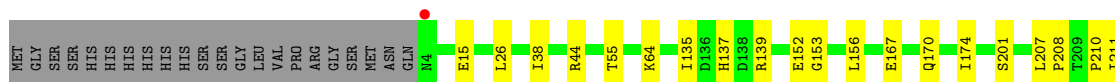
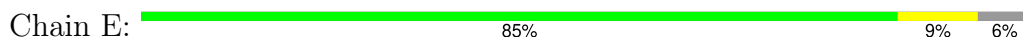




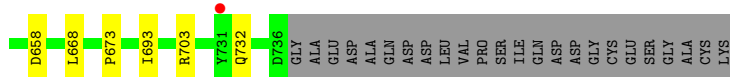
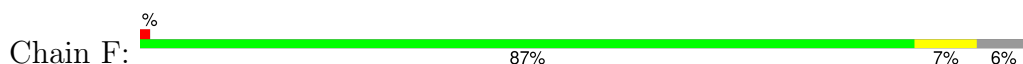
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



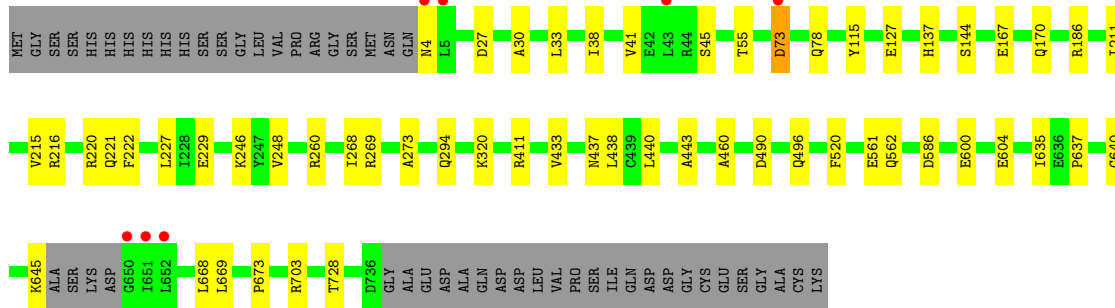
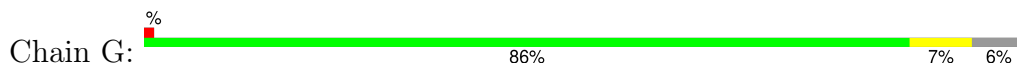
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



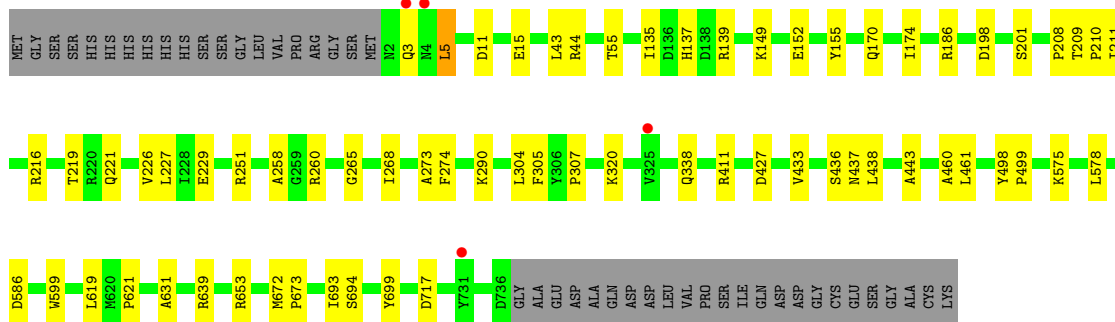
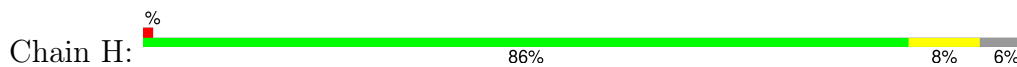
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



● Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	288.72Å 316.61Å 158.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.61 49.74 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.74-2.61) 99.5 (49.74-2.61)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.189 , 0.209 0.197 , 0.218	Depositor DCC
$R_{free}$ test set	217861 reflections (0.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.9	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	0.95	EDS
Total number of atoms	48995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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, CDP, ATP, SO4

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	0.27	0/5942	0.43	0/8047
1	B	0.27	0/5955	0.41	0/8065
1	C	0.26	0/5976	0.41	0/8094
1	D	0.27	0/5914	0.42	0/8009
1	E	0.26	0/5968	0.42	0/8083
1	F	0.26	0/5951	0.41	0/8058
1	G	0.27	0/5926	0.42	0/8025
1	H	0.27	0/5988	0.42	0/8110
All	All	0.27	0/47620	0.42	0/64491

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5817	0	5740	35	0
1	B	5829	0	5758	38	0
1	C	5849	0	5771	34	0
1	D	5789	0	5716	42	0
1	E	5841	0	5766	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5826	0	5753	33	0
1	G	5801	0	5730	36	0
1	H	5861	0	5784	40	0
2	A	40	0	0	1	0
2	B	20	0	0	1	0
2	C	25	0	0	0	0
2	D	35	0	0	4	0
2	E	20	0	0	1	0
2	F	20	0	0	2	0
2	G	15	0	0	2	0
2	H	25	0	0	0	0
3	A	93	0	36	2	0
3	B	93	0	36	2	0
3	C	93	0	36	1	0
3	D	93	0	36	1	0
3	E	93	0	36	2	0
3	F	93	0	36	2	0
3	G	93	0	36	1	0
3	H	93	0	36	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
5	A	25	0	12	2	0
5	B	25	0	12	2	0
5	C	25	0	12	2	0
5	D	25	0	12	2	0
5	E	25	0	12	2	0
5	F	25	0	12	3	0
5	G	25	0	12	2	0
5	H	25	0	12	2	0
6	A	176	0	0	1	0
6	B	138	0	0	3	0
6	C	149	0	0	6	0
6	D	160	0	0	4	0
6	E	118	0	0	4	0
6	F	139	0	0	3	0
6	G	166	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	176	0	0	6	0
All	All	48995	0	46402	289	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.

All (289) 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:260:ARG:HH12	1:B:434:ARG:NH1	1.53	1.05
1:H:229:GLU:OE2	1:H:260:ARG:NH1	1.90	1.03
1:H:427:ASP:OD2	1:H:575:LYS:NZ	1.93	0.99
1:G:127:GLU:OE2	1:G:186:ARG:NH1	2.00	0.94
1:G:127:GLU:CD	1:G:186:ARG:HH12	1.77	0.87
1:A:4:ASN:HD22	1:A:16:ARG:HE	1.24	0.86
1:C:434:ARG:NH1	6:C:901:HOH:O	2.07	0.85
1:B:260:ARG:HH12	1:B:434:ARG:HH12	1.25	0.82
1:E:229:GLU:OE2	1:E:260:ARG:NH1	2.12	0.82
1:B:260:ARG:NH1	1:B:434:ARG:NH1	2.27	0.82
1:E:584:LYS:NZ	1:E:723:LYS:O	2.16	0.77
1:D:16:ARG:HG3	1:D:16:ARG:HH11	1.51	0.75
1:D:229:GLU:OE2	1:D:260:ARG:NH1	2.19	0.75
1:D:227:LEU:HB2	1:D:460:ALA:HB3	1.68	0.75
1:C:670:TRP:O	1:C:703:ARG:NH2	2.20	0.74
1:B:427:ASP:OD2	1:B:575:LYS:NZ	2.20	0.72
1:H:15:GLU:OE2	3:H:803:ATP:N6	2.23	0.72
1:E:607:LYS:NZ	6:E:902:HOH:O	2.22	0.71
1:G:144:SER:OG	6:G:901:HOH:O	2.09	0.69
1:H:639:ARG:NH1	6:H:907:HOH:O	2.26	0.68
1:H:198:ASP:OD2	6:H:901:HOH:O	2.10	0.68
1:C:4:ASN:N	6:C:909:HOH:O	2.27	0.67
1:B:246:LYS:NZ	2:B:801:SO4:O3	2.25	0.67
1:B:127:GLU:OE2	1:B:186:ARG:NH1	2.28	0.67
1:H:227:LEU:HB2	1:H:460:ALA:HB3	1.77	0.66
1:E:636:GLU:OE2	6:E:901:HOH:O	2.14	0.66
1:F:227:LEU:HB2	1:F:460:ALA:HB3	1.79	0.65
1:G:229:GLU:OE2	1:G:260:ARG:NH1	2.29	0.65
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.79	0.64
1:F:703:ARG:NH2	1:H:653:ARG:HH22	1.95	0.64
1:B:497:ASP:OD2	6:B:901:HOH:O	2.16	0.63
1:A:4:ASN:ND2	1:A:16:ARG:HE	1.92	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ARG:N	2:D:810:SO4:O1	2.28	0.63
1:A:246:LYS:NZ	2:A:801:SO4:O3	2.28	0.63
1:B:320:LYS:HE2	1:B:411:ARG:HB2	1.81	0.63
1:D:641:TYR:N	2:D:812:SO4:O2	2.32	0.62
1:F:144:SER:OG	6:F:901:HOH:O	2.13	0.62
1:F:437:ASN:ND2	5:F:809:CDP:O3'	2.33	0.61
1:A:55:THR:HG21	3:A:804:ATP:O2B	2.01	0.60
1:D:26:LEU:HB3	1:D:38:ILE:HD12	1.82	0.60
1:C:437:ASN:ND2	5:C:809:CDP:O3'	2.34	0.60
1:G:227:LEU:HB2	1:G:460:ALA:HB3	1.83	0.60
1:C:226:VAL:HG22	1:C:461:LEU:HD22	1.84	0.60
1:D:246:LYS:NZ	2:D:801:SO4:O1	2.26	0.59
1:B:437:ASN:ND2	5:B:809:CDP:O3'	2.35	0.59
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.84	0.59
1:F:533:ASP:HB2	1:H:43:LEU:HB3	1.85	0.58
1:A:226:VAL:HG22	1:A:461:LEU:HD22	1.84	0.58
1:B:290:LYS:HE3	1:B:332:HIS:HB3	1.86	0.57
1:D:114:LYS:NZ	6:D:902:HOH:O	2.20	0.57
1:F:703:ARG:HH22	1:H:653:ARG:HH22	1.51	0.57
1:E:226:VAL:HG22	1:E:461:LEU:HD22	1.85	0.57
1:G:55:THR:HG21	3:G:803:ATP:O2B	2.05	0.57
1:G:437:ASN:ND2	5:G:808:CDP:O3'	2.38	0.57
1:C:645:LYS:NZ	6:C:906:HOH:O	2.25	0.56
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.86	0.56
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.86	0.56
1:A:4:ASN:HD22	1:A:16:ARG:NE	1.97	0.56
1:B:127:GLU:CD	1:B:186:ARG:HH12	2.08	0.56
1:G:438:LEU:HD23	5:G:808:CDP:H2'	1.88	0.56
1:G:115:TYR:OH	1:G:167:GLU:OE1	2.21	0.56
1:A:229:GLU:OE2	1:A:260:ARG:NH1	2.37	0.55
1:E:320:LYS:HE2	1:E:411:ARG:HB2	1.88	0.55
1:H:226:VAL:HG22	1:H:461:LEU:HD22	1.88	0.55
1:A:15:GLU:OE2	3:A:804:ATP:N6	2.38	0.55
1:A:290:LYS:HE3	1:A:332:HIS:HB3	1.89	0.55
1:B:438:LEU:HD23	5:B:809:CDP:H2'	1.88	0.55
1:B:44:ARG:HG3	1:D:673:PRO:HG3	1.88	0.55
1:D:16:ARG:HG3	1:D:16:ARG:NH1	2.16	0.54
1:D:320:LYS:HE2	1:D:411:ARG:HB2	1.90	0.54
1:E:55:THR:HG21	3:E:804:ATP:O2B	2.08	0.54
1:E:258:ALA:HB3	1:E:304:LEU:HD21	1.89	0.54
1:A:320:LYS:HE2	1:A:411:ARG:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:HIS:HA	1:D:170:GLN:HG3	1.89	0.54
1:B:366:ASP:OD2	6:B:902:HOH:O	2.18	0.54
1:A:576:GLY:O	1:A:603:ARG:NH1	2.39	0.53
1:D:258:ALA:HB3	1:D:304:LEU:HD21	1.90	0.53
1:H:55:THR:HG21	3:H:803:ATP:O2B	2.08	0.53
1:B:35:ASN:ND2	1:B:73:ASP:O	2.41	0.53
1:G:320:LYS:HE2	1:G:411:ARG:HB2	1.90	0.53
1:D:19:LEU:O	1:D:23:HIS:HB2	2.08	0.53
1:E:438:LEU:HD23	5:E:809:CDP:H2'	1.90	0.52
1:H:437:ASN:ND2	5:H:808:CDP:O3'	2.42	0.52
1:C:283:LYS:NZ	6:C:919:HOH:O	2.41	0.52
1:A:438:LEU:HD23	5:A:809:CDP:H2'	1.90	0.52
1:C:55:THR:HG21	3:C:804:ATP:O2B	2.09	0.52
1:H:290:LYS:NZ	6:H:923:HOH:O	2.41	0.52
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.91	0.52
1:D:438:LEU:HD23	5:D:809:CDP:H2'	1.92	0.52
1:H:186:ARG:NH2	6:H:931:HOH:O	2.43	0.52
1:H:320:LYS:HE2	1:H:411:ARG:HB2	1.92	0.51
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.93	0.51
1:G:73:ASP:OD2	1:G:73:ASP:N	2.44	0.51
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.92	0.51
1:E:15:GLU:OE2	3:E:804:ATP:N6	2.37	0.51
1:D:40:GLN:O	1:D:44:ARG:HG3	2.10	0.51
1:C:320:LYS:HE2	1:C:411:ARG:HB2	1.93	0.50
1:H:631:ALA:O	6:H:902:HOH:O	2.19	0.50
1:H:137:HIS:HA	1:H:170:GLN:HG3	1.93	0.50
1:B:510:ARG:NH2	1:B:570:GLU:OE1	2.45	0.50
1:B:26:LEU:HB3	1:B:38:ILE:HD12	1.91	0.50
1:F:433:VAL:HG11	1:F:443:ALA:HB1	1.94	0.50
1:G:30:ALA:HA	1:G:33:LEU:HD12	1.93	0.50
1:C:208:PRO:HD2	1:C:211:ILE:HD12	1.94	0.50
1:F:640:GLY:HA2	1:F:668:LEU:HD13	1.93	0.50
1:A:437:ASN:ND2	5:A:809:CDP:O3'	2.45	0.50
1:D:9:LYS:HD3	1:D:15:GLU:HG2	1.93	0.50
1:D:640:GLY:HA2	1:D:668:LEU:HD13	1.94	0.50
1:F:246:LYS:NZ	2:F:801:SO4:O1	2.44	0.50
1:F:438:LEU:HD23	5:F:809:CDP:H2'	1.93	0.50
1:H:699:TYR:OH	1:H:717:ASP:OD2	2.25	0.50
1:D:210:PRO:HB3	1:D:251:ARG:HB3	1.94	0.49
1:G:433:VAL:HG11	1:G:443:ALA:HB1	1.93	0.49
1:D:4:ASN:HA	1:D:16:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:LYS:HE3	1:F:332:HIS:HB3	1.94	0.49
1:G:268:ILE:HB	1:G:273:ALA:HB3	1.95	0.49
1:H:139:ARG:NH1	1:H:201:SER:OG	2.46	0.49
1:F:520:PHE:HB3	1:F:635:ILE:HA	1.94	0.49
1:E:137:HIS:HA	1:E:170:GLN:HG3	1.95	0.49
1:E:44:ARG:HE	1:G:673:PRO:HG3	1.78	0.49
1:E:227:LEU:HB2	1:E:460:ALA:HB3	1.93	0.49
1:G:490:ASP:OD2	6:G:902:HOH:O	2.20	0.49
1:B:268:ILE:HB	1:B:273:ALA:HB3	1.94	0.49
1:F:208:PRO:HD2	1:F:211:ILE:HD12	1.95	0.49
1:A:530:ARG:HB3	1:A:667:GLU:OE2	2.14	0.48
1:A:26:LEU:HB3	1:A:38:ILE:HD12	1.96	0.48
1:B:55:THR:HG21	3:B:804:ATP:O2B	2.13	0.48
1:F:320:LYS:HE2	1:F:411:ARG:HB2	1.95	0.48
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.95	0.48
1:C:260:ARG:NH1	1:C:434:ARG:NH2	2.61	0.48
1:D:226:VAL:HG22	1:D:461:LEU:HD22	1.95	0.48
1:C:438:LEU:HD23	5:C:809:CDP:H2'	1.96	0.48
1:D:444:LEU:HD22	1:D:512:THR:HG21	1.96	0.48
1:F:55:THR:HG21	3:F:804:ATP:O2B	2.14	0.48
1:D:490:ASP:O	1:D:511:ARG:NH2	2.47	0.47
1:D:433:VAL:HG11	1:D:443:ALA:HB1	1.96	0.47
1:G:640:GLY:HA2	1:G:668:LEU:HD13	1.96	0.47
1:G:38:ILE:N	2:G:809:SO4:O1	2.46	0.47
1:E:139:ARG:NH1	1:E:201:SER:OG	2.47	0.47
1:E:651:ILE:H	1:E:651:ILE:HG13	1.47	0.47
1:H:433:VAL:HG11	1:H:443:ALA:HB1	1.94	0.47
1:E:437:ASN:ND2	5:E:809:CDP:O3'	2.48	0.47
1:D:645:LYS:NZ	6:D:901:HOH:O	2.16	0.47
1:E:26:LEU:HB3	1:E:38:ILE:HD12	1.97	0.47
1:E:248:VAL:O	1:E:294:GLN:HA	2.15	0.47
1:A:248:VAL:O	1:A:294:GLN:HA	2.14	0.47
1:B:260:ARG:NH1	1:B:434:ARG:HH12	2.02	0.47
1:F:258:ALA:HB3	1:F:304:LEU:HD21	1.96	0.47
1:G:246:LYS:NZ	2:G:801:SO4:O1	2.46	0.47
1:A:573:TYR:OH	1:A:690:ASP:OD1	2.28	0.47
1:E:520:PHE:HB3	1:E:635:ILE:HA	1.97	0.47
1:H:438:LEU:HD23	5:H:808:CDP:H2'	1.96	0.47
1:A:384:LYS:N	1:A:384:LYS:HD2	2.30	0.47
1:A:474:ASN:OD1	1:A:477:GLU:HG3	2.15	0.47
1:H:258:ALA:HB3	1:H:304:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.97	0.46
1:F:658:ASP:N	2:F:810:SO4:O3	2.21	0.46
1:C:290:LYS:HE3	1:C:332:HIS:HB3	1.97	0.46
1:A:64:LYS:HB3	1:A:64:LYS:HE3	1.82	0.46
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.97	0.46
1:D:520:PHE:HB3	1:D:635:ILE:HA	1.98	0.46
1:A:210:PRO:HB3	1:A:251:ARG:HB3	1.98	0.46
1:A:458:GLU:OE2	1:A:510:ARG:NE	2.38	0.46
1:D:265:GLY:HA2	1:D:274:PHE:CZ	2.50	0.46
1:D:55:THR:HG21	3:D:804:ATP:O2B	2.16	0.46
1:B:210:PRO:HB3	1:B:251:ARG:HB3	1.96	0.46
1:E:321:ASN:O	1:E:329:ARG:NE	2.38	0.46
1:D:437:ASN:ND2	5:D:809:CDP:O3'	2.48	0.45
1:F:444:LEU:HD22	1:F:512:THR:HG21	1.99	0.45
1:F:651:ILE:H	1:F:651:ILE:HG13	1.55	0.45
1:F:673:PRO:HG3	1:H:44:ARG:CZ	2.47	0.45
1:E:208:PRO:HD2	1:E:211:ILE:HD12	1.98	0.45
1:F:732:GLN:NE2	6:F:929:HOH:O	2.50	0.45
1:G:673:PRO:O	1:G:703:ARG:NH2	2.50	0.45
1:B:265:GLY:HA2	1:B:274:PHE:CZ	2.52	0.45
1:D:290:LYS:HE3	1:D:332:HIS:HB3	1.99	0.45
1:C:381:LYS:NZ	6:C:929:HOH:O	2.49	0.45
1:C:520:PHE:HB3	1:C:635:ILE:HA	1.98	0.45
1:B:91:LYS:NZ	3:B:804:ATP:O3G	2.44	0.45
1:F:619:LEU:HB2	1:F:693:ILE:HG23	1.98	0.45
1:A:194:LYS:NZ	6:A:928:HOH:O	2.50	0.45
1:D:192:TYR:OH	2:D:811:SO4:O4	2.18	0.45
1:C:276:THR:OG1	6:C:902:HOH:O	2.21	0.44
1:C:651:ILE:H	1:C:651:ILE:HG13	1.65	0.44
1:H:305:PHE:CZ	1:H:436:SER:HB3	2.51	0.44
1:B:260:ARG:NH1	1:B:434:ARG:HH11	2.08	0.44
1:H:672:MET:HA	1:H:673:PRO:HD3	1.78	0.44
1:E:135:ILE:HD11	1:E:174:ILE:HG21	1.99	0.44
1:H:11:ASP:OD2	6:H:903:HOH:O	2.21	0.44
1:A:619:LEU:HB2	1:A:693:ILE:HG23	1.99	0.44
1:G:520:PHE:HB3	1:G:635:ILE:HA	1.99	0.44
1:B:672:MET:HA	1:B:673:PRO:HD3	1.86	0.44
1:H:135:ILE:HD11	1:H:174:ILE:HG21	2.00	0.44
1:A:520:PHE:HB3	1:A:635:ILE:HA	2.00	0.44
1:A:673:PRO:HG3	1:C:44:ARG:CZ	2.48	0.44
1:G:78:GLN:OE1	6:G:903:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:VAL:HG11	1:E:443:ALA:HB1	2.00	0.44
1:E:538:ASN:ND2	2:E:802:SO4:O3	2.30	0.44
1:E:700:ASP:HB3	1:E:703:ARG:HD2	2.00	0.43
1:A:578:LEU:HD11	1:A:603:ARG:HB2	2.00	0.43
1:D:248:VAL:O	1:D:294:GLN:HA	2.18	0.43
1:F:265:GLY:HA2	1:F:274:PHE:CZ	2.53	0.43
1:E:268:ILE:HB	1:E:273:ALA:HB3	2.00	0.43
1:G:137:HIS:HA	1:G:170:GLN:HG3	2.00	0.43
1:H:208:PRO:HD2	1:H:211:ILE:HD12	2.00	0.43
1:G:248:VAL:O	1:G:294:GLN:HA	2.18	0.43
1:H:210:PRO:HB3	1:H:251:ARG:HB3	2.00	0.43
1:A:156:LEU:HD22	1:A:167:GLU:HG3	2.01	0.43
1:F:15:GLU:OE2	3:F:804:ATP:N6	2.42	0.43
1:H:307:PRO:HA	1:H:338:GLN:HB2	2.00	0.43
1:H:578:LEU:HD13	1:H:599:TRP:HE3	1.84	0.43
1:A:444:LEU:HD22	1:A:512:THR:HG21	2.01	0.43
1:E:437:ASN:HB2	6:E:976:HOH:O	2.18	0.43
1:B:619:LEU:HB2	1:B:693:ILE:HG23	1.99	0.43
1:E:290:LYS:HE3	1:E:332:HIS:HB3	1.99	0.43
1:G:4:ASN:N	6:G:933:HOH:O	2.51	0.43
1:D:35:ASN:N	1:G:27:ASP:OD2	2.44	0.43
1:F:137:HIS:HA	1:F:170:GLN:HG3	2.00	0.43
1:G:269:ARG:NH2	1:H:219:THR:OG1	2.52	0.43
1:H:621:PRO:HD3	1:H:694:SER:OG	2.19	0.43
1:F:371:ASP:HB3	1:F:374:GLU:HB3	2.00	0.43
1:C:260:ARG:HH12	1:C:434:ARG:NH2	2.17	0.43
1:D:366:ASP:OD1	6:D:904:HOH:O	2.21	0.43
1:E:64:LYS:HE3	1:E:64:LYS:HB3	1.87	0.42
1:E:636:GLU:OE1	1:E:678:TYR:OH	2.22	0.42
1:F:248:VAL:O	1:F:294:GLN:HA	2.19	0.42
1:C:248:VAL:O	1:C:294:GLN:HA	2.19	0.42
1:H:268:ILE:HB	1:H:273:ALA:HB3	2.01	0.42
1:A:321:ASN:O	1:A:329:ARG:NE	2.47	0.42
1:E:269:ARG:NH2	1:F:219:THR:OG1	2.52	0.42
1:C:107:VAL:O	1:C:111:GLU:HG3	2.20	0.42
1:C:137:HIS:HA	1:C:170:GLN:HG3	2.02	0.42
1:D:208:PRO:HD2	1:D:211:ILE:HD12	2.00	0.42
1:F:437:ASN:HB2	6:F:988:HOH:O	2.18	0.42
5:F:809:CDP:O5'	5:F:809:CDP:H6	2.02	0.42
1:G:600:GLU:O	1:G:604:GLU:HG2	2.19	0.42
1:H:619:LEU:HB2	1:H:693:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ILE:HB	1:A:273:ALA:HB3	2.02	0.42
1:B:305:PHE:CZ	1:B:436:SER:HB3	2.55	0.42
1:D:311:LEU:HA	1:D:355:LEU:HB3	2.02	0.42
1:G:561:GLU:HG2	1:G:562:GLN:HG3	2.02	0.42
1:H:155:TYR:HE1	1:H:209:THR:HG23	1.84	0.42
1:H:265:GLY:HA2	1:H:274:PHE:CE2	2.55	0.42
1:D:685:MET:O	1:D:689:ILE:HG12	2.19	0.42
1:D:123:TYR:O	6:D:903:HOH:O	2.21	0.41
1:F:139:ARG:NH1	1:F:201:SER:OG	2.53	0.41
1:C:621:PRO:HD3	1:C:694:SER:OG	2.19	0.41
1:E:456:ASN:ND2	6:E:932:HOH:O	2.53	0.41
1:F:463:THR:HG21	1:F:492:LEU:HD22	2.02	0.41
1:F:552:LEU:HD23	1:F:616:LEU:HD12	2.01	0.41
1:B:150:GLN:NE2	1:B:627:GLN:OE1	2.53	0.41
1:D:619:LEU:HB2	1:D:693:ILE:HG23	2.02	0.41
1:A:533:ASP:HB2	1:C:43:LEU:HB3	2.02	0.41
1:D:207:LEU:HA	1:D:208:PRO:HD3	1.90	0.41
1:G:41:VAL:O	1:G:45:SER:OG	2.36	0.41
1:C:260:ARG:HH12	1:C:434:ARG:HH22	1.68	0.41
1:E:156:LEU:HD22	1:E:167:GLU:HG3	2.02	0.41
1:E:207:LEU:HA	1:E:208:PRO:HD3	1.90	0.41
1:E:640:GLY:HA2	1:E:668:LEU:HD13	2.03	0.41
1:H:498:TYR:HA	1:H:499:PRO:HD2	1.93	0.41
1:B:437:ASN:HB2	6:B:993:HOH:O	2.19	0.41
1:C:463:THR:HG22	1:C:489:LEU:HD22	2.03	0.41
1:E:406:ARG:HG2	1:E:732:GLN:OE1	2.21	0.41
1:G:220:ARG:HB3	1:G:496:GLN:HA	2.03	0.41
1:B:137:HIS:HA	1:B:170:GLN:HG3	2.02	0.41
1:E:444:LEU:HD22	1:E:512:THR:HG21	2.02	0.41
1:G:211:ILE:HA	1:G:215:VAL:HG23	2.03	0.41
1:G:637:PRO:HG2	1:G:669:LEU:HD13	2.02	0.41
1:G:645:LYS:NZ	6:G:905:HOH:O	2.23	0.41
1:B:107:VAL:O	1:B:111:GLU:HG3	2.21	0.41
1:C:210:PRO:HB3	1:C:251:ARG:HB3	2.02	0.41
1:H:3:GLN:C	1:H:5:LEU:H	2.23	0.41
1:B:207:LEU:HA	1:B:208:PRO:HD3	1.90	0.41
1:B:730:TYR:CG	1:B:731:TYR:N	2.88	0.41
1:C:20:ASP:HB3	1:C:24:ARG:NH2	2.36	0.40
1:C:265:GLY:HA2	1:C:274:PHE:CZ	2.56	0.40
1:E:672:MET:HA	1:E:673:PRO:HD3	1.86	0.40
1:G:440:LEU:HD12	1:G:728:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:669:LEU:HD23	1:E:670:TRP:CE2	2.56	0.40
1:F:156:LEU:HD22	1:F:167:GLU:HG3	2.03	0.40
1:B:30:ALA:HA	1:B:33:LEU:HD12	2.03	0.40
1:B:371:ASP:HB3	1:B:374:GLU:HB3	2.04	0.40
1:D:340:ASN:OD1	1:D:343:MET:HG2	2.22	0.40
1:E:210:PRO:HB3	1:E:251:ARG:HB3	2.04	0.40
1:H:149:LYS:NZ	1:H:152:GLU:OE2	2.37	0.40
1:C:311:LEU:HA	1:C:355:LEU:HB3	2.04	0.40
1:D:30:ALA:HA	1:D:33:LEU:HD12	2.02	0.40
1:E:152:GLU:HG3	1:E:153:GLY:N	2.37	0.40
1:G:220:ARG:HA	1:G:222:PHE:CZ	2.57	0.40

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	727/779 (93%)	711 (98%)	15 (2%)	1 (0%)	48 71
1	B	731/779 (94%)	716 (98%)	14 (2%)	1 (0%)	48 71
1	C	733/779 (94%)	719 (98%)	13 (2%)	1 (0%)	48 71
1	D	723/779 (93%)	707 (98%)	15 (2%)	1 (0%)	48 71
1	E	732/779 (94%)	717 (98%)	14 (2%)	1 (0%)	48 71
1	F	728/779 (94%)	714 (98%)	13 (2%)	1 (0%)	48 71
1	G	725/779 (93%)	709 (98%)	15 (2%)	1 (0%)	48 71
1	H	734/779 (94%)	718 (98%)	15 (2%)	1 (0%)	48 71
All	All	5833/6232 (94%)	5711 (98%)	114 (2%)	8 (0%)	48 71

All (8) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	216	ARG
1	B	216	ARG
1	C	216	ARG
1	D	216	ARG
1	E	216	ARG
1	F	216	ARG
1	G	216	ARG
1	H	216	ARG

### 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	626/665 (94%)	624 (100%)	2 (0%)	91	97
1	B	627/665 (94%)	625 (100%)	2 (0%)	91	97
1	C	629/665 (95%)	627 (100%)	2 (0%)	91	97
1	D	623/665 (94%)	620 (100%)	3 (0%)	86	95
1	E	628/665 (94%)	626 (100%)	2 (0%)	91	97
1	F	627/665 (94%)	625 (100%)	2 (0%)	91	97
1	G	624/665 (94%)	621 (100%)	3 (0%)	86	95
1	H	631/665 (95%)	628 (100%)	3 (0%)	86	95
All	All	5015/5320 (94%)	4996 (100%)	19 (0%)	89	96

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	A	586	ASP
1	B	221	GLN
1	B	586	ASP
1	C	221	GLN
1	C	586	ASP
1	D	17	ILE
1	D	221	GLN

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Mol	Chain	Res	Type
1	D	586	ASP
1	E	221	GLN
1	E	586	ASP
1	F	221	GLN
1	F	586	ASP
1	G	73	ASP
1	G	221	GLN
1	G	586	ASP
1	H	5	LEU
1	H	221	GLN
1	H	586	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	F	732	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 16 are monoatomic - leaving 72 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	C	807	4	28,33,33	0.71	0	34,52,52	0.66	1 (2%)
2	SO4	C	802	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	D	802	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	C	810	-	4,4,4	0.23	0	6,6,6	0.13	0
3	ATP	G	803	4	28,33,33	0.69	0	34,52,52	0.69	1 (2%)
2	SO4	A	813	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	H	801	-	4,4,4	0.22	0	6,6,6	0.12	0
2	SO4	B	803	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	E	803	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	F	803	-	4,4,4	0.23	0	6,6,6	0.10	0
3	ATP	F	806	4	28,33,33	0.66	0	34,52,52	0.65	1 (2%)
3	ATP	H	803	4	28,33,33	0.67	0	34,52,52	0.71	1 (2%)
2	SO4	A	810	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	803	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	811	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	D	812	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	D	803	-	4,4,4	0.23	0	6,6,6	0.07	0
3	ATP	B	804	4	28,33,33	0.67	0	34,52,52	0.70	1 (2%)
2	SO4	C	803	-	4,4,4	0.22	0	6,6,6	0.09	0
3	ATP	C	804	4	28,33,33	0.67	0	34,52,52	0.71	1 (2%)
3	ATP	G	806	4	28,33,33	0.65	0	34,52,52	0.64	1 (2%)
2	SO4	D	813	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	E	810	-	4,4,4	0.23	0	6,6,6	0.08	0
3	ATP	C	806	4	28,33,33	0.66	0	34,52,52	0.68	1 (2%)
5	CDP	E	809	-	25,26,26	0.88	0	38,40,40	0.94	1 (2%)
2	SO4	F	810	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	G	802	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	E	801	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	D	810	-	4,4,4	0.23	0	6,6,6	0.09	0
5	CDP	A	809	-	25,26,26	0.93	1 (4%)	38,40,40	0.96	1 (2%)
5	CDP	C	809	-	25,26,26	0.89	0	38,40,40	1.01	1 (2%)
5	CDP	D	809	-	25,26,26	0.89	0	38,40,40	0.96	2 (5%)
3	ATP	D	806	4	28,33,33	0.66	0	34,52,52	0.66	1 (2%)
3	ATP	A	804	4	28,33,33	0.72	0	34,52,52	0.68	1 (2%)
5	CDP	F	809	-	25,26,26	0.90	1 (4%)	38,40,40	1.01	1 (2%)
2	SO4	E	802	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	E	804	4	28,33,33	0.69	0	34,52,52	0.67	1 (2%)
5	CDP	G	808	-	25,26,26	0.90	1 (4%)	38,40,40	0.94	1 (2%)
2	SO4	A	812	-	4,4,4	0.22	0	6,6,6	0.08	0
3	ATP	F	804	4	28,33,33	0.66	0	34,52,52	0.66	1 (2%)
2	SO4	H	809	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	B	802	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	G	809	-	4,4,4	0.21	0	6,6,6	0.11	0
3	ATP	D	804	4	28,33,33	0.67	0	34,52,52	0.67	1 (2%)
2	SO4	F	801	-	4,4,4	0.24	0	6,6,6	0.09	0
3	ATP	H	806	4	28,33,33	0.70	0	34,52,52	0.65	1 (2%)
5	CDP	B	809	-	25,26,26	0.91	1 (4%)	38,40,40	0.94	0
2	SO4	G	801	-	4,4,4	0.23	0	6,6,6	0.06	0
5	CDP	H	808	-	25,26,26	0.90	0	38,40,40	0.93	2 (5%)
2	SO4	A	811	-	4,4,4	0.23	0	6,6,6	0.07	0
3	ATP	B	806	4	28,33,33	0.66	0	34,52,52	0.62	1 (2%)
2	SO4	A	802	-	4,4,4	0.23	0	6,6,6	0.10	0
3	ATP	E	807	4	28,33,33	0.66	0	34,52,52	0.67	1 (2%)
2	SO4	A	814	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	D	811	-	4,4,4	0.24	0	6,6,6	0.09	0
3	ATP	D	807	4	28,33,33	0.69	0	34,52,52	0.62	1 (2%)
3	ATP	E	806	4	28,33,33	0.66	0	34,52,52	0.70	1 (2%)
3	ATP	G	805	4	28,33,33	0.69	0	34,52,52	0.69	1 (2%)
2	SO4	H	802	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	H	811	-	4,4,4	0.22	0	6,6,6	0.12	0
3	ATP	B	807	4	28,33,33	0.72	0	34,52,52	0.64	1 (2%)
3	ATP	A	807	4	28,33,33	0.72	0	34,52,52	0.68	1 (2%)
3	ATP	H	805	4	28,33,33	0.67	0	34,52,52	0.68	1 (2%)
2	SO4	A	801	-	4,4,4	0.22	0	6,6,6	0.12	0
2	SO4	B	810	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	C	801	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	D	801	-	4,4,4	0.23	0	6,6,6	0.07	0
3	ATP	F	807	4	28,33,33	0.71	0	34,52,52	0.68	1 (2%)
3	ATP	A	806	4	28,33,33	0.70	0	34,52,52	0.67	1 (2%)
2	SO4	F	802	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	H	810	-	4,4,4	0.23	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	C	807	4	-	5/18/38/38	0/3/3/3
3	ATP	G	803	4	-	0/18/38/38	0/3/3/3
3	ATP	F	806	4	-	4/18/38/38	0/3/3/3
3	ATP	H	803	4	-	2/18/38/38	0/3/3/3
3	ATP	B	804	4	-	2/18/38/38	0/3/3/3
3	ATP	C	804	4	-	2/18/38/38	0/3/3/3
5	CDP	E	809	-	-	4/16/32/32	0/2/2/2
3	ATP	G	806	4	-	6/18/38/38	0/3/3/3
3	ATP	C	806	4	-	7/18/38/38	0/3/3/3
5	CDP	A	809	-	-	7/16/32/32	0/2/2/2
5	CDP	C	809	-	-	7/16/32/32	0/2/2/2
5	CDP	D	809	-	-	5/16/32/32	0/2/2/2
3	ATP	D	806	4	-	7/18/38/38	0/3/3/3
3	ATP	A	804	4	-	0/18/38/38	0/3/3/3
5	CDP	F	809	-	-	7/16/32/32	0/2/2/2
3	ATP	E	804	4	-	0/18/38/38	0/3/3/3
5	CDP	G	808	-	-	7/16/32/32	0/2/2/2
3	ATP	F	804	4	-	0/18/38/38	0/3/3/3
5	CDP	B	809	-	-	6/16/32/32	0/2/2/2
3	ATP	H	806	4	-	7/18/38/38	0/3/3/3
3	ATP	D	804	4	-	0/18/38/38	0/3/3/3
5	CDP	H	808	-	-	5/16/32/32	0/2/2/2
3	ATP	B	806	4	-	8/18/38/38	0/3/3/3
3	ATP	E	806	4	-	6/18/38/38	0/3/3/3
3	ATP	G	805	4	-	8/18/38/38	0/3/3/3
3	ATP	B	807	4	-	6/18/38/38	0/3/3/3
3	ATP	A	807	4	-	7/18/38/38	0/3/3/3
3	ATP	H	805	4	-	5/18/38/38	0/3/3/3
3	ATP	E	807	4	-	7/18/38/38	0/3/3/3
3	ATP	F	807	4	-	7/18/38/38	0/3/3/3
3	ATP	A	806	4	-	5/18/38/38	0/3/3/3
3	ATP	D	807	4	-	6/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	809	CDP	PA-O3A	2.26	1.61	1.59
5	B	809	CDP	PA-O3A	2.09	1.61	1.59
5	F	809	CDP	PA-O3A	2.06	1.61	1.59
5	G	808	CDP	PA-O3A	2.04	1.61	1.59

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	803	ATP	C5-C6-N6	2.57	124.23	120.31
3	G	806	ATP	C5-C6-N6	2.55	124.19	120.31
3	E	807	ATP	C5-C6-N6	2.50	124.11	120.31
3	A	807	ATP	C5-C6-N6	2.46	124.06	120.31
3	A	804	ATP	C5-C6-N6	2.46	124.06	120.31
3	B	804	ATP	C5-C6-N6	2.46	124.06	120.31
3	B	807	ATP	C5-C6-N6	2.43	124.02	120.31
3	E	806	ATP	C5-C6-N6	2.42	123.99	120.31
3	E	804	ATP	C5-C6-N6	2.42	123.99	120.31
3	G	803	ATP	C5-C6-N6	2.41	123.98	120.31
3	F	804	ATP	C5-C6-N6	2.40	123.96	120.31
3	D	806	ATP	C5-C6-N6	2.39	123.96	120.31
3	A	806	ATP	C5-C6-N6	2.39	123.95	120.31
3	H	805	ATP	C5-C6-N6	2.38	123.94	120.31
3	F	807	ATP	C5-C6-N6	2.38	123.94	120.31
3	C	807	ATP	C5-C6-N6	2.38	123.93	120.31
3	F	806	ATP	C5-C6-N6	2.37	123.92	120.31
3	C	806	ATP	C5-C6-N6	2.36	123.91	120.31
3	H	806	ATP	C5-C6-N6	2.36	123.90	120.31
5	C	809	CDP	C3'-C2'-C1'	2.35	105.91	101.46
3	C	804	ATP	C5-C6-N6	2.35	123.89	120.31
3	G	805	ATP	C5-C6-N6	2.34	123.88	120.31
3	D	804	ATP	C5-C6-N6	2.32	123.85	120.31
3	B	806	ATP	C5-C6-N6	2.30	123.81	120.31
5	F	809	CDP	C3'-C2'-C1'	2.29	105.79	101.46
3	D	807	ATP	C5-C6-N6	2.26	123.75	120.31
5	E	809	CDP	C3'-C2'-C1'	2.19	105.61	101.46
5	D	809	CDP	O2-C2-N3	-2.17	118.91	122.33
5	A	809	CDP	C3'-C2'-C1'	2.03	105.31	101.46
5	H	808	CDP	O2-C2-N3	-2.01	119.16	122.33
5	H	808	CDP	C3'-C2'-C1'	2.01	105.26	101.46
5	D	809	CDP	O2A-PA-O1A	2.01	121.78	112.44
5	G	808	CDP	O2B-PB-O3B	2.00	115.30	107.80

There are no chirality outliers.

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	806	ATP	PB-O3B-PG-O3G
3	A	807	ATP	C5'-O5'-PA-O2A
3	B	806	ATP	PB-O3B-PG-O3G
3	B	806	ATP	C5'-O5'-PA-O1A
3	C	806	ATP	PB-O3B-PG-O3G
3	C	806	ATP	C5'-O5'-PA-O1A
3	D	806	ATP	PB-O3B-PG-O2G
3	D	806	ATP	PB-O3B-PG-O3G
3	D	806	ATP	C5'-O5'-PA-O1A
3	D	807	ATP	C5'-O5'-PA-O1A
3	D	807	ATP	C5'-O5'-PA-O2A
3	D	807	ATP	C5'-O5'-PA-O3A
3	E	806	ATP	PB-O3B-PG-O3G
3	E	807	ATP	C5'-O5'-PA-O2A
3	F	807	ATP	C5'-O5'-PA-O2A
3	G	805	ATP	PB-O3B-PG-O3G
3	G	805	ATP	C5'-O5'-PA-O1A
3	G	806	ATP	C5'-O5'-PA-O2A
3	H	805	ATP	PB-O3B-PG-O3G
3	H	806	ATP	C5'-O5'-PA-O1A
3	H	806	ATP	C5'-O5'-PA-O2A
3	H	806	ATP	C5'-O5'-PA-O3A
5	A	809	CDP	C5'-O5'-PA-O3A
5	A	809	CDP	C5'-O5'-PA-O1A
5	B	809	CDP	PA-O3A-PB-O3B
5	B	809	CDP	PA-O3A-PB-O2B
5	B	809	CDP	C5'-O5'-PA-O1A
5	C	809	CDP	PA-O3A-PB-O3B
5	C	809	CDP	C5'-O5'-PA-O3A
5	C	809	CDP	C5'-O5'-PA-O2A
5	D	809	CDP	PA-O3A-PB-O3B
5	D	809	CDP	C5'-O5'-PA-O3A
5	D	809	CDP	C5'-O5'-PA-O1A
5	E	809	CDP	C5'-O5'-PA-O2A
5	F	809	CDP	C5'-O5'-PA-O3A
5	F	809	CDP	C5'-O5'-PA-O1A
5	F	809	CDP	C5'-O5'-PA-O2A
5	G	808	CDP	PA-O3A-PB-O3B
5	G	808	CDP	C5'-O5'-PA-O3A
5	G	808	CDP	C5'-O5'-PA-O2A
5	H	808	CDP	PA-O3A-PB-O3B
5	H	808	CDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	H	808	CDP	C5'-O5'-PA-O1A
5	C	809	CDP	O4'-C4'-C5'-O5'
5	F	809	CDP	O4'-C4'-C5'-O5'
5	A	809	CDP	O4'-C4'-C5'-O5'
5	G	808	CDP	O4'-C4'-C5'-O5'
5	H	808	CDP	O4'-C4'-C5'-O5'
5	F	809	CDP	PA-O3A-PB-O1B
5	C	809	CDP	C3'-C4'-C5'-O5'
3	B	806	ATP	PG-O3B-PB-O1B
3	B	806	ATP	PA-O3A-PB-O1B
3	C	806	ATP	PA-O3A-PB-O1B
3	G	805	ATP	PA-O3A-PB-O1B
5	F	809	CDP	C3'-C4'-C5'-O5'
3	G	805	ATP	PB-O3B-PG-O2G
5	E	809	CDP	PA-O3A-PB-O3B
3	B	804	ATP	PB-O3A-PA-O1A
3	B	807	ATP	PG-O3B-PB-O2B
3	B	807	ATP	PB-O3A-PA-O2A
3	C	807	ATP	PG-O3B-PB-O2B
3	D	807	ATP	PG-O3B-PB-O2B
3	F	807	ATP	PG-O3B-PB-O2B
3	G	806	ATP	PG-O3B-PB-O2B
3	H	803	ATP	PB-O3A-PA-O1A
3	H	805	ATP	PA-O3A-PB-O2B
5	D	809	CDP	O4'-C4'-C5'-O5'
5	E	809	CDP	O4'-C4'-C5'-O5'
3	A	806	ATP	C5'-O5'-PA-O1A
3	A	807	ATP	C5'-O5'-PA-O1A
3	A	807	ATP	C5'-O5'-PA-O3A
3	B	807	ATP	C5'-O5'-PA-O1A
3	B	807	ATP	C5'-O5'-PA-O2A
3	C	807	ATP	C5'-O5'-PA-O1A
3	D	806	ATP	C5'-O5'-PA-O3A
3	E	806	ATP	C5'-O5'-PA-O1A
3	E	807	ATP	C5'-O5'-PA-O1A
3	E	807	ATP	C5'-O5'-PA-O3A
3	F	806	ATP	C5'-O5'-PA-O1A
3	F	807	ATP	C5'-O5'-PA-O1A
3	F	807	ATP	C5'-O5'-PA-O3A
3	G	806	ATP	C5'-O5'-PA-O1A
3	H	805	ATP	C5'-O5'-PA-O1A
5	A	809	CDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	B	809	CDP	C5'-O5'-PA-O3A
5	C	809	CDP	C5'-O5'-PA-O1A
5	D	809	CDP	C5'-O5'-PA-O2A
5	E	809	CDP	C5'-O5'-PA-O3A
5	G	808	CDP	C5'-O5'-PA-O1A
5	H	808	CDP	C5'-O5'-PA-O2A
3	A	806	ATP	PA-O3A-PB-O2B
3	A	807	ATP	PG-O3B-PB-O2B
3	A	807	ATP	PB-O3A-PA-O2A
3	B	807	ATP	PA-O3A-PB-O1B
3	C	807	ATP	PB-O3A-PA-O2A
3	D	806	ATP	PG-O3B-PB-O1B
3	D	807	ATP	PB-O3A-PA-O2A
3	E	806	ATP	PA-O3A-PB-O1B
3	E	807	ATP	PG-O3B-PB-O2B
3	F	806	ATP	PA-O3A-PB-O2B
3	F	807	ATP	PB-O3A-PA-O2A
3	G	806	ATP	PB-O3A-PA-O2A
3	H	806	ATP	PG-O3B-PB-O1B
3	H	806	ATP	PB-O3A-PA-O2A
3	F	806	ATP	PB-O3B-PG-O1G
5	B	809	CDP	O4'-C4'-C5'-O5'
3	B	806	ATP	PA-O3A-PB-O2B
3	C	804	ATP	PB-O3A-PA-O1A
3	D	806	ATP	PA-O3A-PB-O1B
3	E	806	ATP	PA-O3A-PB-O2B
3	E	807	ATP	PB-O3A-PA-O1A
3	E	807	ATP	PB-O3A-PA-O2A
3	G	805	ATP	PG-O3B-PB-O1B
3	G	805	ATP	PA-O3A-PB-O2B
3	C	806	ATP	PB-O3B-PG-O1G
3	E	806	ATP	PB-O3B-PG-O1G
3	G	805	ATP	PB-O3B-PG-O1G
5	B	809	CDP	PA-O3A-PB-O1B
5	C	809	CDP	PA-O3A-PB-O1B
5	G	808	CDP	PA-O3A-PB-O1B
3	B	806	ATP	PB-O3B-PG-O2G
3	C	806	ATP	PB-O3B-PG-O2G
3	H	805	ATP	PB-O3B-PG-O2G
5	A	809	CDP	PA-O3A-PB-O3B
5	A	809	CDP	PA-O3A-PB-O2B
5	F	809	CDP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	B	806	ATP	PB-O3A-PA-O2A
3	B	807	ATP	PG-O3B-PB-O1B
3	C	806	ATP	PA-O3A-PB-O2B
3	C	806	ATP	PB-O3A-PA-O2A
3	C	807	ATP	PG-O3B-PB-O1B
3	C	807	ATP	PB-O3A-PA-O1A
3	F	807	ATP	PG-O3B-PB-O1B
3	F	807	ATP	PB-O3A-PA-O1A
3	G	805	ATP	PB-O3A-PA-O2A
3	G	806	ATP	PG-O3B-PB-O1B
3	G	806	ATP	PB-O3A-PA-O1A
3	H	805	ATP	PA-O3A-PB-O1B
3	H	806	ATP	PG-O3B-PB-O2B
3	H	806	ATP	PB-O3A-PA-O1A
5	A	809	CDP	C3'-C4'-C5'-O5'
5	G	808	CDP	C3'-C4'-C5'-O5'
3	A	806	ATP	PA-O3A-PB-O1B
3	A	806	ATP	PB-O3A-PA-O2A
3	A	807	ATP	PG-O3B-PB-O1B
3	A	807	ATP	PB-O3A-PA-O1A
3	B	804	ATP	PB-O3A-PA-O2A
3	B	806	ATP	PG-O3B-PB-O2B
3	C	804	ATP	PB-O3A-PA-O2A
3	D	806	ATP	PB-O3A-PA-O2A
3	D	807	ATP	PB-O3A-PA-O1A
3	E	806	ATP	PB-O3A-PA-O2A
3	E	807	ATP	PG-O3B-PB-O1B
3	F	806	ATP	PA-O3A-PB-O1B
3	H	803	ATP	PB-O3A-PA-O2A

There are no ring outliers.

27 monomers are involved in 41 short contacts:

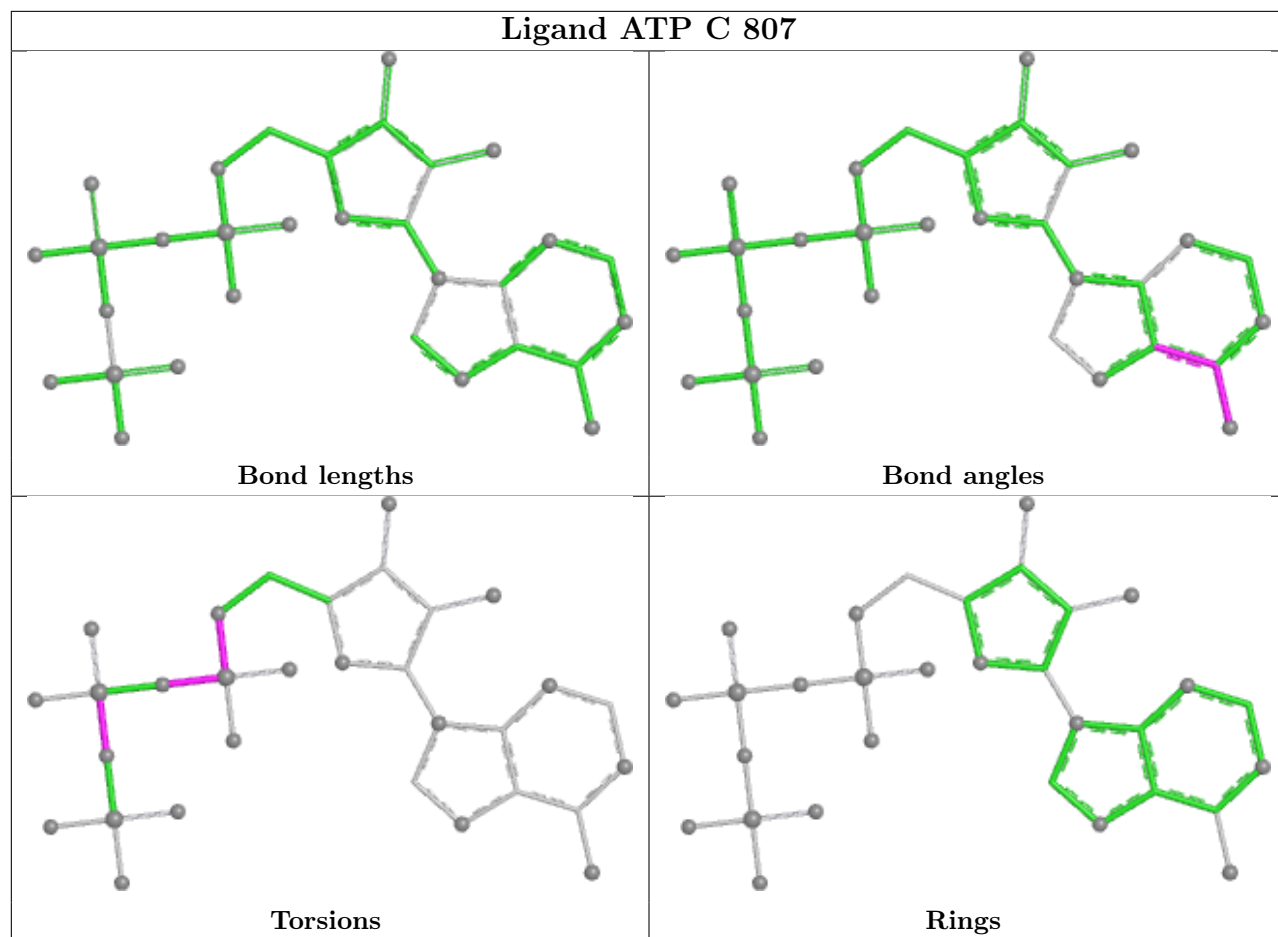
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	803	ATP	1	0
3	H	803	ATP	2	0
2	D	812	SO4	1	0
3	B	804	ATP	2	0
3	C	804	ATP	1	0
5	E	809	CDP	2	0
2	F	810	SO4	1	0
2	D	810	SO4	1	0

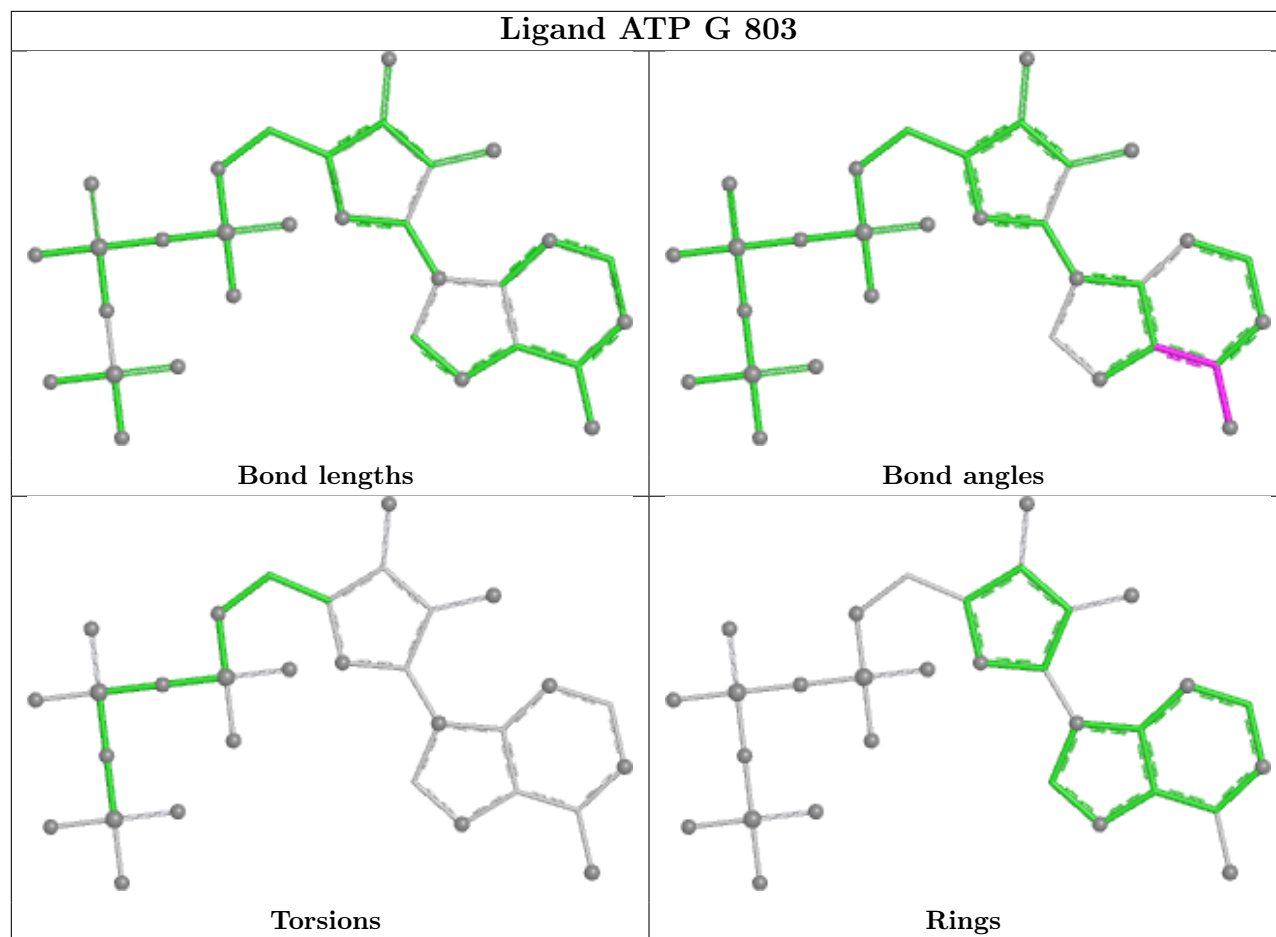
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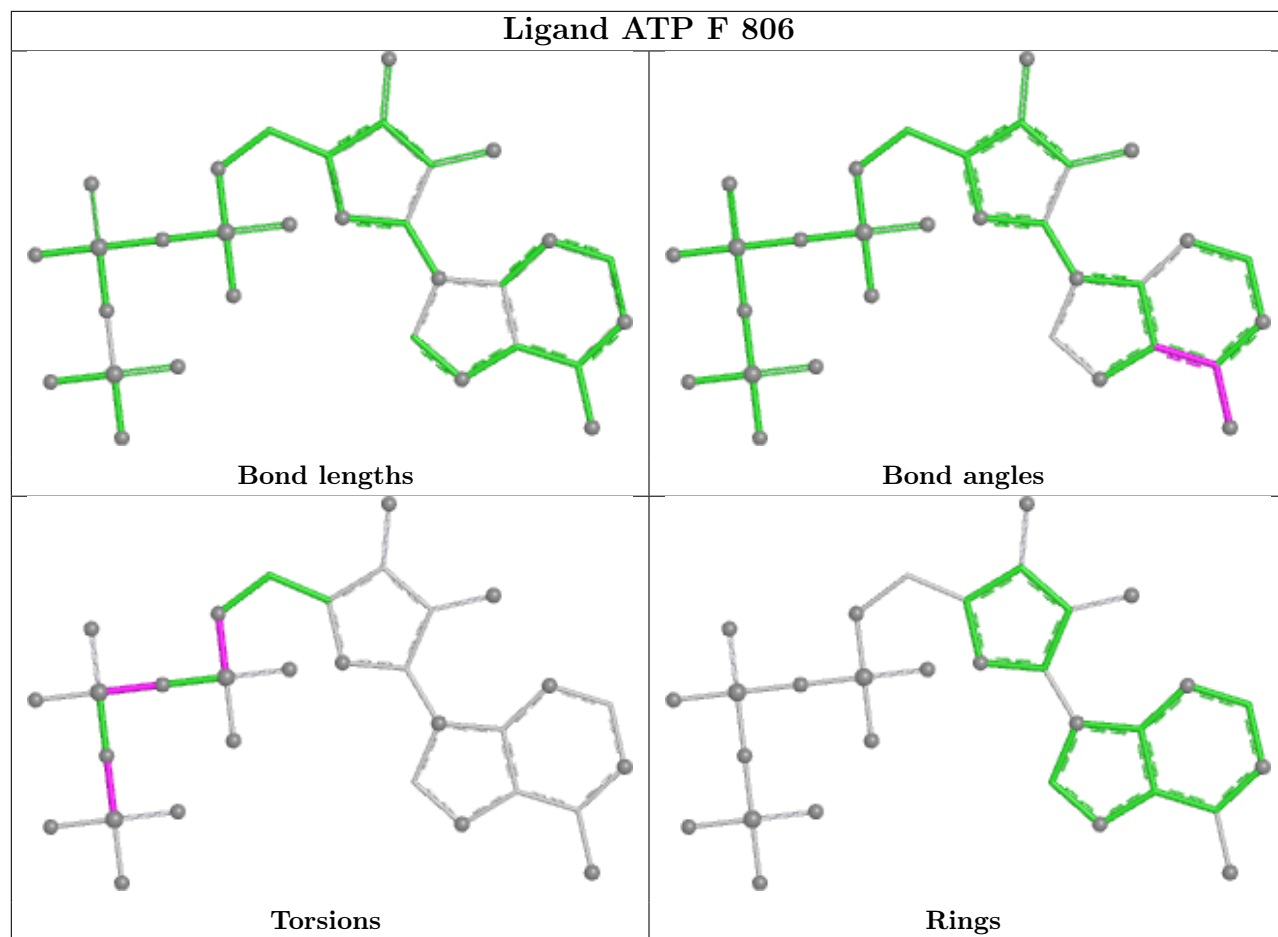
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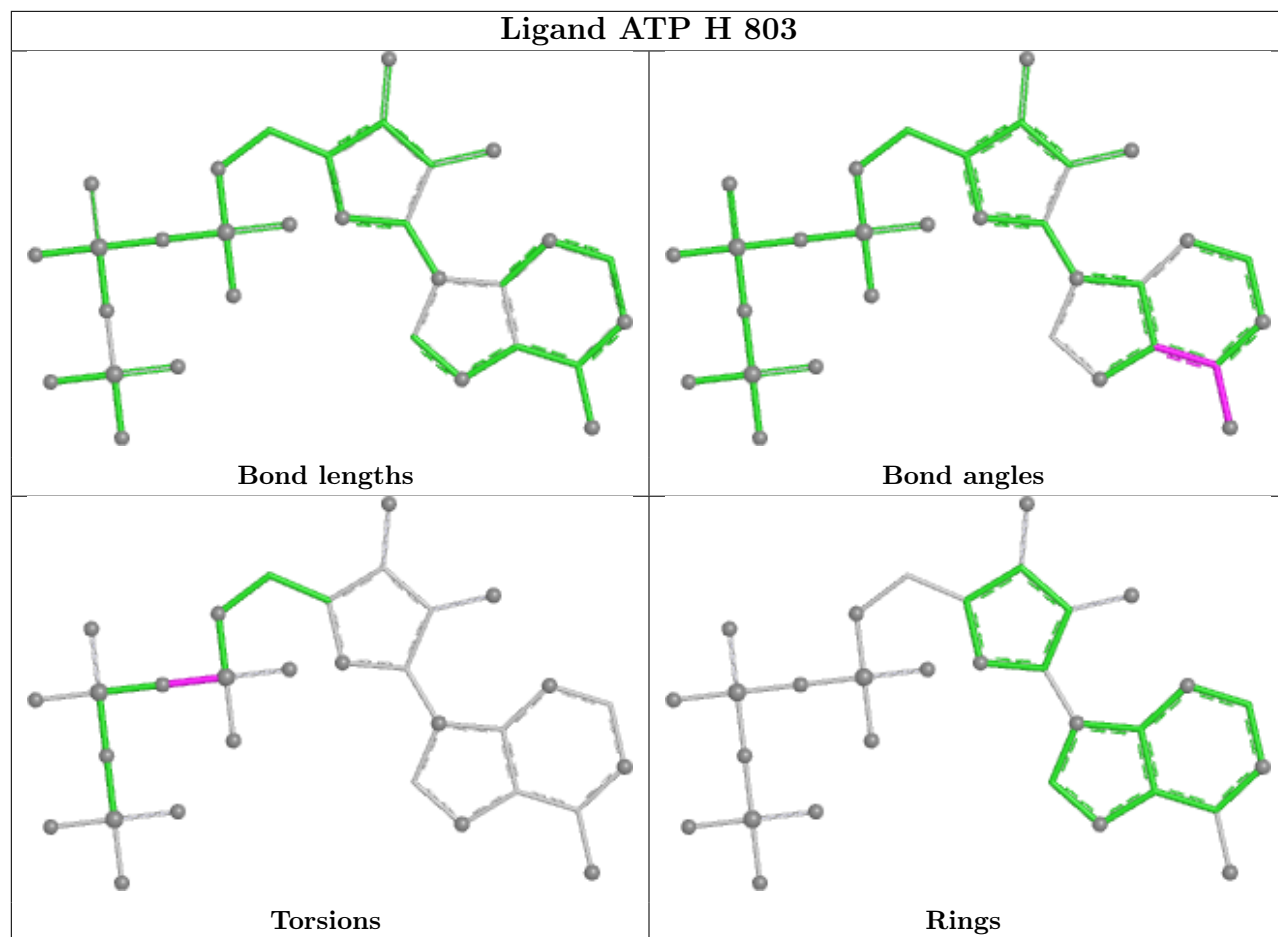
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	809	CDP	2	0
5	C	809	CDP	2	0
5	D	809	CDP	2	0
3	A	804	ATP	2	0
5	F	809	CDP	3	0
2	E	802	SO4	1	0
2	B	801	SO4	1	0
3	E	804	ATP	2	0
5	G	808	CDP	2	0
3	F	804	ATP	2	0
2	G	809	SO4	1	0
3	D	804	ATP	1	0
2	F	801	SO4	1	0
5	B	809	CDP	2	0
2	G	801	SO4	1	0
5	H	808	CDP	2	0
2	D	811	SO4	1	0
2	A	801	SO4	1	0
2	D	801	SO4	1	0

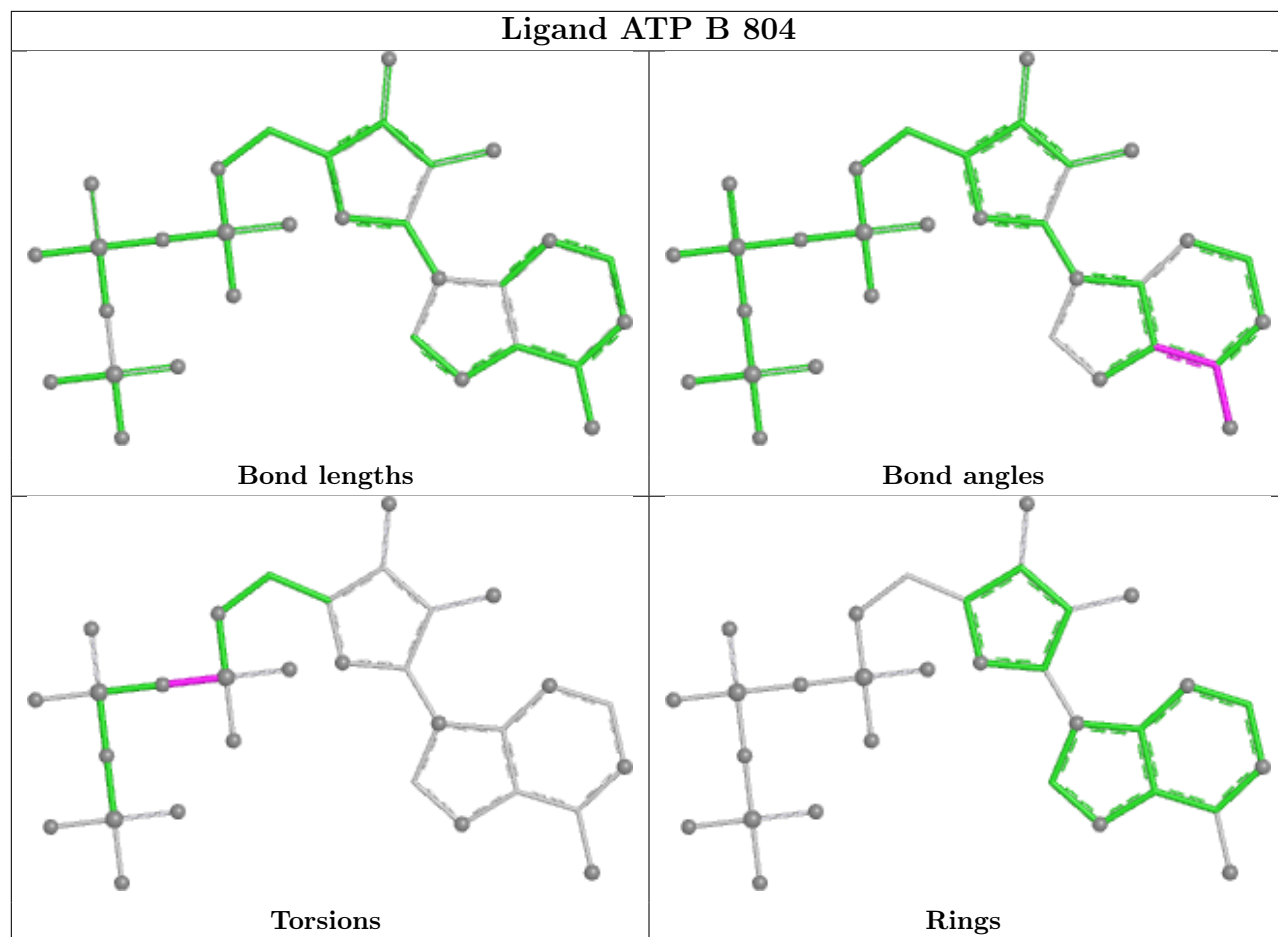
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



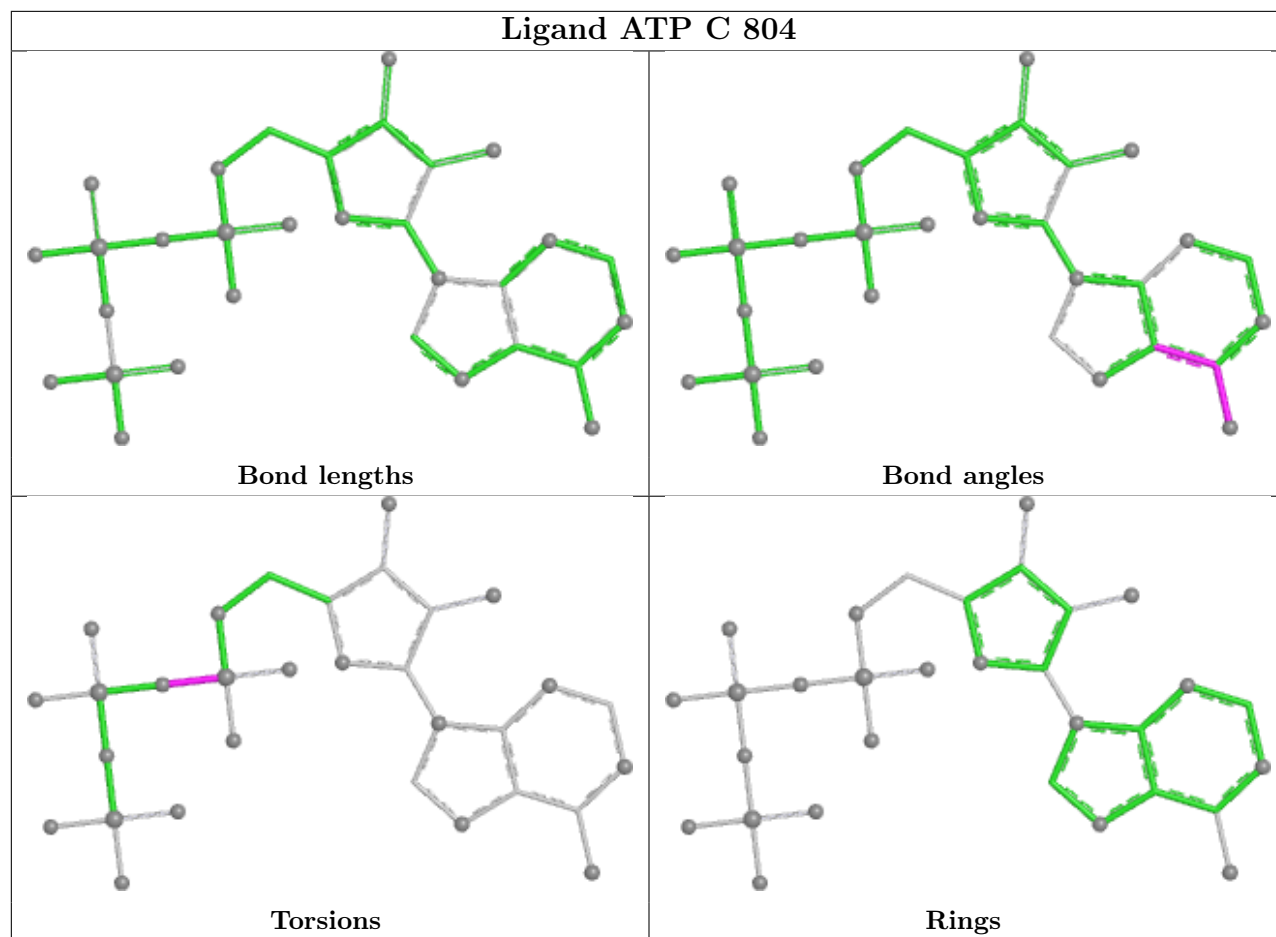


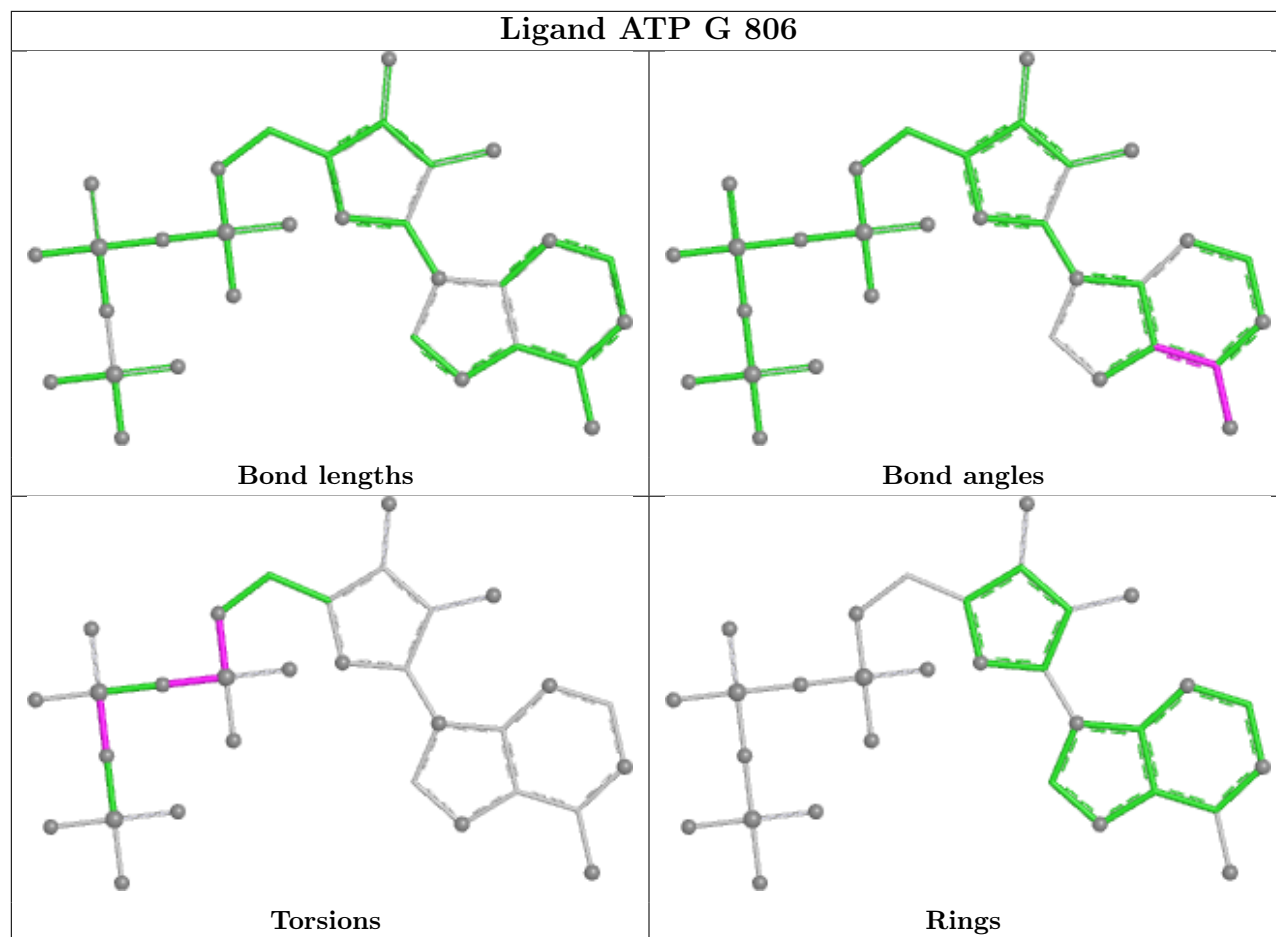


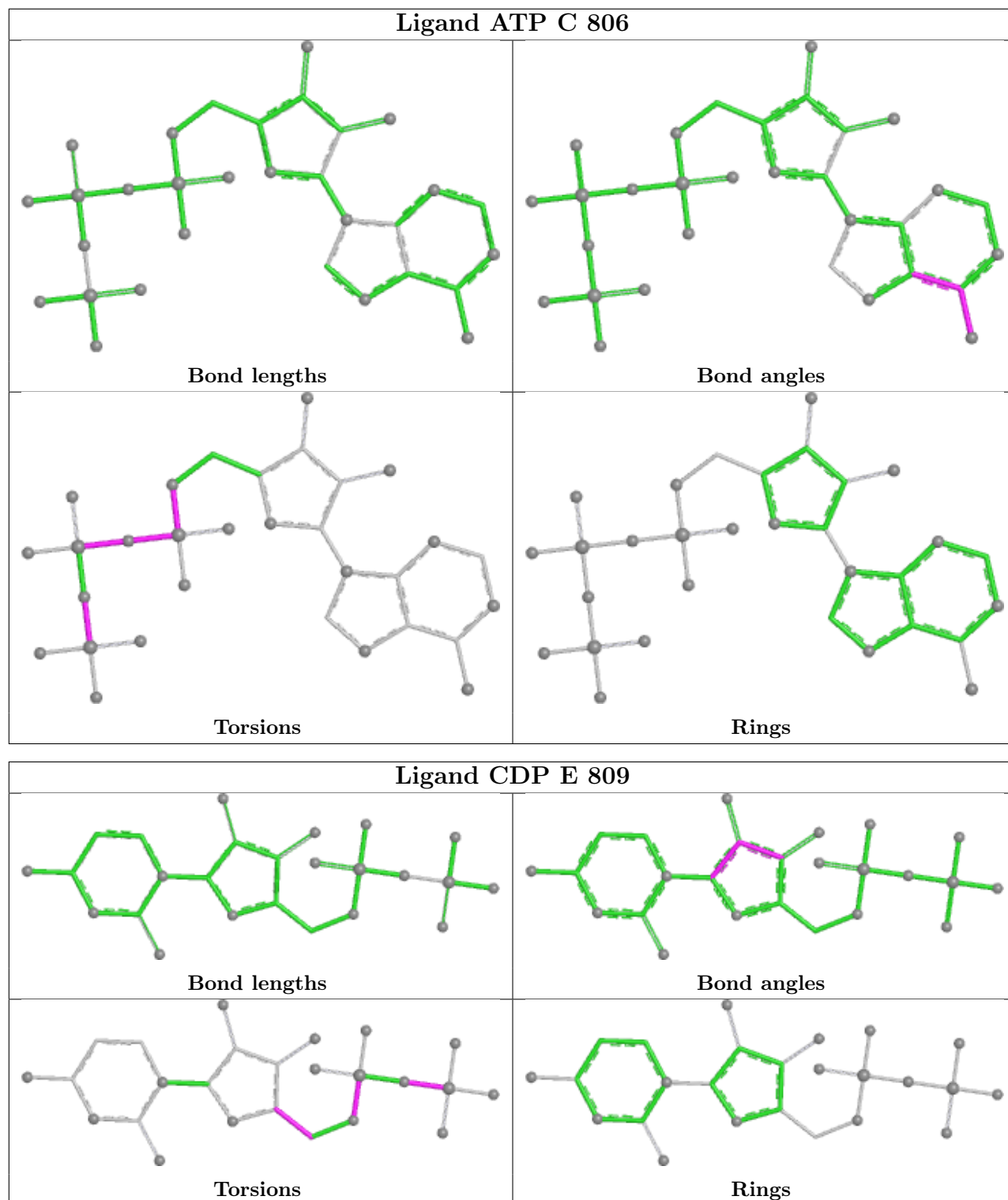


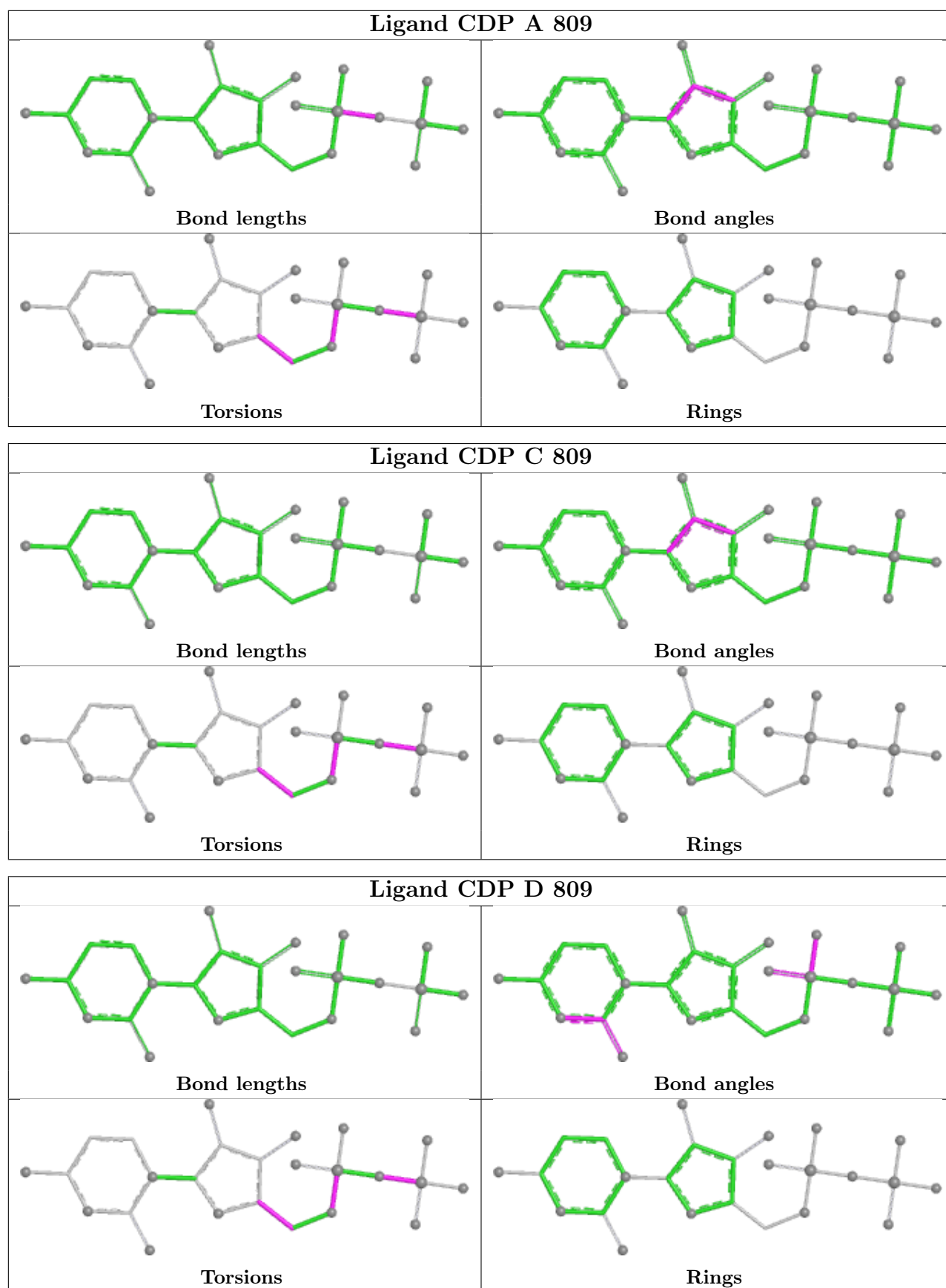


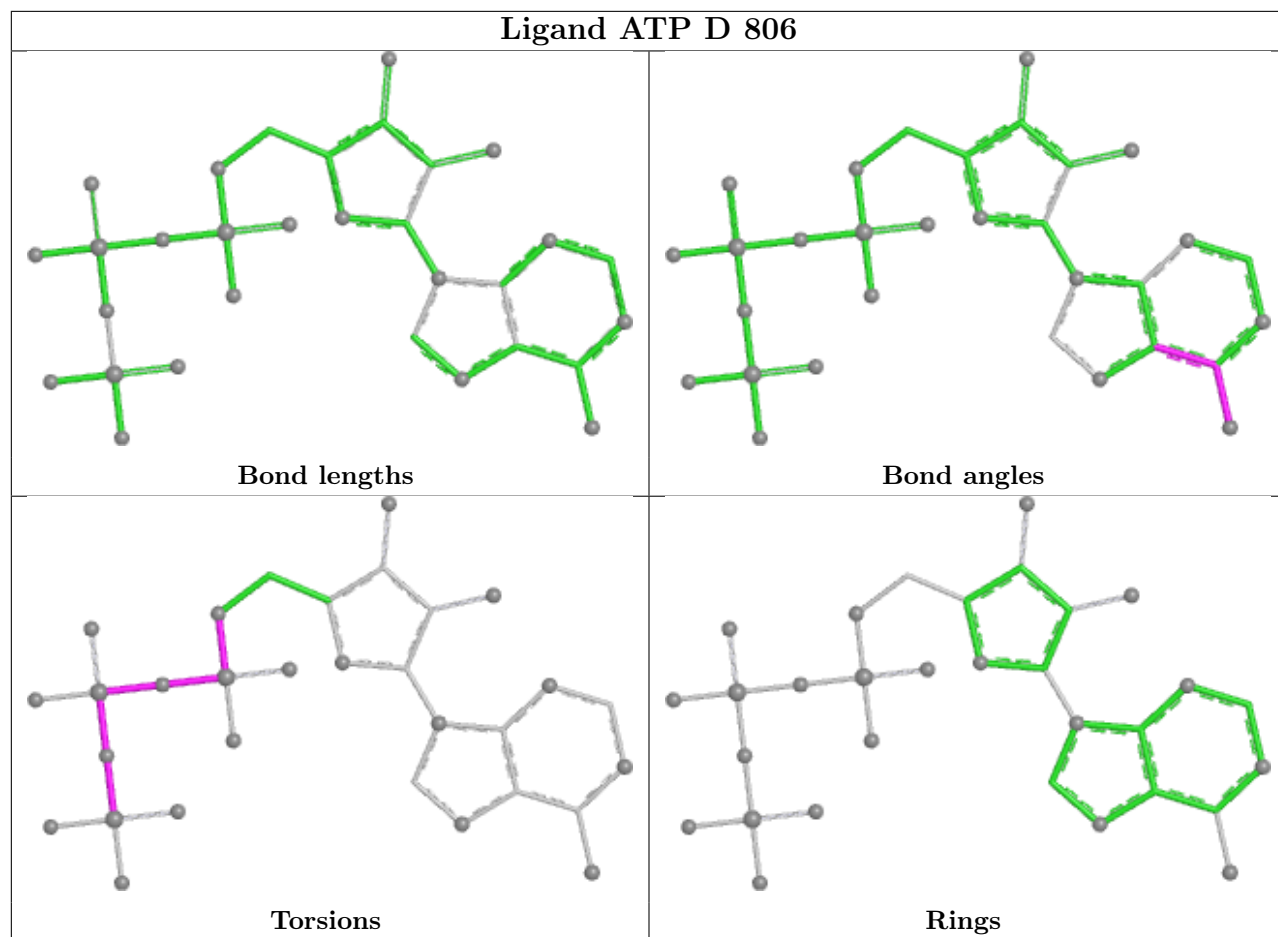


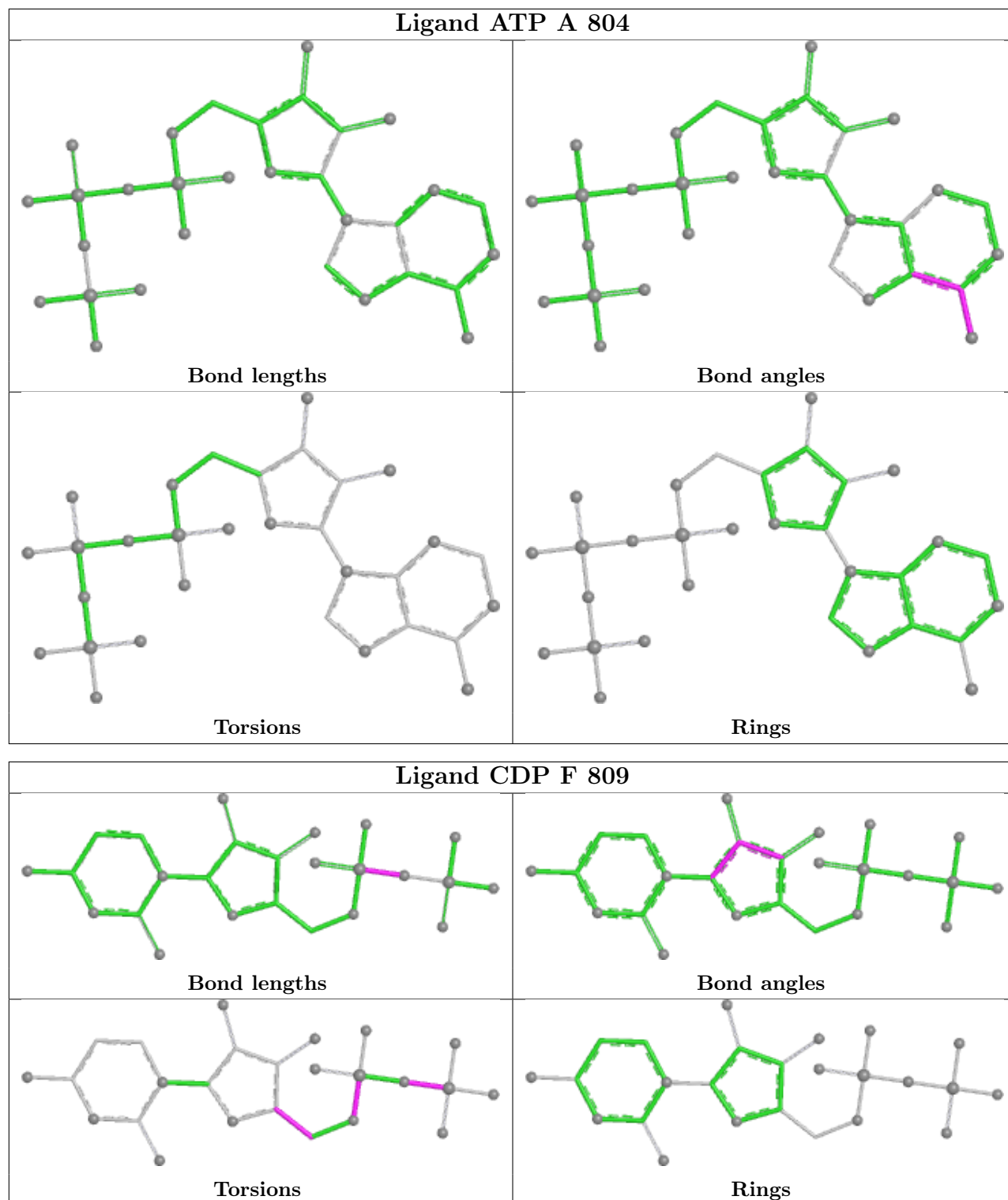


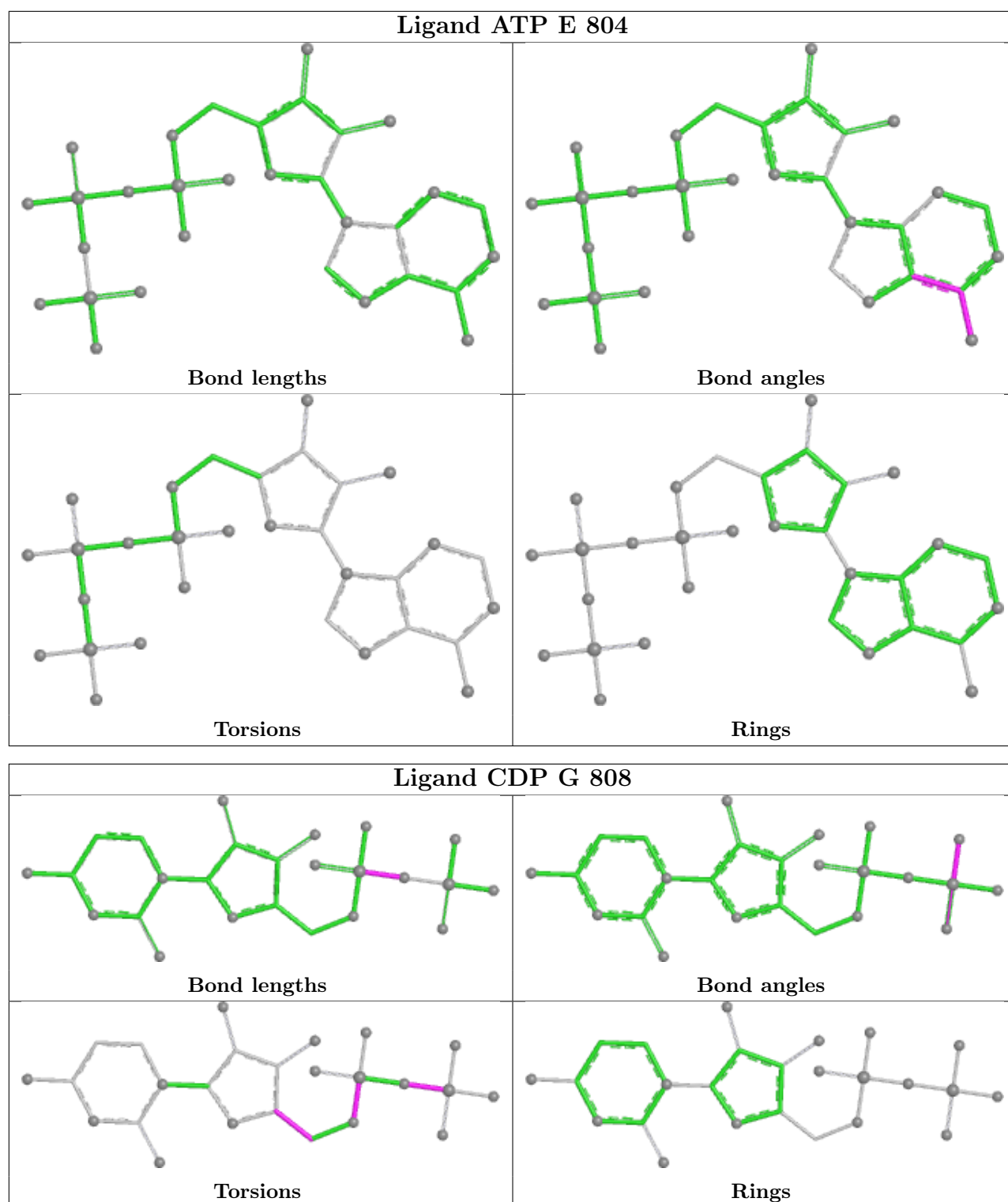


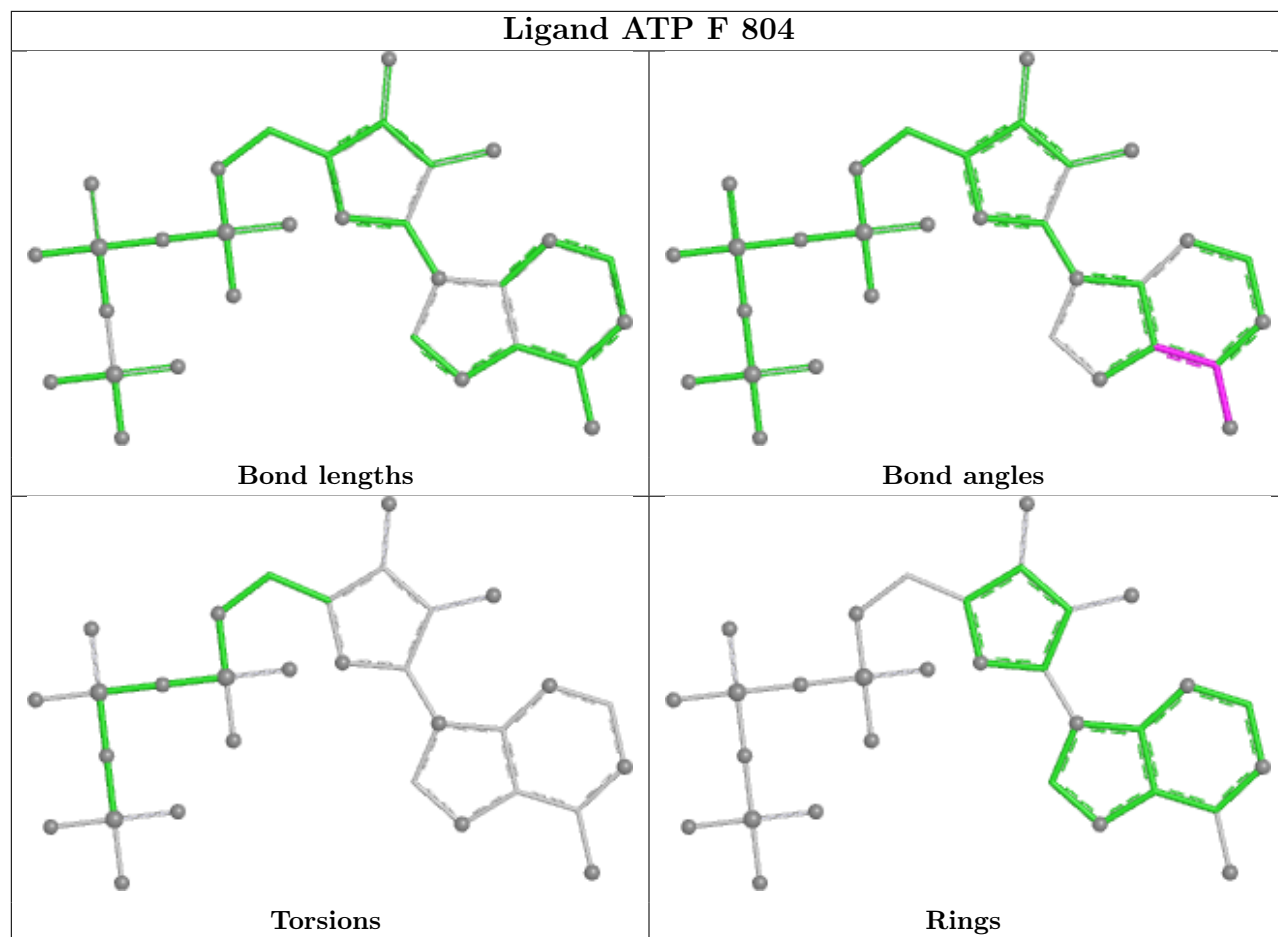




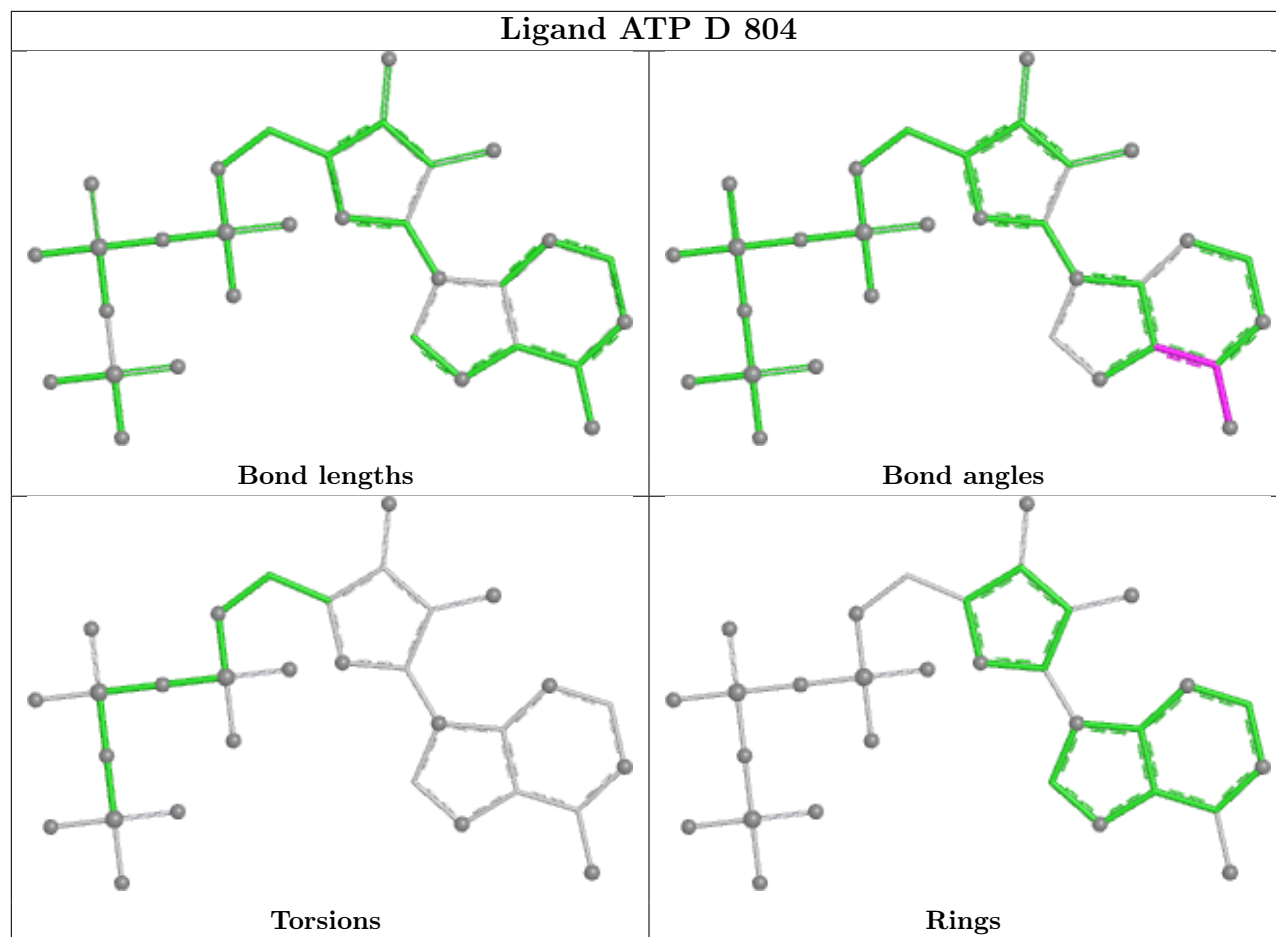


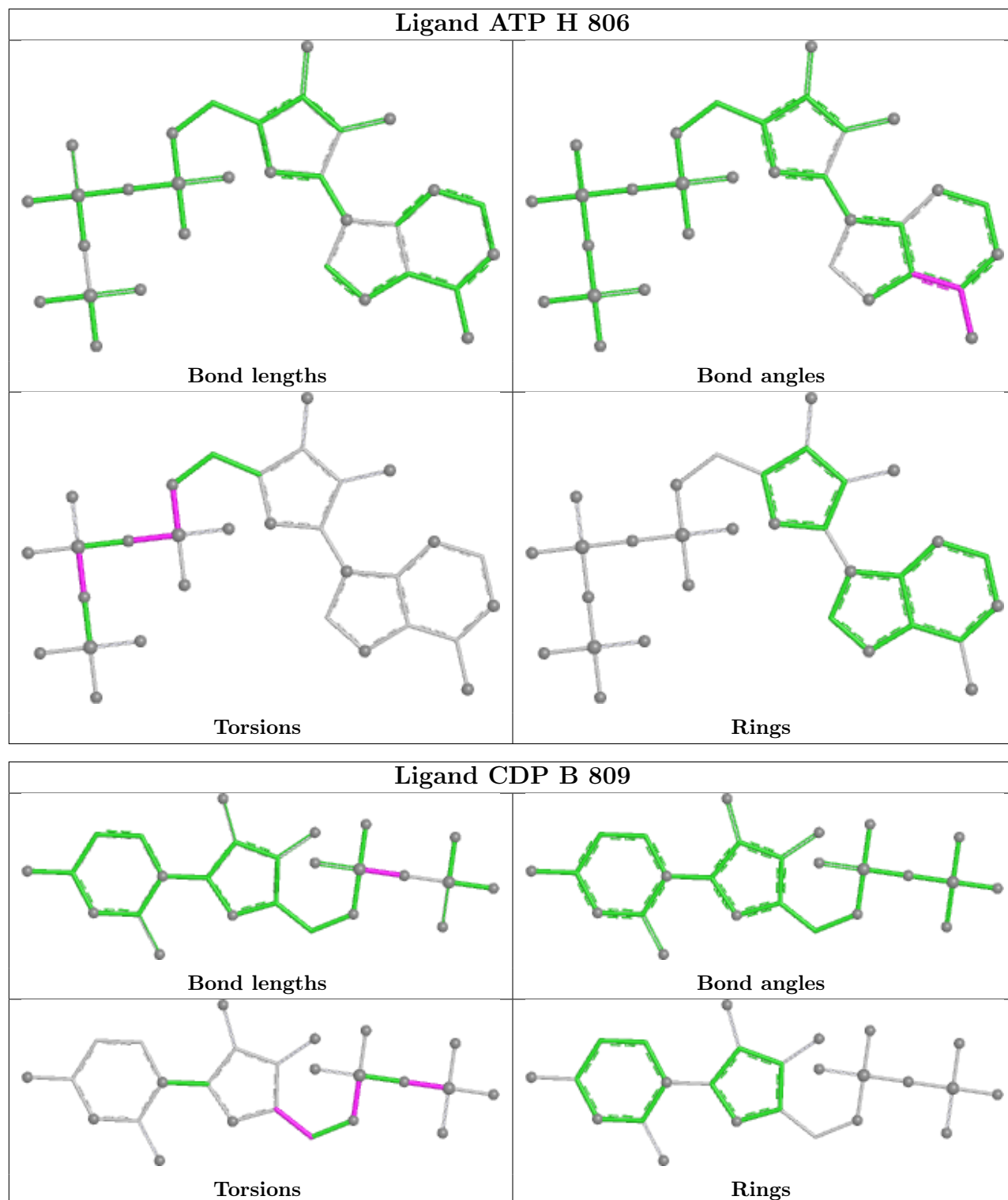


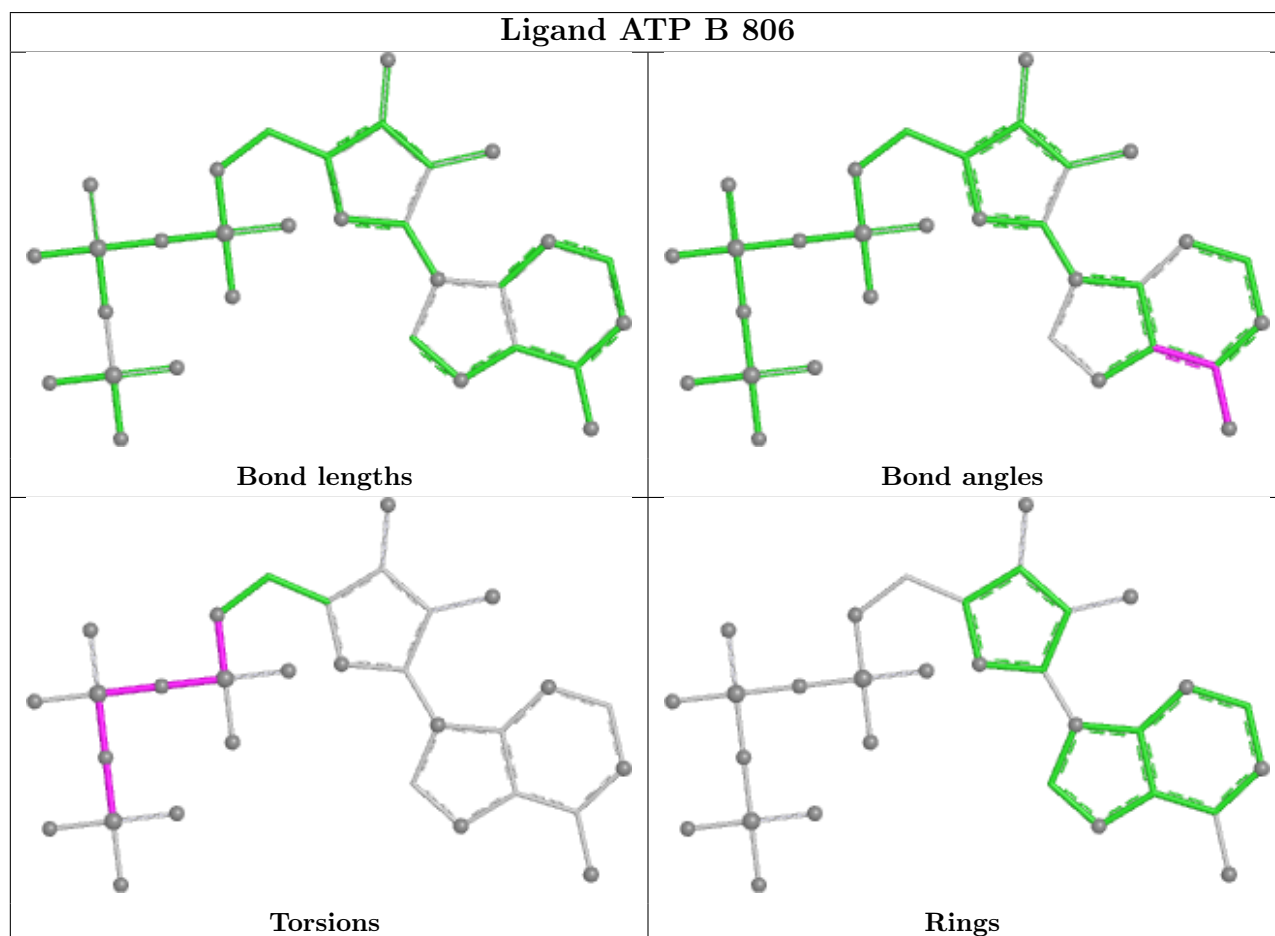
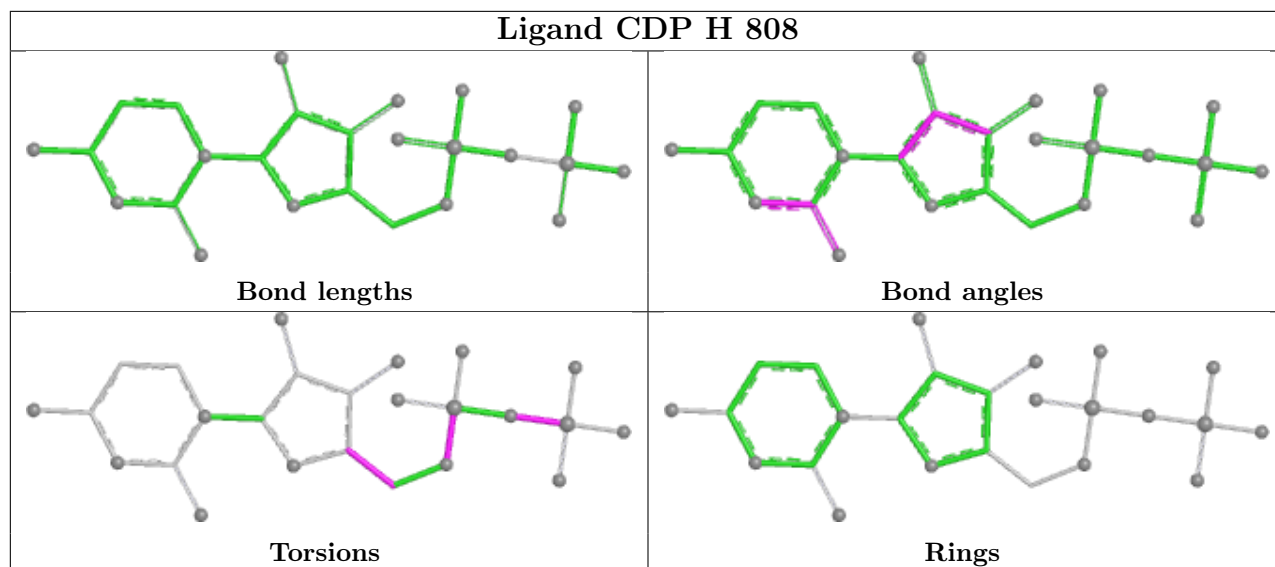


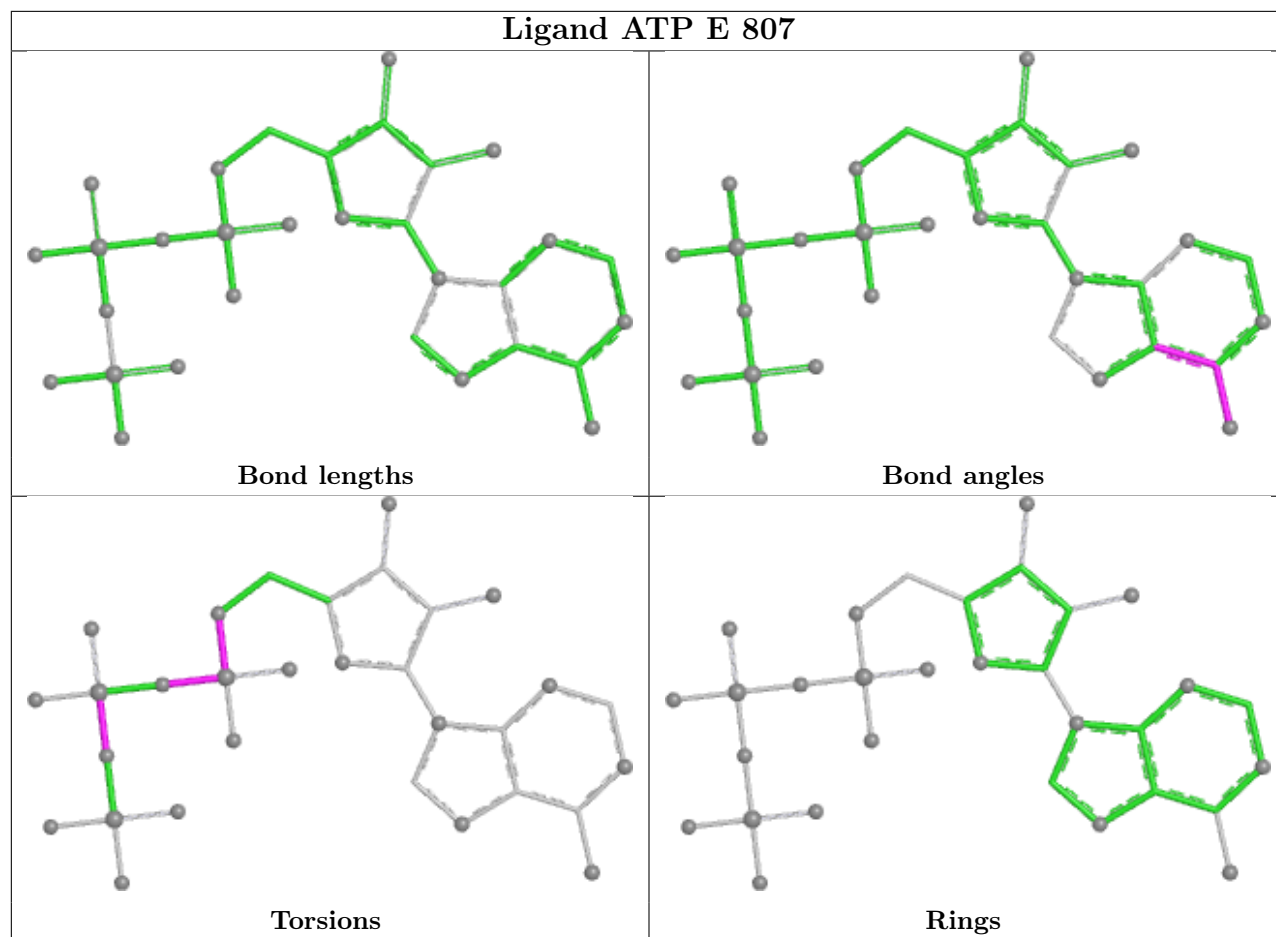


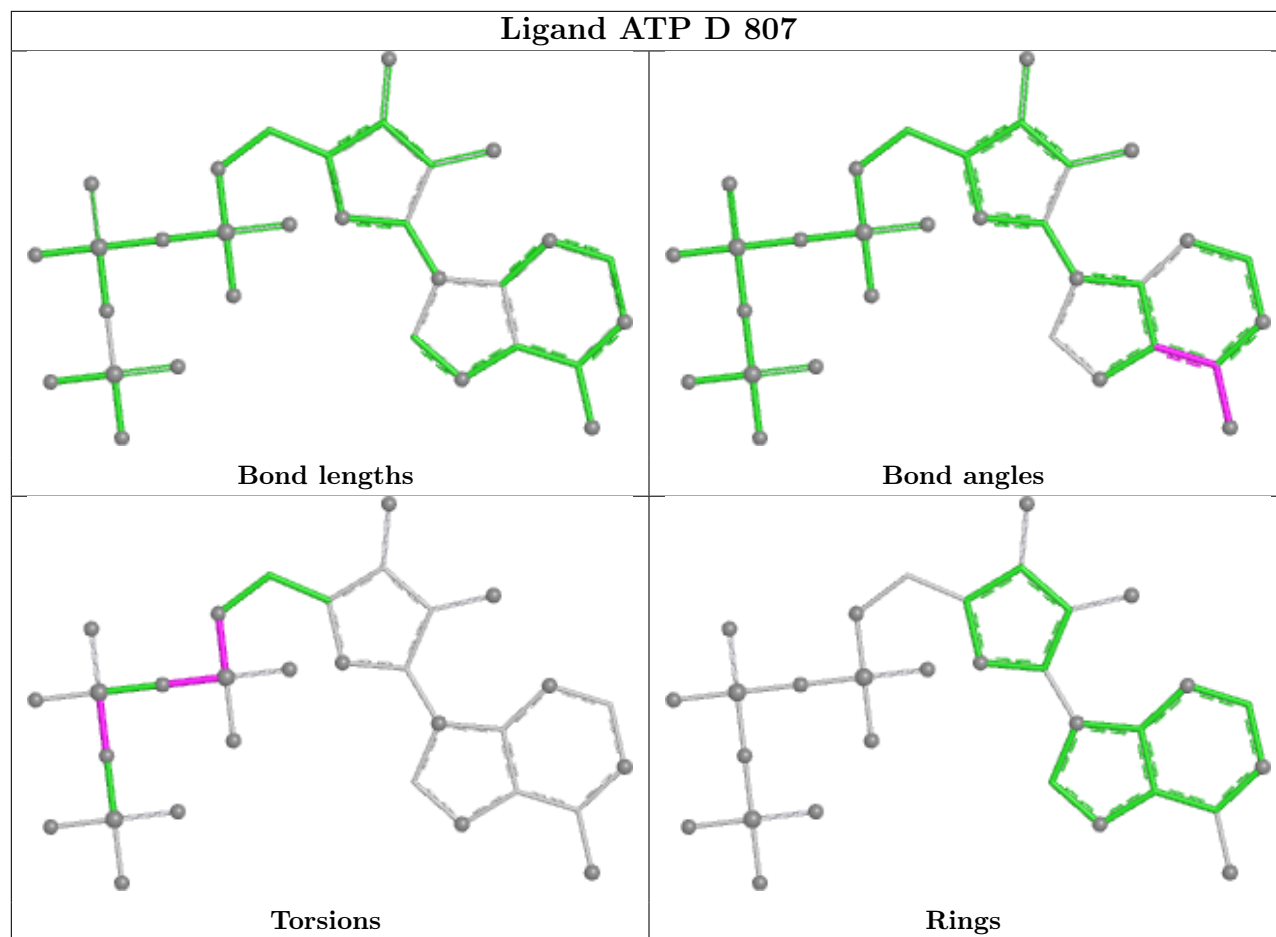


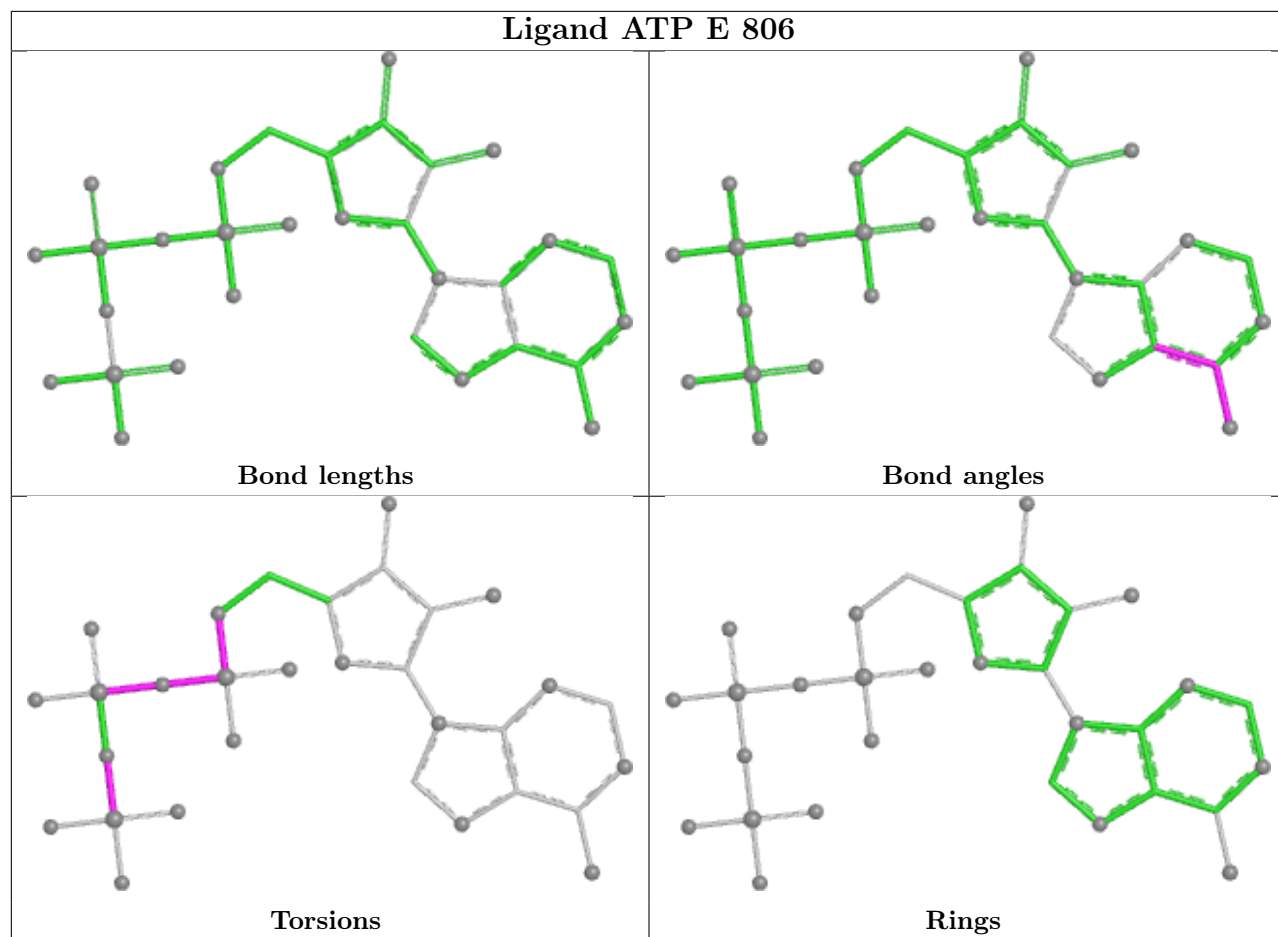


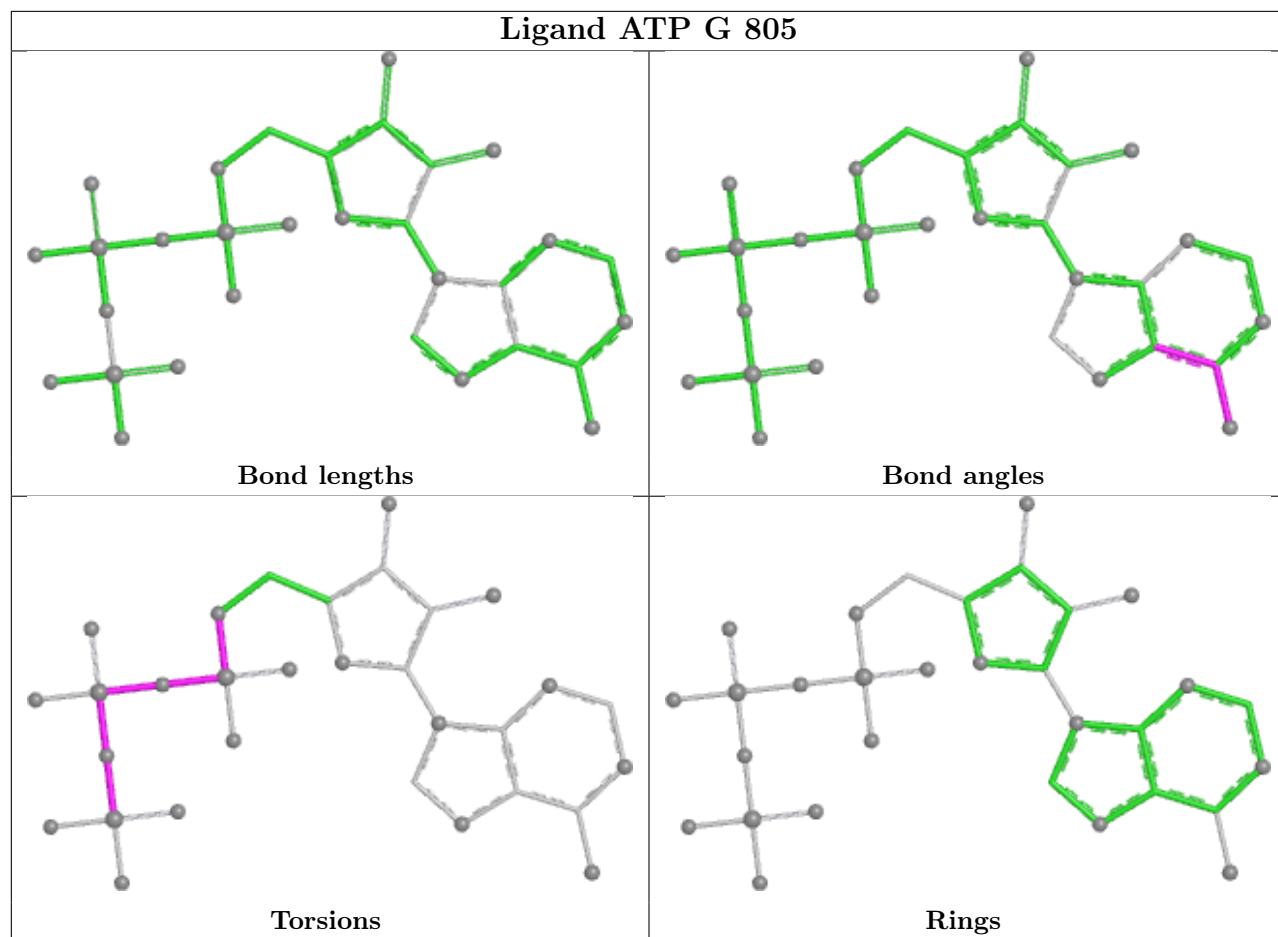


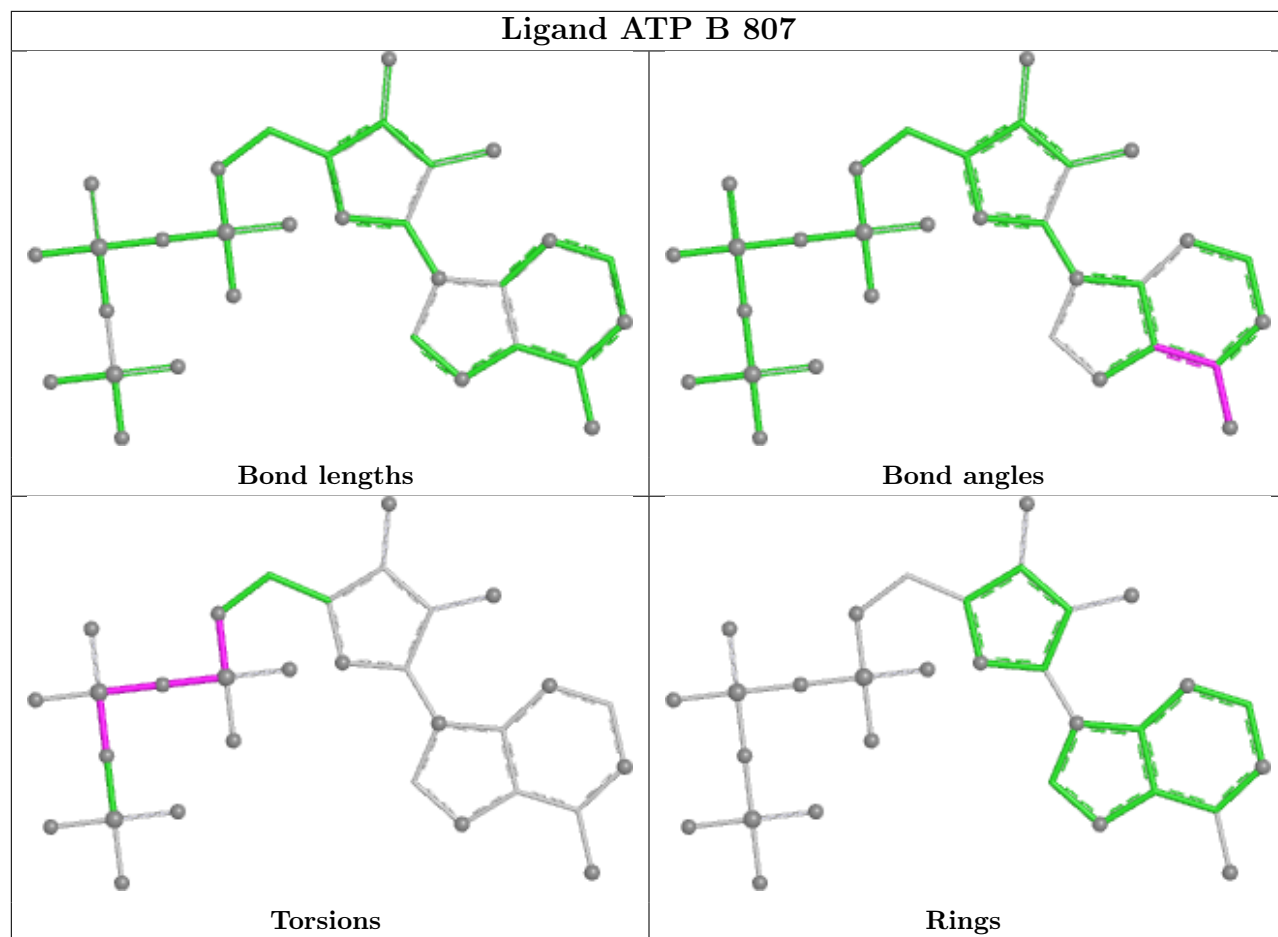




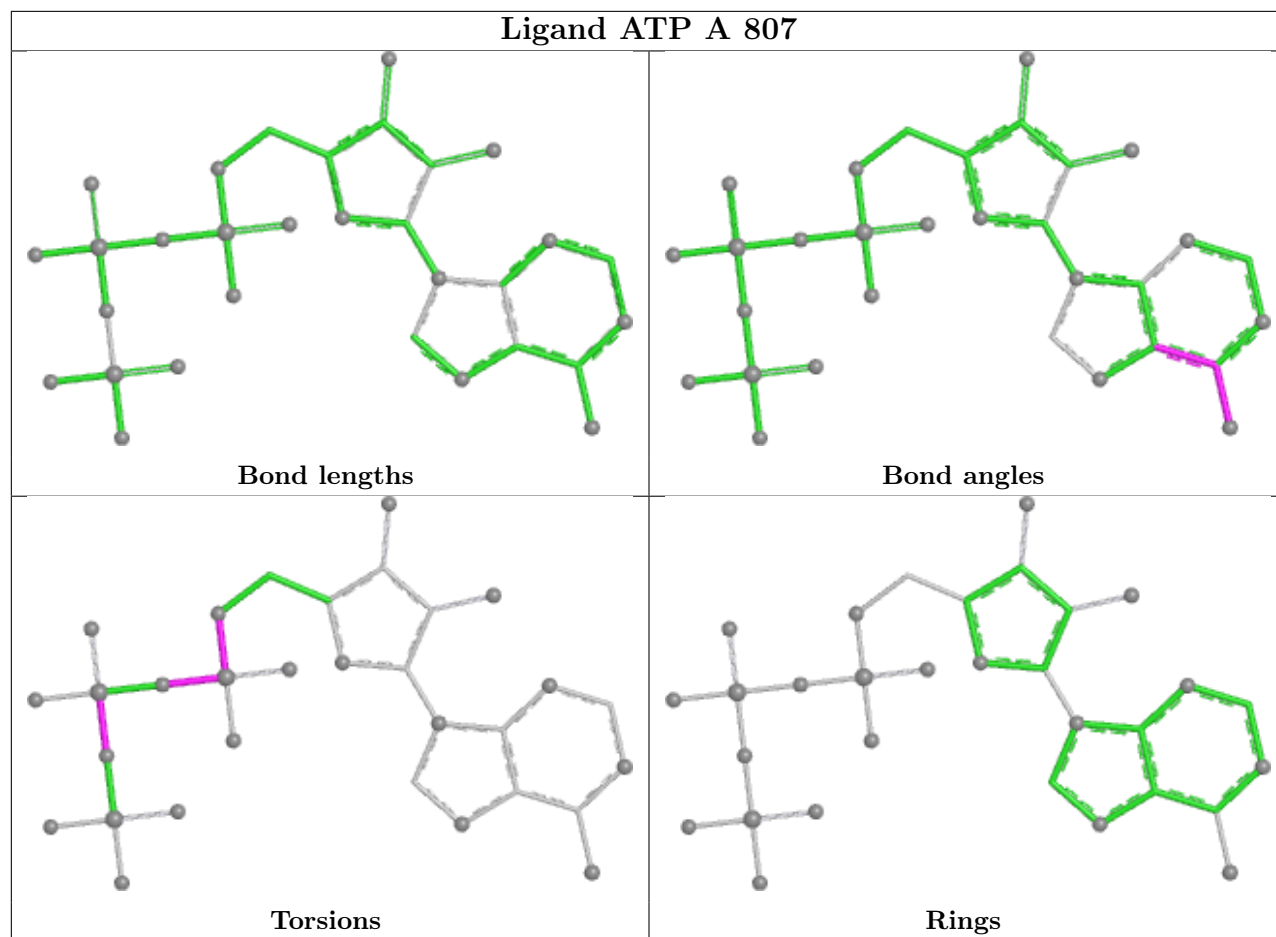


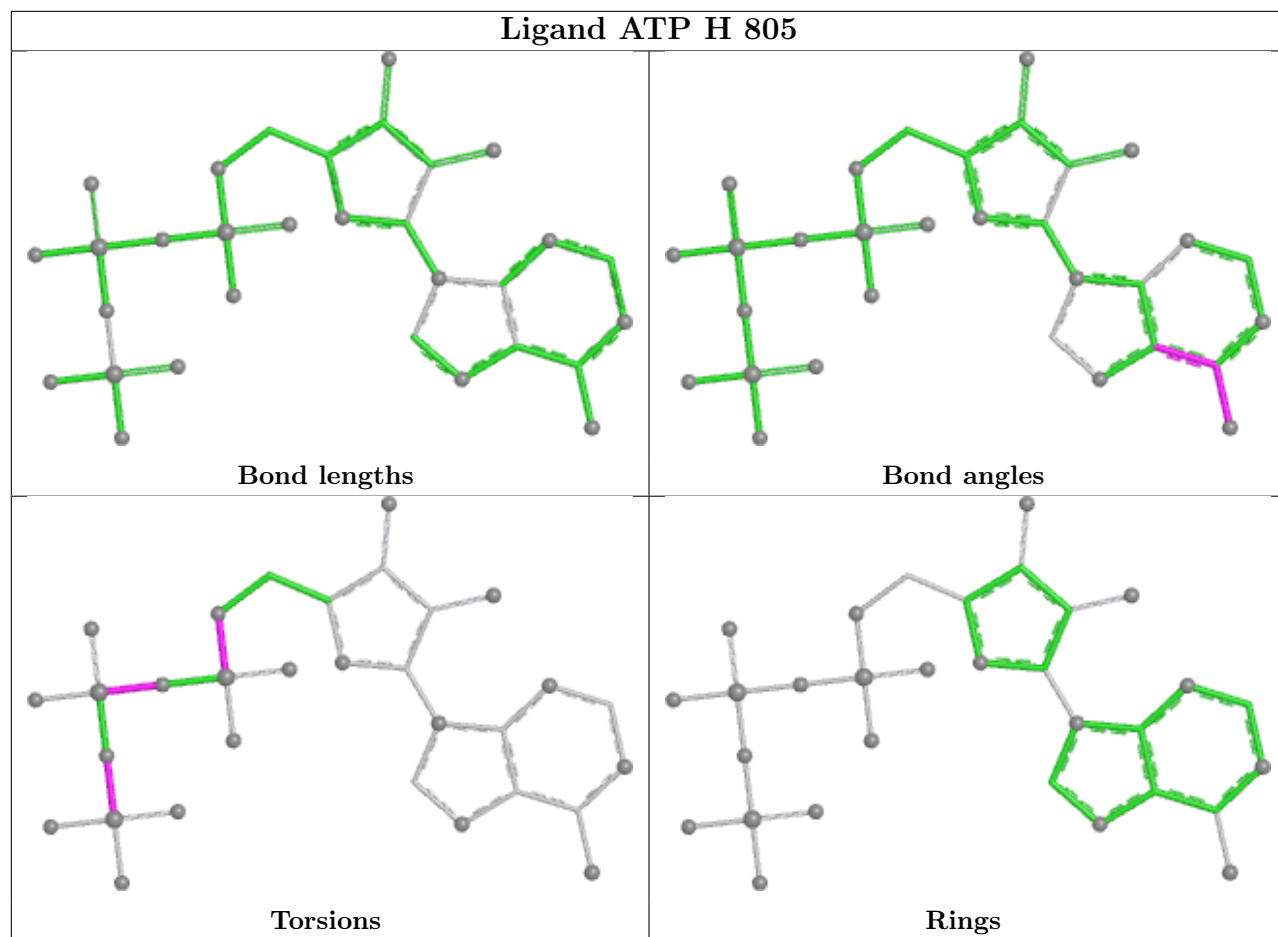


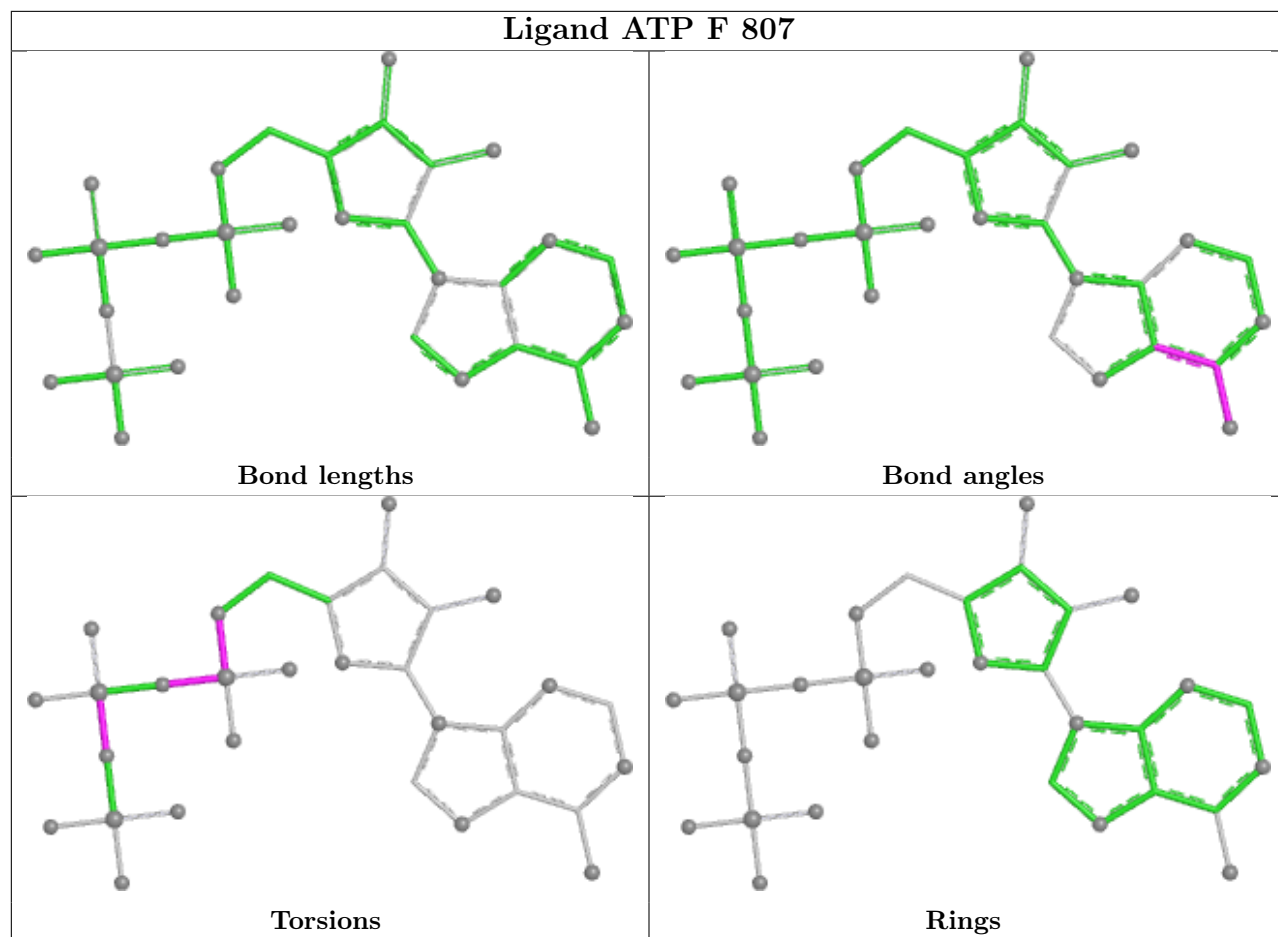


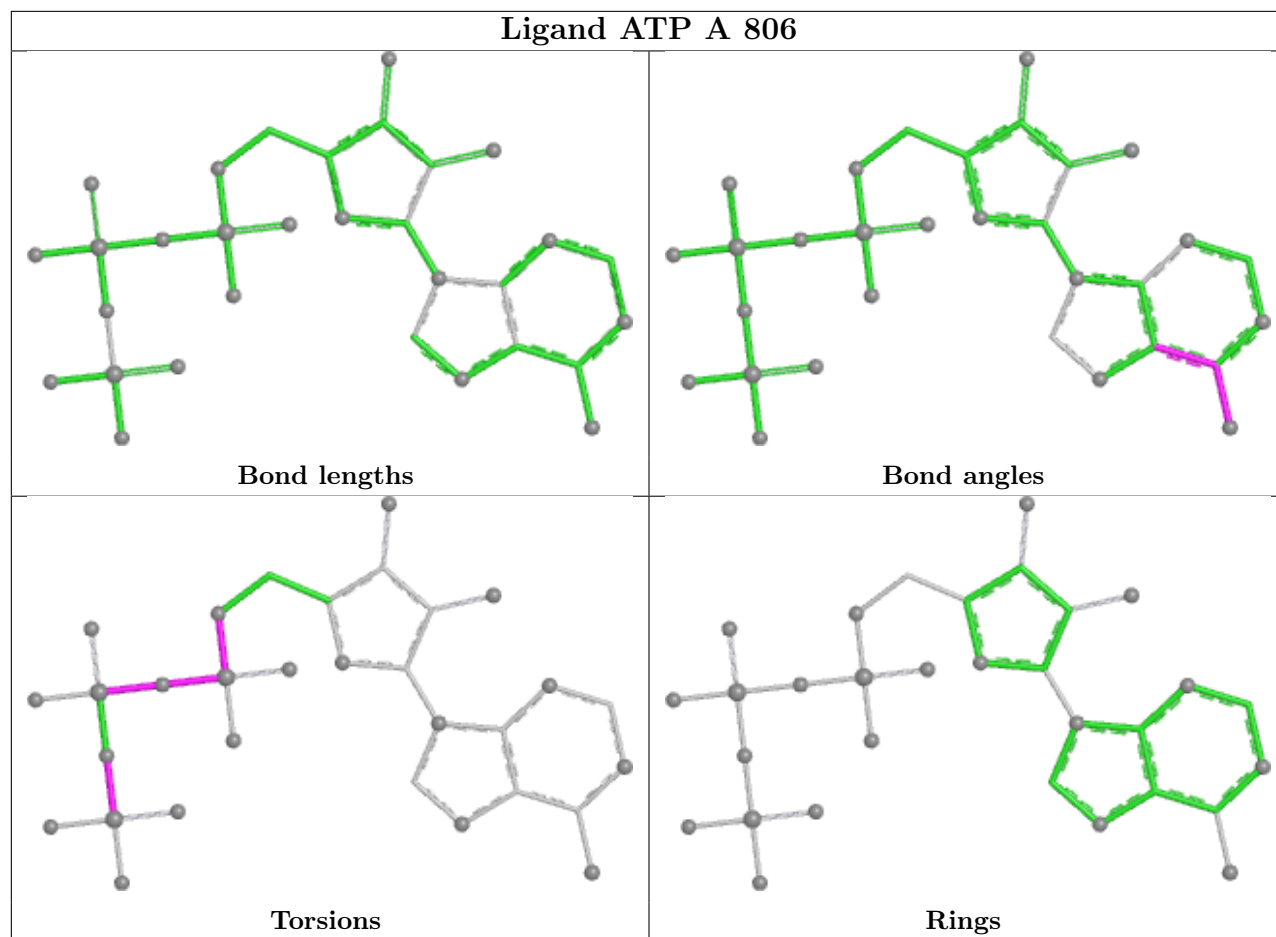












## 5.7 Other polymers [i](#)

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, 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	731/779 (93%)	-0.35	4 (0%) 87 84	42, 49, 67, 115	0
1	B	733/779 (94%)	-0.27	3 (0%) 89 86	43, 52, 69, 96	0
1	C	733/779 (94%)	-0.20	6 (0%) 82 79	26, 54, 71, 103	2 (0%)
1	D	727/779 (93%)	-0.29	7 (0%) 79 75	38, 48, 75, 102	0
1	E	733/779 (94%)	-0.12	3 (0%) 89 86	38, 57, 77, 105	1 (0%)
1	F	732/779 (93%)	-0.17	6 (0%) 82 79	44, 54, 75, 121	0
1	G	729/779 (93%)	-0.30	7 (0%) 79 75	41, 49, 72, 111	0
1	H	735/779 (94%)	-0.30	4 (0%) 87 84	34, 50, 70, 104	1 (0%)
All	All	5853/6232 (93%)	-0.25	40 (0%) 84 81	26, 52, 73, 121	4 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	731[A]	TYR	5.5
1	H	731[A]	TYR	4.7
1	E	4	ASN	4.7
1	G	650	GLY	4.6
1	C	731[A]	TYR	4.4
1	F	651	ILE	4.3
1	A	651	ILE	4.3
1	B	4	ASN	4.3
1	G	4	ASN	3.6
1	G	651	ILE	3.5
1	D	4	ASN	3.1
1	C	4	ASN	3.1
1	D	644	ILE	2.8
1	F	3	GLN	2.8
1	A	325	VAL	2.7
1	F	648	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	325	VAL	2.6
1	B	325	VAL	2.6
1	H	4	ASN	2.6
1	C	703	ARG	2.6
1	F	325	VAL	2.5
1	D	5	LEU	2.5
1	D	327	GLY	2.5
1	D	652	LEU	2.4
1	E	325	VAL	2.3
1	D	325	VAL	2.2
1	A	650	GLY	2.2
1	G	73	ASP	2.2
1	D	43	LEU	2.2
1	G	43	LEU	2.2
1	C	322	ASN	2.2
1	C	325	VAL	2.1
1	B	646	ALA	2.1
1	C	648	LYS	2.1
1	H	3	GLN	2.1
1	G	652	LEU	2.1
1	F	644	ILE	2.1
1	A	623	GLU	2.0
1	G	5	LEU	2.0
1	F	731	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
2	SO4	G	809	5/5	0.39	0.31	65,66,66,70	5
2	SO4	A	814	5/5	0.62	0.21	59,62,63,65	5
2	SO4	H	801	5/5	0.63	0.23	55,55,57,61	5
2	SO4	H	809	5/5	0.63	0.32	60,60,60,61	5
2	SO4	C	810	5/5	0.65	0.28	60,60,61,61	5
2	SO4	D	812	5/5	0.65	0.22	60,61,62,65	5
2	SO4	G	802	5/5	0.65	0.26	54,54,57,66	5
2	SO4	H	811	5/5	0.66	0.21	62,62,63,64	5
2	SO4	D	802	5/5	0.67	0.21	53,54,59,65	5
2	SO4	A	802	5/5	0.68	0.27	52,53,53,61	5
2	SO4	A	812	5/5	0.68	0.22	59,60,62,65	5
2	SO4	A	813	5/5	0.68	0.22	62,62,63,69	5
2	SO4	D	803	5/5	0.69	0.22	59,60,63,64	5
2	SO4	E	803	5/5	0.70	0.24	65,66,72,100	5
2	SO4	C	802	5/5	0.72	0.24	56,56,58,59	5
2	SO4	E	810	5/5	0.73	0.29	61,61,61,62	5
2	SO4	B	802	5/5	0.74	0.22	53,53,54,62	5
2	SO4	A	811	5/5	0.75	0.24	56,56,57,59	5
2	SO4	B	810	5/5	0.75	0.30	60,60,60,61	5
2	SO4	F	803	5/5	0.77	0.27	51,52,53,56	5
2	SO4	C	811	5/5	0.77	0.23	60,60,61,66	5
2	SO4	F	802	5/5	0.77	0.18	55,55,56,64	5
2	SO4	F	810	5/5	0.78	0.17	58,58,59,63	5
2	SO4	E	802	5/5	0.78	0.25	58,58,59,70	5
2	SO4	H	810	5/5	0.81	0.21	59,59,61,63	5
2	SO4	A	810	5/5	0.81	0.20	57,57,58,65	5
2	SO4	B	803	5/5	0.82	0.17	53,54,54,58	5
2	SO4	G	801	5/5	0.82	0.21	46,47,49,49	5
2	SO4	H	802	5/5	0.83	0.19	54,54,57,61	5
2	SO4	B	801	5/5	0.83	0.22	49,51,53,53	5
2	SO4	A	803	5/5	0.84	0.20	53,53,55,56	5
2	SO4	D	811	5/5	0.85	0.20	51,52,53,57	5
2	SO4	D	810	5/5	0.86	0.19	64,65,65,65	5
2	SO4	C	803	5/5	0.87	0.15	53,53,54,54	5
2	SO4	C	801	5/5	0.87	0.17	54,57,57,58	5
2	SO4	F	801	5/5	0.88	0.17	52,53,55,56	5
2	SO4	E	801	5/5	0.89	0.16	50,51,52,57	5
2	SO4	D	801	5/5	0.89	0.19	49,51,51,52	5
2	SO4	A	801	5/5	0.91	0.16	44,44,45,46	5
3	ATP	B	806	31/31	0.93	0.08	54,57,65,70	0
3	ATP	F	804	31/31	0.94	0.08	61,64,66,72	0
2	SO4	D	813	5/5	0.95	0.13	54,55,58,59	5
3	ATP	C	806	31/31	0.95	0.07	55,57,68,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ATP	D	806	31/31	0.95	0.07	55,58,64,70	0
3	ATP	E	804	31/31	0.95	0.07	57,59,61,63	0
3	ATP	E	806	31/31	0.95	0.07	55,57,64,66	0
3	ATP	B	804	31/31	0.95	0.07	56,59,62,64	0
3	ATP	F	806	31/31	0.95	0.07	56,58,62,66	0
3	ATP	G	805	31/31	0.95	0.07	51,53,56,59	0
3	ATP	A	804	31/31	0.96	0.07	52,53,55,57	0
3	ATP	E	807	31/31	0.96	0.07	50,53,62,82	0
3	ATP	D	804	31/31	0.96	0.06	62,64,68,72	0
3	ATP	B	807	31/31	0.96	0.06	41,43,50,51	0
3	ATP	G	803	31/31	0.96	0.07	56,58,60,68	0
3	ATP	C	804	31/31	0.96	0.06	57,59,61,62	0
3	ATP	H	803	31/31	0.96	0.07	54,56,58,62	0
3	ATP	H	805	31/31	0.96	0.07	52,53,54,65	0
3	ATP	H	806	31/31	0.96	0.07	42,44,48,70	0
4	MG	H	804	1/1	0.96	0.05	54,54,54,54	0
5	CDP	B	809	25/25	0.96	0.07	42,43,44,51	0
5	CDP	C	809	25/25	0.96	0.07	42,44,47,64	0
5	CDP	F	809	25/25	0.96	0.07	45,47,51,62	0
3	ATP	C	807	31/31	0.97	0.06	44,45,48,60	0
3	ATP	F	807	31/31	0.97	0.06	46,47,50,80	0
3	ATP	A	807	31/31	0.97	0.06	44,45,51,58	0
5	CDP	A	809	25/25	0.97	0.06	42,44,47,52	0
3	ATP	A	806	31/31	0.97	0.06	48,49,54,55	0
3	ATP	G	806	31/31	0.97	0.06	40,41,49,52	0
5	CDP	D	809	25/25	0.97	0.05	40,41,45,49	0
5	CDP	E	809	25/25	0.97	0.06	43,45,47,63	0
3	ATP	D	807	31/31	0.97	0.06	45,45,48,59	0
5	CDP	G	808	25/25	0.97	0.06	41,42,43,55	0
5	CDP	H	808	25/25	0.97	0.06	41,43,45,60	0
4	MG	A	808	1/1	0.98	0.04	51,51,51,51	0
4	MG	B	805	1/1	0.98	0.03	62,62,62,62	0
4	MG	D	805	1/1	0.98	0.04	62,62,62,62	0
4	MG	B	808	1/1	0.99	0.02	42,42,42,42	0
4	MG	C	805	1/1	0.99	0.02	58,58,58,58	0
4	MG	C	808	1/1	0.99	0.03	45,45,45,45	0
4	MG	A	805	1/1	0.99	0.04	55,55,55,55	0
4	MG	D	808	1/1	0.99	0.04	47,47,47,47	0
4	MG	E	805	1/1	0.99	0.03	58,58,58,58	0
4	MG	E	808	1/1	0.99	0.03	55,55,55,55	0
4	MG	F	805	1/1	0.99	0.03	62,62,62,62	0
4	MG	G	804	1/1	0.99	0.03	56,56,56,56	0

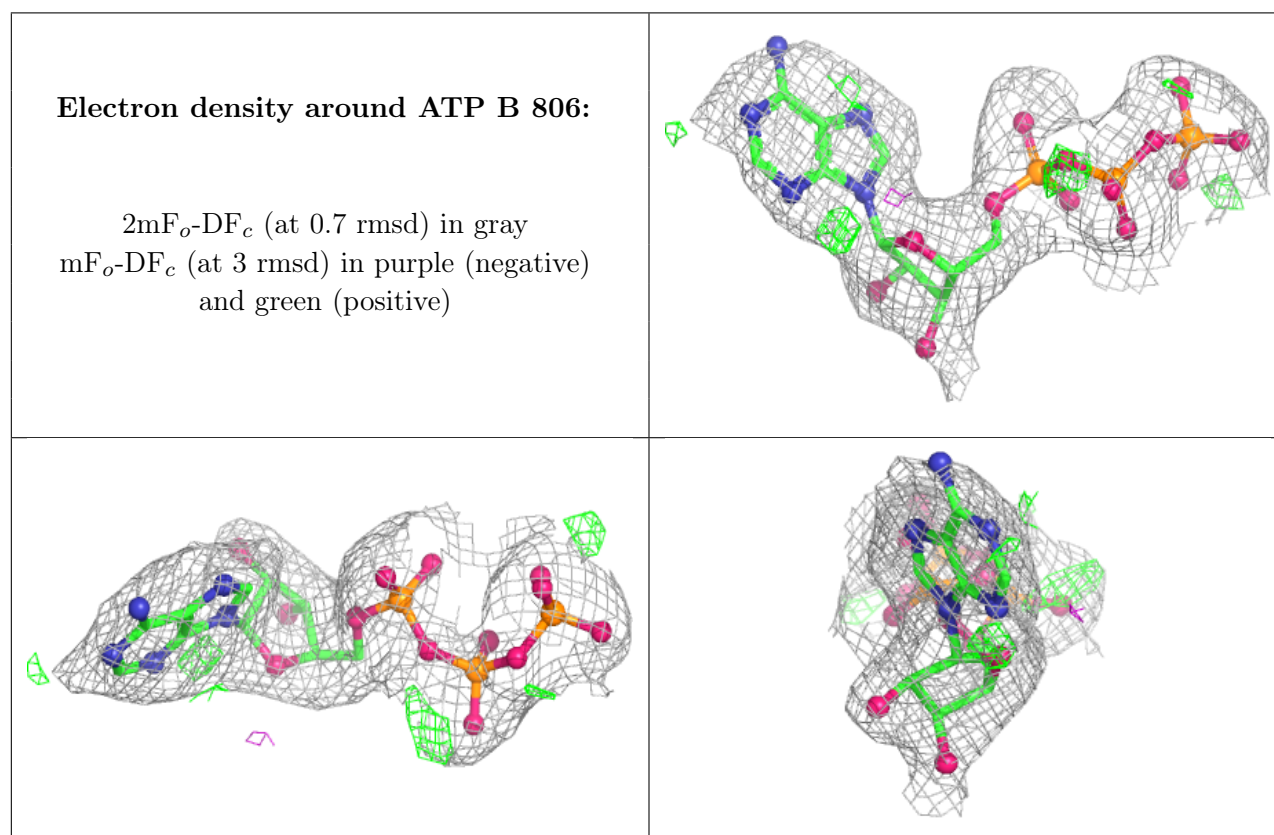
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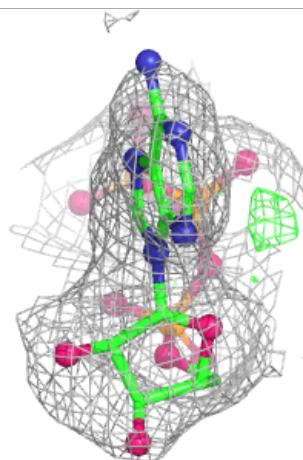
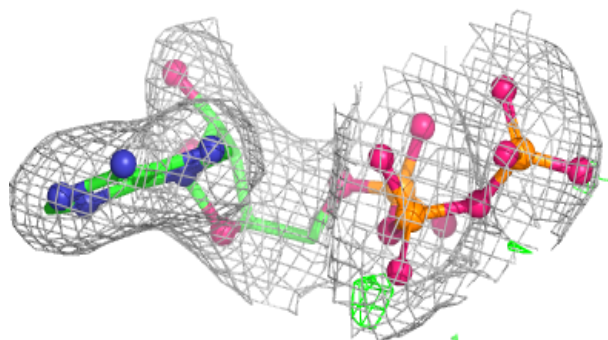
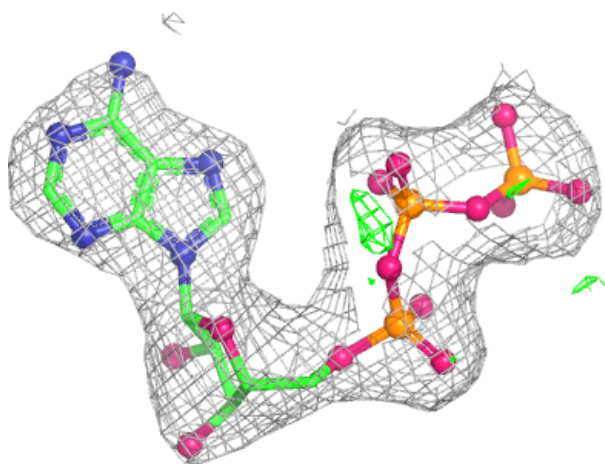
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	H	807	1/1	1.00	0.03	43,43,43,43	0
4	MG	G	807	1/1	1.00	0.02	45,45,45,45	0
4	MG	F	808	1/1	1.00	0.03	50,50,50,50	0

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.



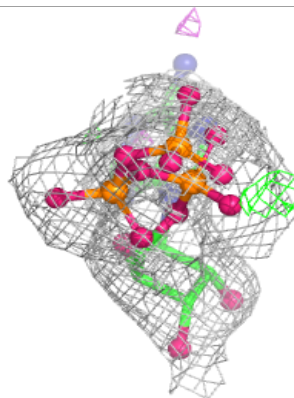
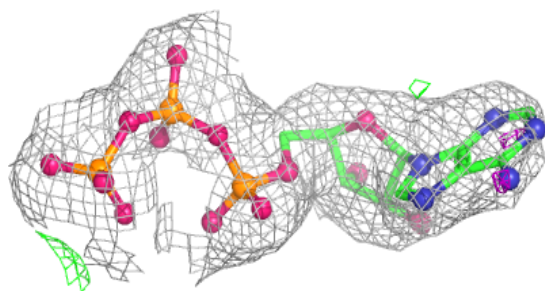
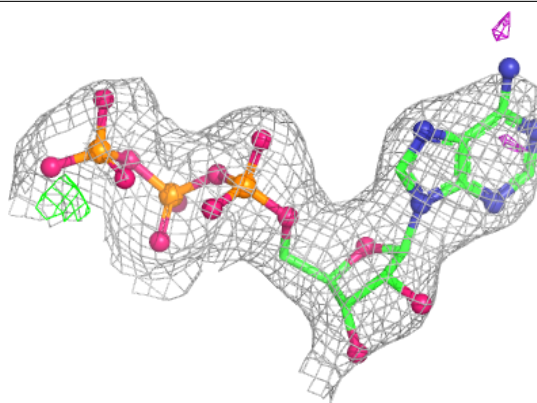
**Electron density around ATP F 804:**

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

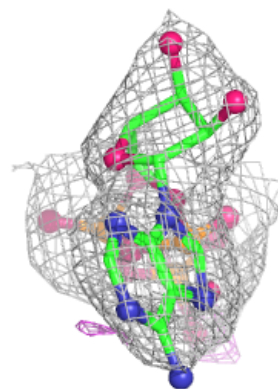
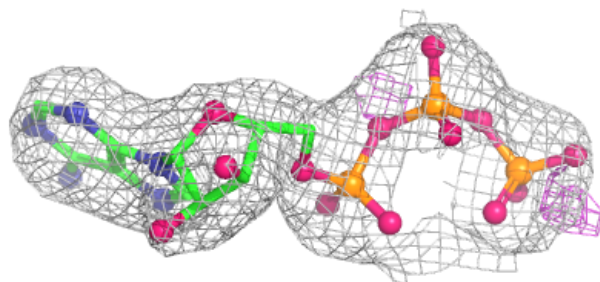
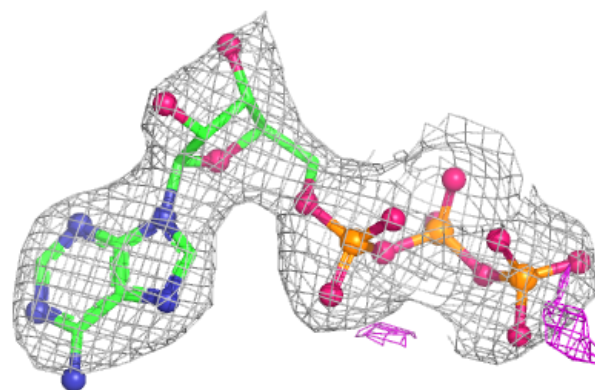


**Electron density around ATP C 806:**

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

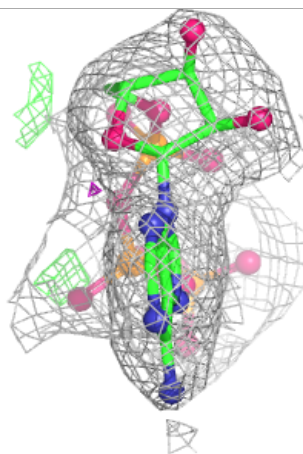
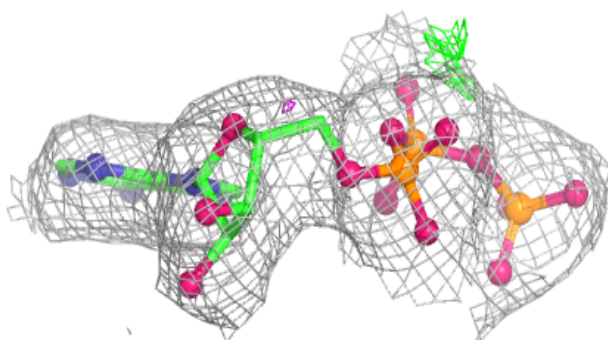
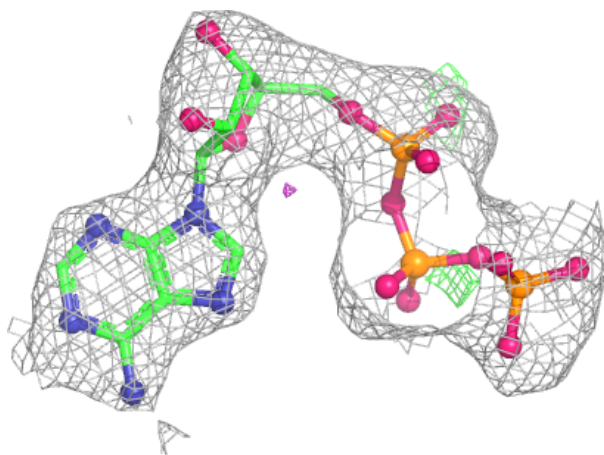
**Electron density around ATP D 806:**

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



**Electron density around ATP E 804:**

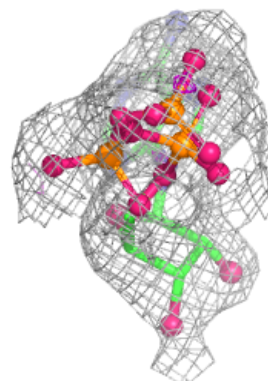
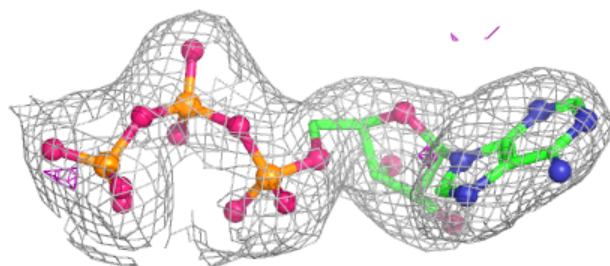
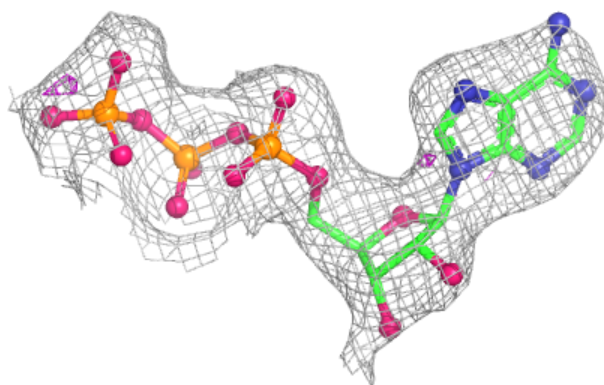
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



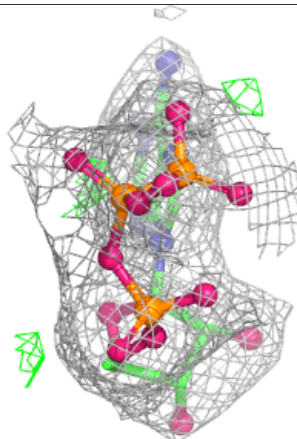
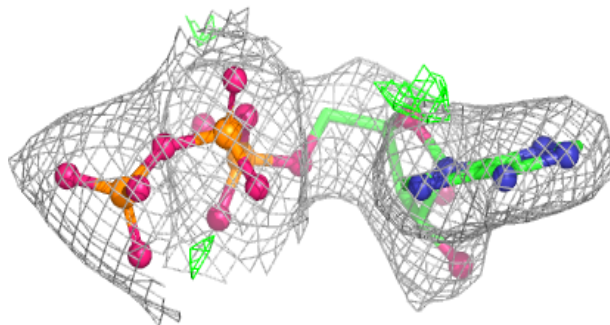
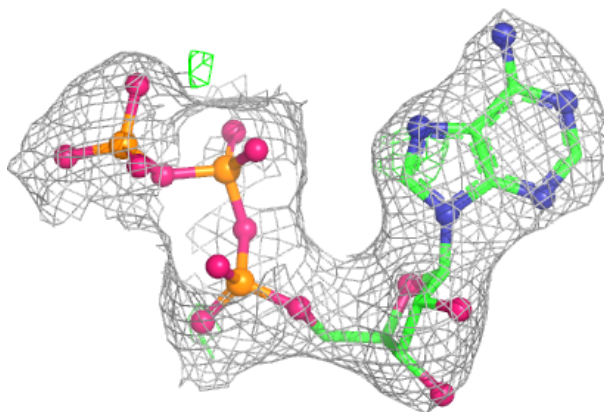


**Electron density around ATP E 806:**

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

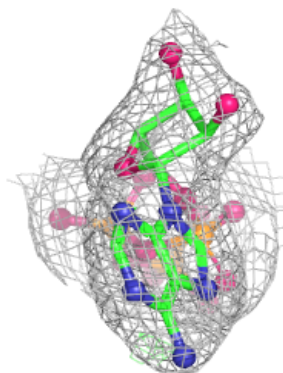
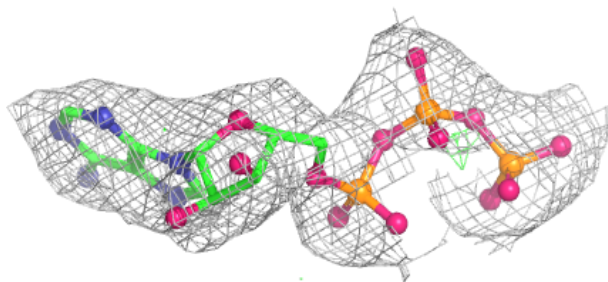
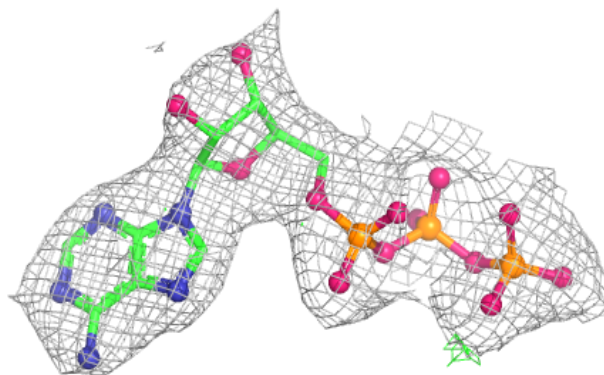
**Electron density around ATP B 804:**

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

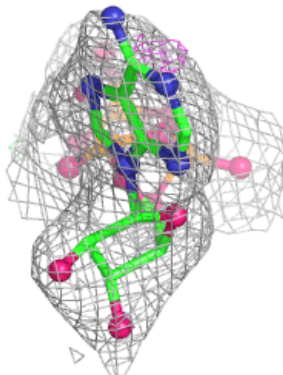
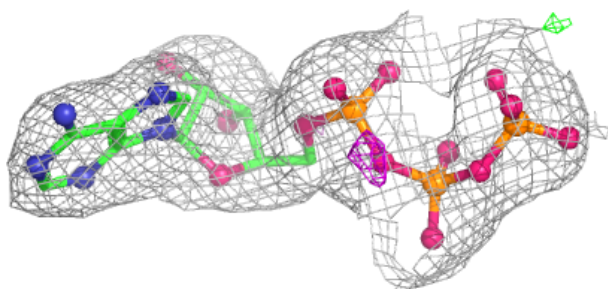
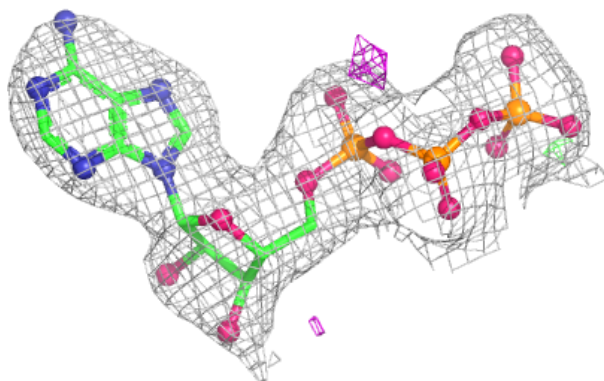


**Electron density around ATP F 806:**

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

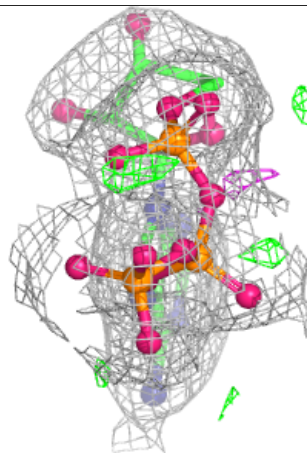
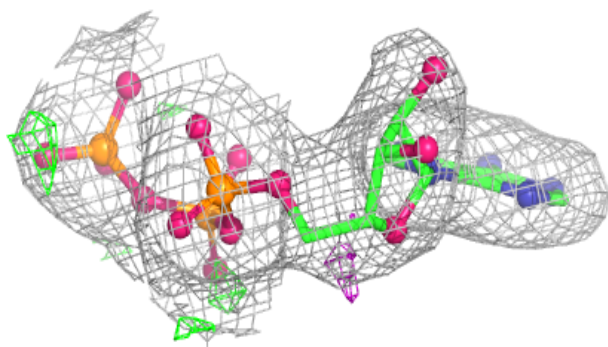
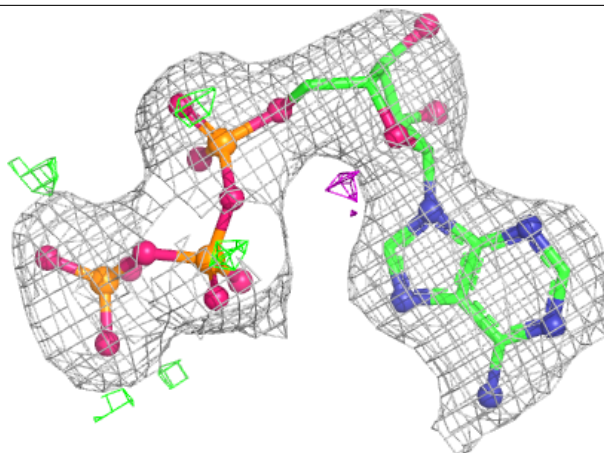
**Electron density around ATP G 805:**

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



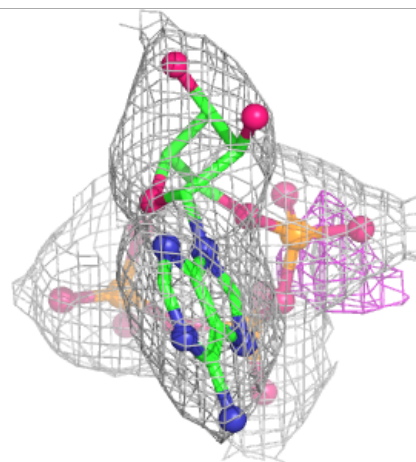
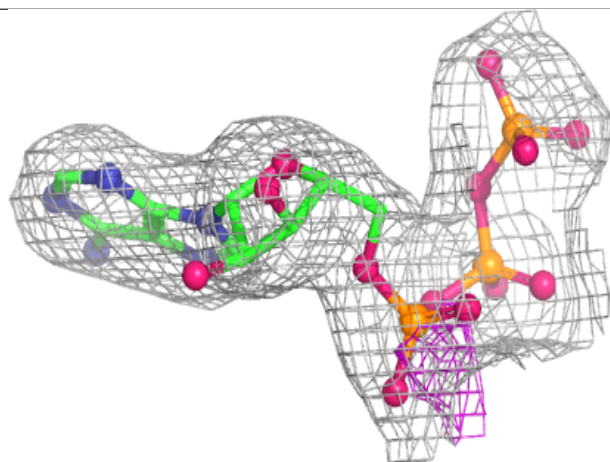
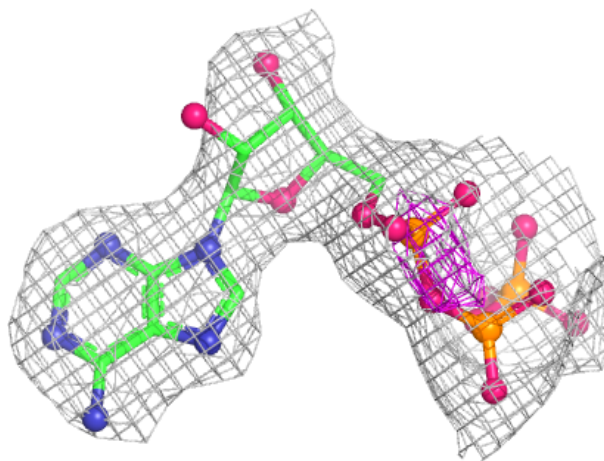
**Electron density around ATP A 804:**

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



**Electron density around ATP E 807:**

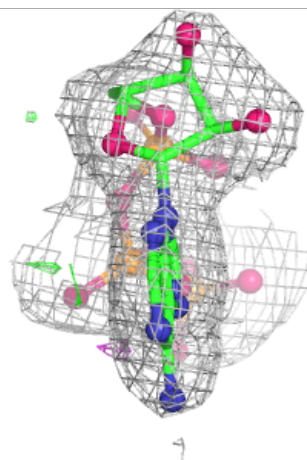
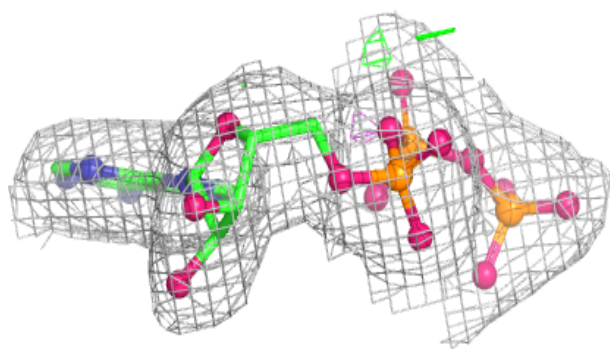
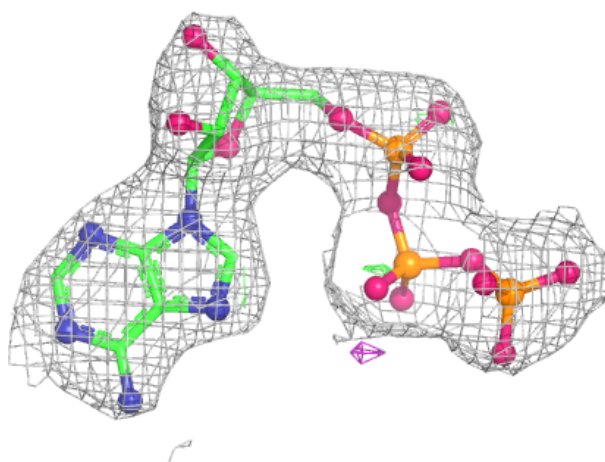
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





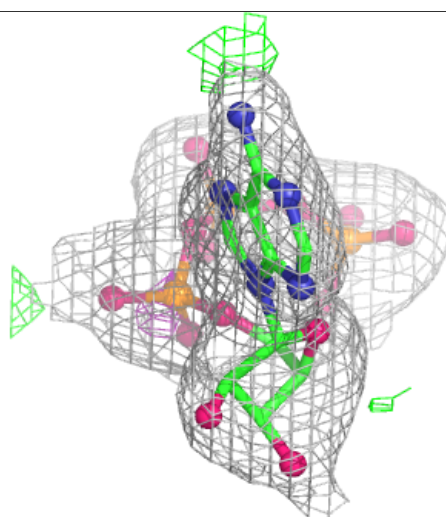
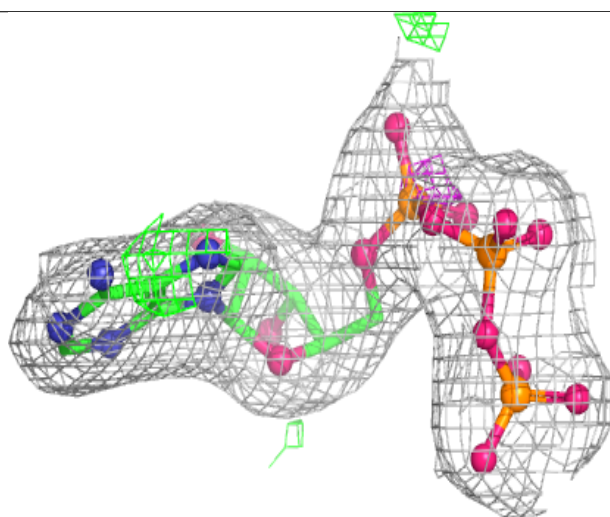
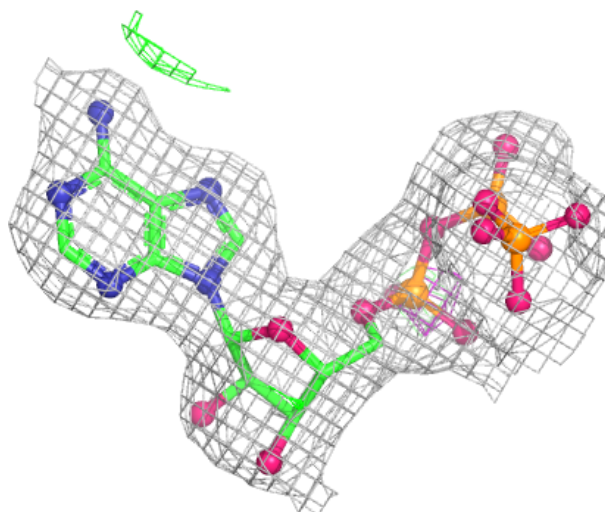
**Electron density around ATP D 804:**

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



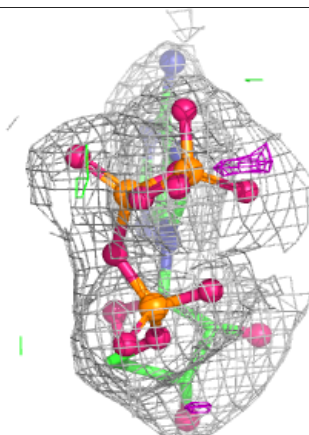
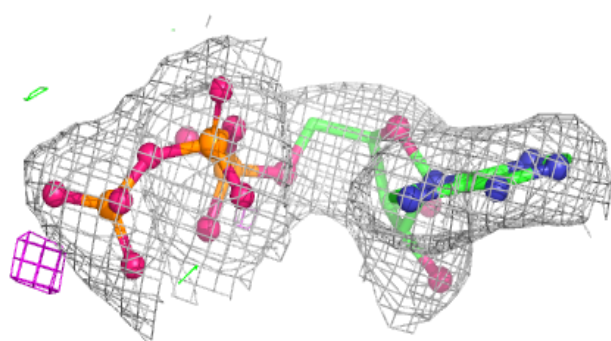
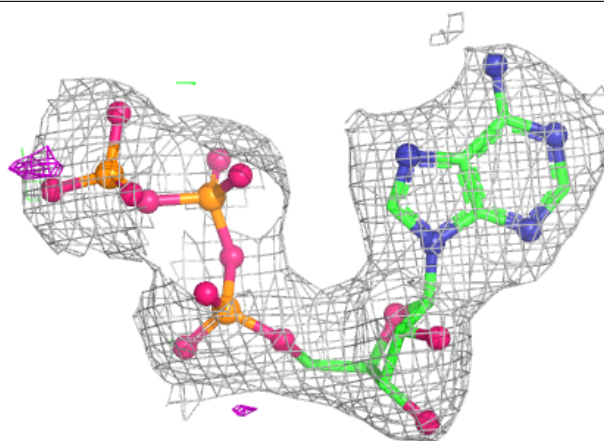
**Electron density around ATP B 807:**

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

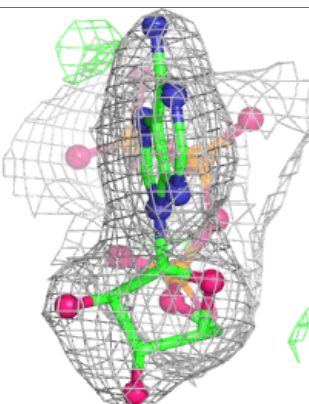
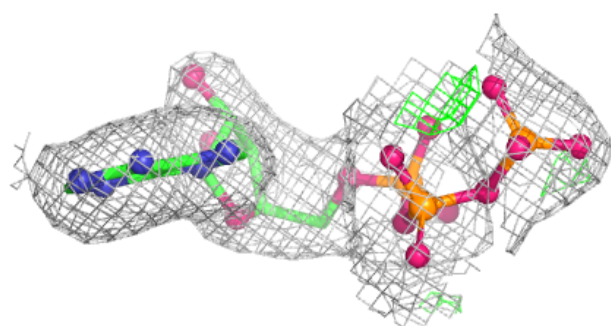
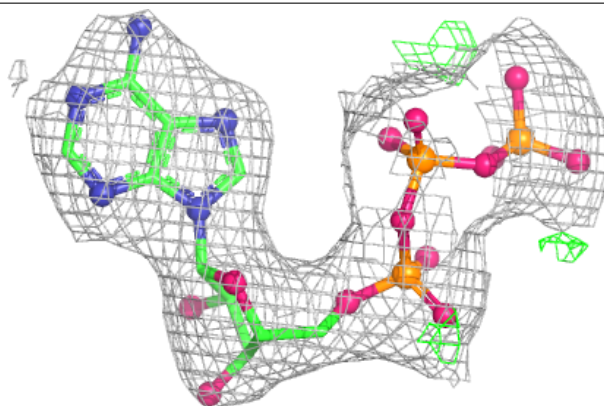


**Electron density around ATP G 803:**

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

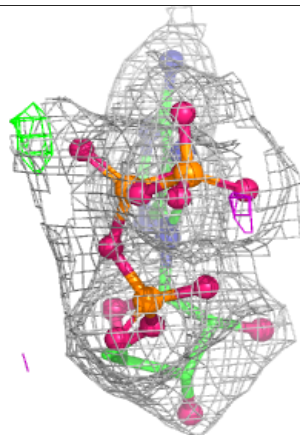
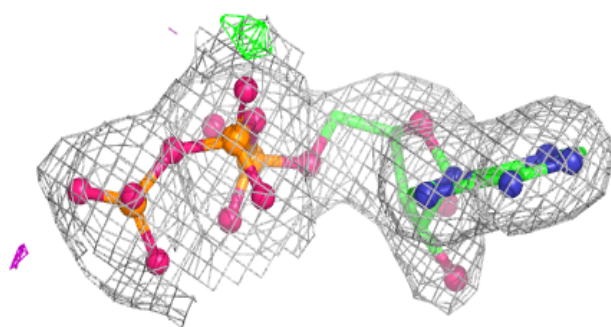
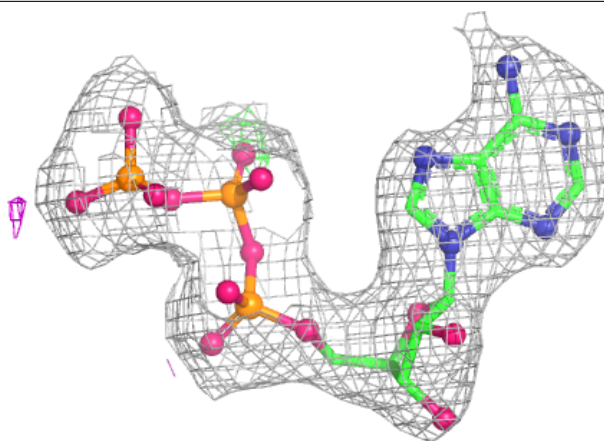
**Electron density around ATP C 804:**

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

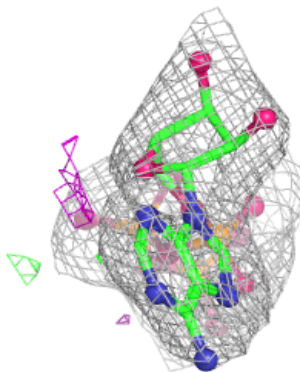
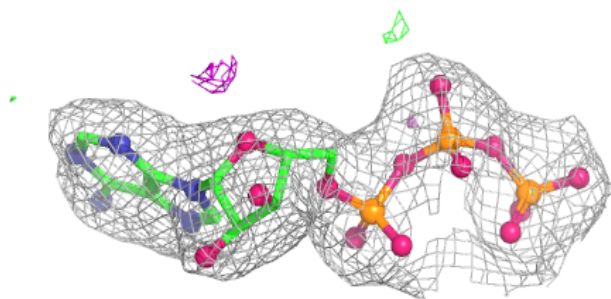
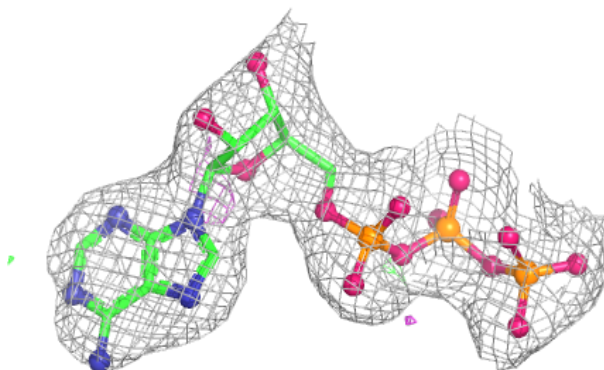


**Electron density around ATP H 803:**

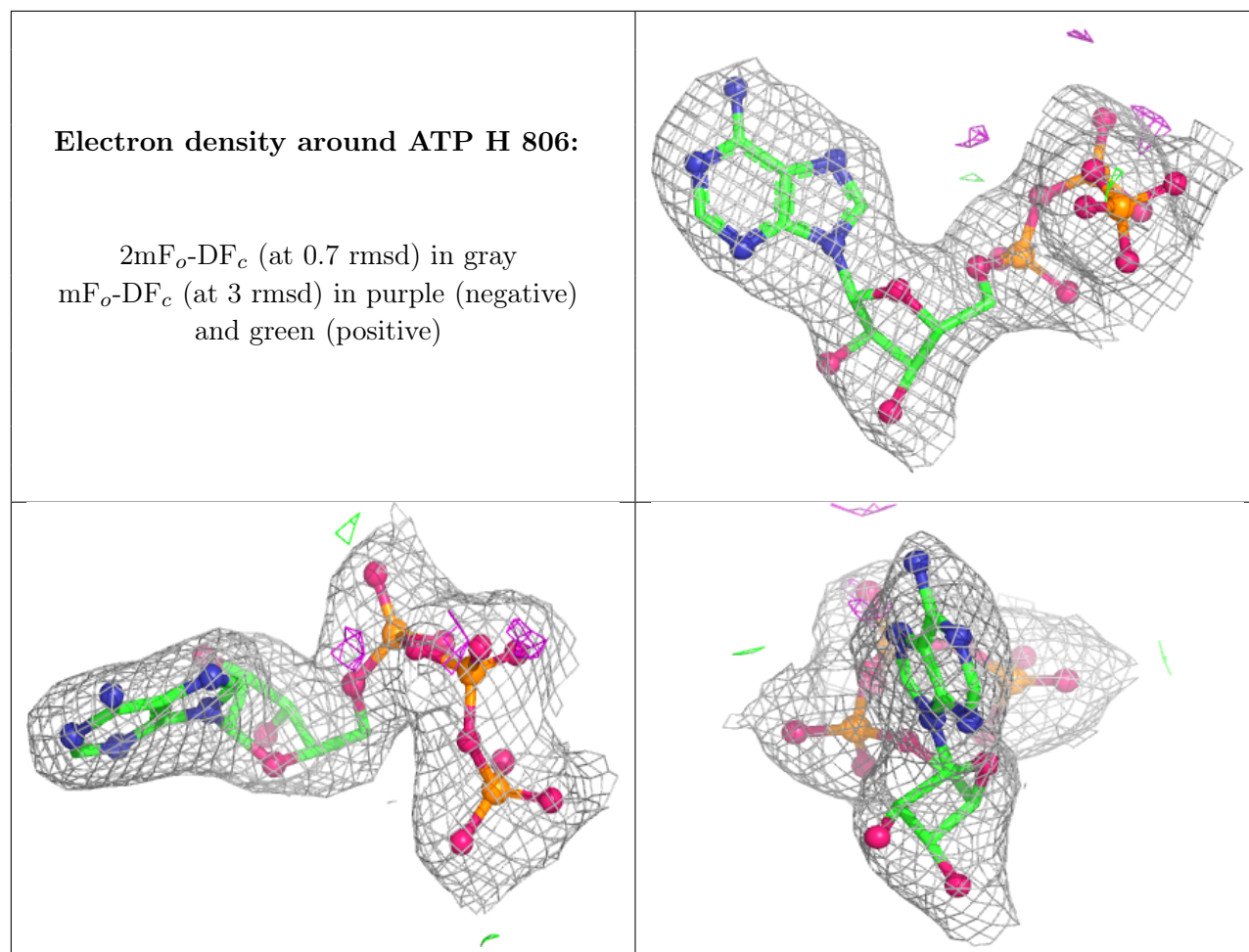
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

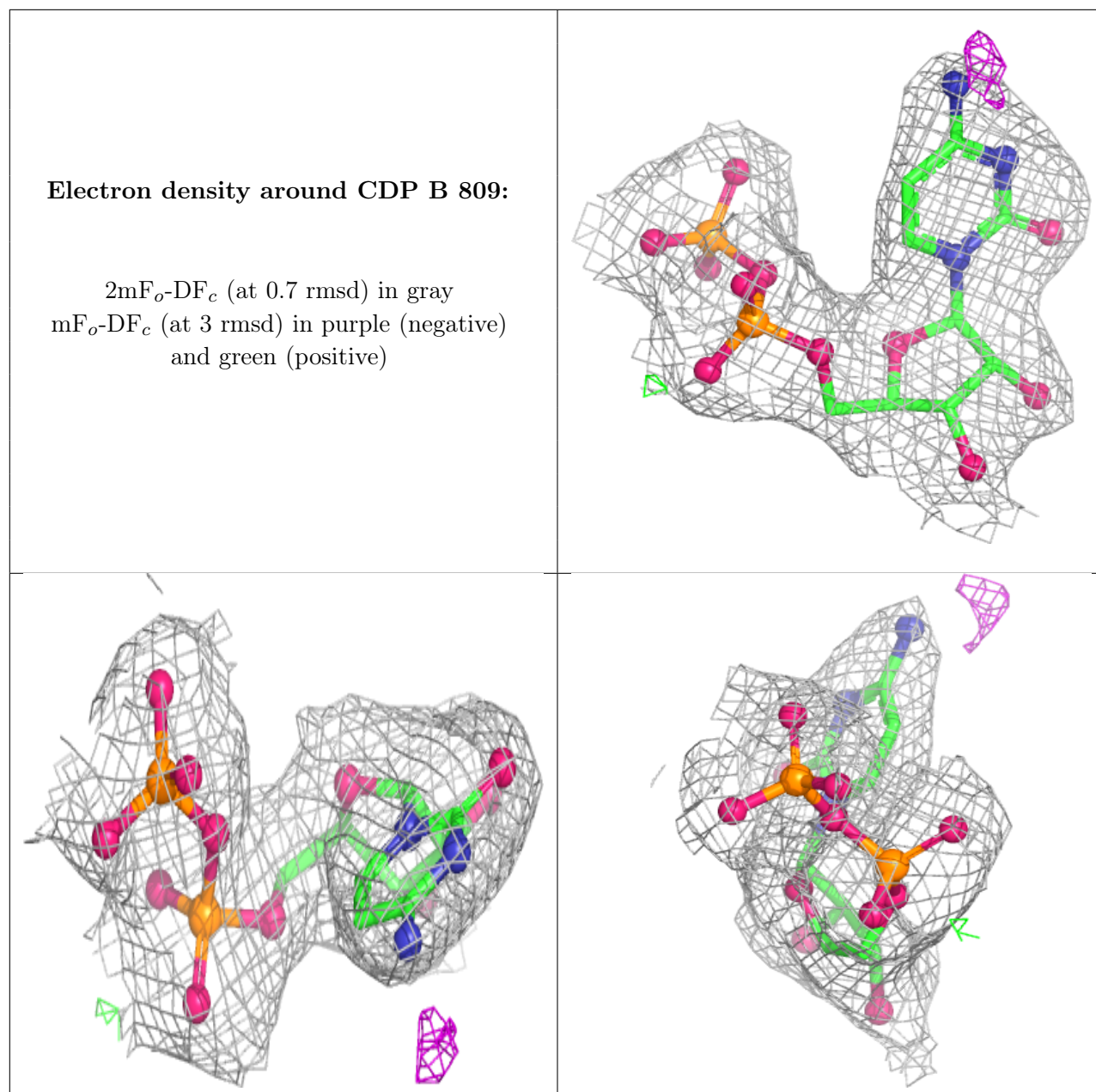
**Electron density around ATP H 805:**

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



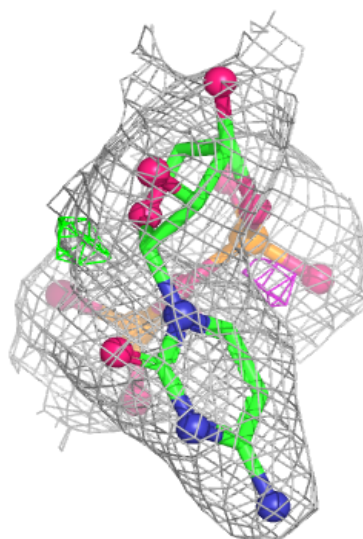
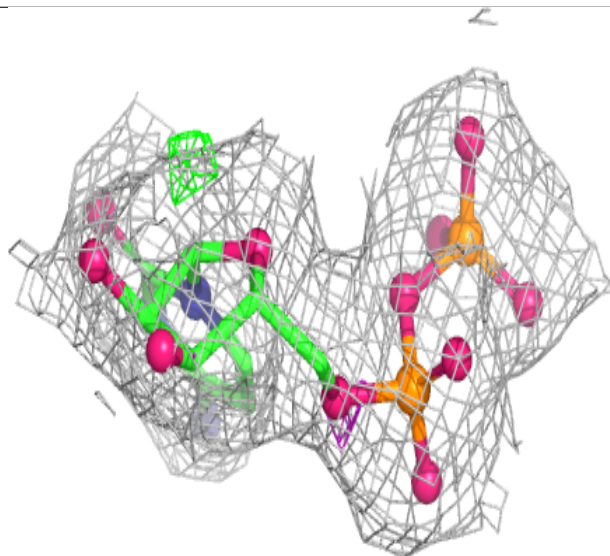
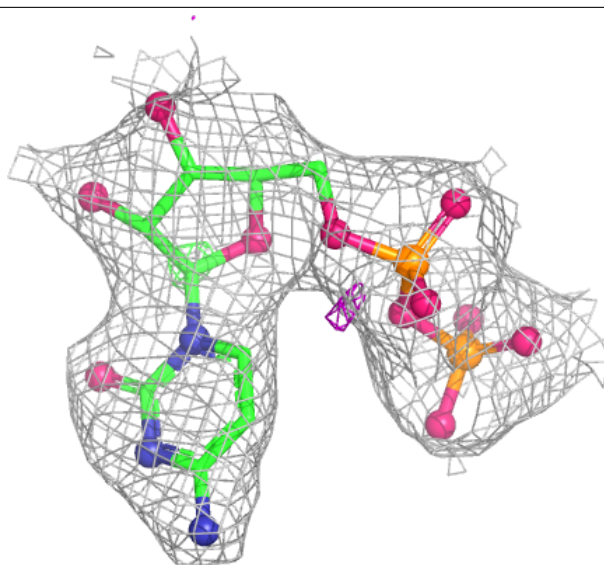






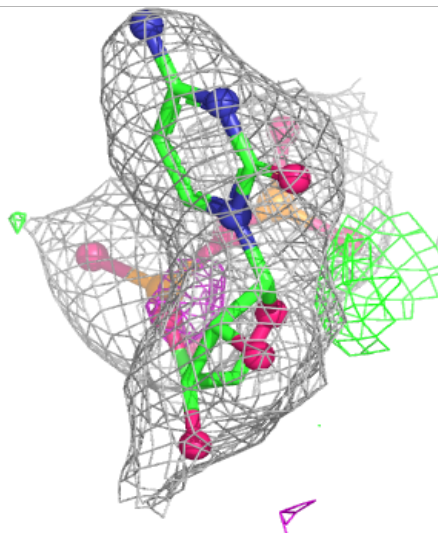
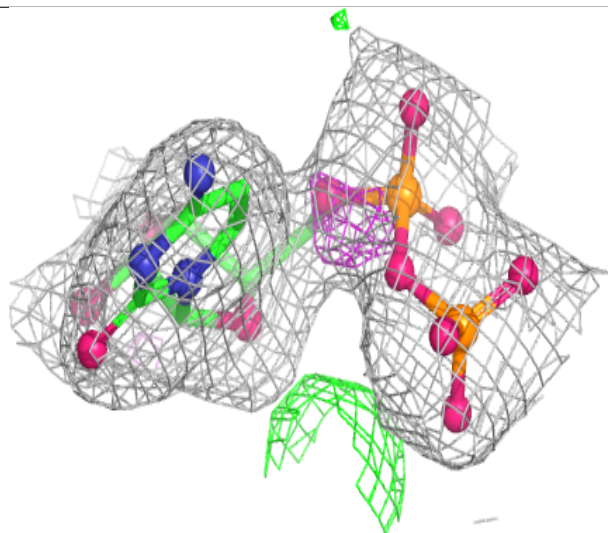
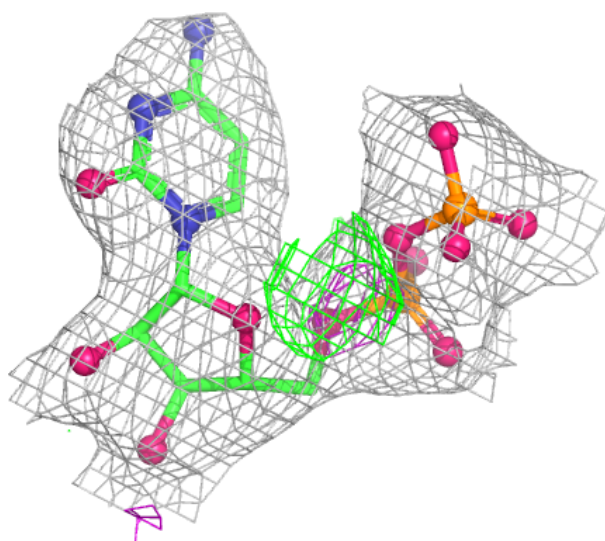
**Electron density around CDP C 809:**

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



**Electron density around CDP F 809:**

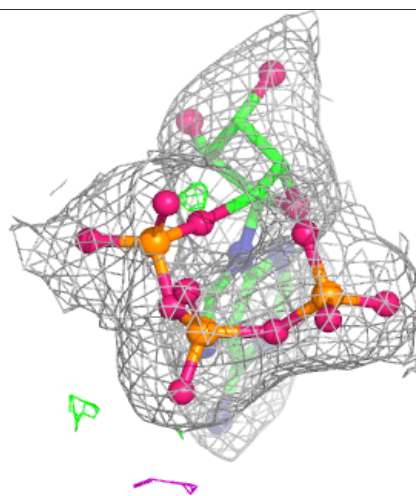
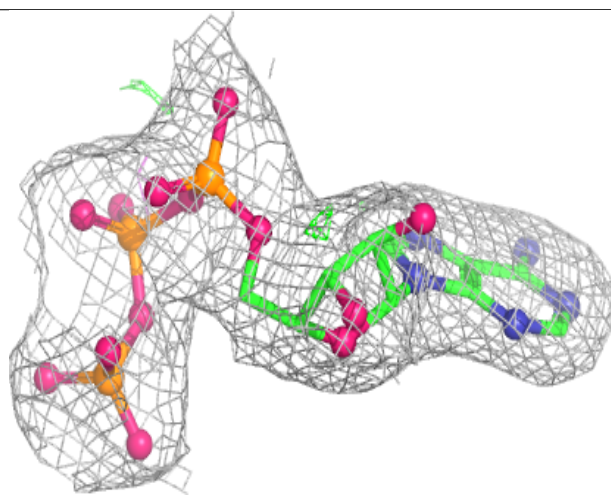
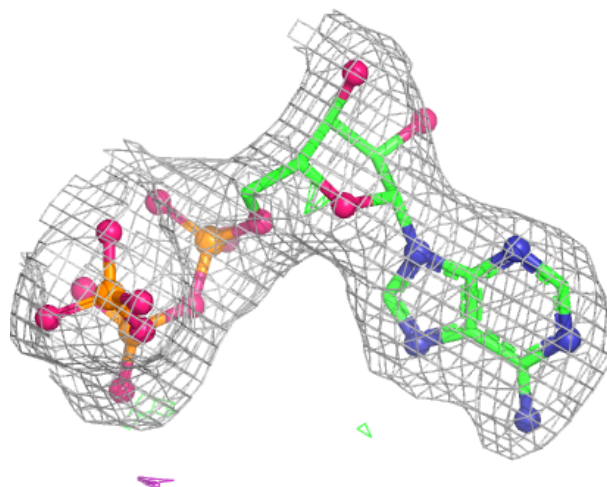
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





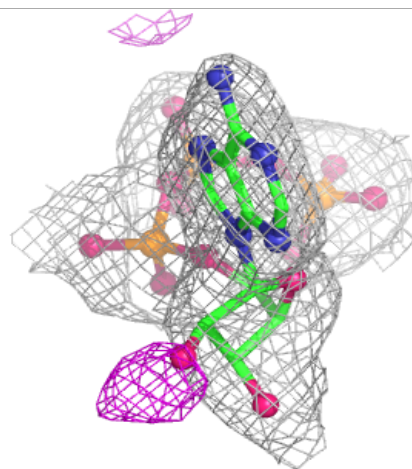
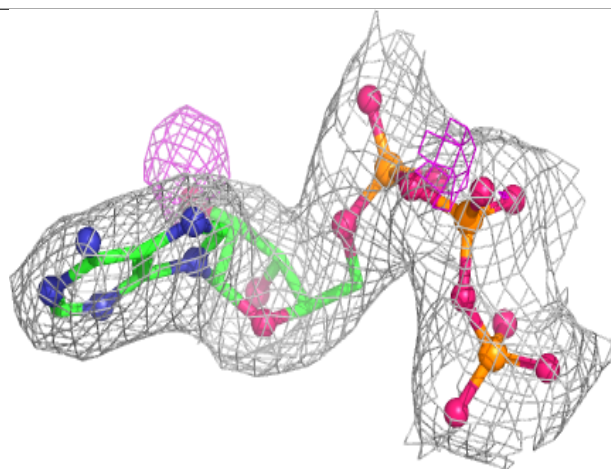
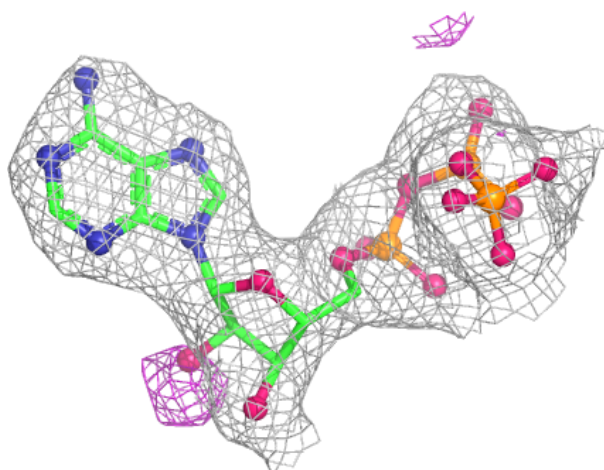
**Electron density around ATP C 807:**

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



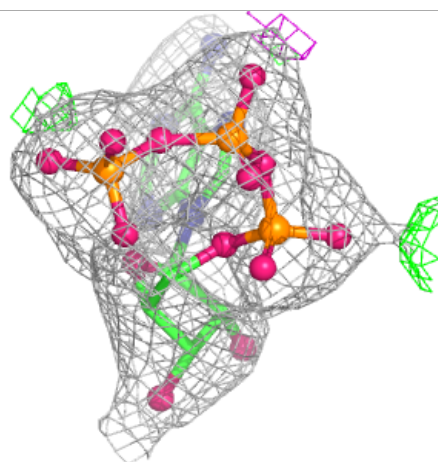
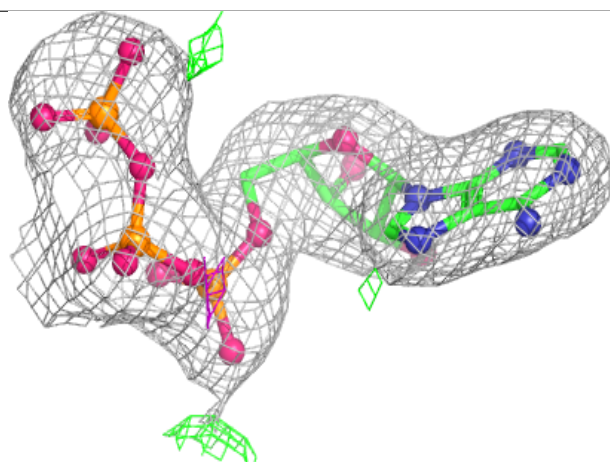
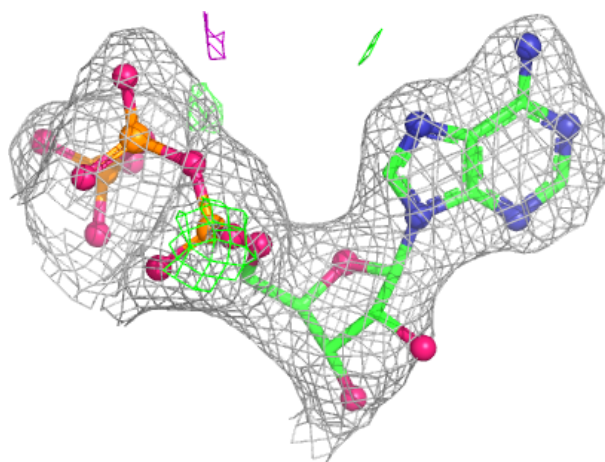
**Electron density around ATP F 807:**

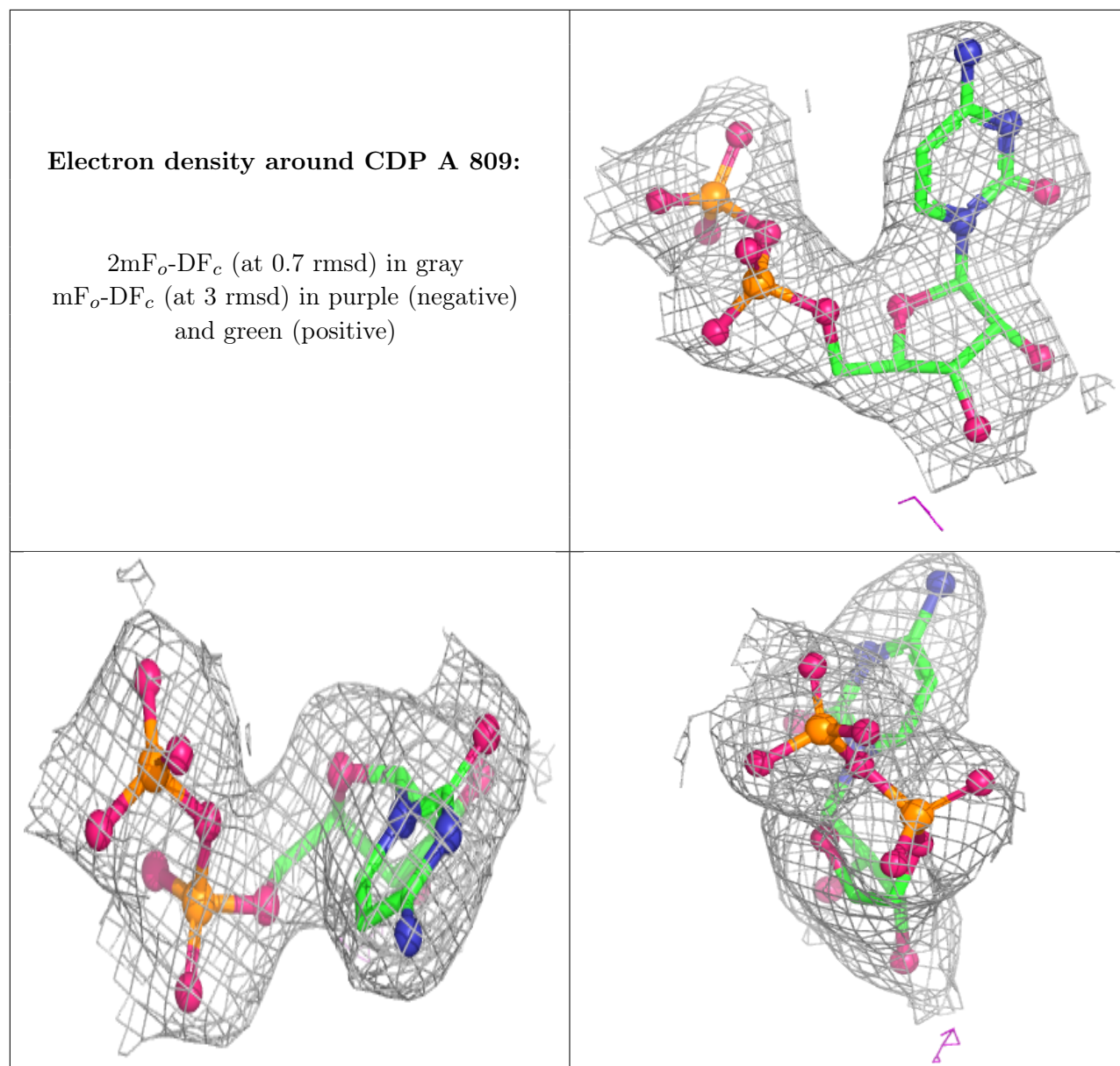
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ATP A 807:**

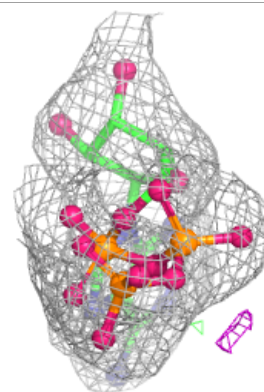
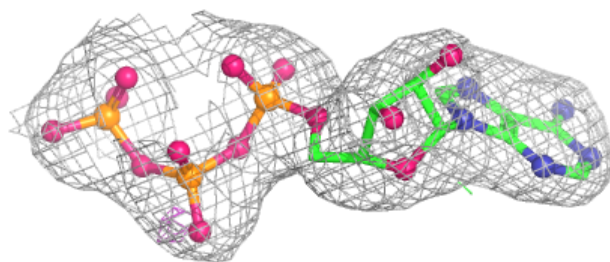
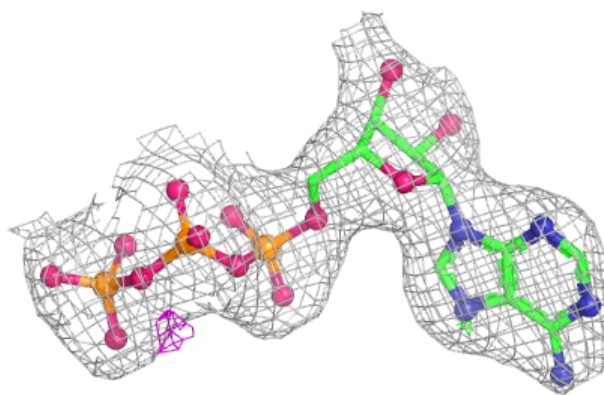
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



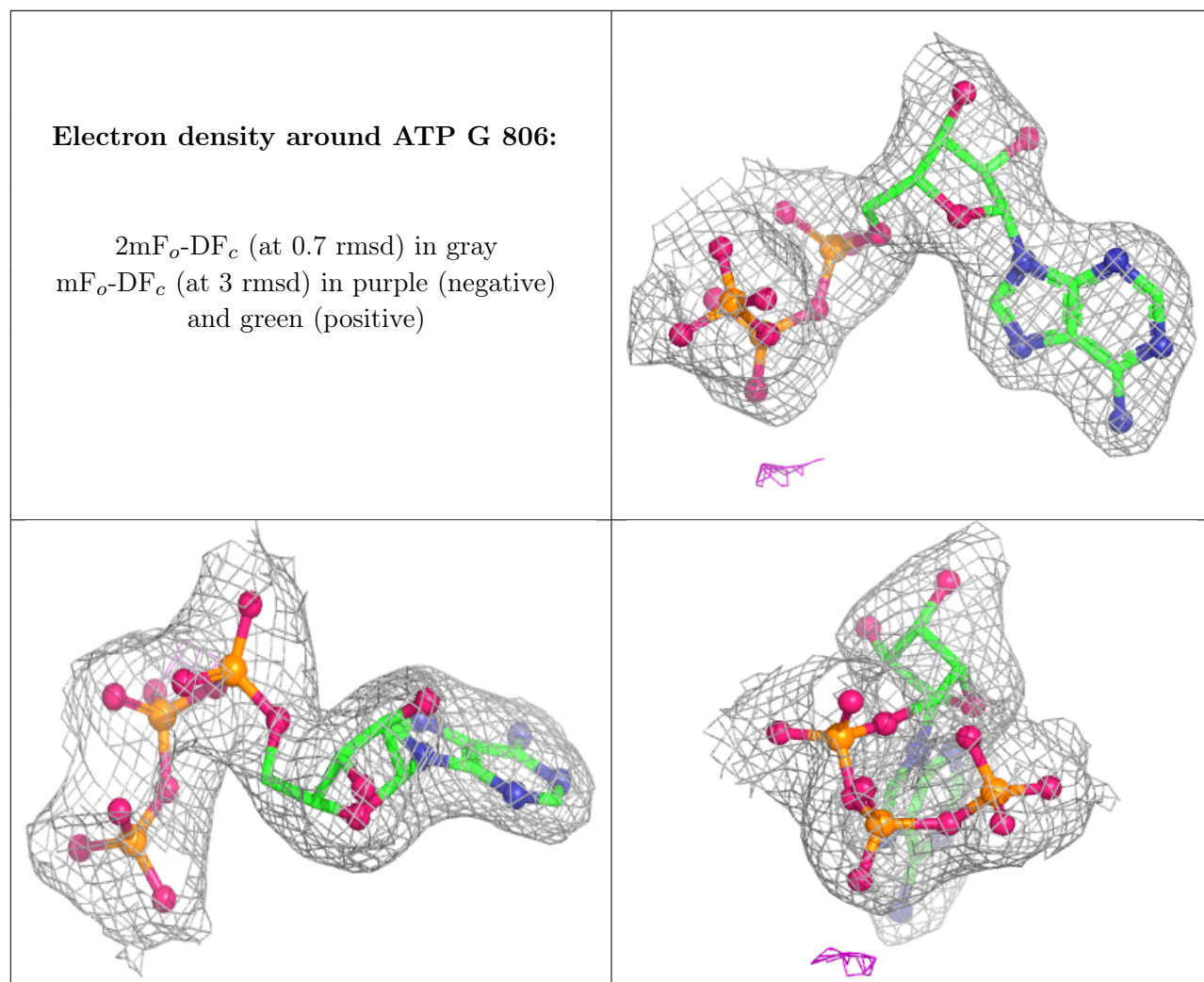


**Electron density around ATP A 806:**

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

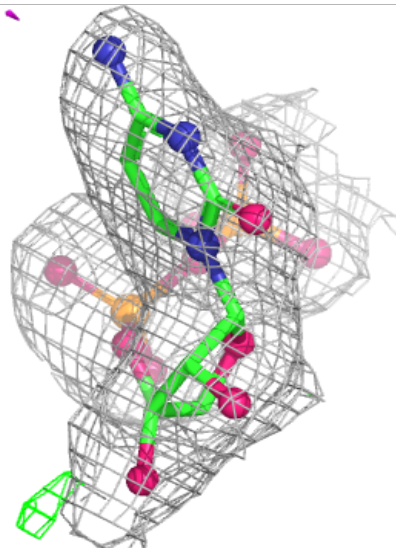
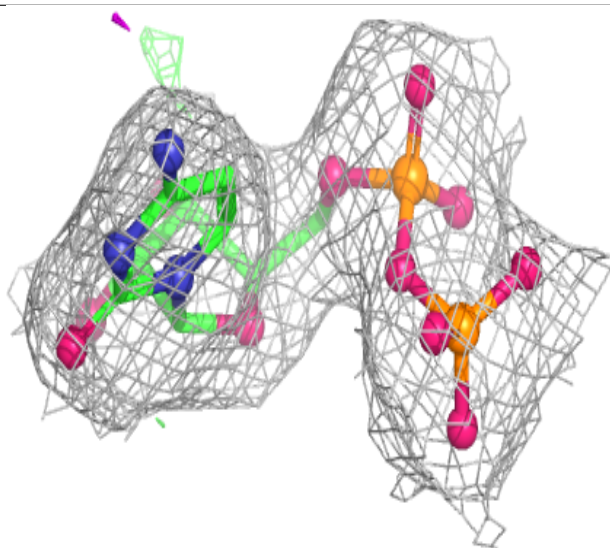
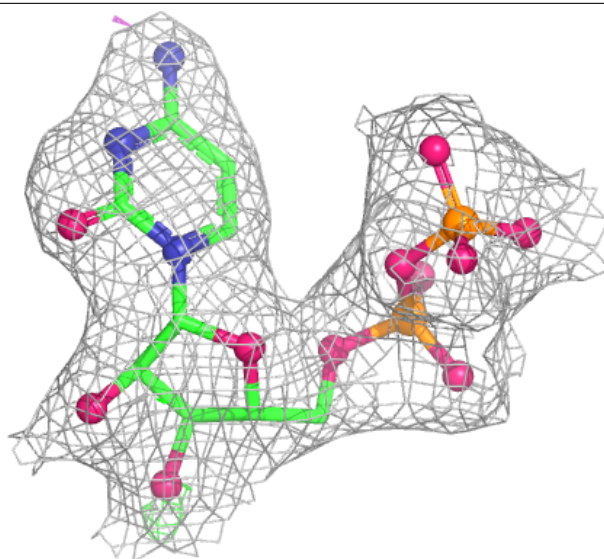






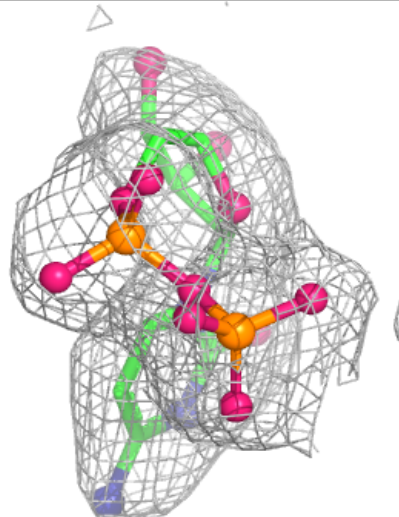
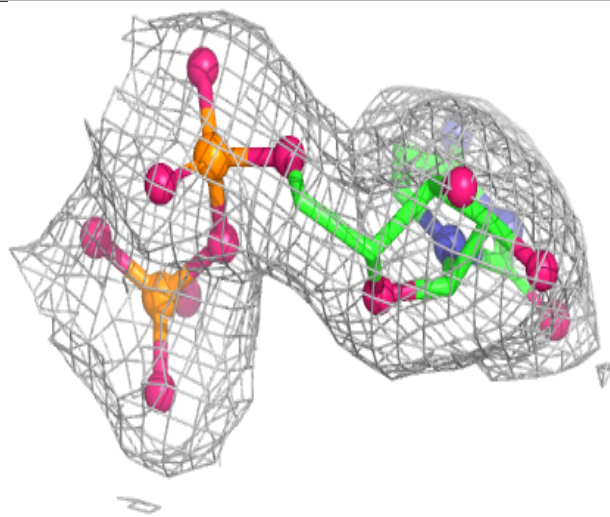
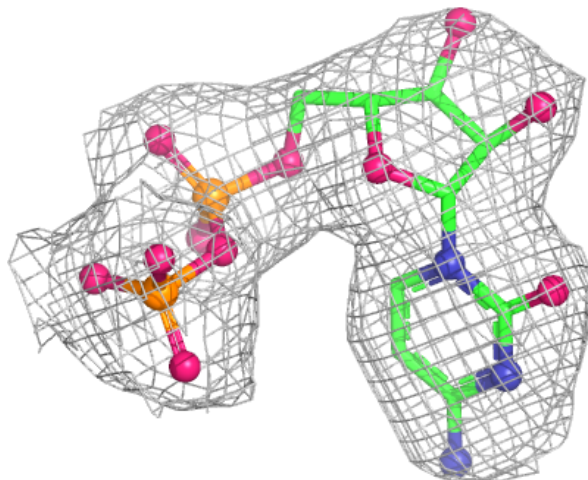
**Electron density around CDP D 809:**

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

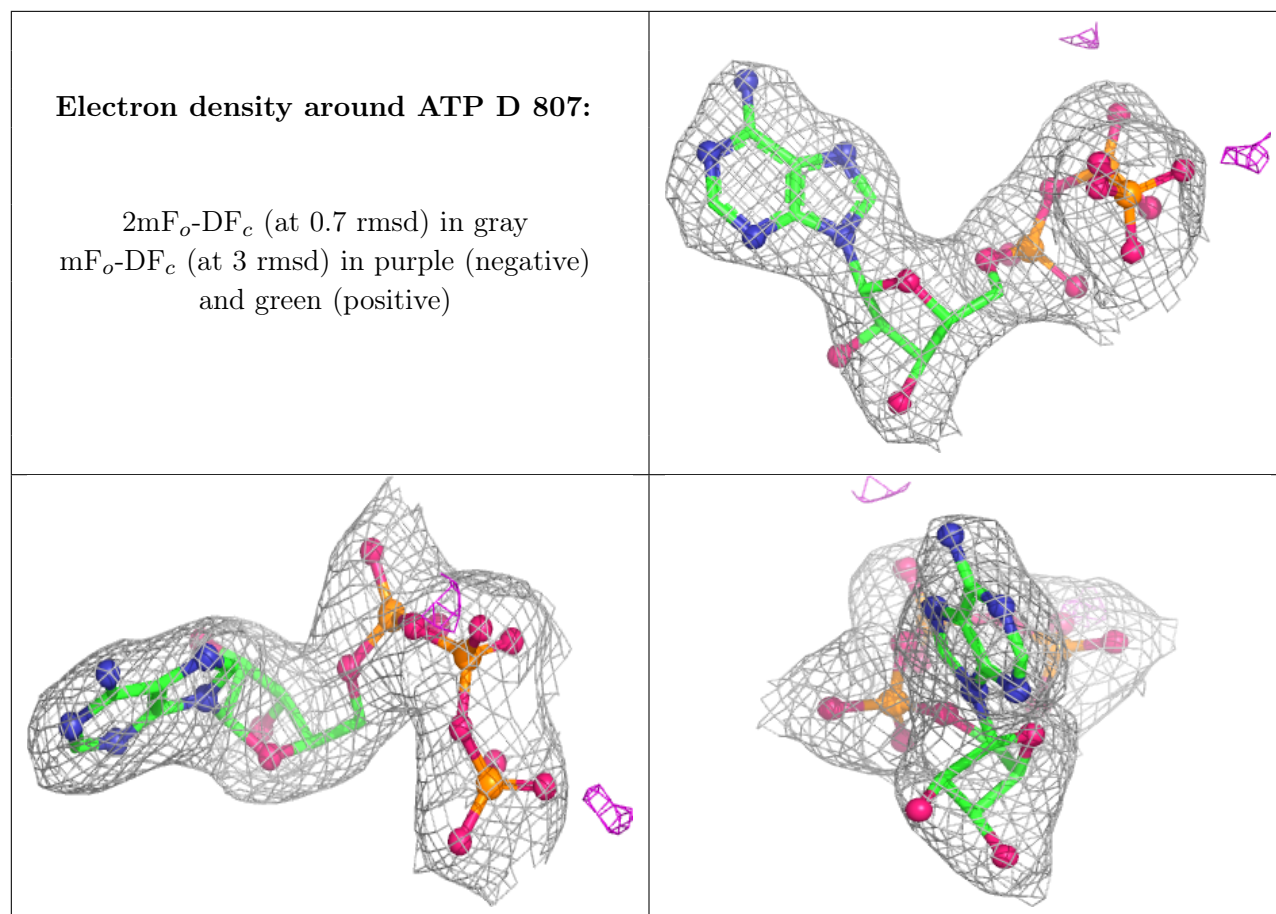


**Electron density around CDP E 809:**

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

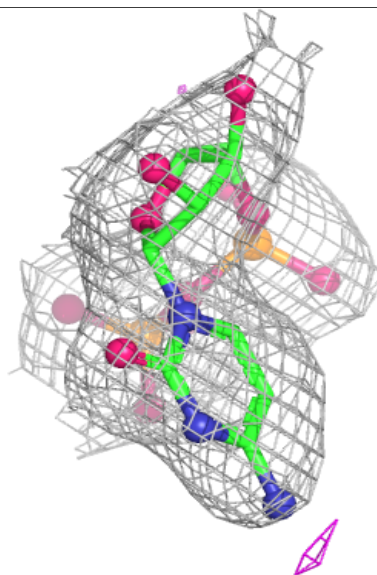
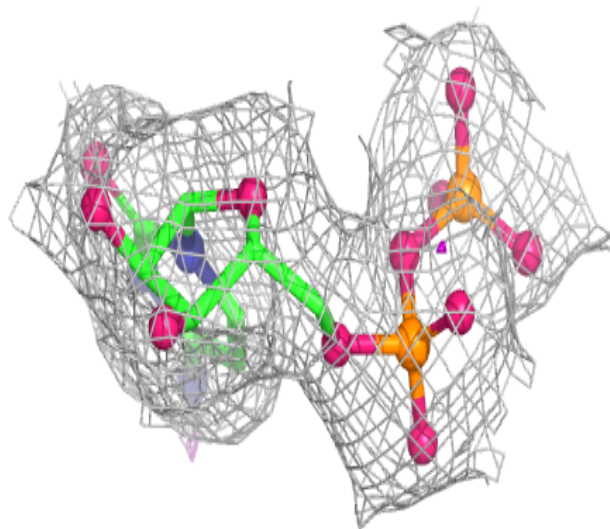
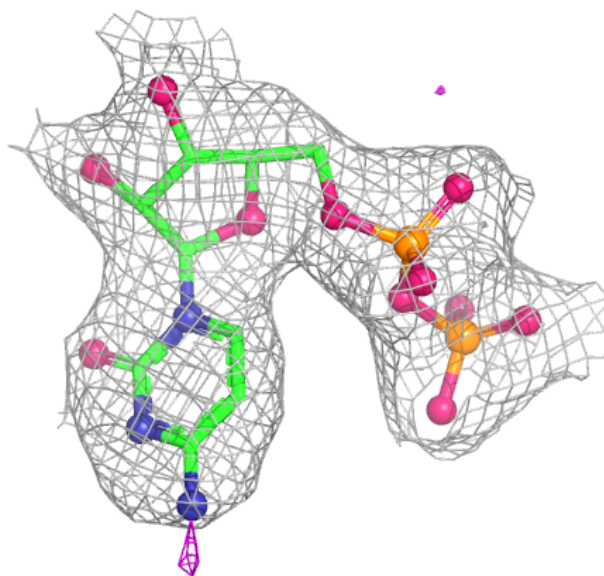


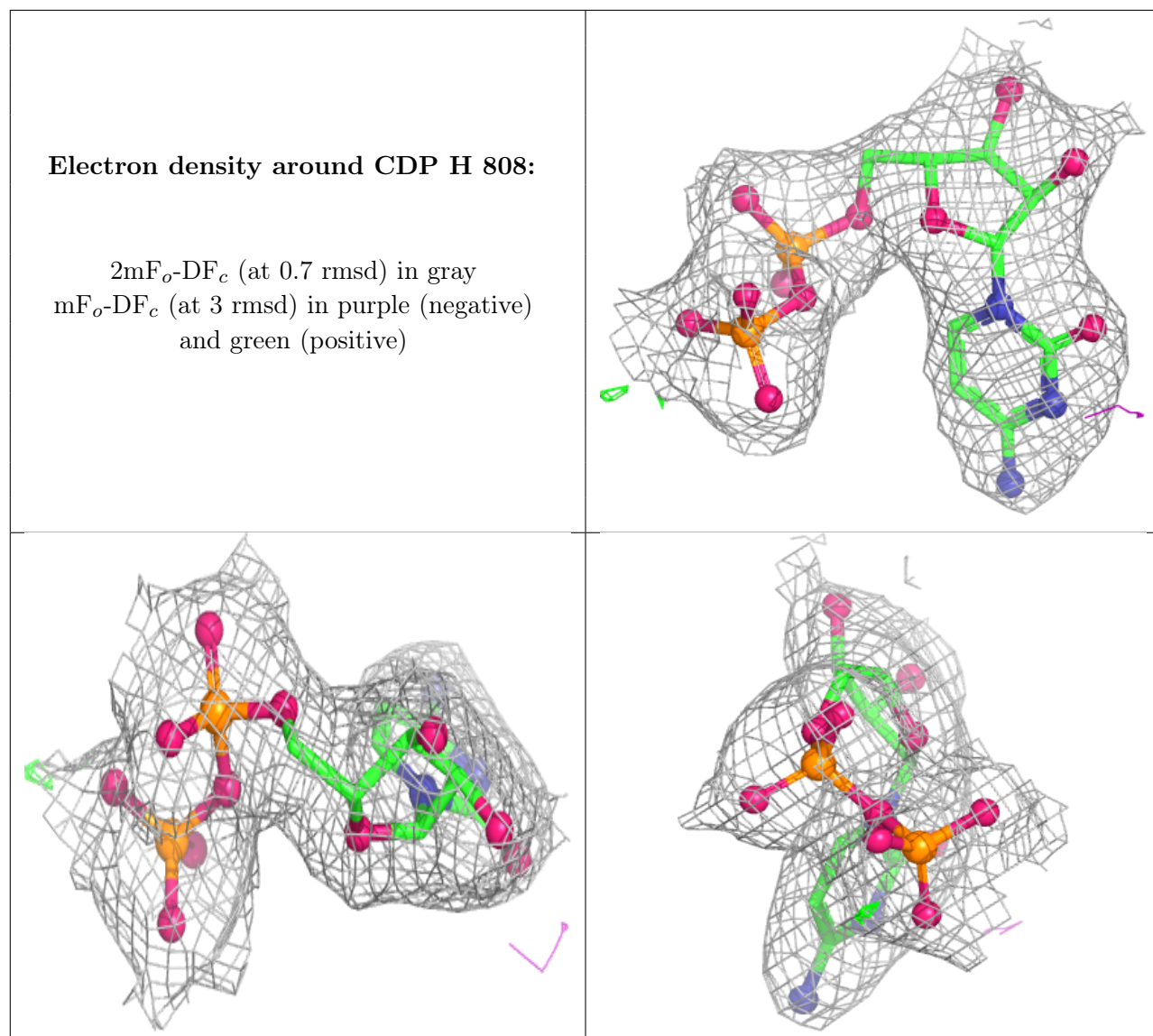




**Electron density around CDP G 808:**

$2mF_o-DF_c$  (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.