



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 03:38 AM UTC

PDB ID : 8VHP / pdb_00008vhp
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

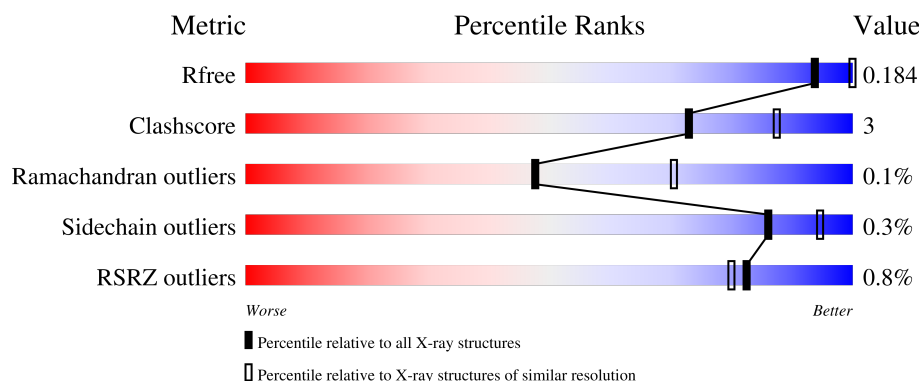
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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% 8% 6%
1	B	779	86% 8% 6%
1	C	779	87% 7% 6%
1	D	779	84% 9% 7%
1	E	779	84% 9% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	779	% 87% 7% 6%
1	G	779	% 86% 7% 6%
1	H	779	% 85% 9% 6%

2 Entry composition

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

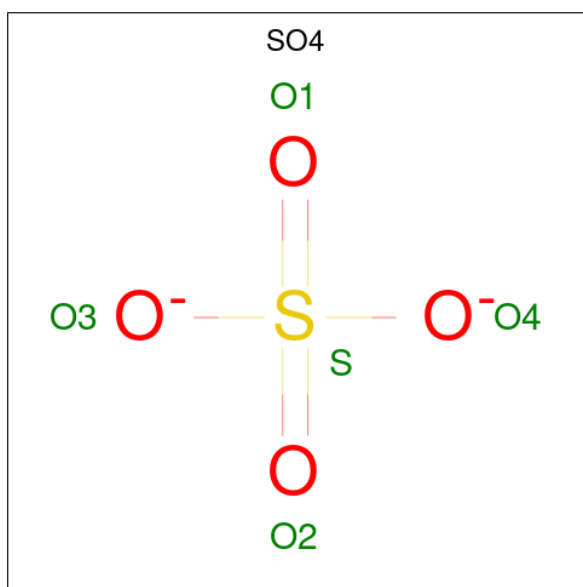
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP P00452
E	0	SER	-	expression tag	UNP P00452
E	28	ALA	TRP	engineered mutation	UNP P00452
F	-18	MET	-	initiating methionine	UNP P00452
F	-17	GLY	-	expression tag	UNP P00452
F	-16	SER	-	expression tag	UNP P00452
F	-15	SER	-	expression 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

Continued on next page...

Continued from previous page...

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 (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

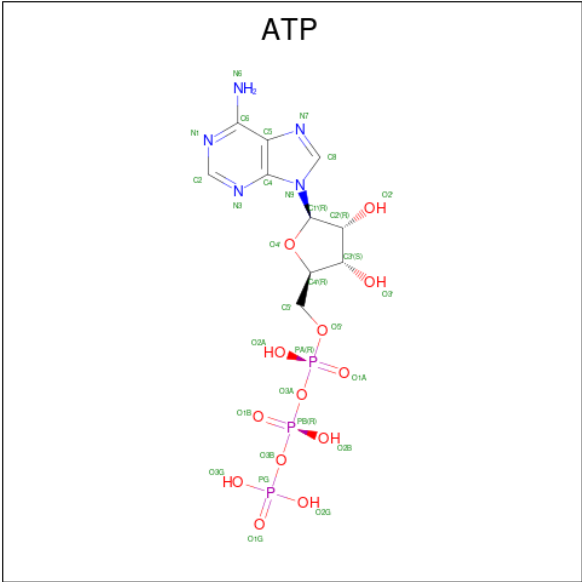
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

Continued on next page...

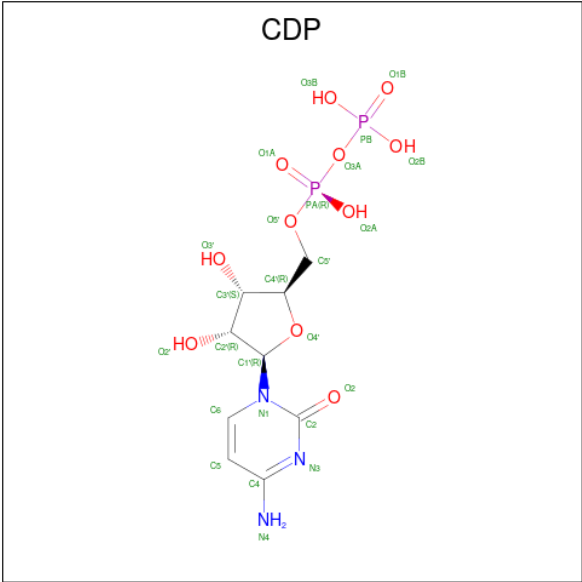
Continued from previous page...

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 (CCD ID: 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 (CCD ID: CDP) (formula: C₉H₁₅N₃O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is water.

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

Continued on next page...

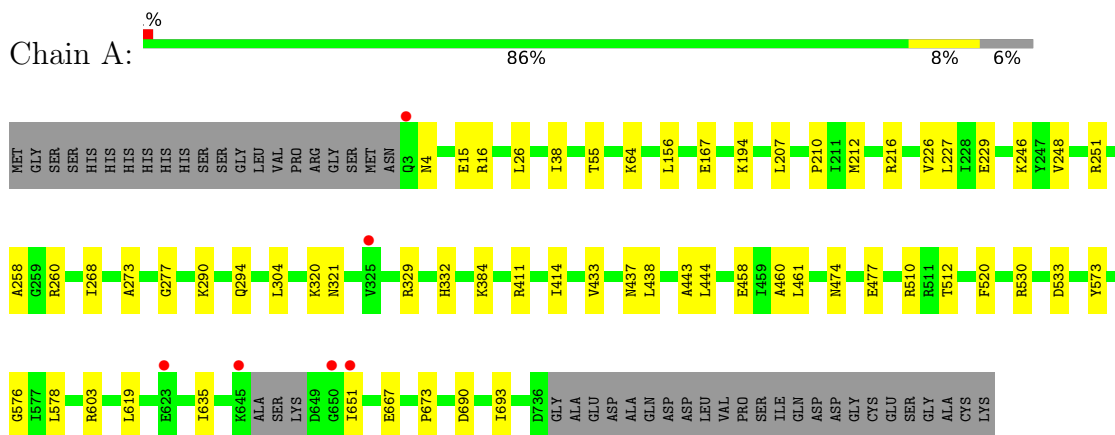
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

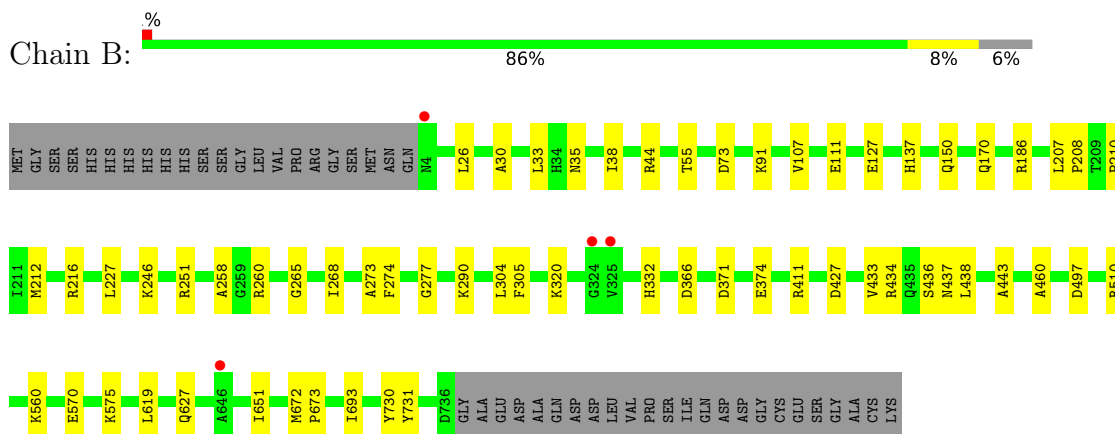
3 Residue-property plots [i](#)

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.

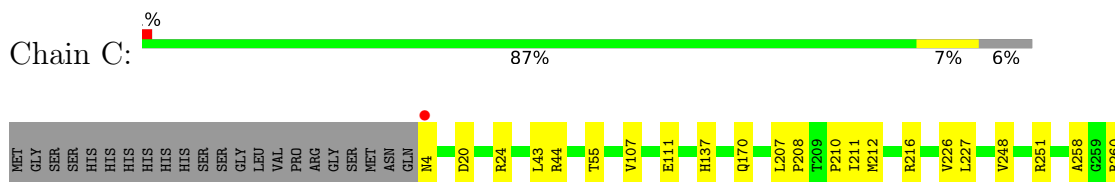
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

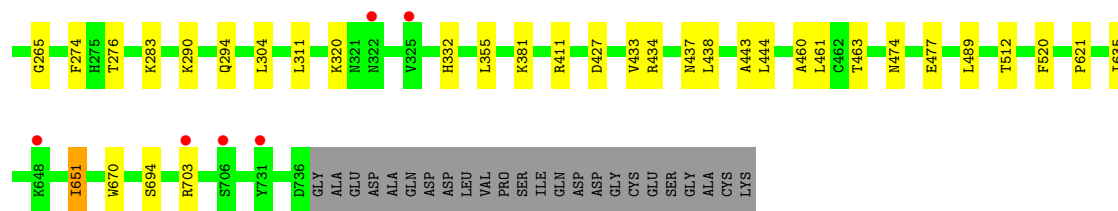


- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

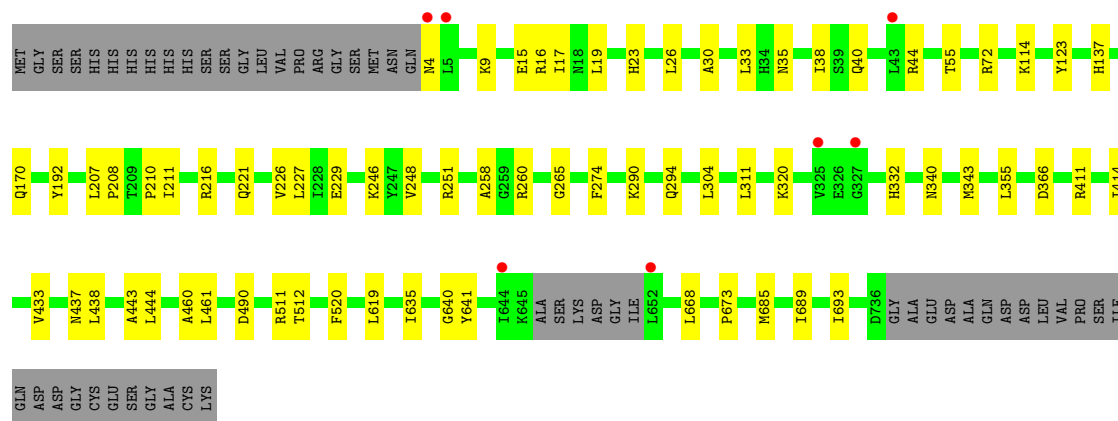
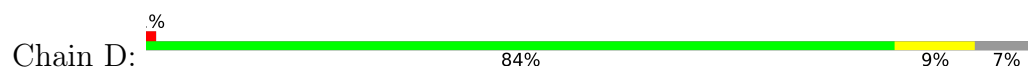


- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

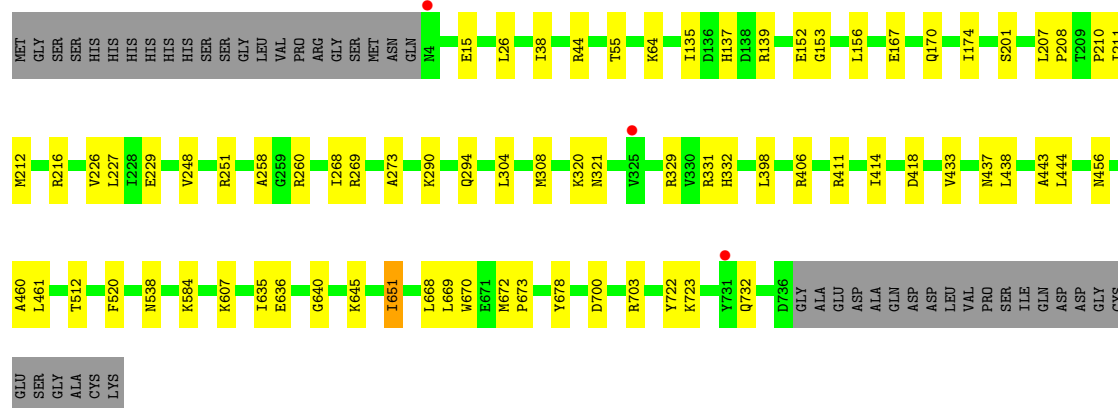
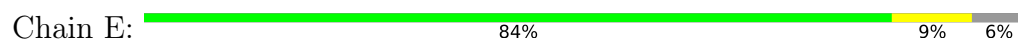




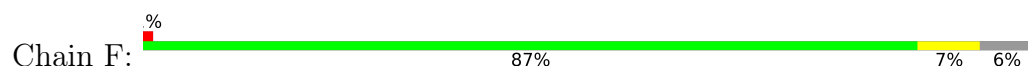
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

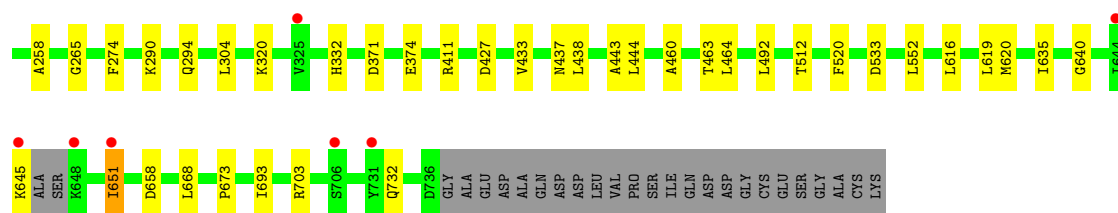


• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

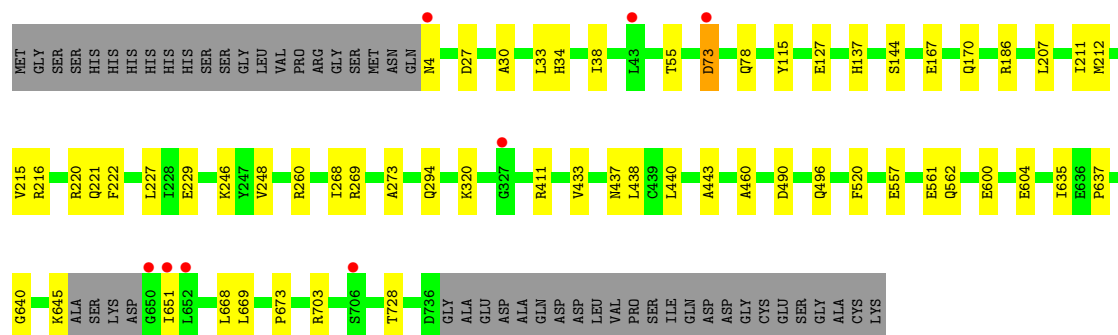
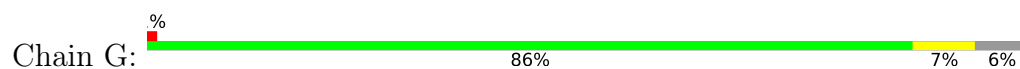


• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

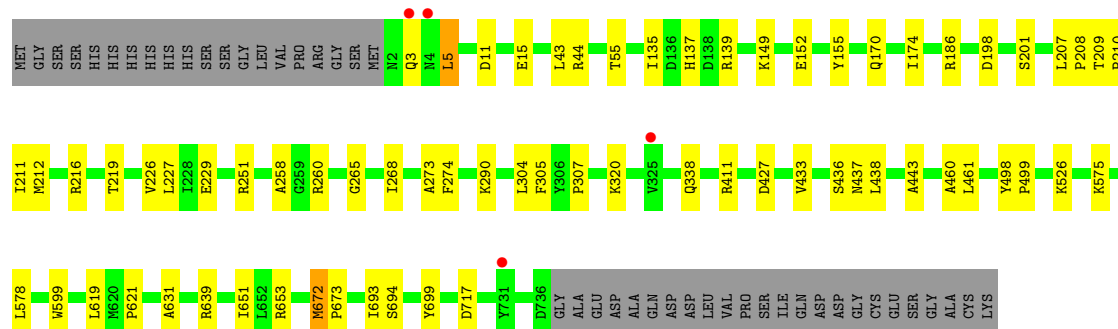
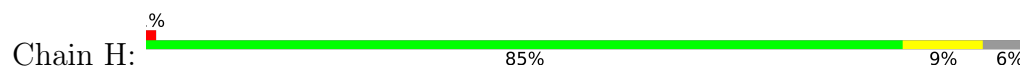




● Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.189 , 0.209 (Not available) , 0.184	Depositor DCC
R_{free} test set	2000 reflections (0.91%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	48995	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CDP, ATP, MG, 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	0.37	0/5942	0.72	1/8047 (0.0%)
1	B	0.36	0/5955	0.70	1/8065 (0.0%)
1	C	0.35	0/5976	0.71	2/8094 (0.0%)
1	D	0.37	0/5914	0.72	0/8009
1	E	0.35	0/5968	0.71	0/8083
1	F	0.34	0/5951	0.71	2/8058 (0.0%)
1	G	0.37	0/5926	0.72	1/8025 (0.0%)
1	H	0.36	0/5988	0.71	2/8110 (0.0%)
All	All	0.36	0/47620	0.71	9/64491 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	672	MET	CA-C-N	6.09	125.64	119.19
1	H	672	MET	C-N-CA	6.09	125.64	119.19
1	G	34	HIS	N-CA-C	5.58	118.31	109.50
1	A	277	GLY	N-CA-C	5.38	117.53	112.04
1	C	427	ASP	CA-C-N	5.28	124.94	119.56

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	36	0
1	B	5829	0	5758	40	0
1	C	5849	0	5771	35	0
1	D	5789	0	5716	41	0
1	E	5841	0	5766	46	0
1	F	5826	0	5753	38	0
1	G	5801	0	5730	36	0
1	H	5861	0	5784	42	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	3	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	4	0
6	C	149	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	160	0	0	3	0
6	E	118	0	0	5	0
6	F	139	0	0	4	0
6	G	166	0	0	5	0
6	H	176	0	0	7	0
All	All	48995	0	46402	304	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 304 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	0.92

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	70
1	B	731/779 (94%)	716 (98%)	14 (2%)	1 (0%)	48	70
1	C	733/779 (94%)	719 (98%)	13 (2%)	1 (0%)	48	70
1	D	723/779 (93%)	707 (98%)	15 (2%)	1 (0%)	48	70
1	E	732/779 (94%)	717 (98%)	14 (2%)	1 (0%)	48	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	728/779 (94%)	714 (98%)	13 (2%)	1 (0%)	48	70
1	G	725/779 (93%)	709 (98%)	15 (2%)	1 (0%)	48	70
1	H	734/779 (94%)	718 (98%)	15 (2%)	1 (0%)	48	70
All	All	5833/6232 (94%)	5711 (98%)	114 (2%)	8 (0%)	48	70

5 of 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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	626/665 (94%)	624 (100%)	2 (0%)	86	94
1	B	627/665 (94%)	626 (100%)	1 (0%)	87	95
1	C	629/665 (95%)	628 (100%)	1 (0%)	87	95
1	D	623/665 (94%)	620 (100%)	3 (0%)	81	92
1	E	628/665 (94%)	626 (100%)	2 (0%)	86	94
1	F	627/665 (94%)	626 (100%)	1 (0%)	87	95
1	G	624/665 (94%)	620 (99%)	4 (1%)	78	91
1	H	631/665 (95%)	629 (100%)	2 (0%)	86	94
All	All	5015/5320 (94%)	4999 (100%)	16 (0%)	86	94

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	5	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	651	ILE
1	E	651	ILE
1	G	557	GLU
1	E	414	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	732	GLN
1	G	654	GLN
1	G	435	GLN
1	H	170	GLN
1	C	609	HIS

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
2	SO4	H	810	-	4,4,4	0.23	0	6,6,6	0.08	0
3	ATP	G	805	4	32,33,33	0.36	0	48,52,52	0.41	0
5	CDP	H	808	-	25,26,26	0.90	0	38,40,40	0.93	2 (5%)
2	SO4	C	802	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	F	810	-	4,4,4	0.23	0	6,6,6	0.08	0
3	ATP	C	804	4	32,33,33	0.34	0	48,52,52	0.42	0
3	ATP	B	804	4	32,33,33	0.36	0	48,52,52	0.40	0
3	ATP	E	806	4	32,33,33	0.32	0	48,52,52	0.41	0
5	CDP	A	809	-	25,26,26	0.93	1 (4%)	38,40,40	0.96	1 (2%)
3	ATP	B	807	4	32,33,33	0.41	0	48,52,52	0.35	0
2	SO4	B	810	-	4,4,4	0.23	0	6,6,6	0.11	0
3	ATP	A	806	4	32,33,33	0.38	0	48,52,52	0.36	0
3	ATP	H	805	4	32,33,33	0.35	0	48,52,52	0.37	0
2	SO4	F	801	-	4,4,4	0.24	0	6,6,6	0.09	0
3	ATP	C	807	4	32,33,33	0.40	0	48,52,52	0.36	0
2	SO4	C	810	-	4,4,4	0.23	0	6,6,6	0.13	0
3	ATP	A	807	4	32,33,33	0.43	0	48,52,52	0.36	0
2	SO4	A	810	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	803	-	4,4,4	0.23	0	6,6,6	0.08	0
3	ATP	E	807	4	32,33,33	0.37	0	48,52,52	0.35	0
3	ATP	G	803	4	32,33,33	0.40	0	48,52,52	0.42	0
2	SO4	F	802	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	811	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	813	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	B	802	-	4,4,4	0.24	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	803	-	4,4,4	0.22	0	6,6,6	0.09	0
5	CDP	E	809	-	25,26,26	0.88	0	38,40,40	0.94	1 (2%)
2	SO4	C	801	-	4,4,4	0.24	0	6,6,6	0.07	0
3	ATP	C	806	4	32,33,33	0.34	0	48,52,52	0.41	0
3	ATP	E	804	4	32,33,33	0.37	0	48,52,52	0.38	0
2	SO4	G	809	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	H	809	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	H	802	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	E	802	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	812	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	D	812	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	E	803	-	4,4,4	0.22	0	6,6,6	0.09	0
3	ATP	H	806	4	32,33,33	0.37	0	48,52,52	0.37	0
5	CDP	C	809	-	25,26,26	0.89	0	38,40,40	1.01	1 (2%)
3	ATP	F	806	4	32,33,33	0.30	0	48,52,52	0.36	0
2	SO4	E	810	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	F	807	4	32,33,33	0.39	0	48,52,52	0.38	0
3	ATP	B	806	4	32,33,33	0.32	0	48,52,52	0.32	0
2	SO4	D	810	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	G	801	-	4,4,4	0.23	0	6,6,6	0.06	0
3	ATP	D	804	4	32,33,33	0.36	0	48,52,52	0.39	0
2	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	G	802	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	H	801	-	4,4,4	0.22	0	6,6,6	0.12	0
2	SO4	H	811	-	4,4,4	0.22	0	6,6,6	0.12	0
3	ATP	D	806	4	32,33,33	0.33	0	48,52,52	0.37	0
3	ATP	D	807	4	32,33,33	0.38	0	48,52,52	0.33	0
2	SO4	D	813	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	F	803	-	4,4,4	0.23	0	6,6,6	0.10	0
5	CDP	B	809	-	25,26,26	0.91	1 (4%)	38,40,40	0.94	0
2	SO4	D	801	-	4,4,4	0.23	0	6,6,6	0.07	0
5	CDP	D	809	-	25,26,26	0.89	0	38,40,40	0.96	2 (5%)
5	CDP	F	809	-	25,26,26	0.90	1 (4%)	38,40,40	1.01	1 (2%)
3	ATP	H	803	4	32,33,33	0.39	0	48,52,52	0.40	0
5	CDP	G	808	-	25,26,26	0.90	1 (4%)	38,40,40	0.94	1 (2%)
2	SO4	D	803	-	4,4,4	0.23	0	6,6,6	0.07	0
3	ATP	F	804	4	32,33,33	0.35	0	48,52,52	0.37	0
2	SO4	D	811	-	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	A	814	-	4,4,4	0.23	0	6,6,6	0.12	0
3	ATP	G	806	4	32,33,33	0.37	0	48,52,52	0.34	0
2	SO4	C	811	-	4,4,4	0.23	0	6,6,6	0.09	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	G	805	4	-	9/22/38/38	0/3/3/3
5	CDP	H	808	-	-	5/16/32/32	0/2/2/2
3	ATP	C	804	4	-	2/22/38/38	0/3/3/3
3	ATP	B	804	4	-	2/22/38/38	0/3/3/3
3	ATP	E	806	4	-	6/22/38/38	0/3/3/3
5	CDP	A	809	-	-	7/16/32/32	0/2/2/2
3	ATP	B	807	4	-	6/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	806	4	-	5/22/38/38	0/3/3/3
3	ATP	H	805	4	-	6/22/38/38	0/3/3/3
3	ATP	C	807	4	-	5/22/38/38	0/3/3/3
3	ATP	E	807	4	-	7/22/38/38	0/3/3/3
3	ATP	A	807	4	-	7/22/38/38	0/3/3/3
3	ATP	G	803	4	-	0/22/38/38	0/3/3/3
5	CDP	E	809	-	-	4/16/32/32	0/2/2/2
3	ATP	C	806	4	-	7/22/38/38	0/3/3/3
3	ATP	E	804	4	-	0/22/38/38	0/3/3/3
3	ATP	H	806	4	-	7/22/38/38	0/3/3/3
3	ATP	F	806	4	-	4/22/38/38	0/3/3/3
3	ATP	F	807	4	-	7/22/38/38	0/3/3/3
3	ATP	B	806	4	-	9/22/38/38	0/3/3/3
3	ATP	D	804	4	-	0/22/38/38	0/3/3/3
5	CDP	D	809	-	-	5/16/32/32	0/2/2/2
3	ATP	D	806	4	-	8/22/38/38	0/3/3/3
3	ATP	D	807	4	-	6/22/38/38	0/3/3/3
5	CDP	B	809	-	-	6/16/32/32	0/2/2/2
5	CDP	F	809	-	-	7/16/32/32	0/2/2/2
3	ATP	H	803	4	-	2/22/38/38	0/3/3/3
5	CDP	G	808	-	-	7/16/32/32	0/2/2/2
3	ATP	F	804	4	-	0/22/38/38	0/3/3/3
5	CDP	C	809	-	-	7/16/32/32	0/2/2/2
3	ATP	G	806	4	-	6/22/38/38	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

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	809	CDP	C3'-C2'-C1'	2.35	105.91	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	809	CDP	C3'-C2'-C1'	2.29	105.79	101.46
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

There are no chirality outliers.

5 of 159 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

There are no ring outliers.

26 monomers are involved in 39 short contacts:

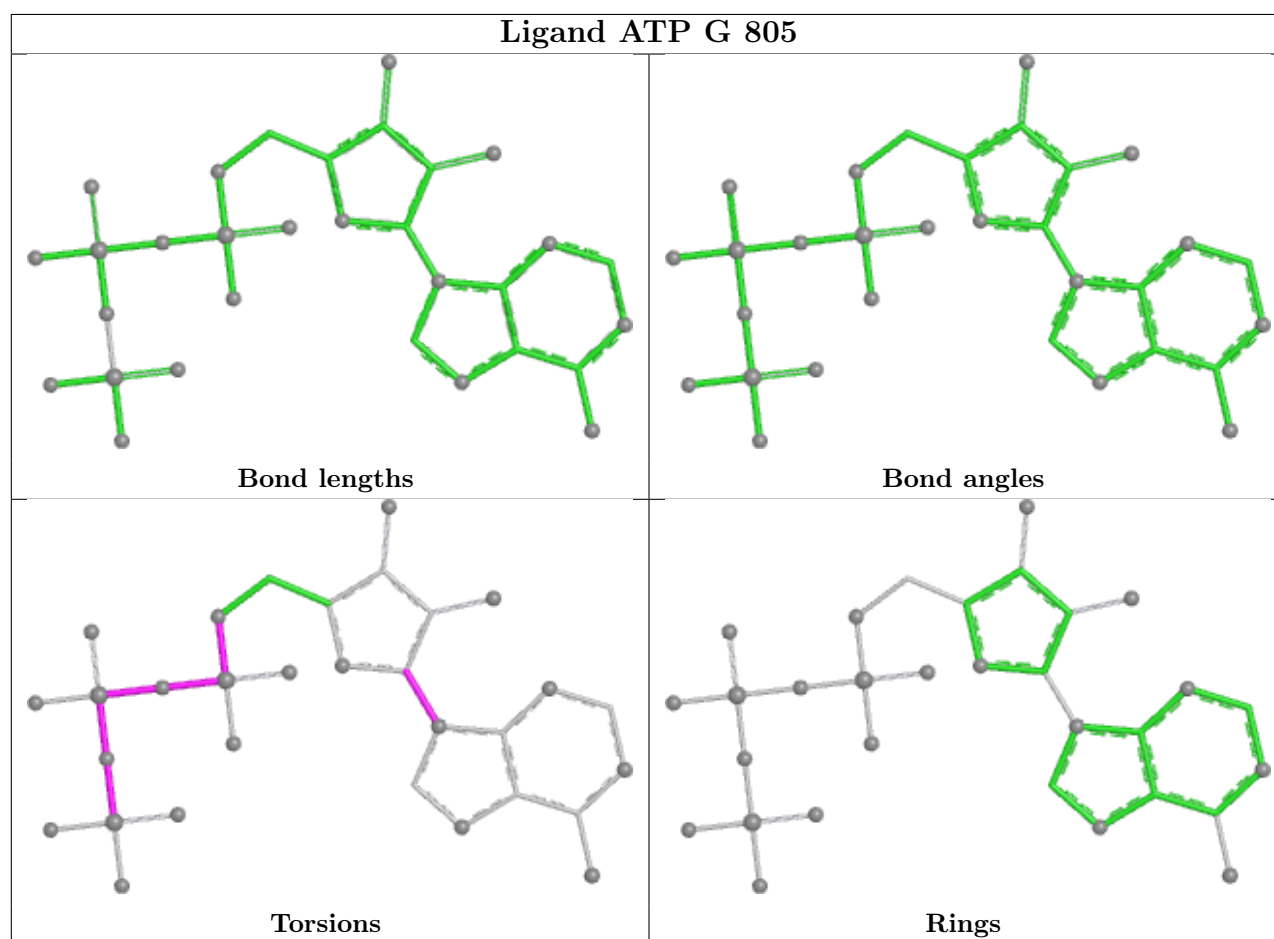
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	808	CDP	2	0
2	F	810	SO4	1	0
3	C	804	ATP	1	0
3	B	804	ATP	2	0
5	A	809	CDP	2	0
2	F	801	SO4	1	0
3	G	803	ATP	1	0
5	E	809	CDP	2	0
3	E	804	ATP	2	0
2	G	809	SO4	1	0
2	E	802	SO4	1	0
2	D	812	SO4	1	0
5	C	809	CDP	2	0
3	F	806	ATP	1	0
2	D	810	SO4	1	0
2	G	801	SO4	1	0
3	D	804	ATP	1	0
2	B	801	SO4	1	0
5	B	809	CDP	2	0
2	D	801	SO4	1	0
5	D	809	CDP	2	0
5	F	809	CDP	3	0

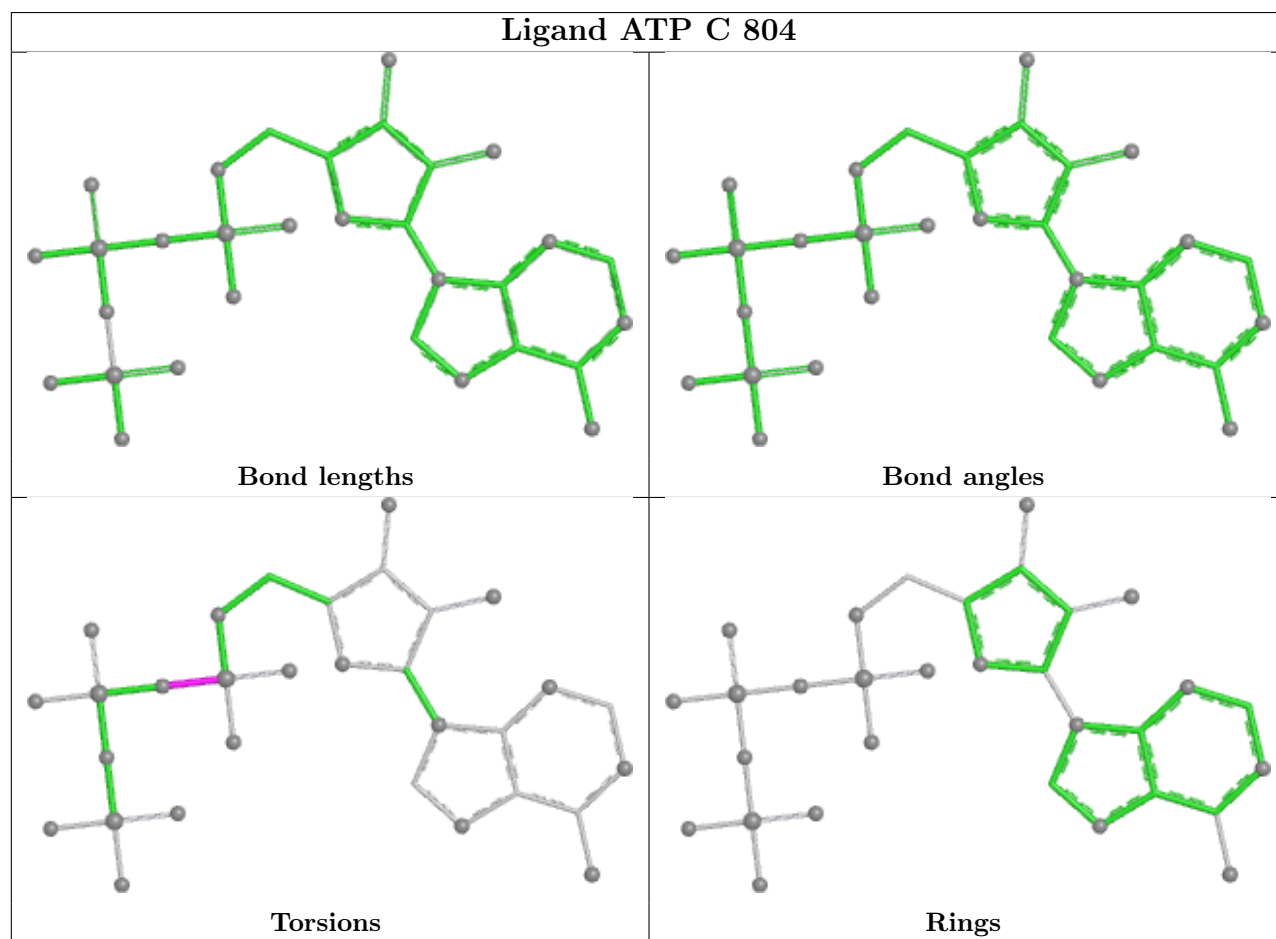
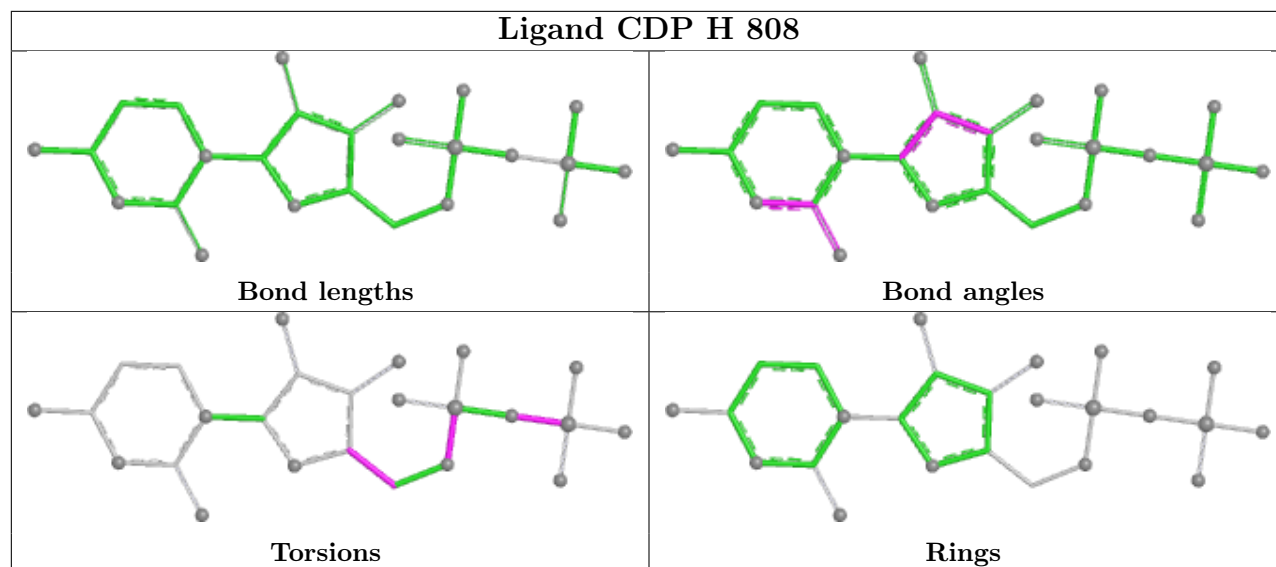
Continued on next page...

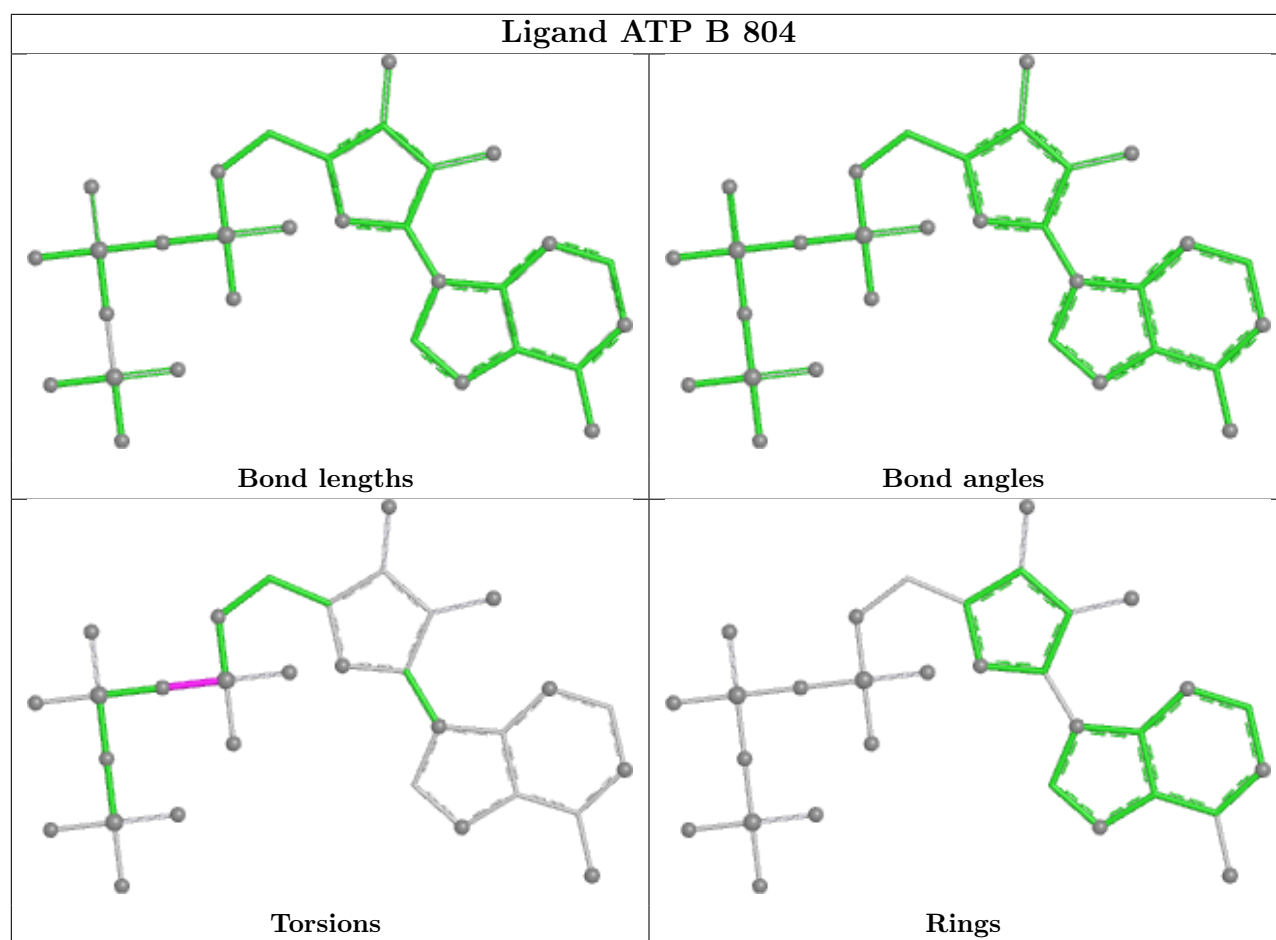
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	803	ATP	2	0
5	G	808	CDP	2	0
3	F	804	ATP	2	0
2	D	811	SO4	1	0

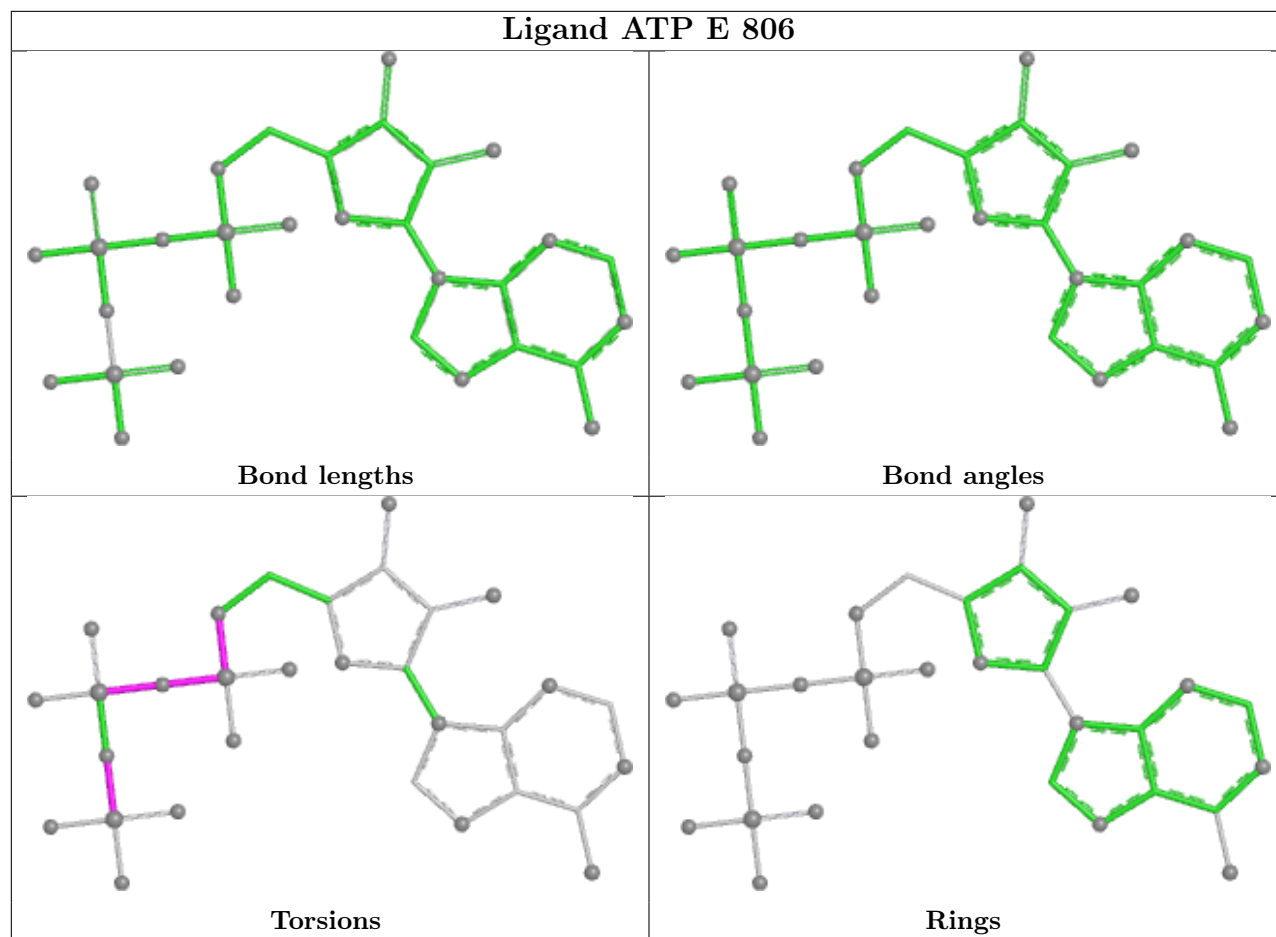
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



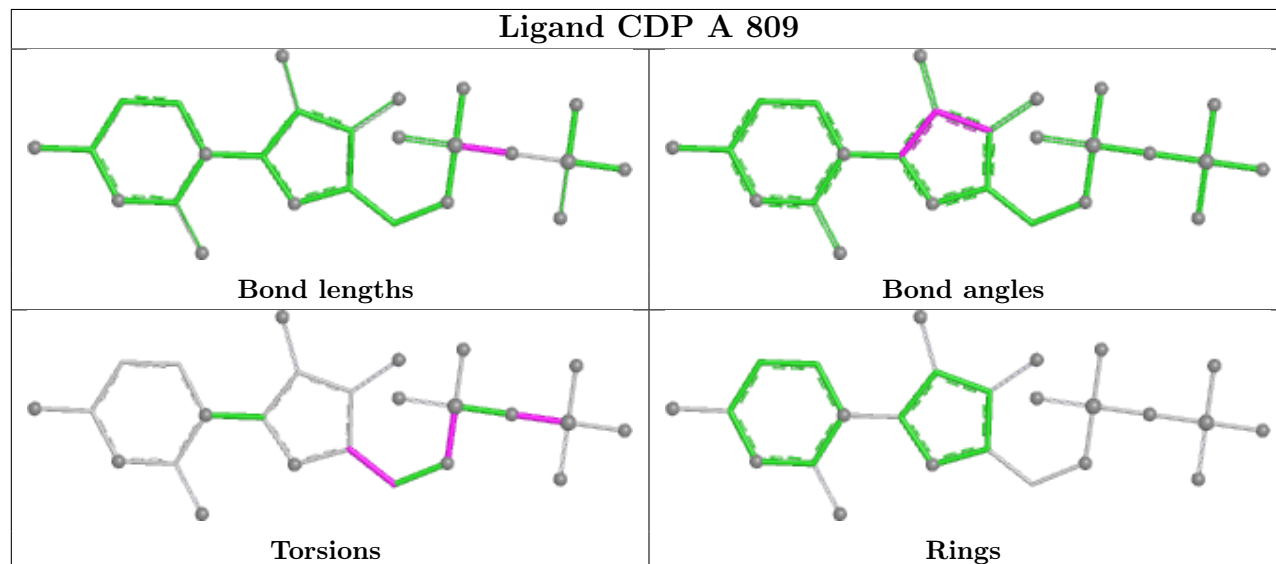


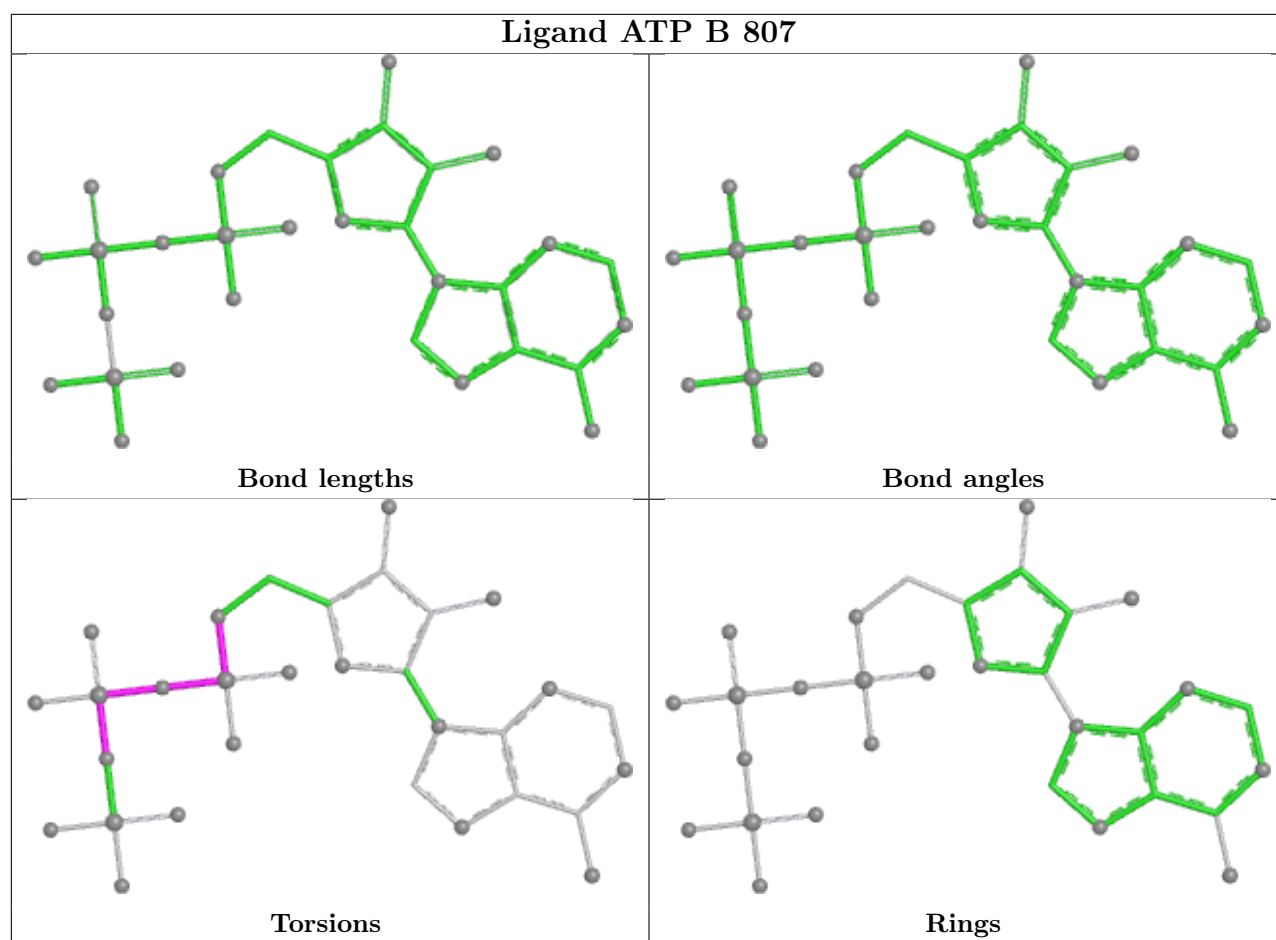


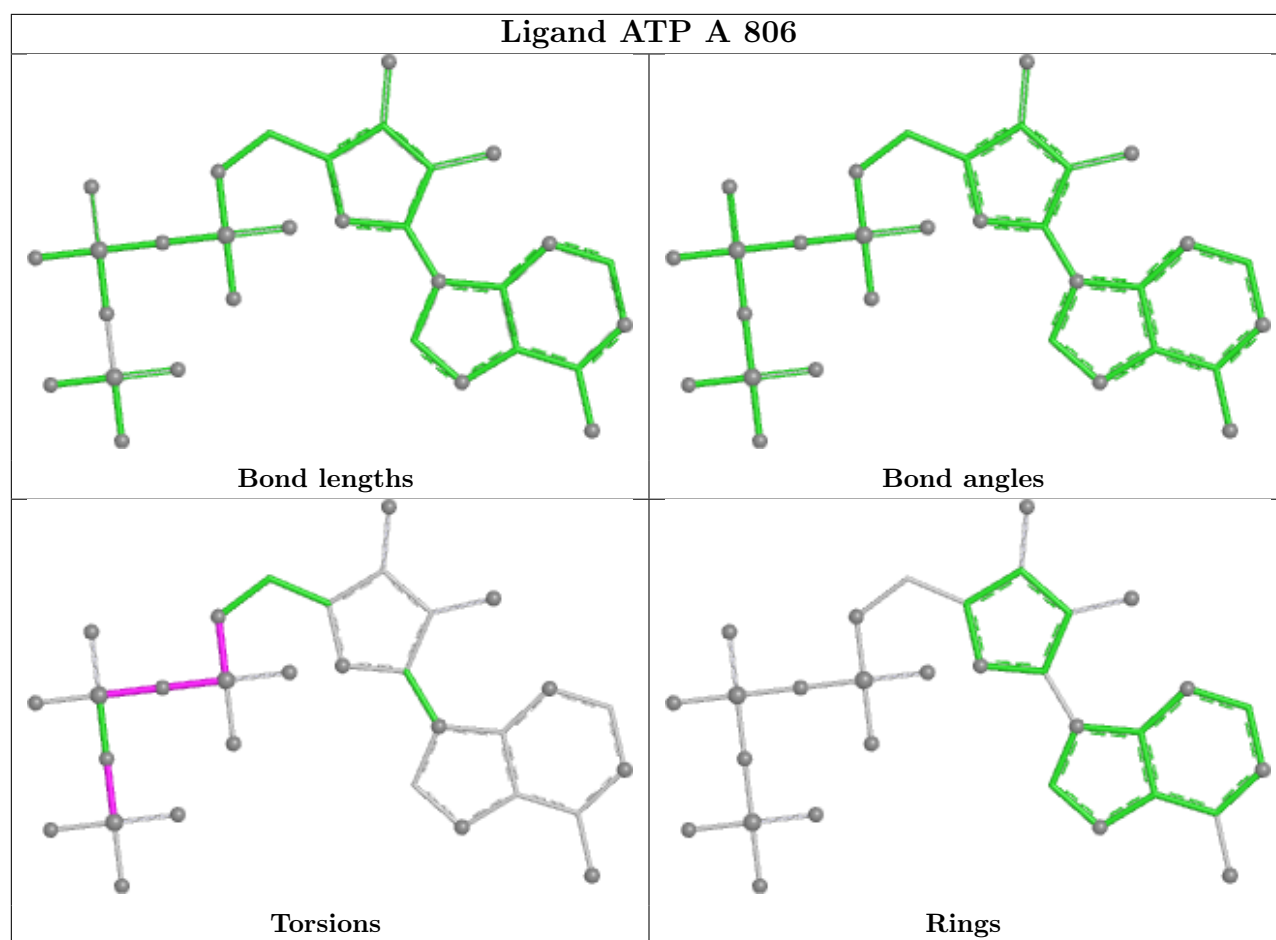
Ligand ATP E 806

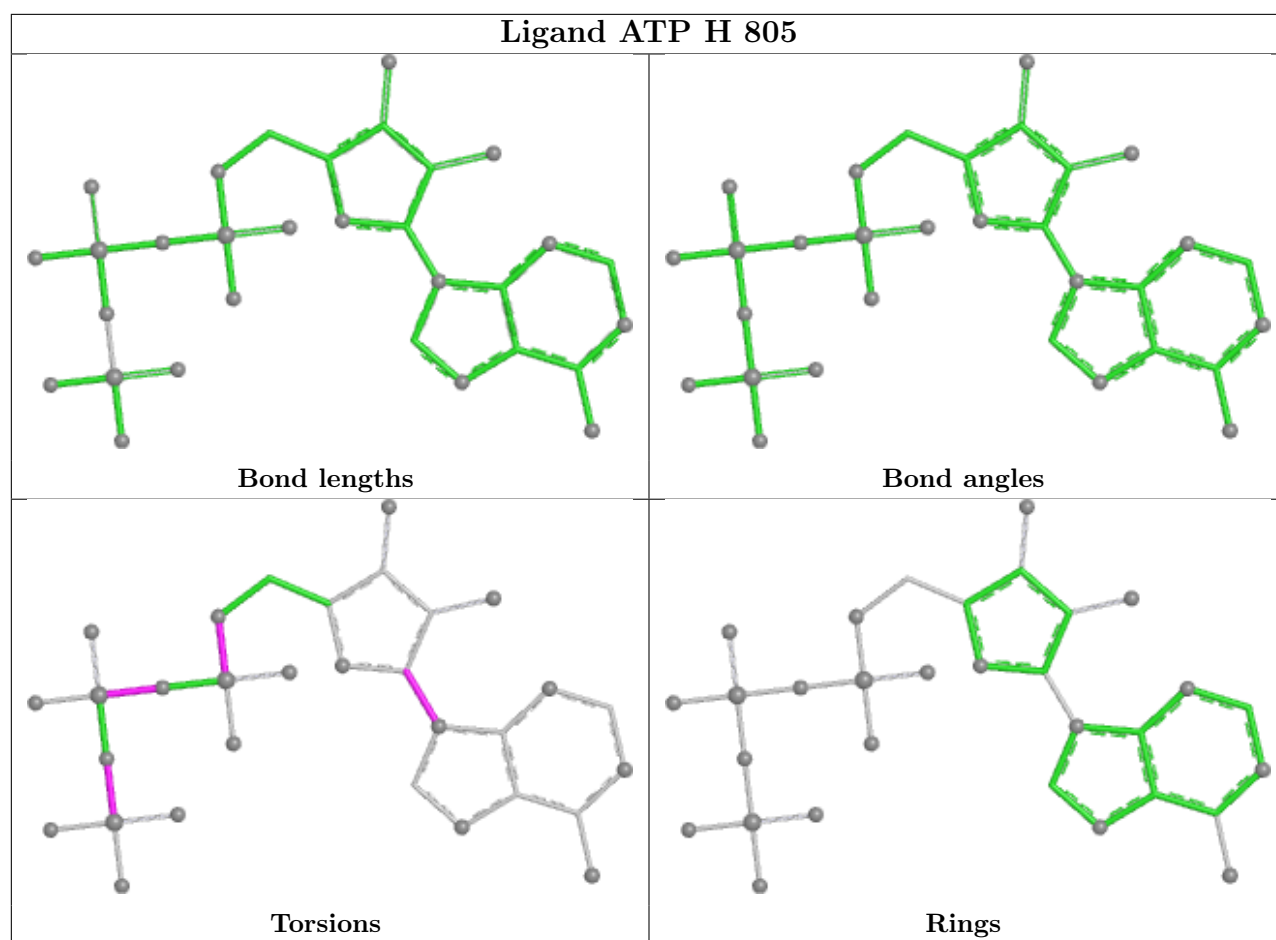


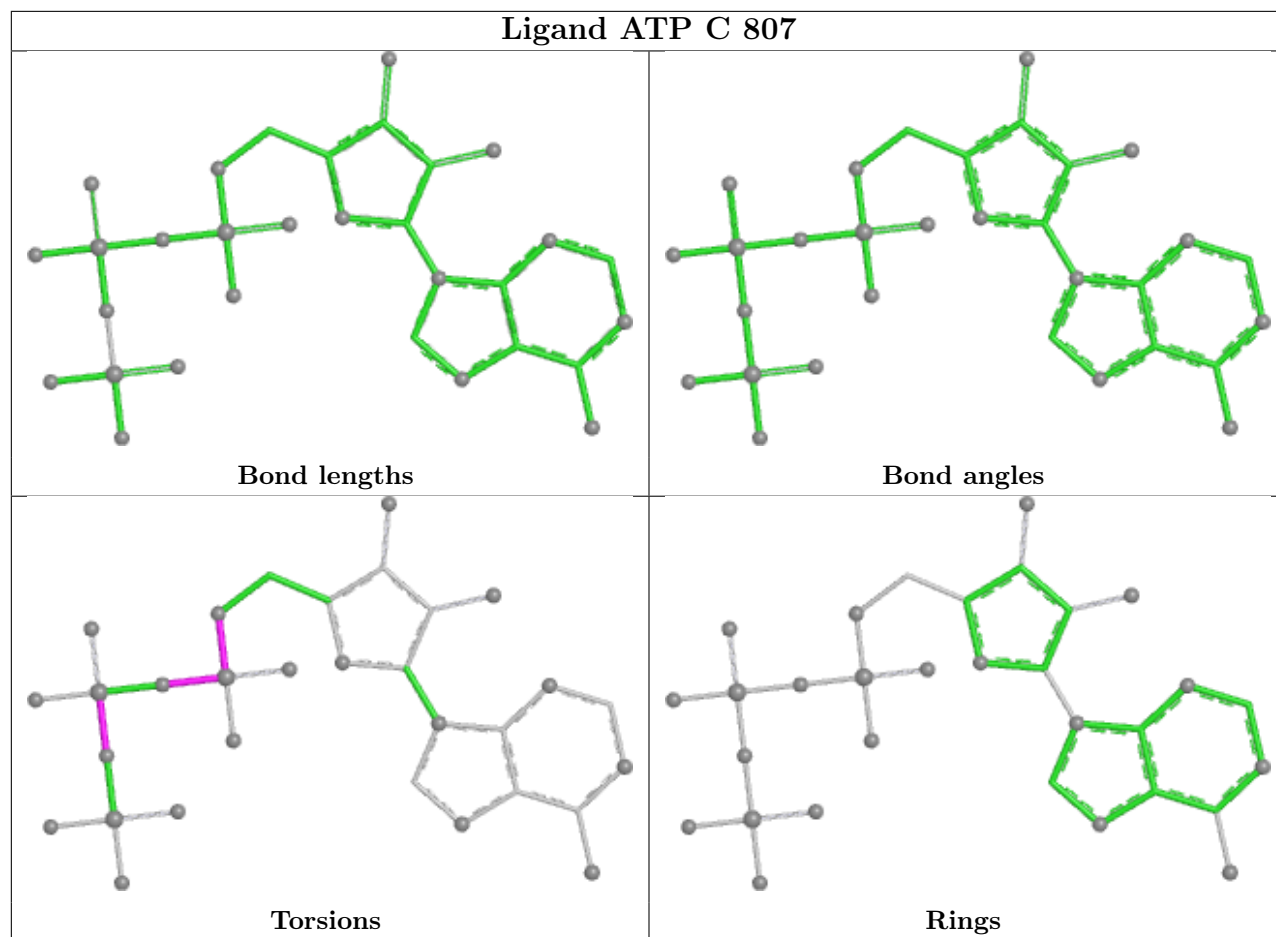
Ligand CDP A 809

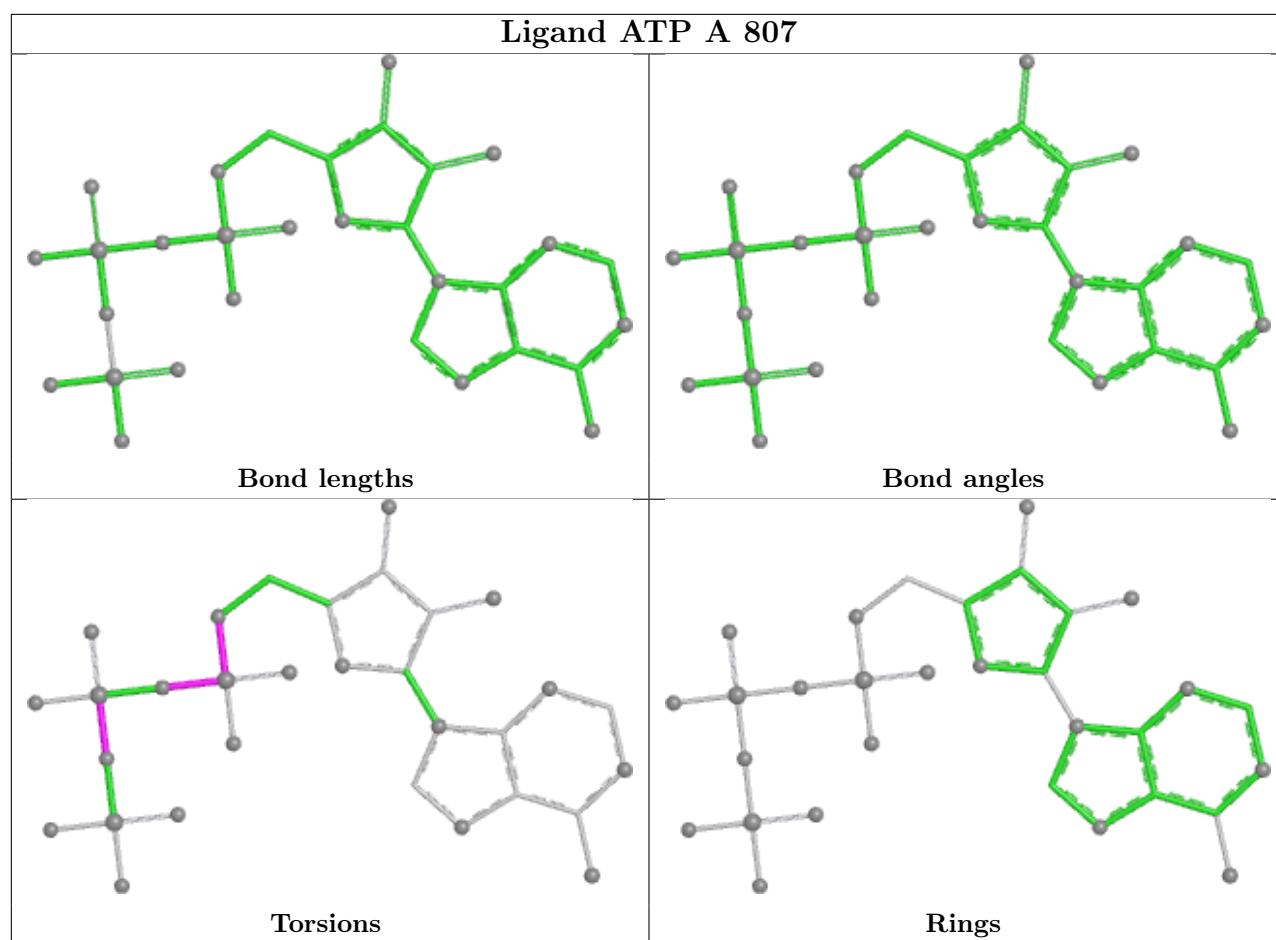


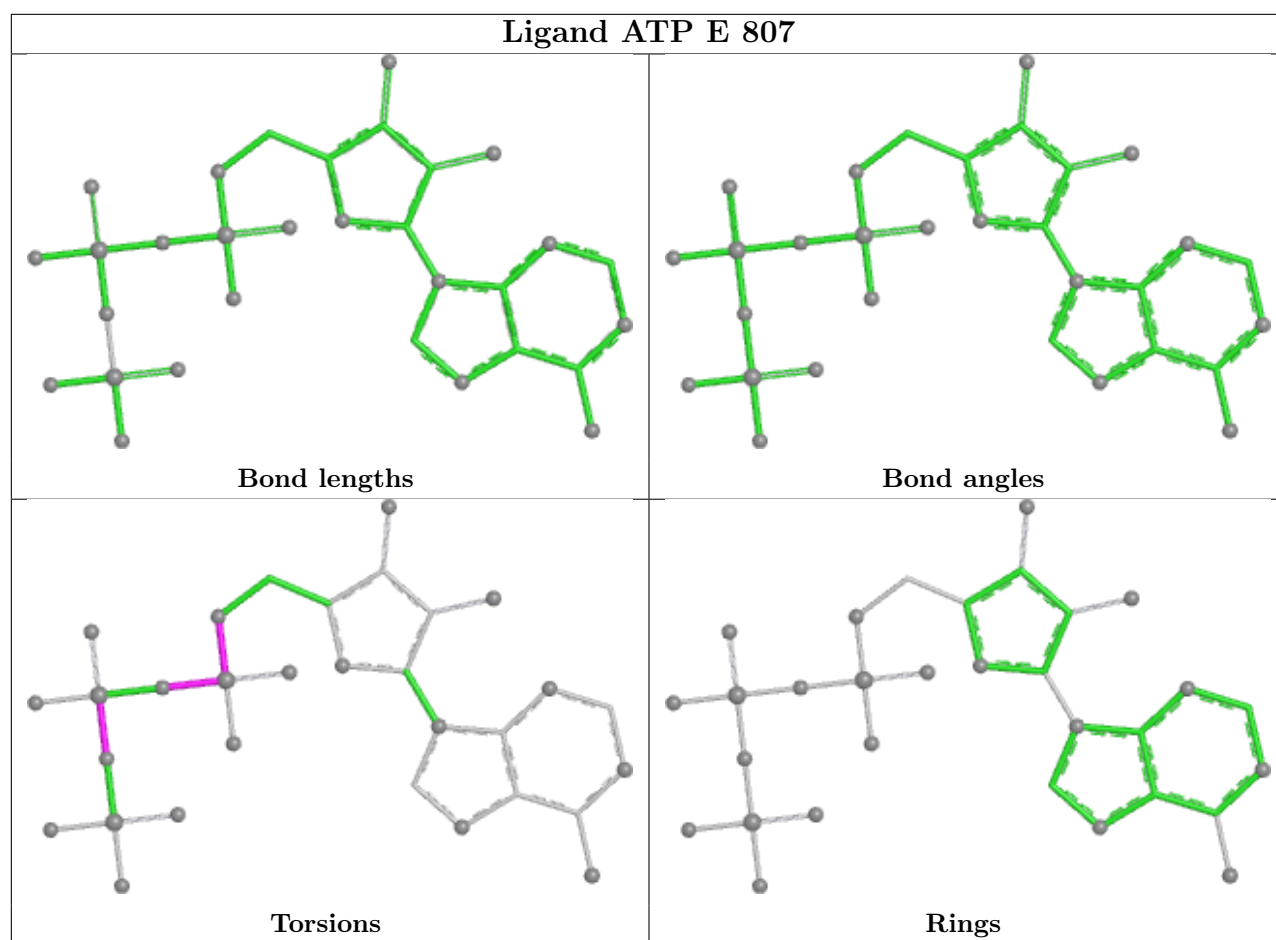


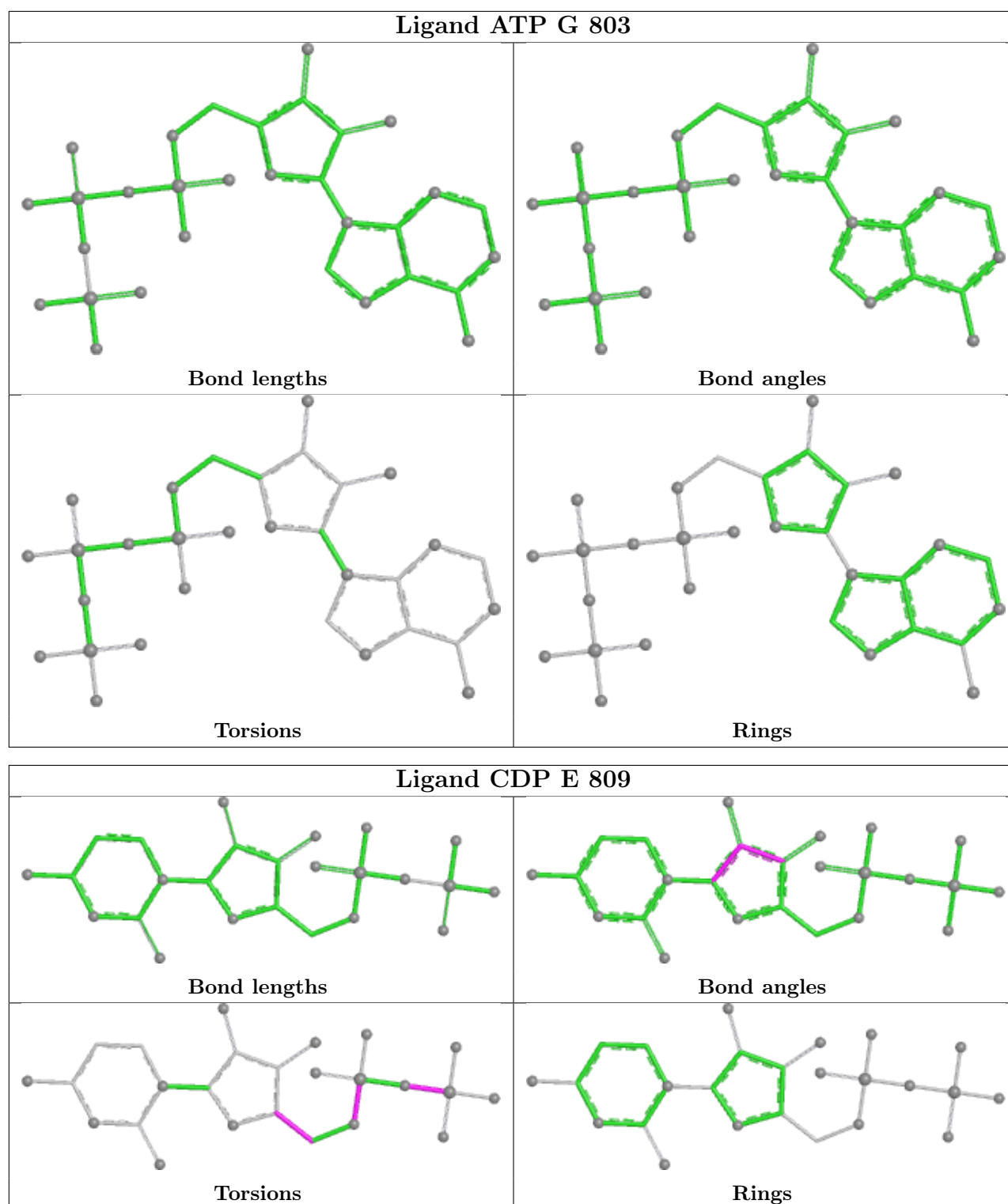


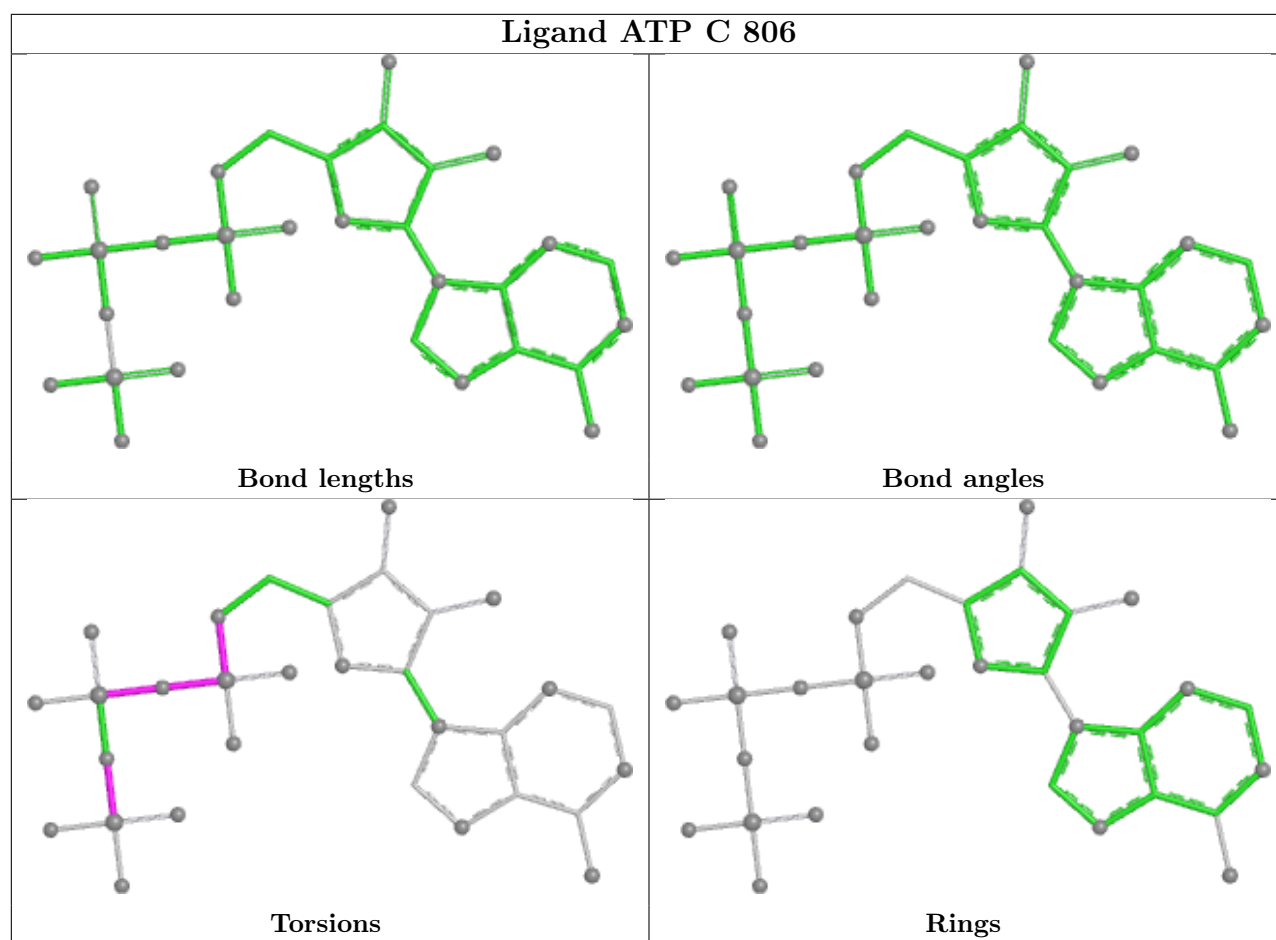


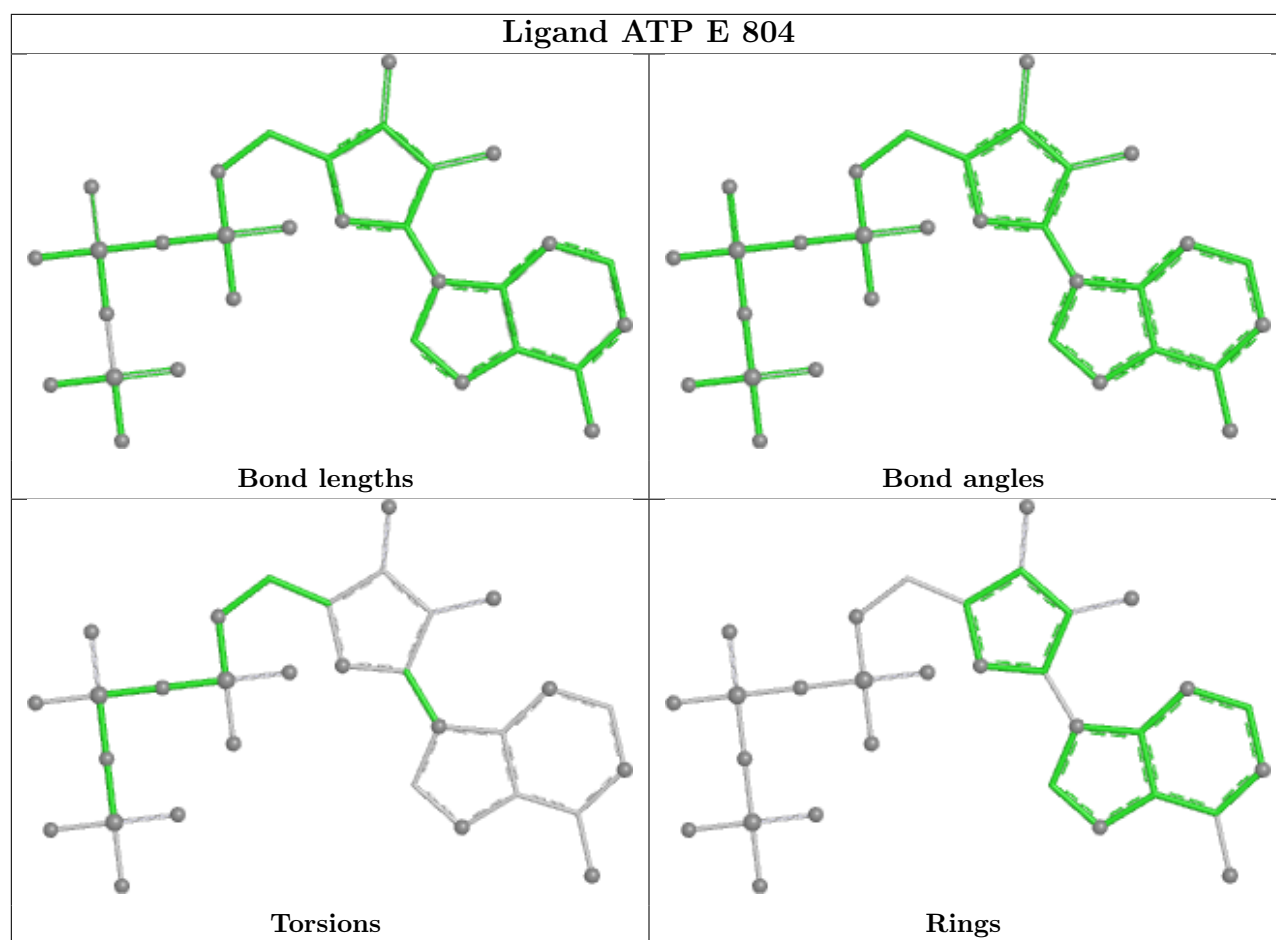


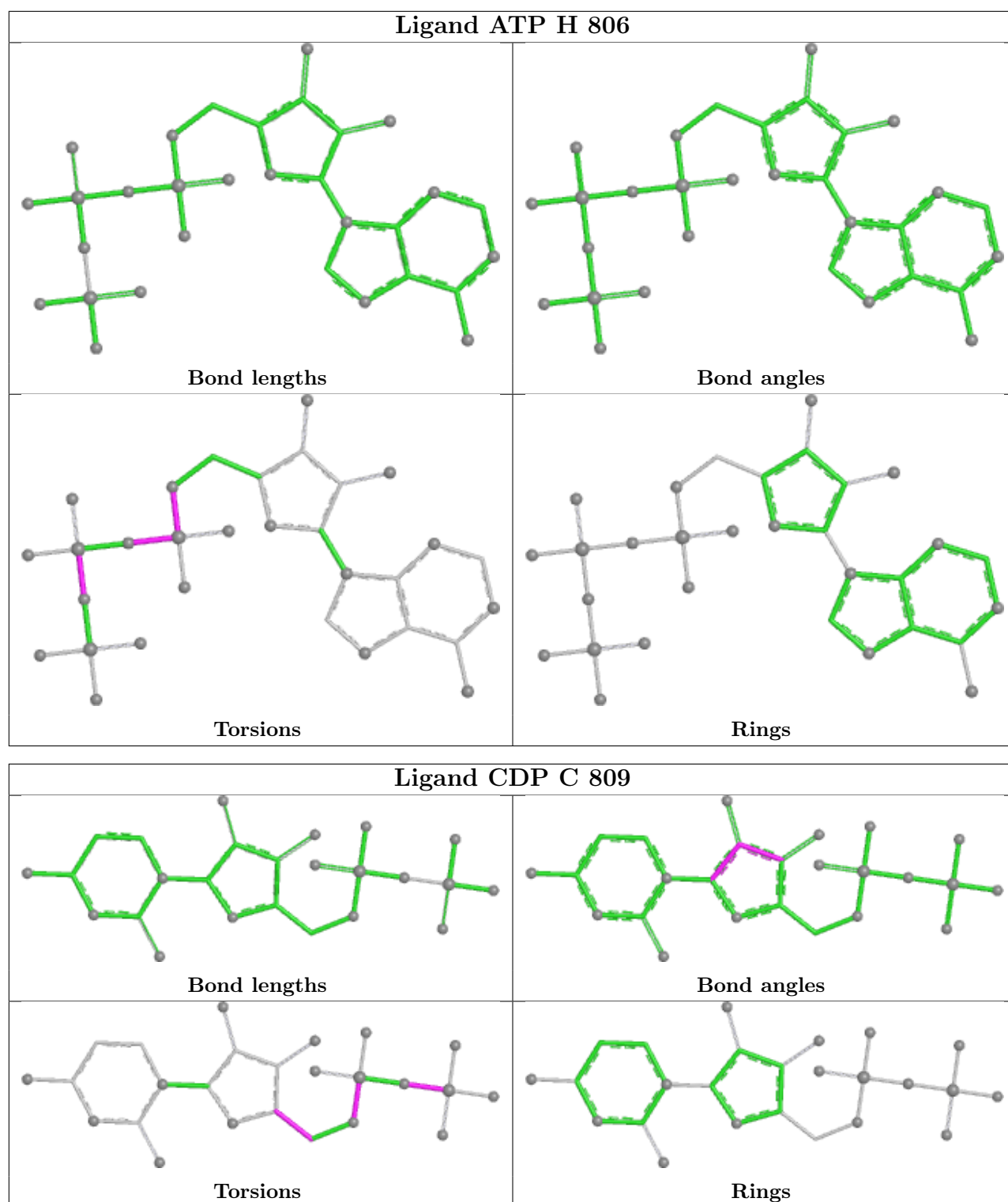


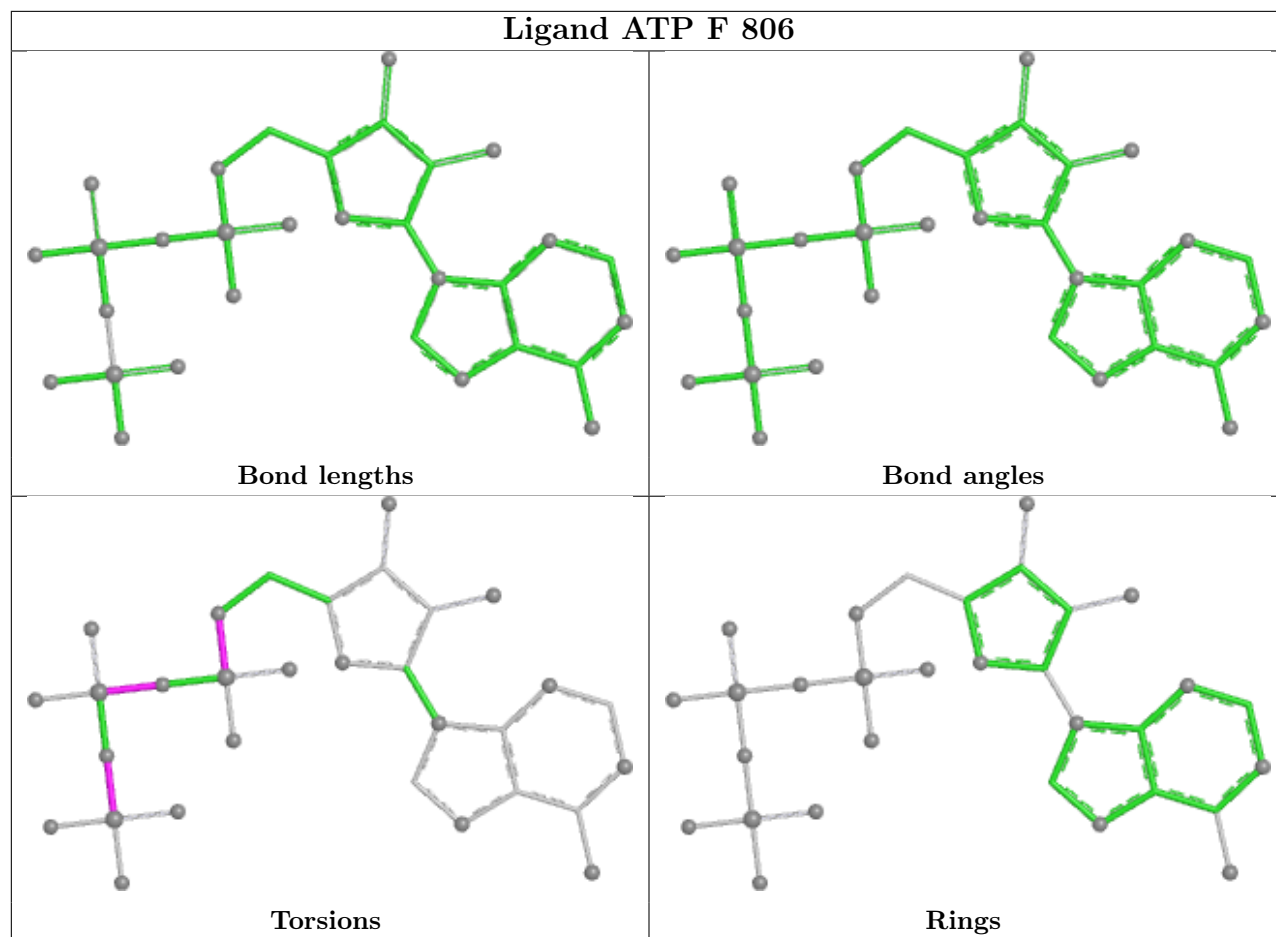


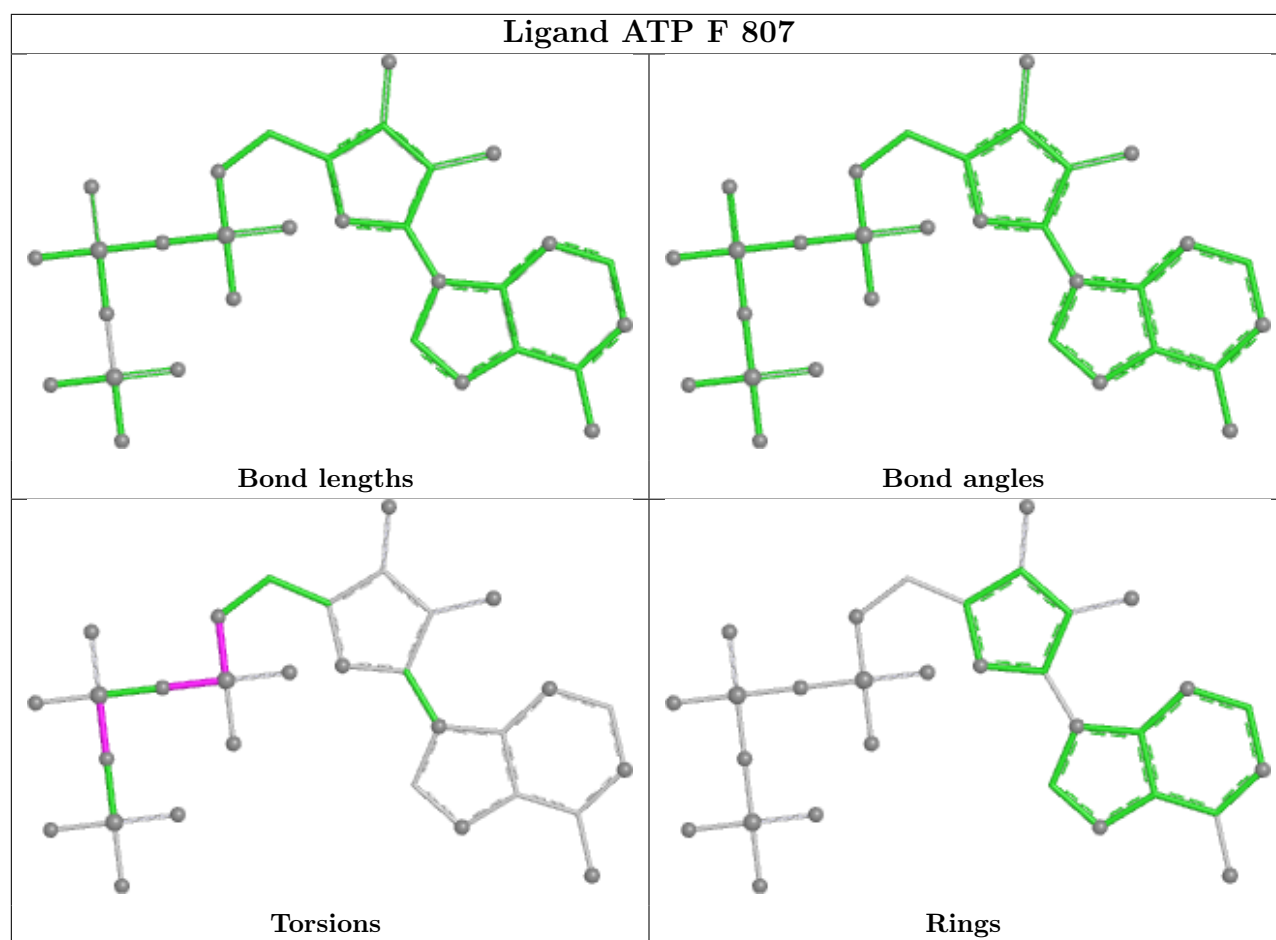


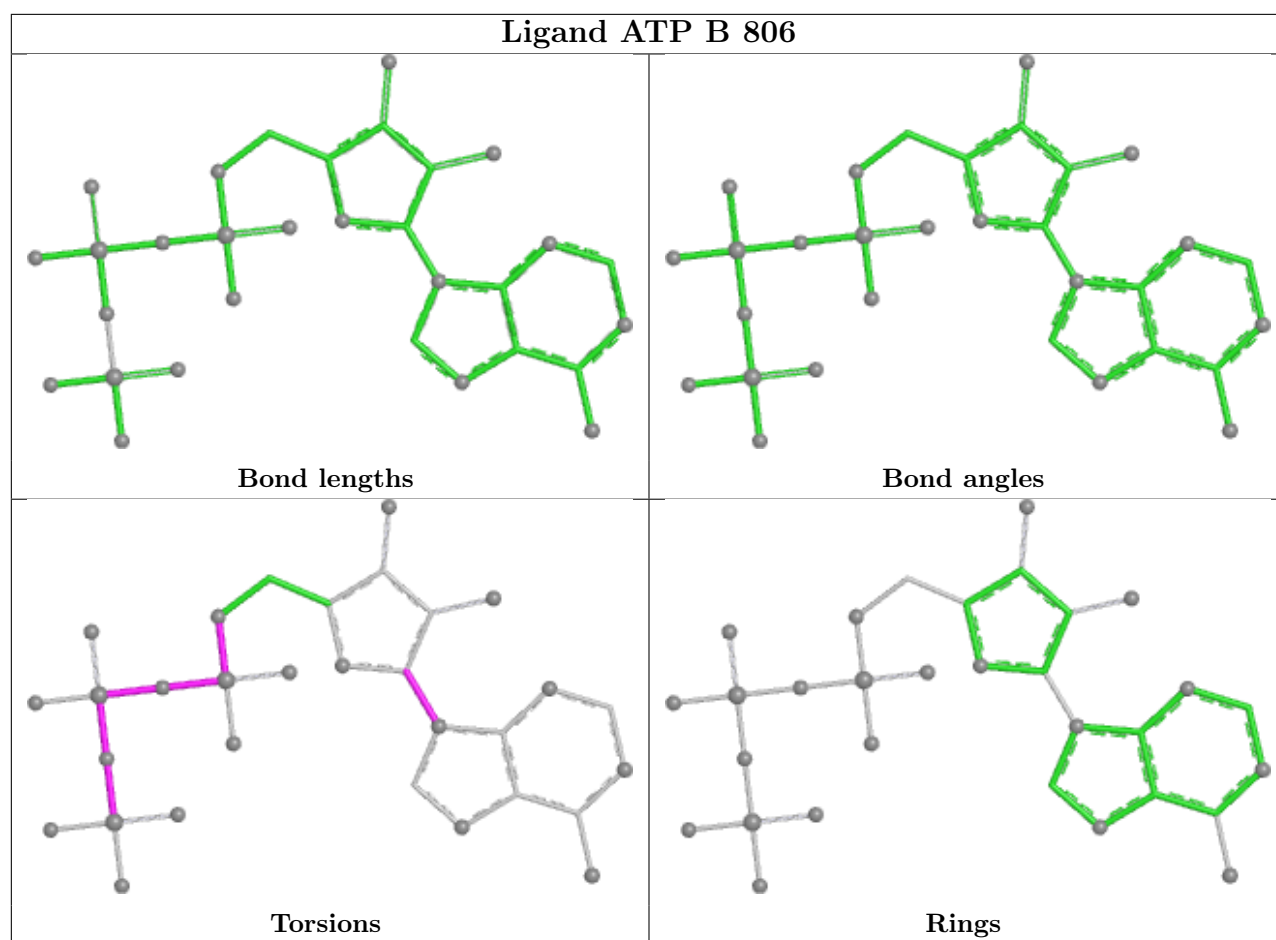


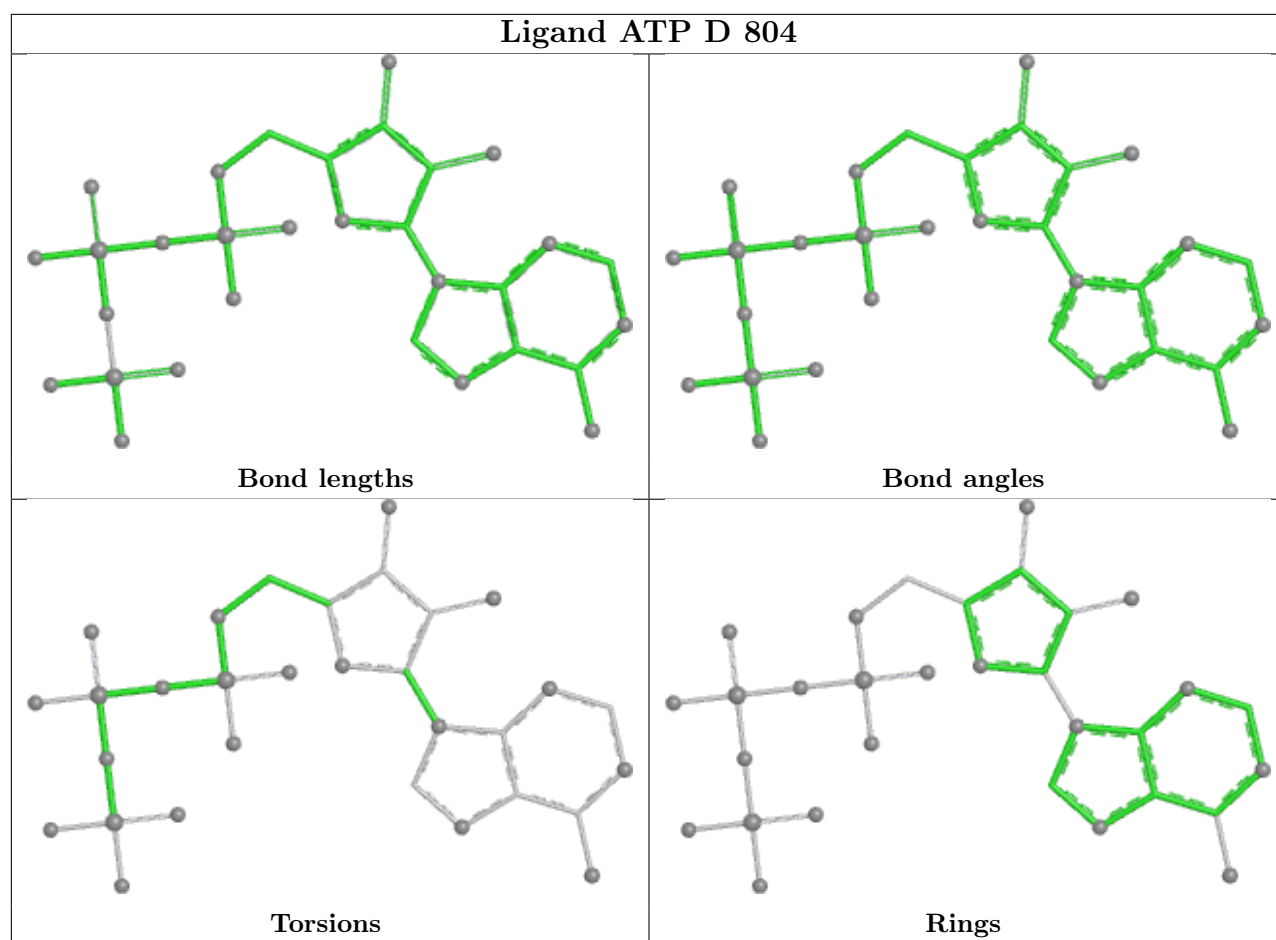


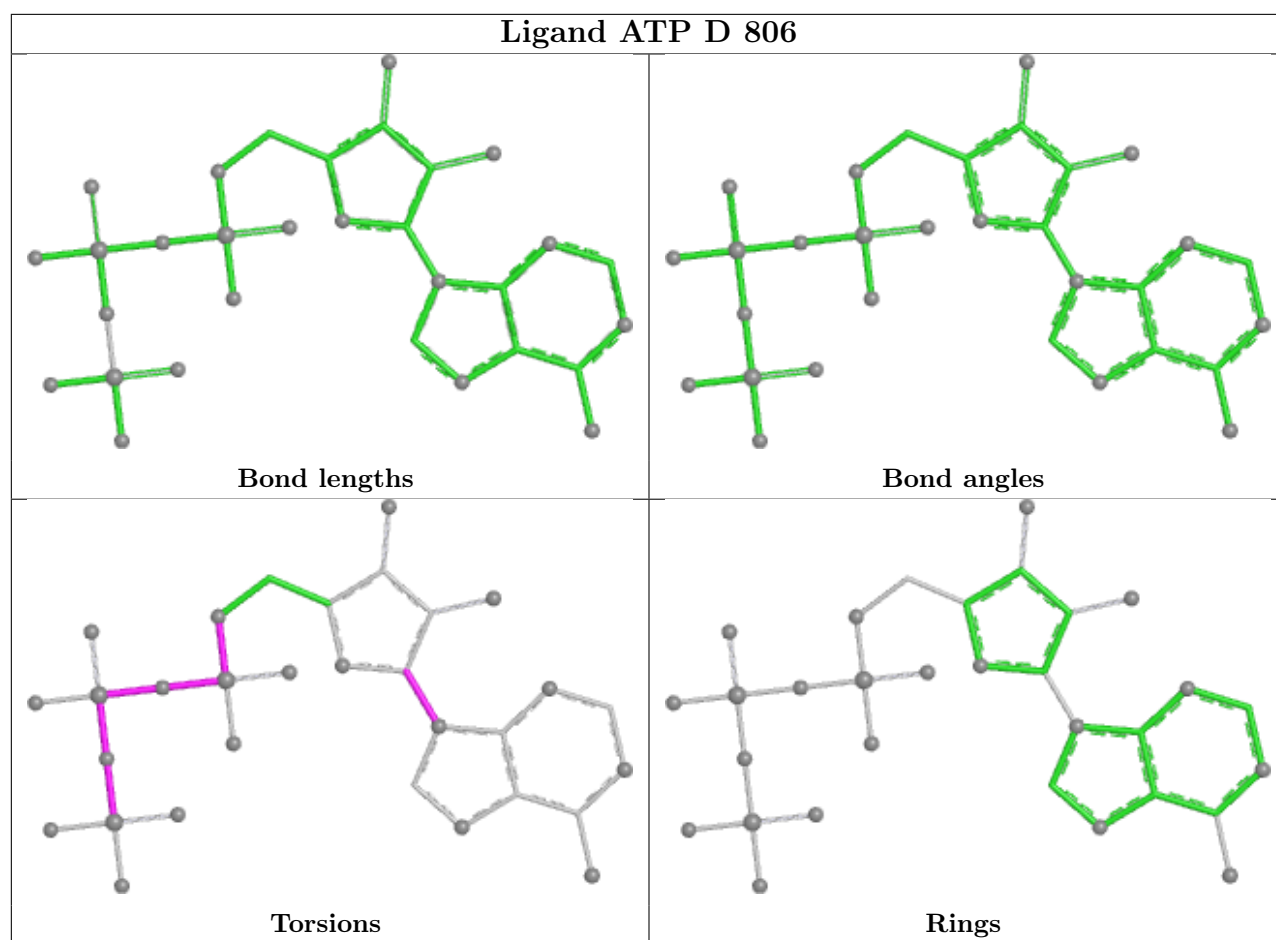




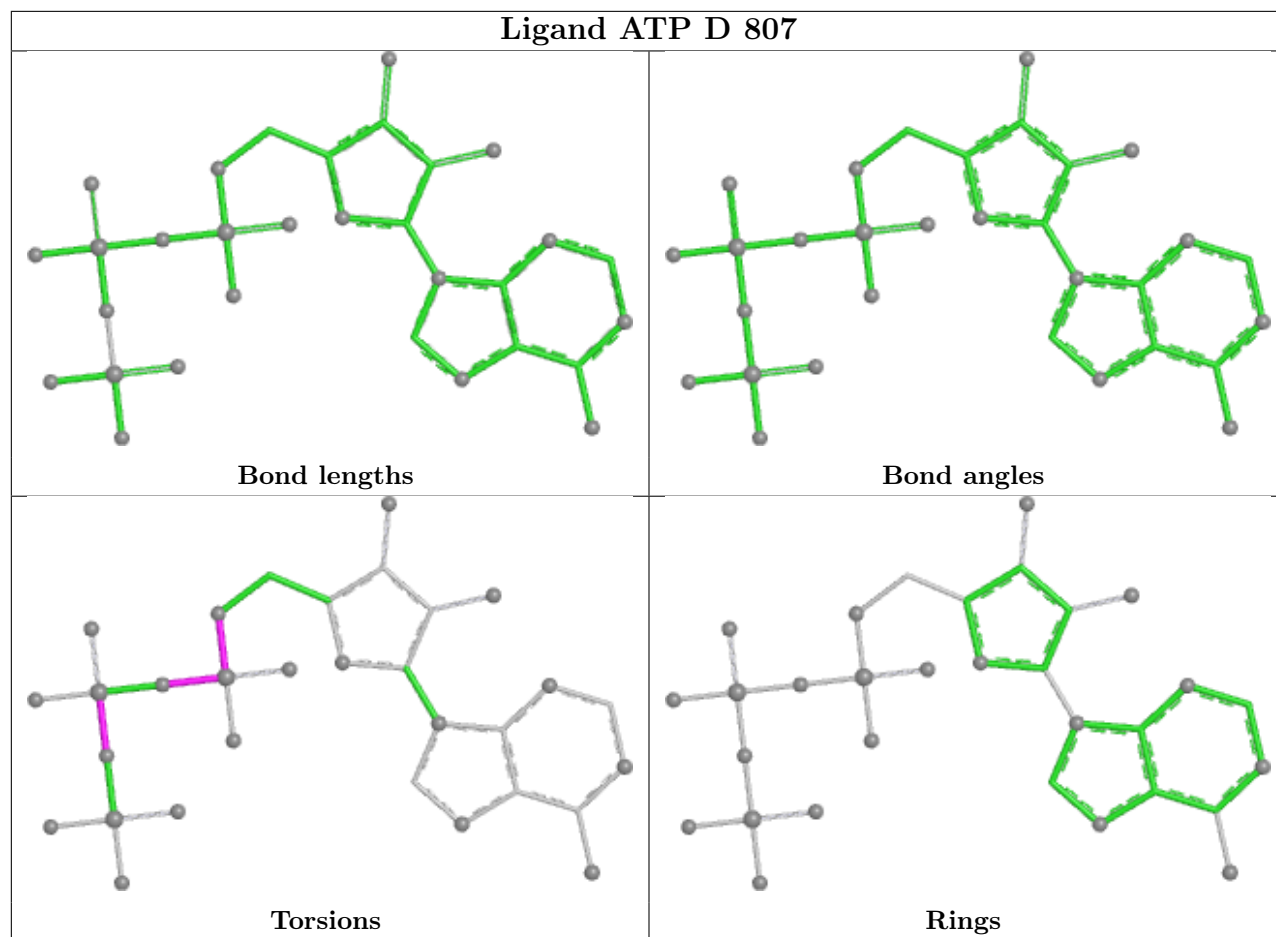




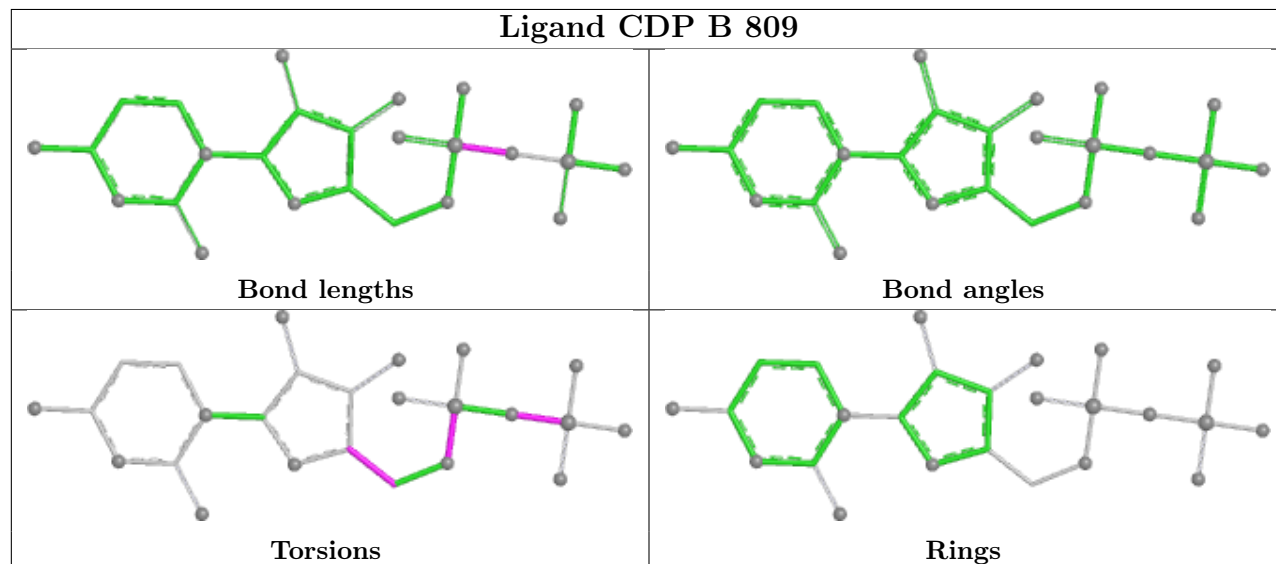


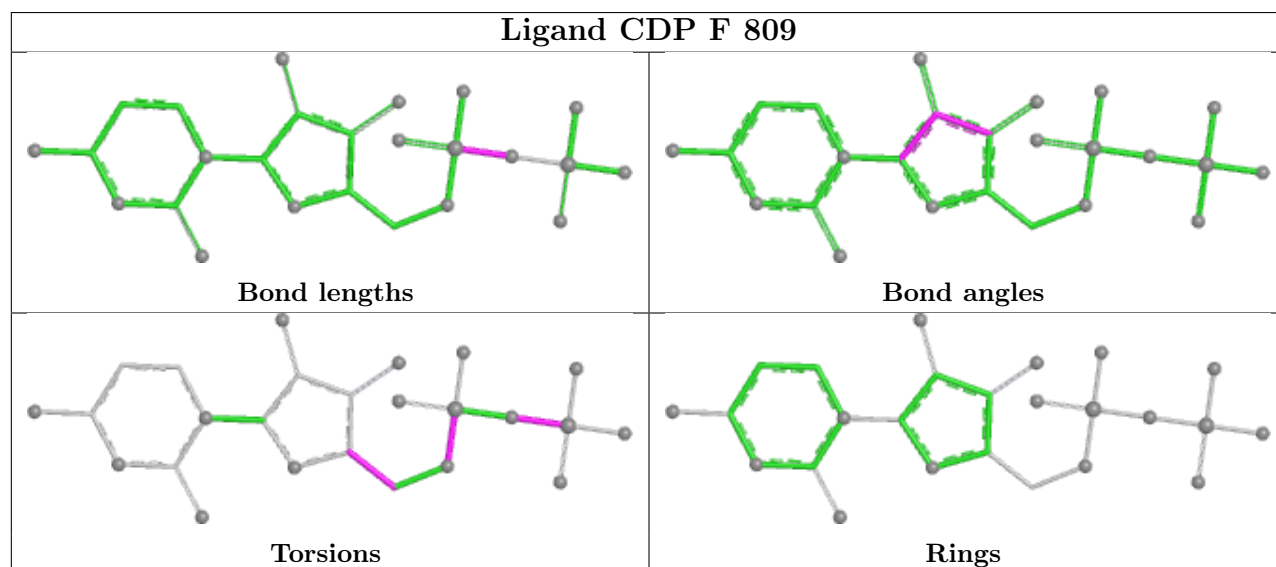
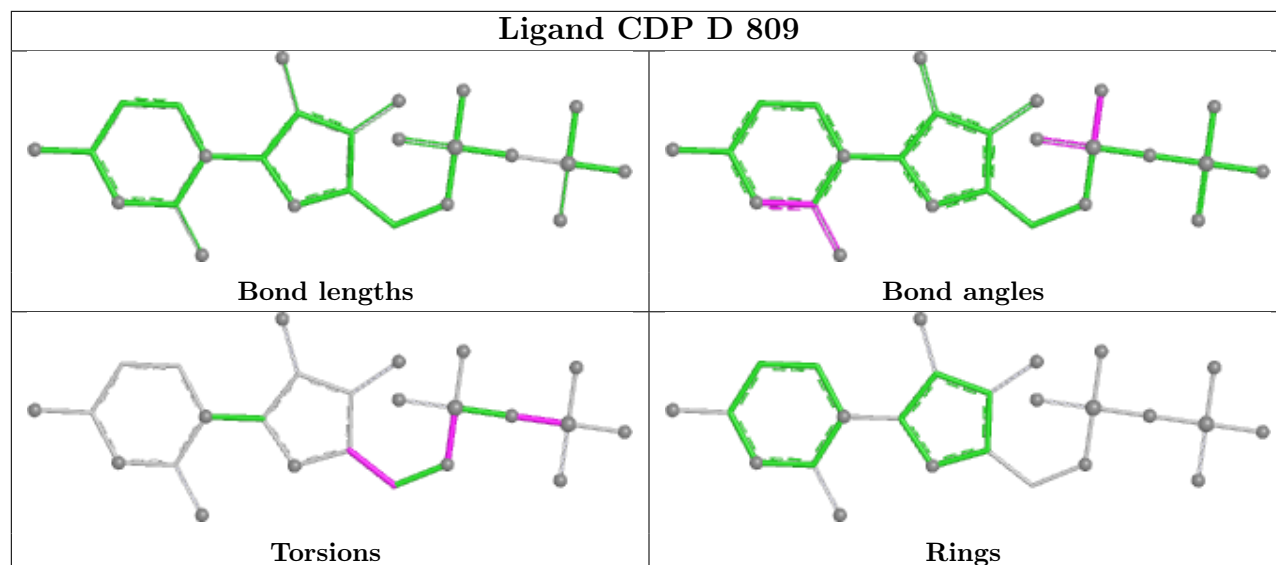


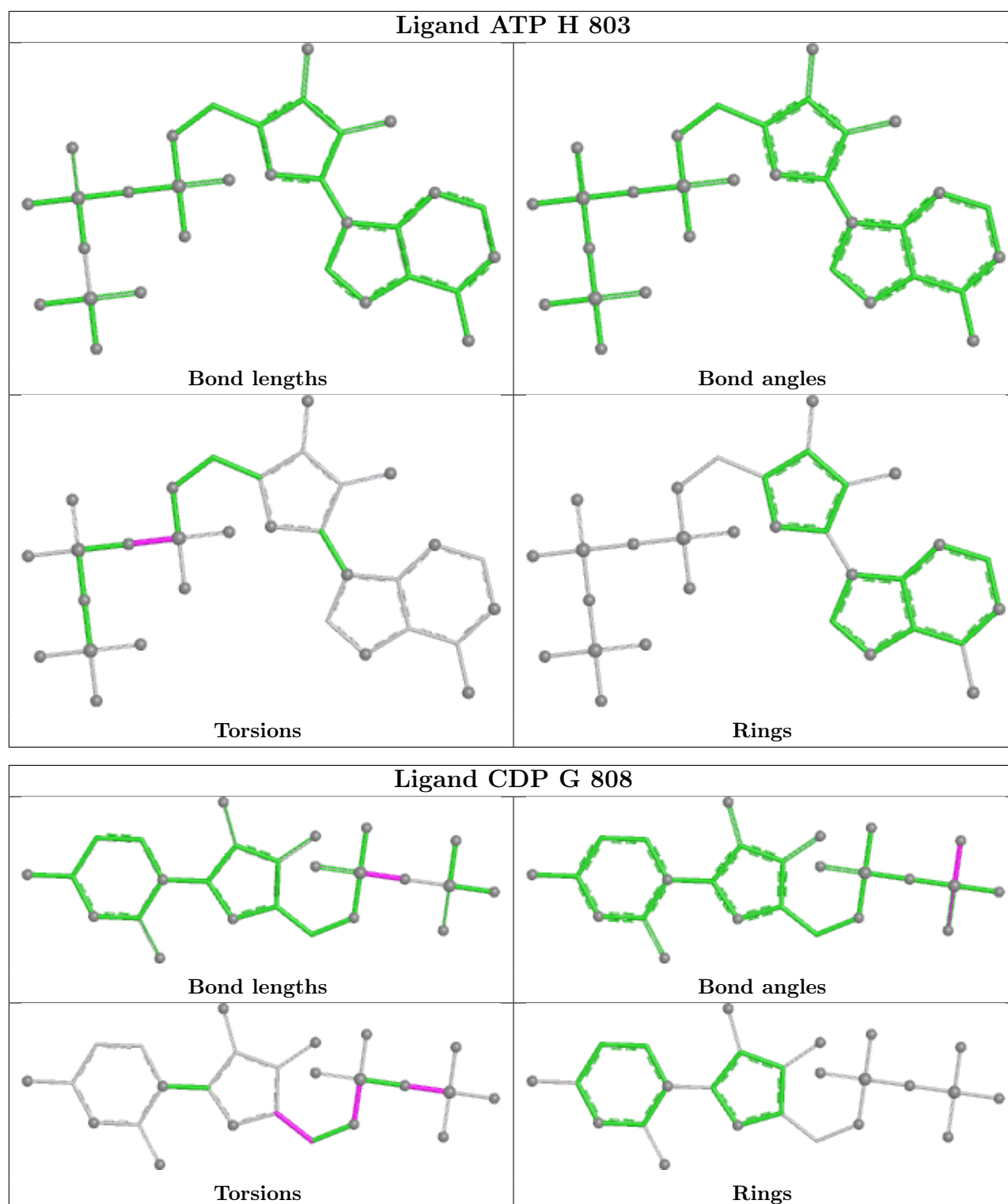
Ligand ATP D 807



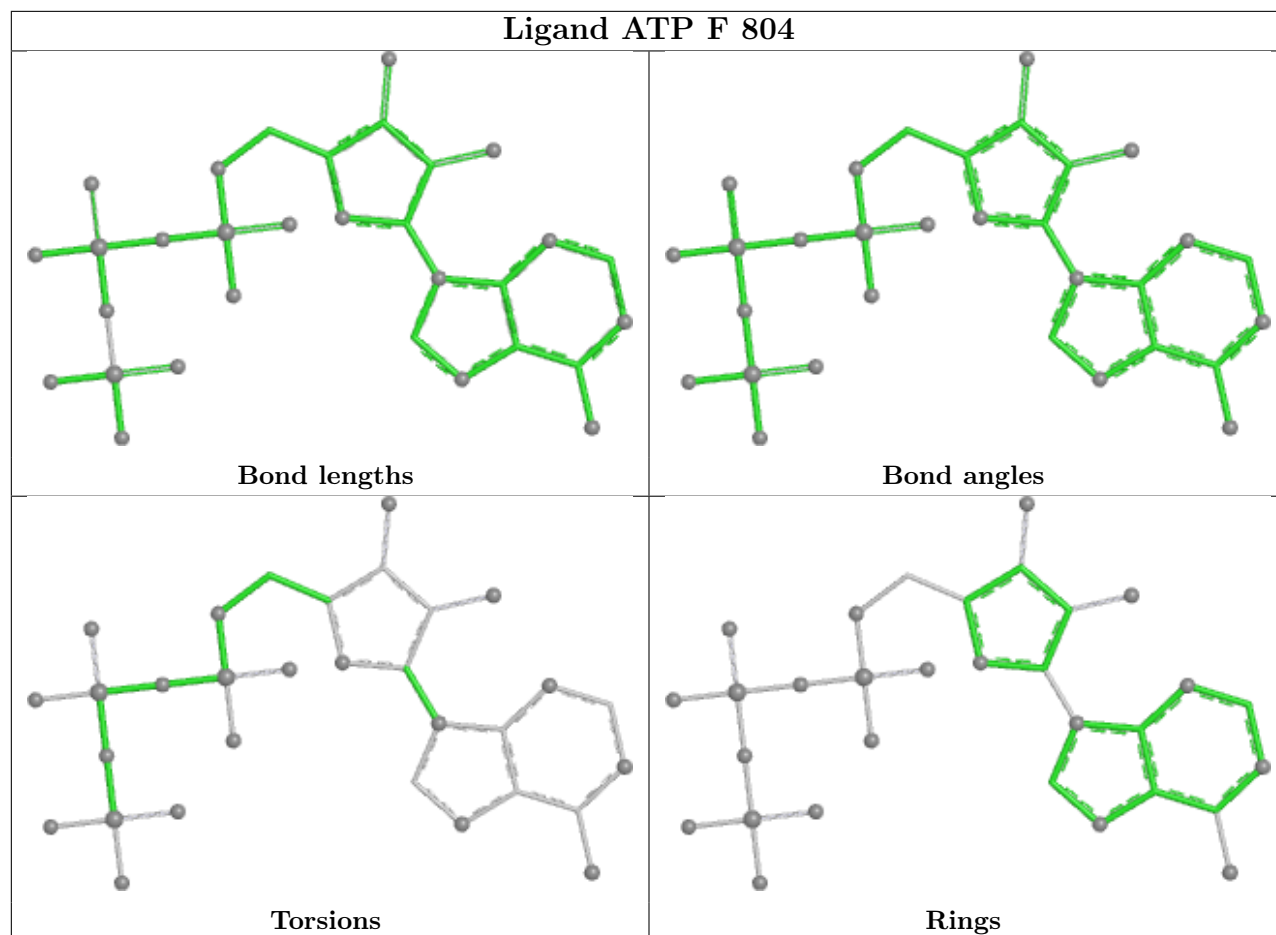
Ligand CDP B 809

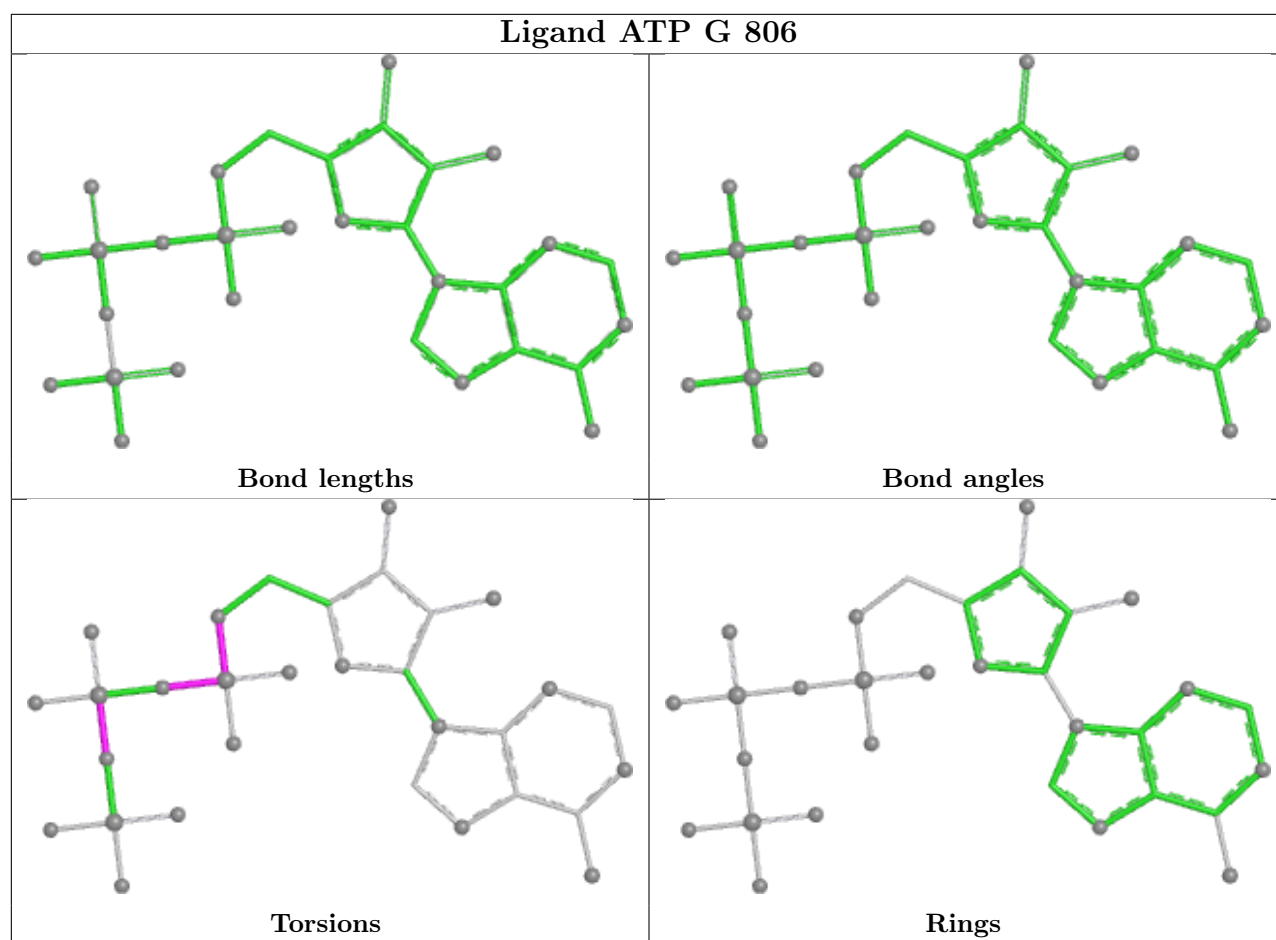


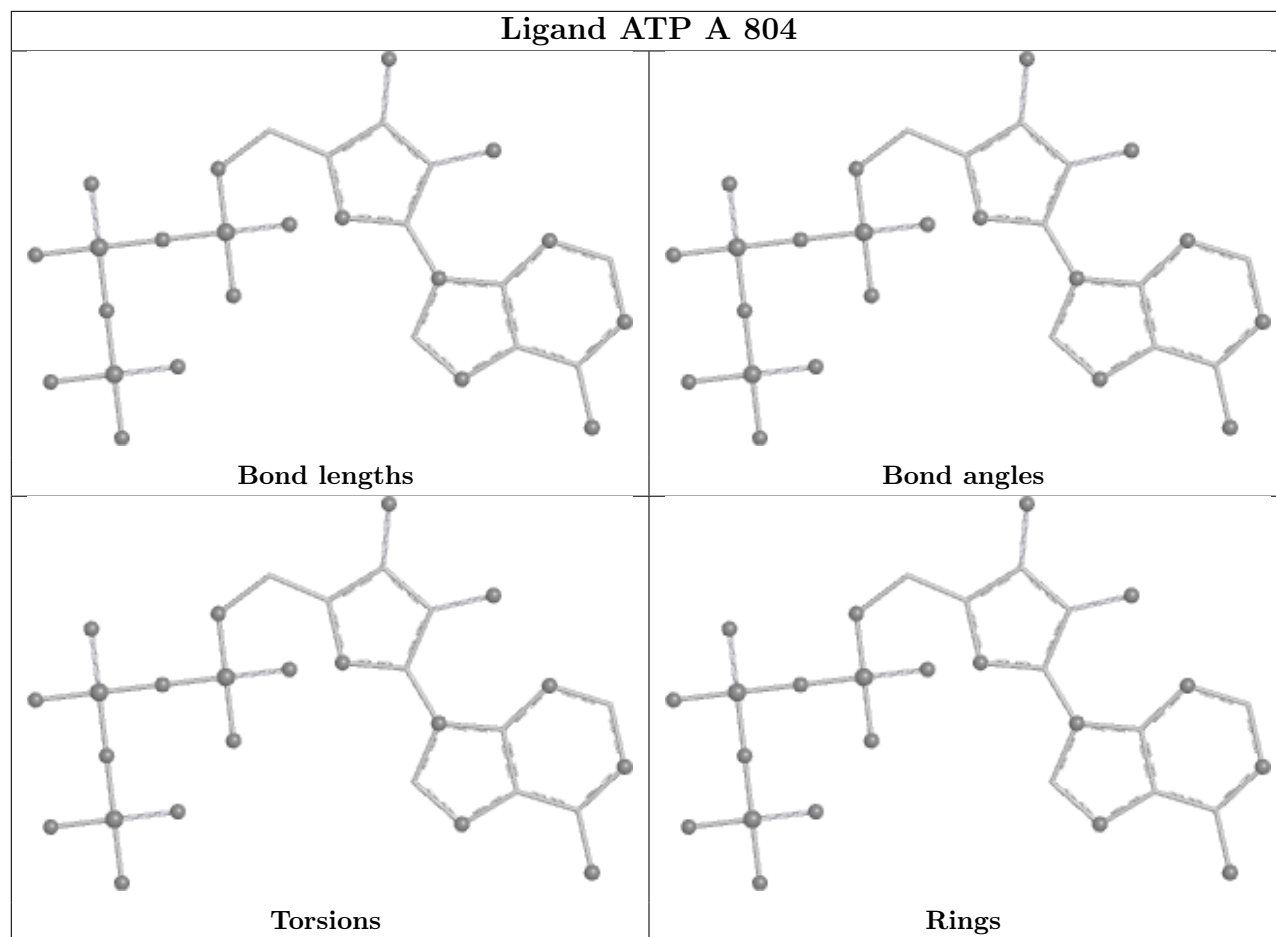




Ligand ATP F 804







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	731/779 (93%)	-0.25	6 (0%) 82 80	42, 49, 67, 115	0
1	B	733/779 (94%)	-0.21	4 (0%) 87 85	43, 52, 69, 96	0
1	C	733/779 (94%)	-0.17	7 (0%) 79 76	26, 54, 71, 103	2 (0%)
1	D	727/779 (93%)	-0.21	7 (0%) 79 76	38, 48, 75, 102	0
1	E	733/779 (94%)	-0.12	3 (0%) 88 86	38, 57, 77, 105	1 (0%)
1	F	732/779 (93%)	-0.12	8 (1%) 78 74	44, 54, 75, 121	0
1	G	729/779 (93%)	-0.25	8 (1%) 78 74	41, 49, 72, 111	0
1	H	735/779 (94%)	-0.24	4 (0%) 87 85	34, 50, 70, 104	1 (0%)
All	All	5853/6232 (93%)	-0.20	47 (0%) 82 80	26, 52, 73, 121	4 (0%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	731[A]	TYR	5.5
1	E	4	ASN	4.8
1	H	731[A]	TYR	4.8
1	G	650	GLY	4.7
1	A	651	ILE	4.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	G	809	5/5	0.39	0.31	65,66,66,70	5
2	SO4	A	814	5/5	0.60	0.21	59,62,63,65	5
2	SO4	H	809	5/5	0.62	0.33	60,60,60,61	5
2	SO4	H	801	5/5	0.63	0.23	55,55,57,61	5
2	SO4	G	802	5/5	0.65	0.25	54,54,57,66	5
2	SO4	D	802	5/5	0.65	0.22	53,54,59,65	5
2	SO4	C	810	5/5	0.66	0.28	60,60,61,61	5
2	SO4	A	812	5/5	0.66	0.23	59,60,62,65	5
2	SO4	H	811	5/5	0.66	0.21	62,62,63,64	5
2	SO4	D	812	5/5	0.67	0.23	60,61,62,65	5
2	SO4	A	802	5/5	0.69	0.27	52,53,53,61	5
2	SO4	D	803	5/5	0.69	0.23	59,60,63,64	5
2	SO4	C	802	5/5	0.70	0.25	56,56,58,59	5
2	SO4	E	803	5/5	0.70	0.24	65,66,72,100	5
2	SO4	E	810	5/5	0.70	0.30	61,61,61,62	5
2	SO4	A	813	5/5	0.70	0.21	62,62,63,69	5
2	SO4	B	802	5/5	0.71	0.21	53,53,54,62	5
2	SO4	F	803	5/5	0.76	0.28	51,52,53,56	5
2	SO4	B	810	5/5	0.76	0.30	60,60,60,61	5
2	SO4	A	811	5/5	0.76	0.24	56,56,57,59	5
2	SO4	F	802	5/5	0.77	0.18	55,55,56,64	5
2	SO4	E	802	5/5	0.78	0.25	58,58,59,70	5
2	SO4	C	811	5/5	0.78	0.23	60,60,61,66	5
2	SO4	F	810	5/5	0.80	0.16	58,58,59,63	5
2	SO4	H	810	5/5	0.81	0.20	59,59,61,63	5
2	SO4	H	802	5/5	0.81	0.19	54,54,57,61	5
2	SO4	G	801	5/5	0.82	0.21	46,47,49,49	5
2	SO4	B	803	5/5	0.82	0.17	53,54,54,58	5
2	SO4	A	810	5/5	0.83	0.19	57,57,58,65	5
2	SO4	A	803	5/5	0.83	0.20	53,53,55,56	5
2	SO4	B	801	5/5	0.84	0.23	49,51,53,53	5
2	SO4	E	801	5/5	0.85	0.17	50,51,52,57	5
2	SO4	C	801	5/5	0.87	0.17	54,57,57,58	5
2	SO4	C	803	5/5	0.87	0.15	53,53,54,54	5
2	SO4	D	810	5/5	0.87	0.18	64,65,65,65	5
2	SO4	D	811	5/5	0.87	0.20	51,52,53,57	5
2	SO4	F	801	5/5	0.88	0.17	52,53,55,56	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
2	SO4	D	813	5/5	0.94	0.13	54,55,58,59	5
3	ATP	B	804	31/31	0.95	0.07	56,59,62,64	0
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	F	804	31/31	0.95	0.07	61,64,66,72	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	C	804	31/31	0.96	0.06	57,59,61,62	0
3	ATP	E	807	31/31	0.96	0.07	50,53,62,82	0
3	ATP	C	806	31/31	0.96	0.07	55,57,68,76	0
3	ATP	A	804	31/31	0.96	0.07	52,53,55,57	0
3	ATP	G	803	31/31	0.96	0.07	56,58,60,68	0
3	ATP	B	807	31/31	0.96	0.06	41,43,50,51	0
3	ATP	H	803	31/31	0.96	0.06	54,56,58,62	0
3	ATP	H	805	31/31	0.96	0.06	52,53,54,65	0
3	ATP	H	806	31/31	0.96	0.07	42,44,48,70	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	G	806	31/31	0.97	0.06	40,41,49,52	0
3	ATP	D	804	31/31	0.97	0.06	62,64,68,72	0
3	ATP	A	807	31/31	0.97	0.06	44,45,51,58	0
3	ATP	D	807	31/31	0.97	0.06	45,45,48,59	0
4	MG	H	804	1/1	0.97	0.04	54,54,54,54	0
5	CDP	A	809	25/25	0.97	0.06	42,44,47,52	0
3	ATP	F	807	31/31	0.97	0.06	46,47,50,80	0
3	ATP	A	806	31/31	0.97	0.06	48,49,54,55	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	C	807	31/31	0.97	0.06	44,45,48,60	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	E	808	1/1	0.98	0.04	55,55,55,55	0
4	MG	G	804	1/1	0.99	0.02	56,56,56,56	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

Continued on next page...

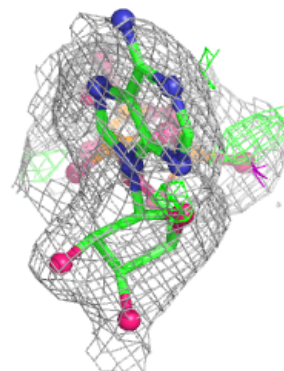
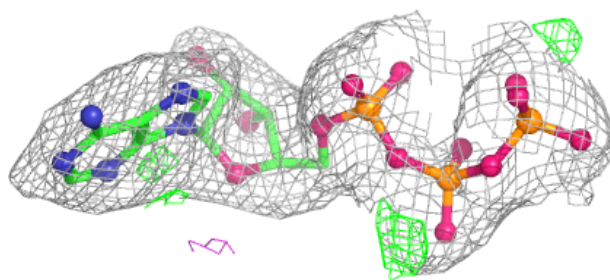
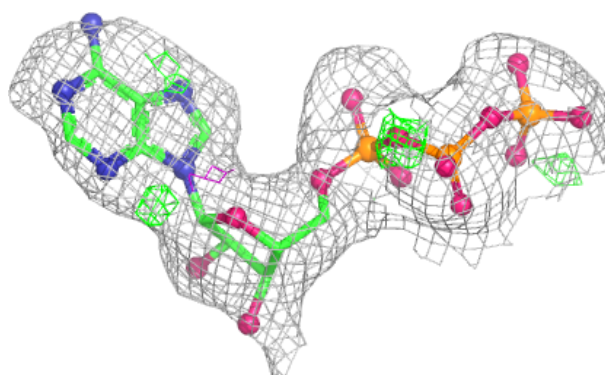
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	C	808	1/1	0.99	0.03	45,45,45,45	0
4	MG	D	805	1/1	0.99	0.03	62,62,62,62	0
4	MG	D	808	1/1	0.99	0.04	47,47,47,47	0
4	MG	E	805	1/1	0.99	0.02	58,58,58,58	0
4	MG	A	805	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	F	808	1/1	0.99	0.03	50,50,50,50	0
4	MG	G	807	1/1	1.00	0.02	45,45,45,45	0
4	MG	H	807	1/1	1.00	0.02	43,43,43,43	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.

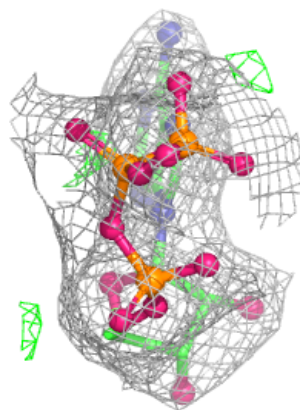
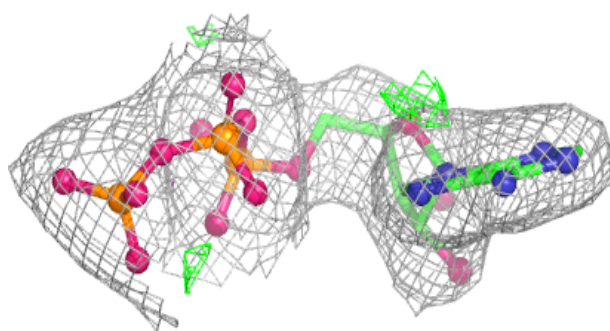
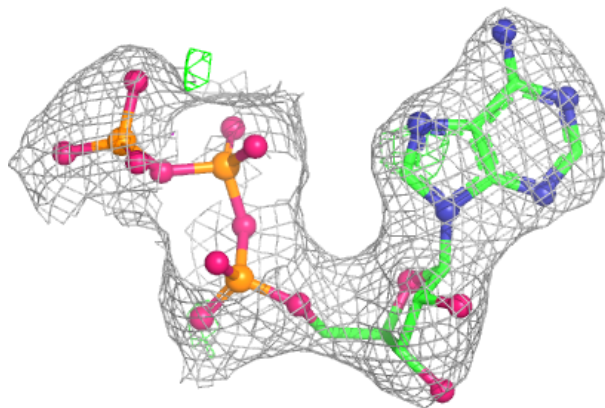
Electron density around ATP B 806:

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



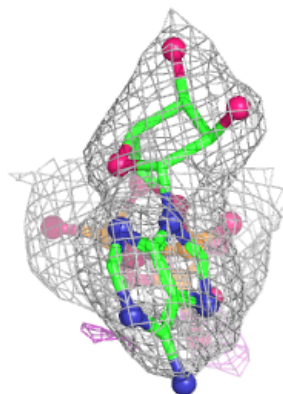
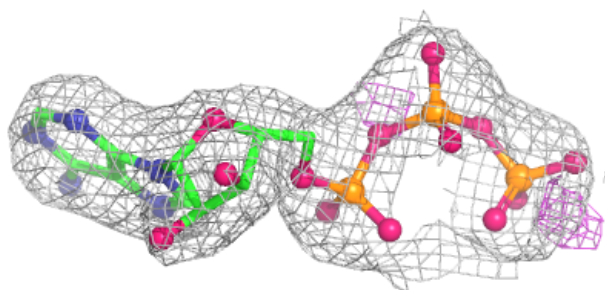
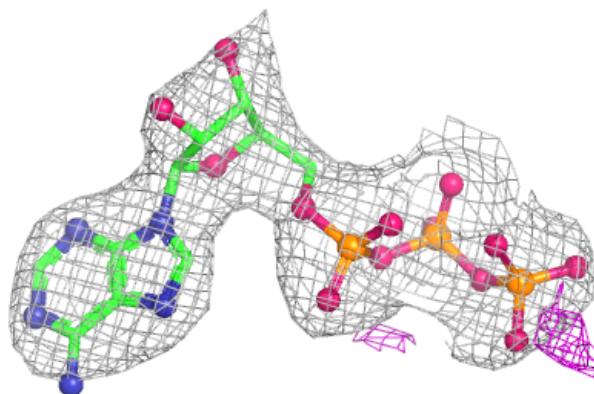
Electron density around ATP B 804:

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



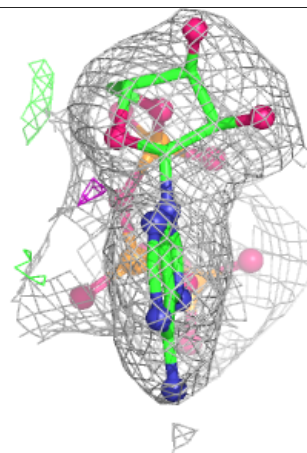
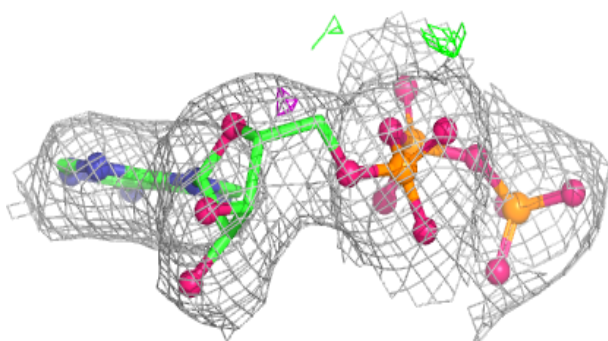
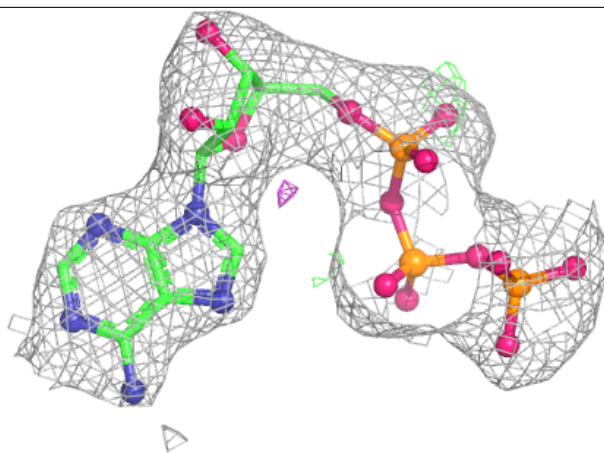
Electron density around ATP D 806:

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

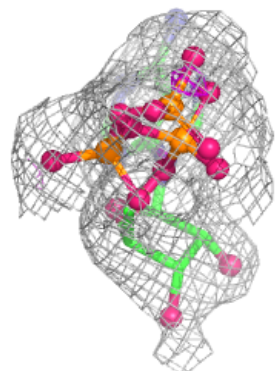
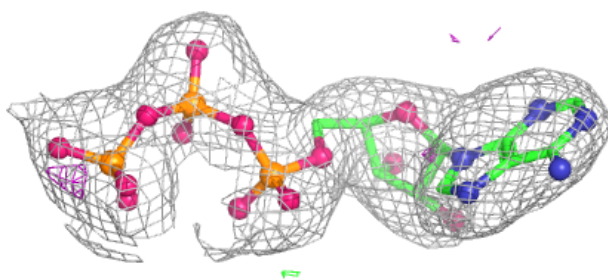
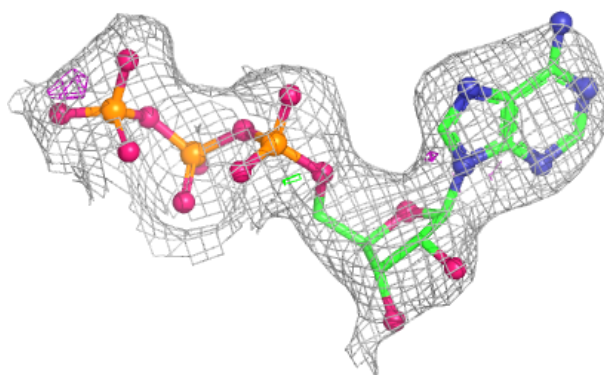


Electron density around ATP E 804:

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

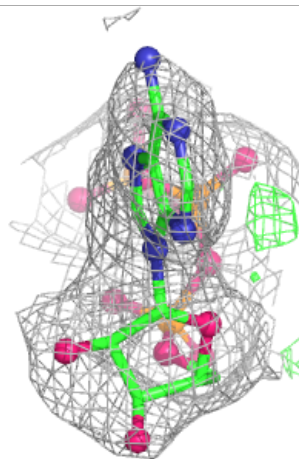
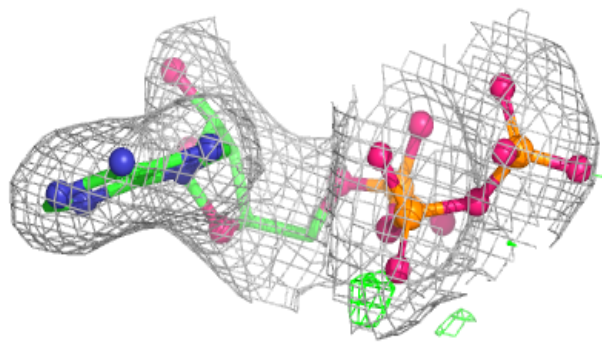
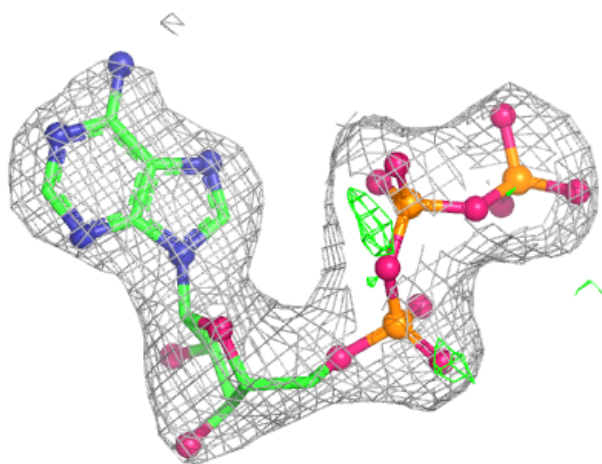
**Electron density around ATP E 806:**

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



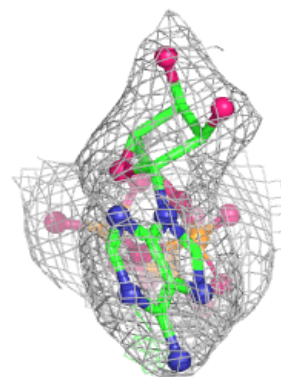
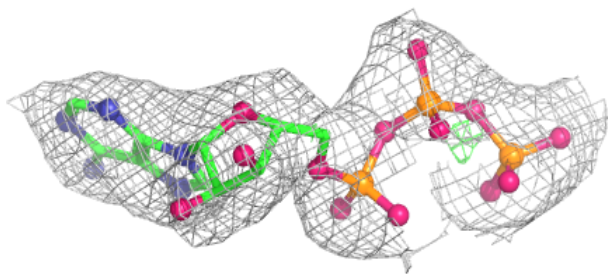
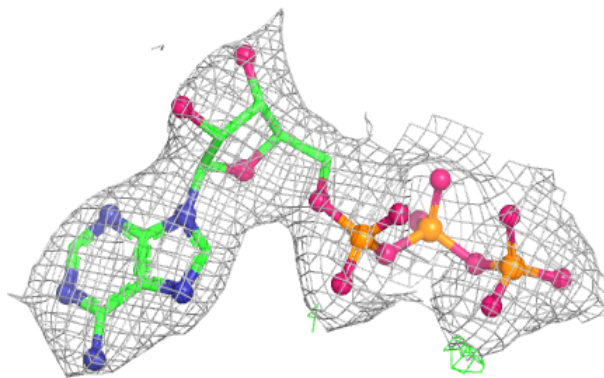
Electron density around ATP F 804:

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

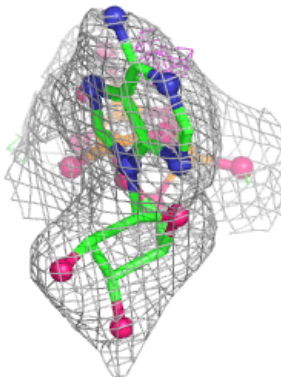
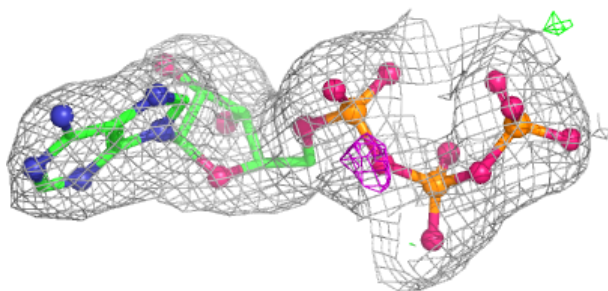
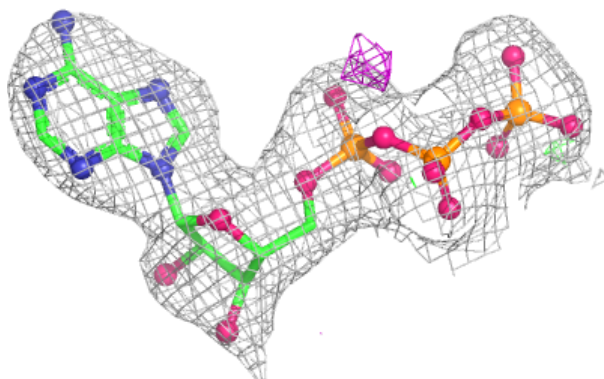


Electron density around ATP F 806:

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

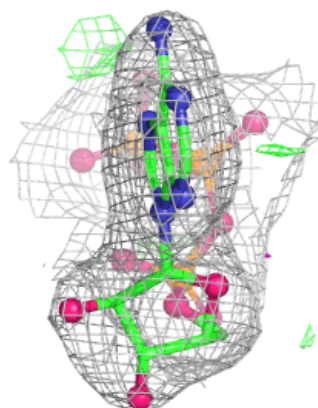
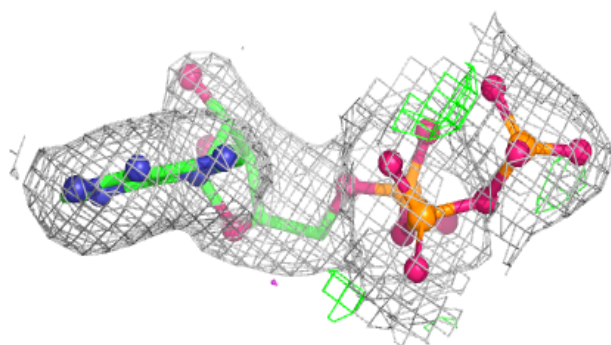
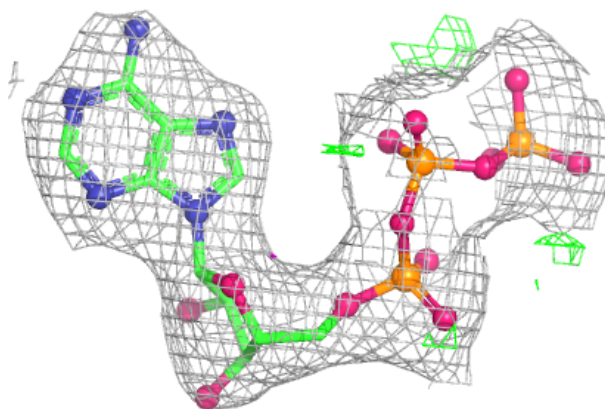
**Electron density around ATP G 805:**

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



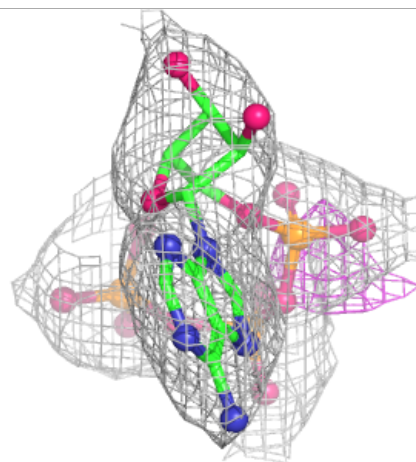
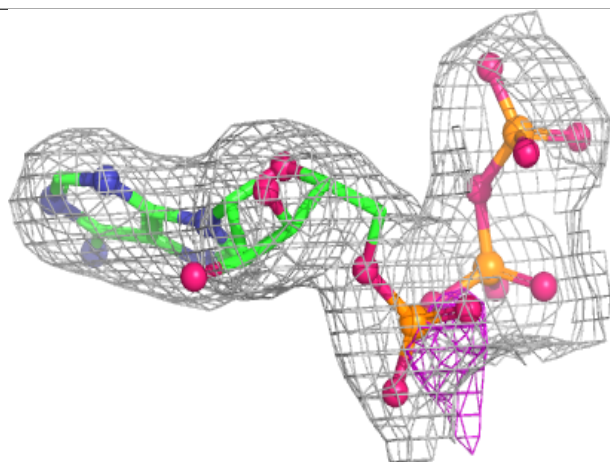
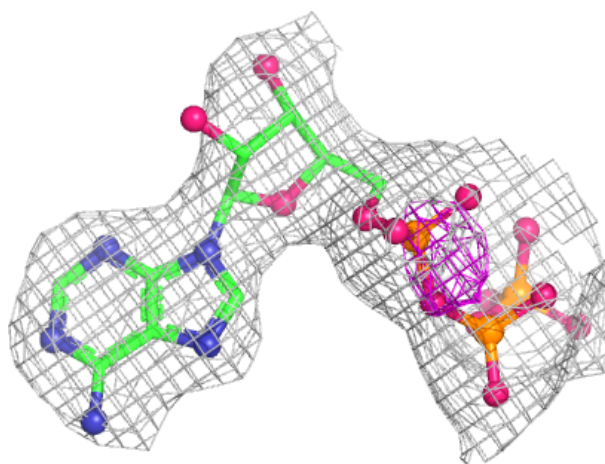
Electron density around ATP C 804:

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



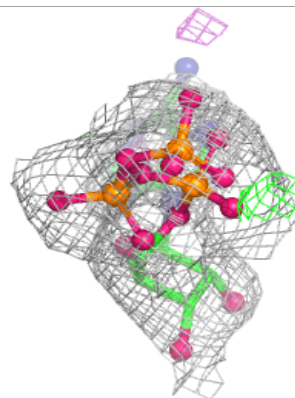
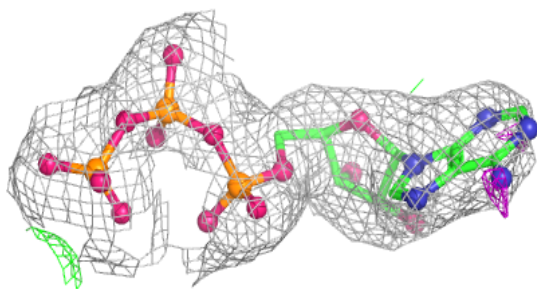
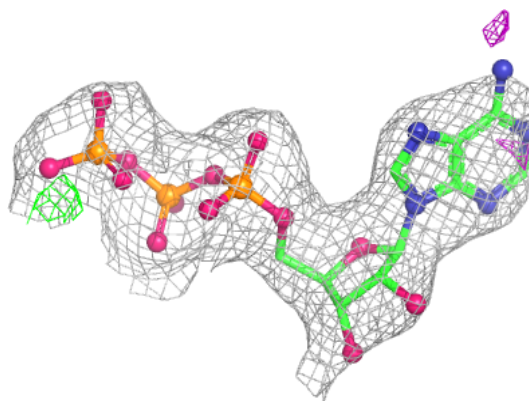
Electron density around ATP E 807:

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



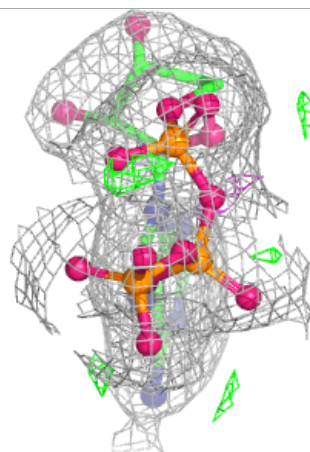
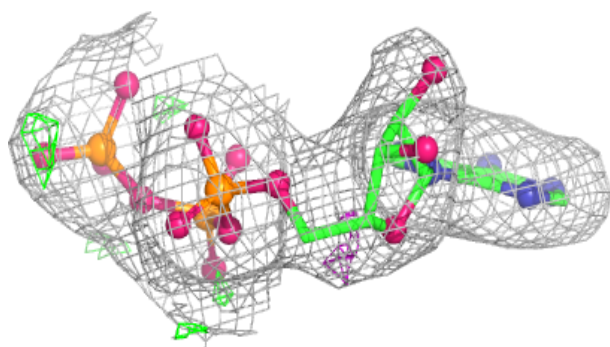
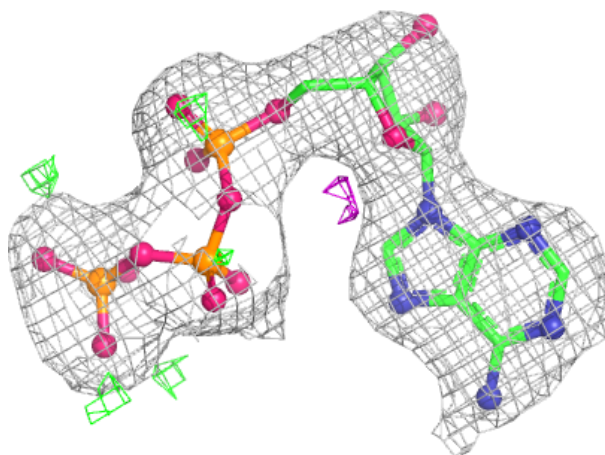
Electron density around ATP C 806:

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



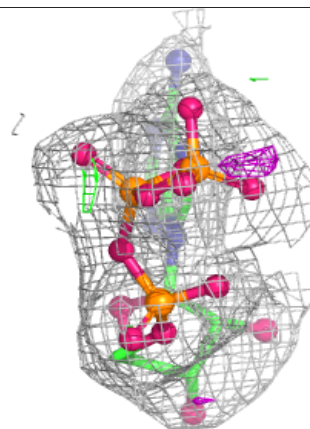
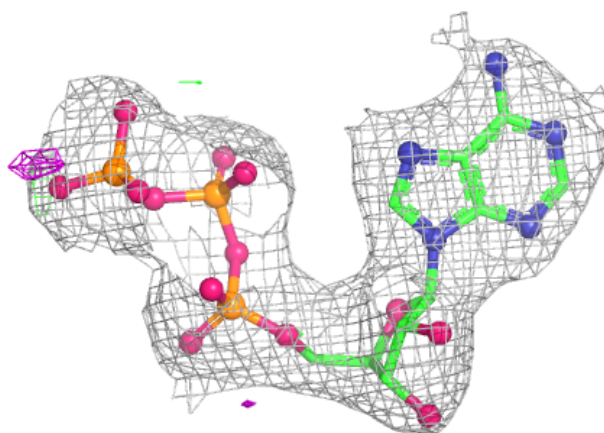
Electron density around ATP A 804:

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



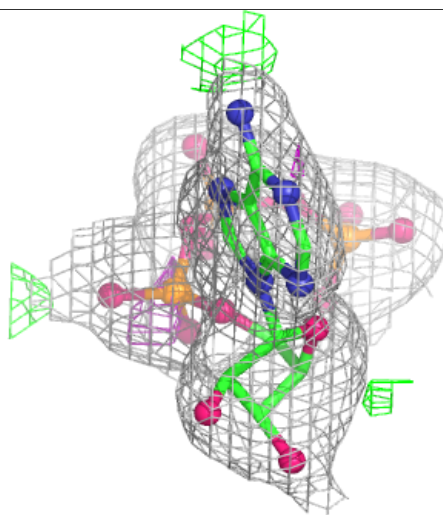
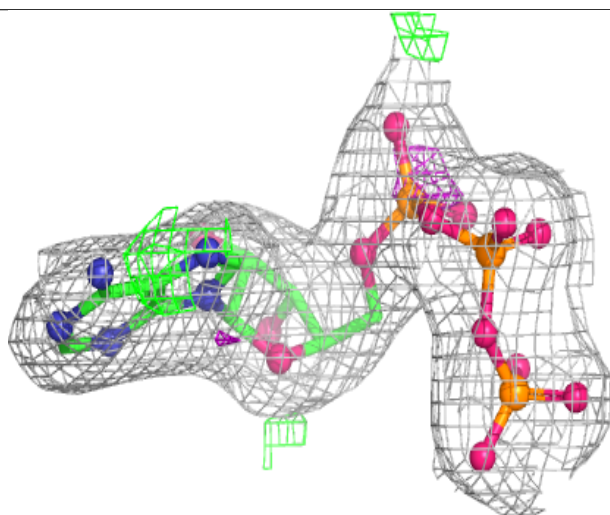
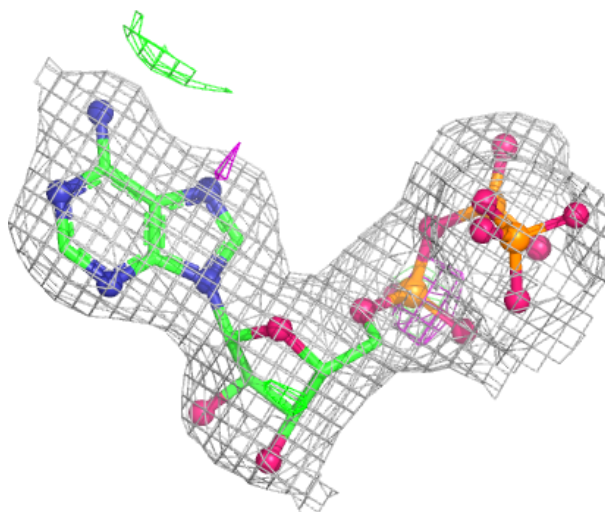
Electron density around ATP G 803:

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



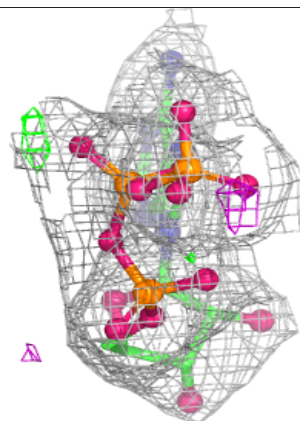
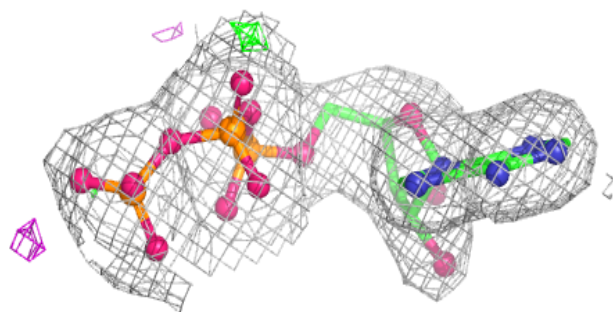
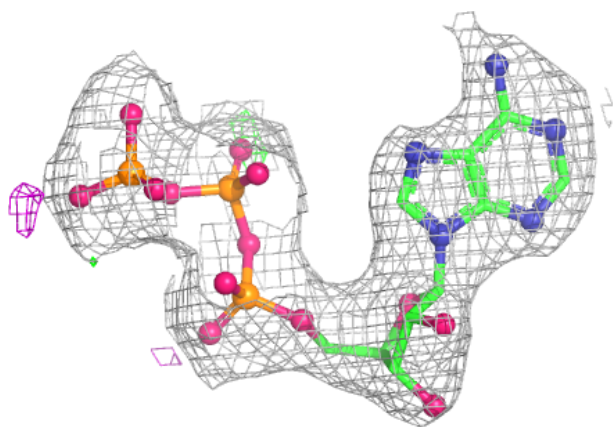
Electron density around ATP B 807:

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

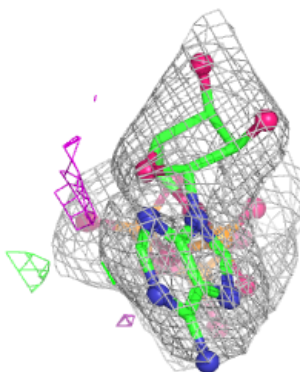
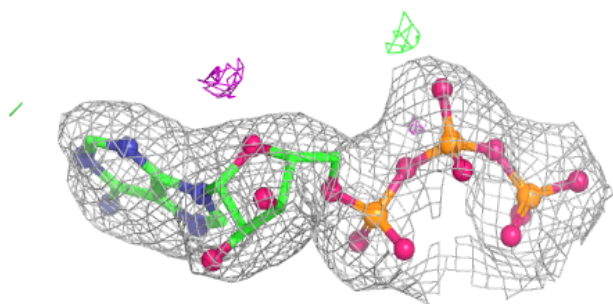
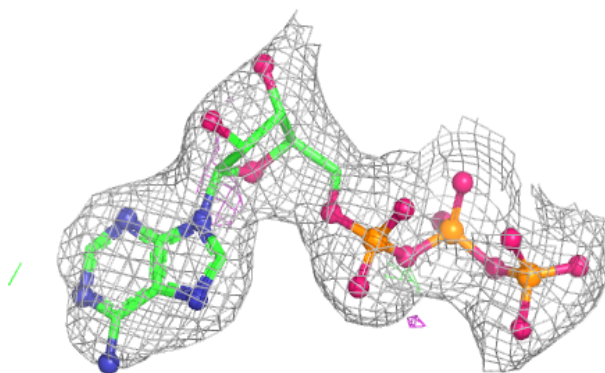


Electron density around ATP H 803:

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

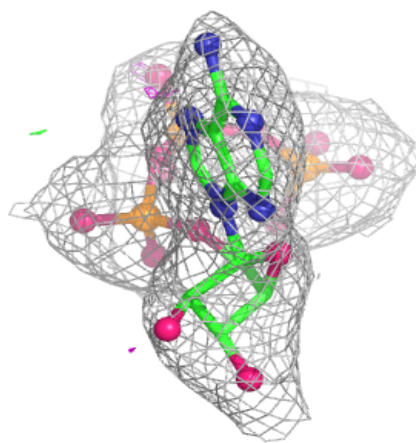
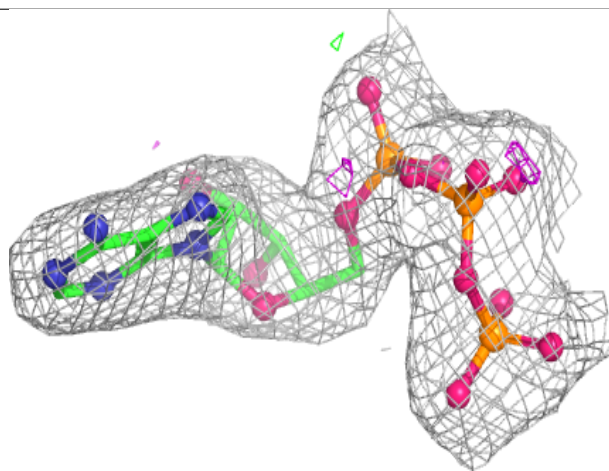
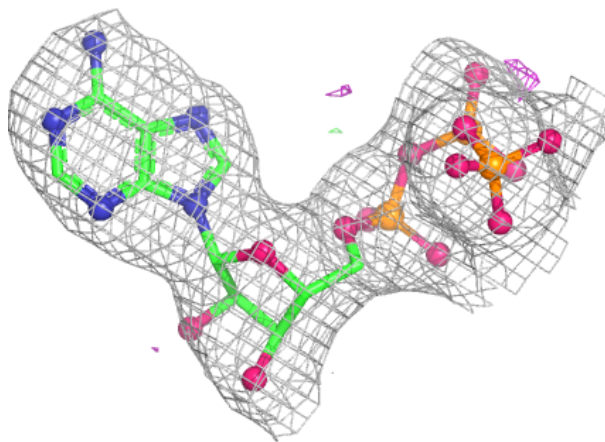
**Electron density around ATP H 805:**

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



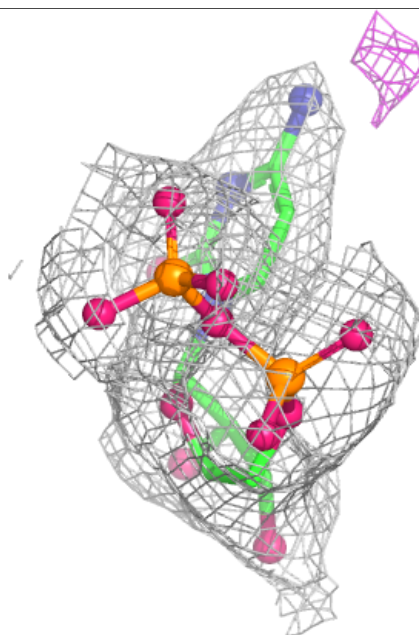
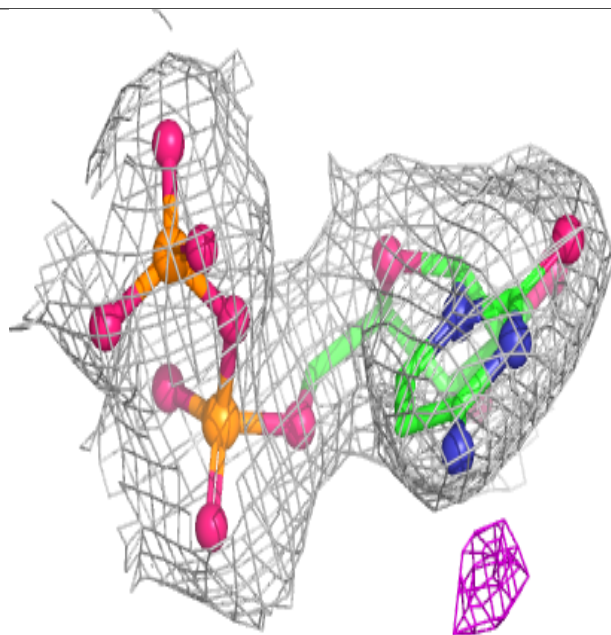
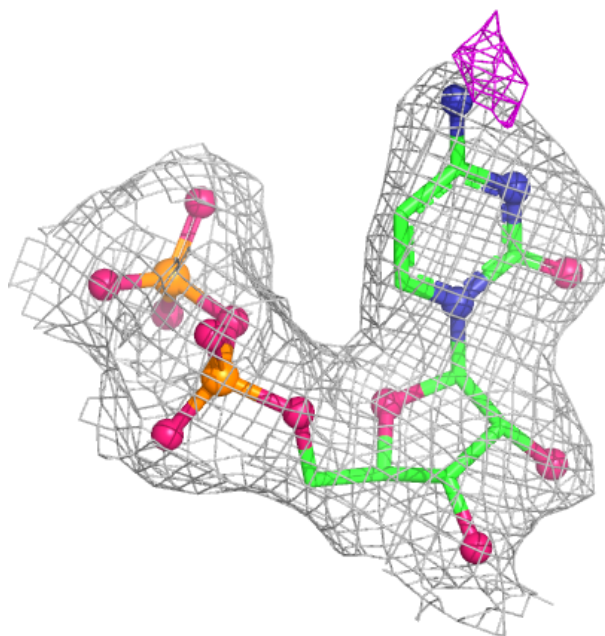
Electron density around ATP H 806:

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



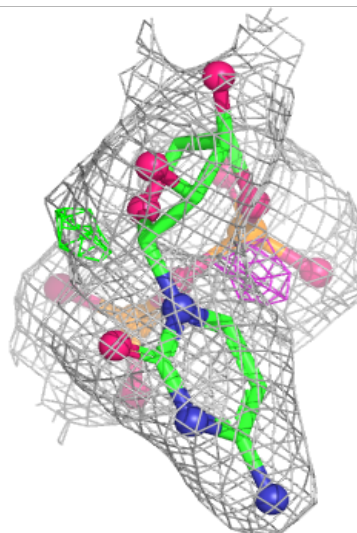
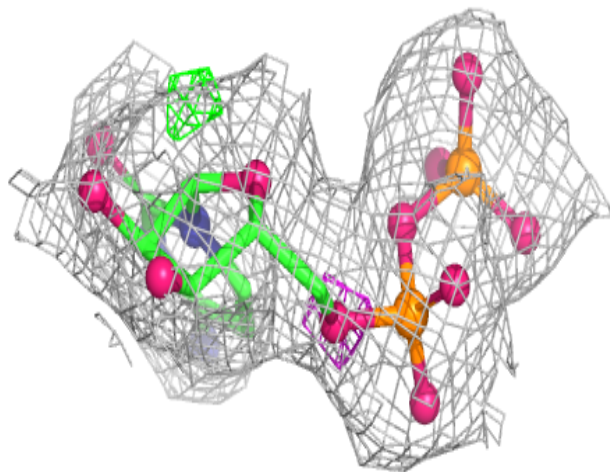
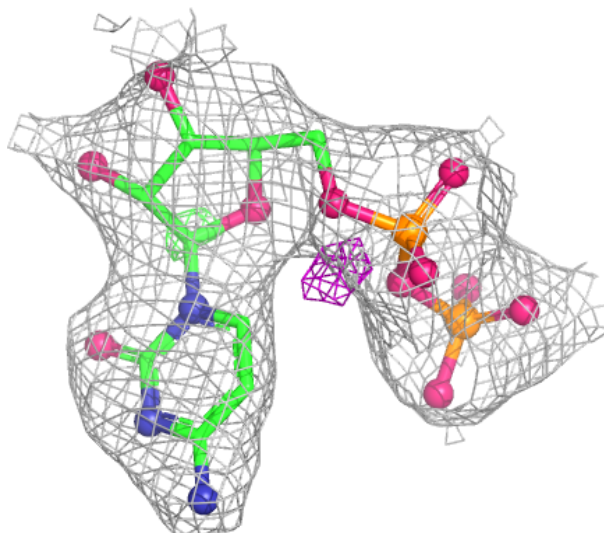
Electron density around CDP B 809:

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



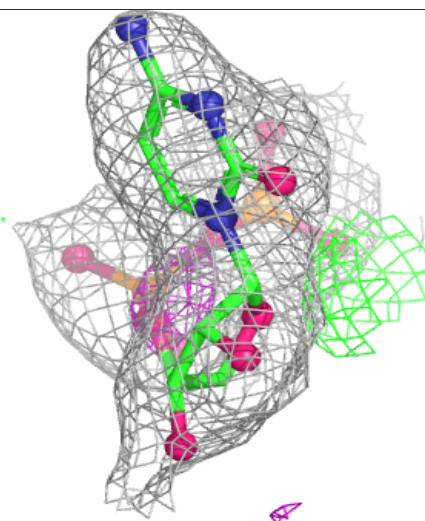
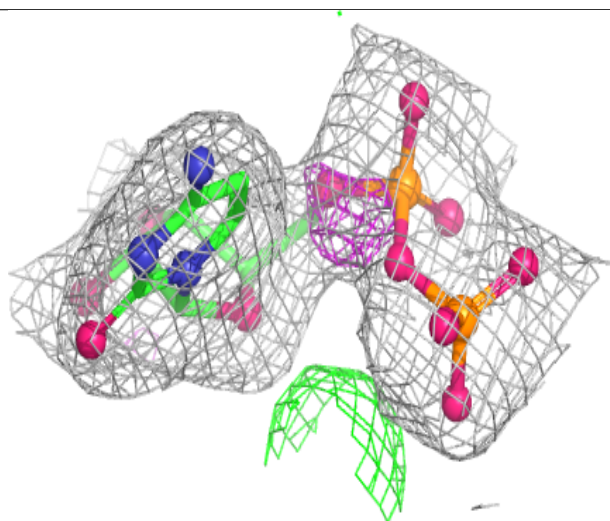
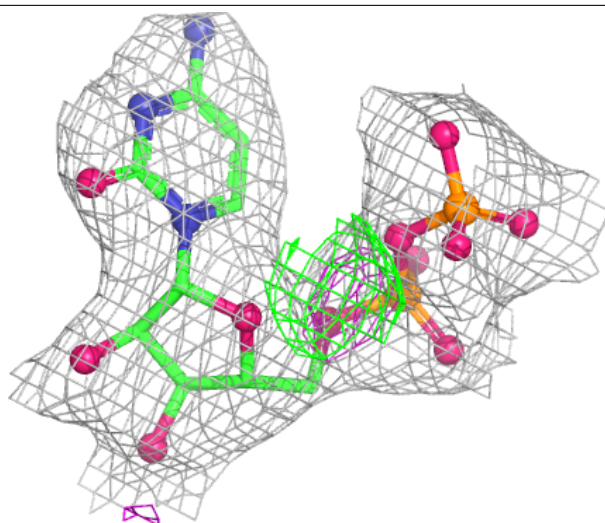
Electron density around CDP C 809:

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



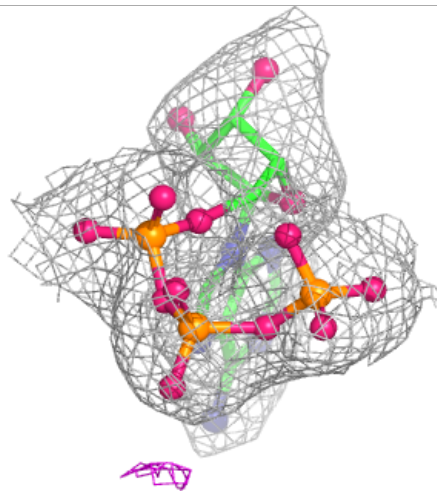
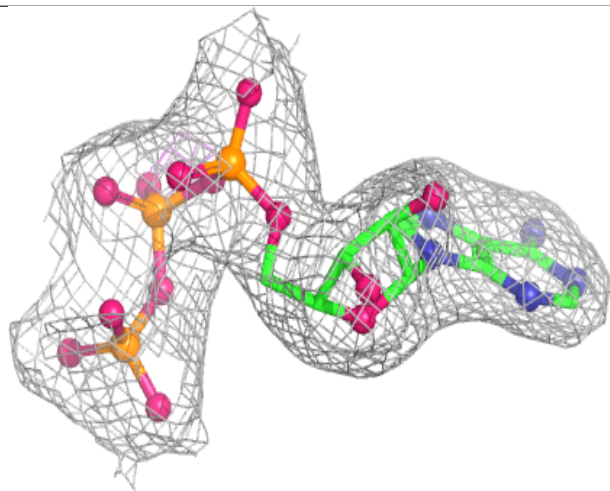
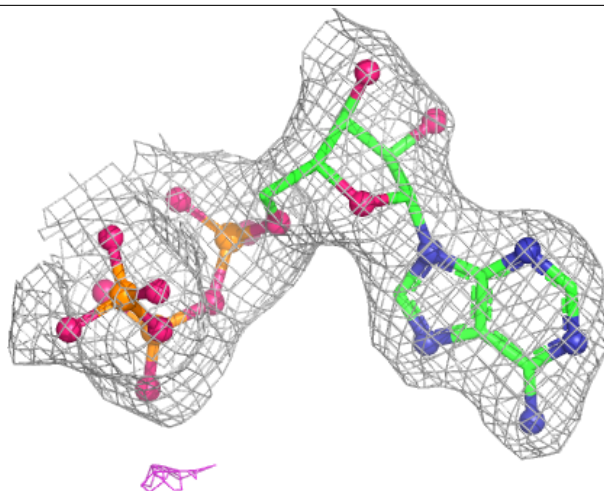
Electron density around CDP F 809:

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



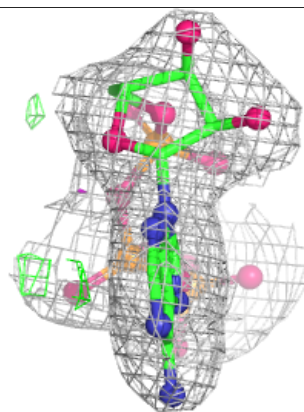
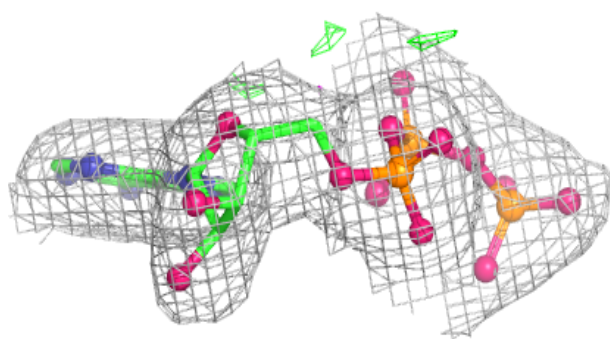
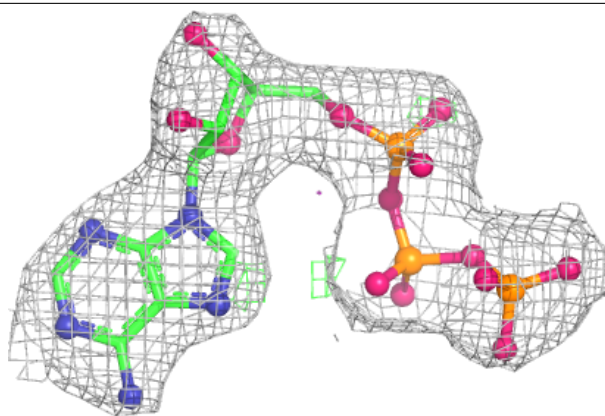
Electron density around ATP G 806:

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



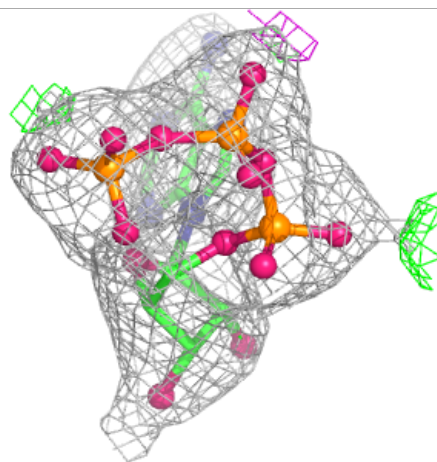
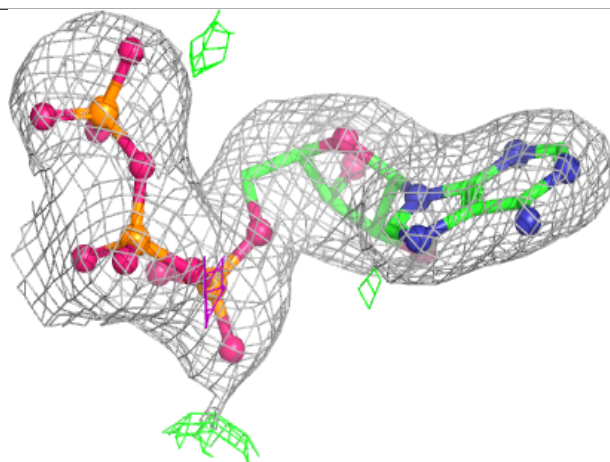
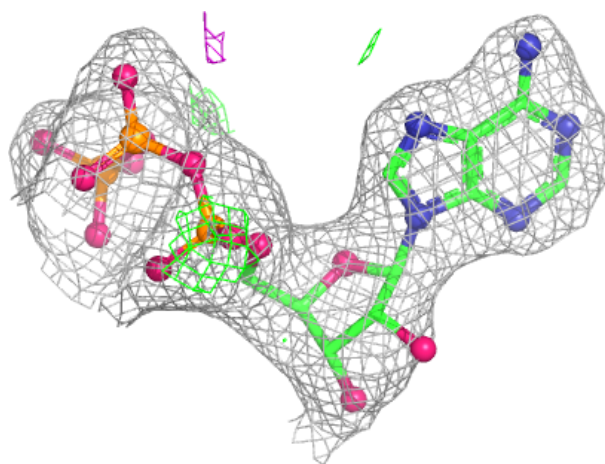
Electron density around ATP D 804:

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



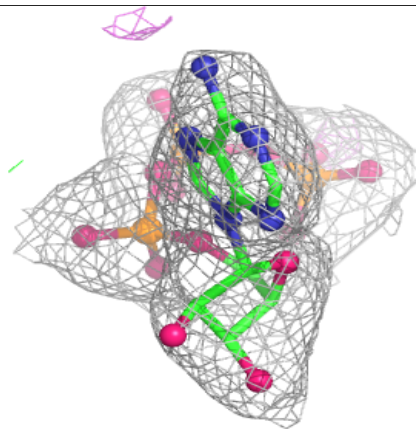
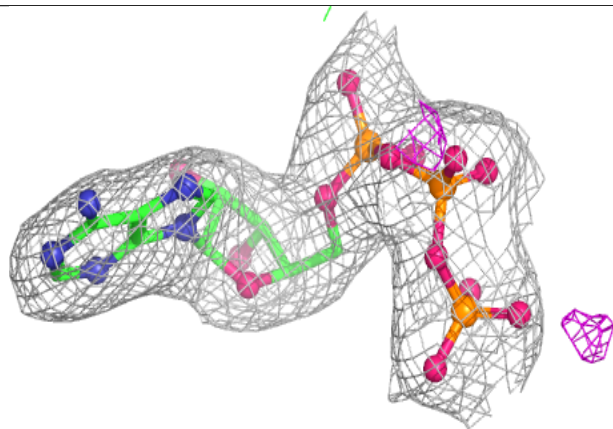
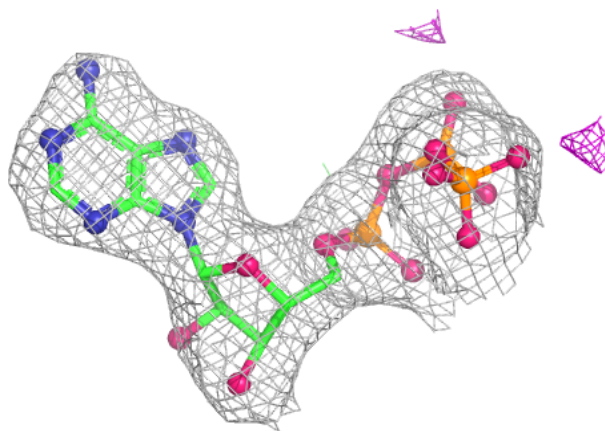
Electron density around ATP A 807:

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



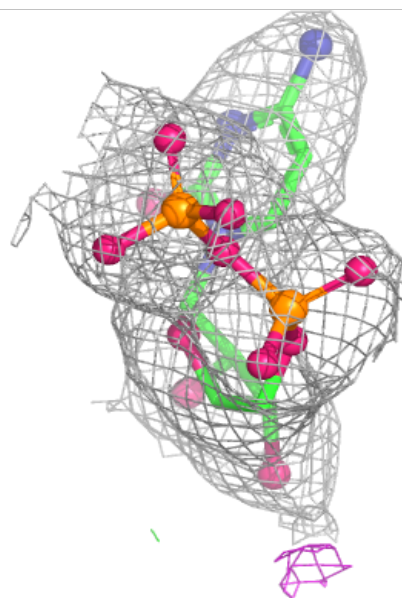
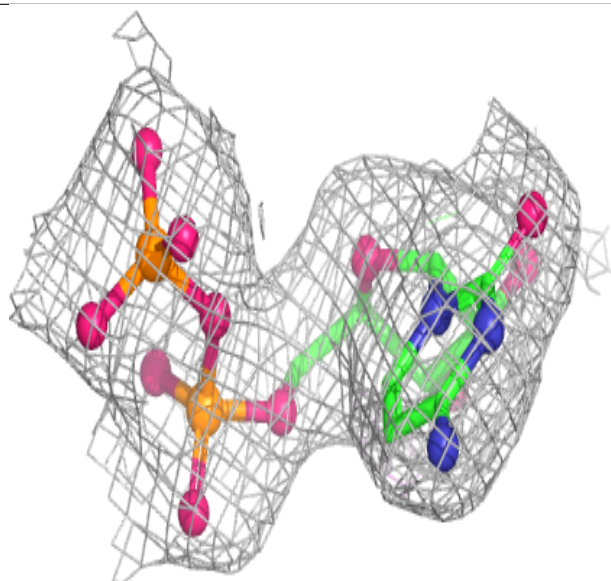
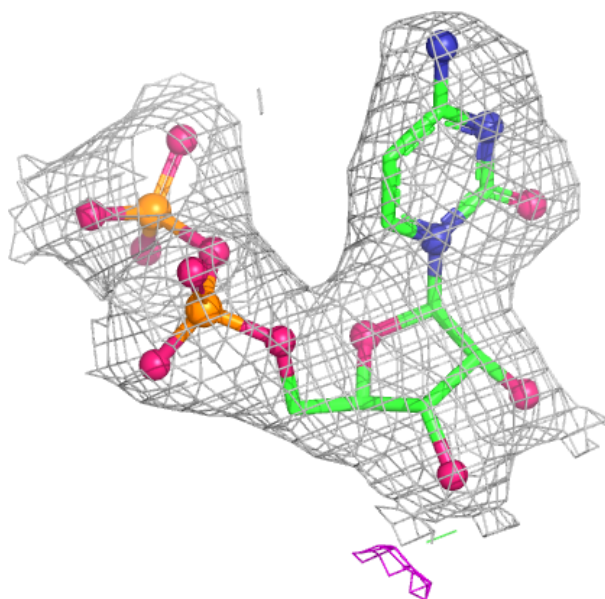
Electron density around ATP D 807:

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



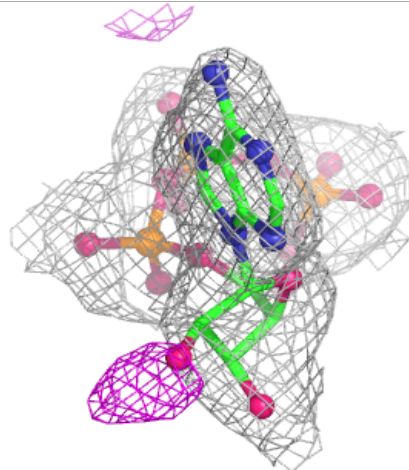
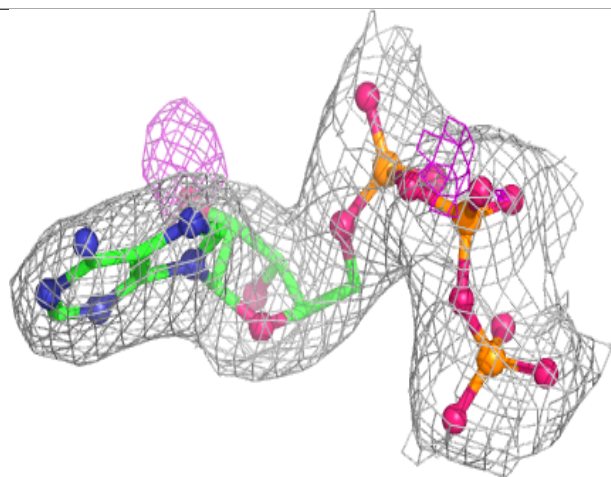
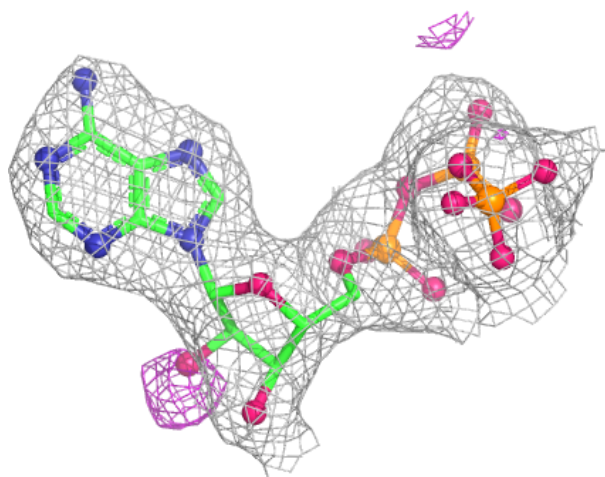
Electron density around CDP A 809:

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



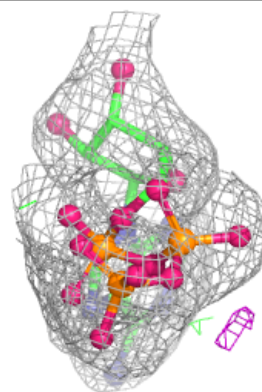
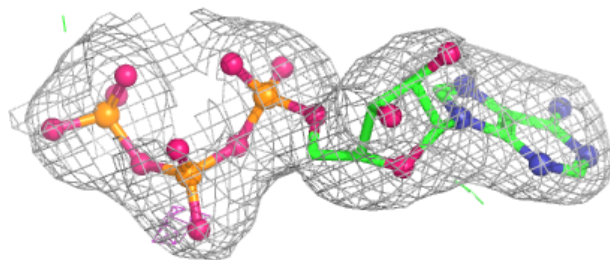
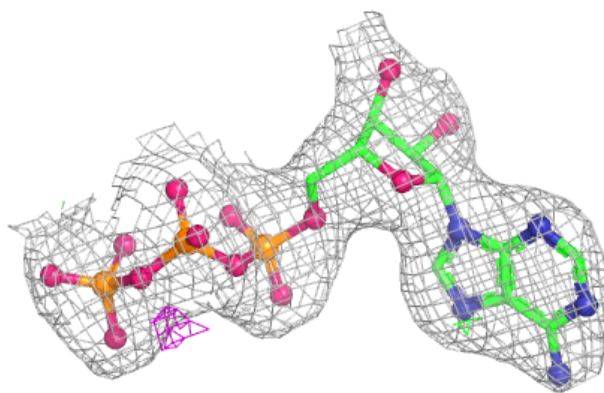
Electron density around ATP F 807:

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



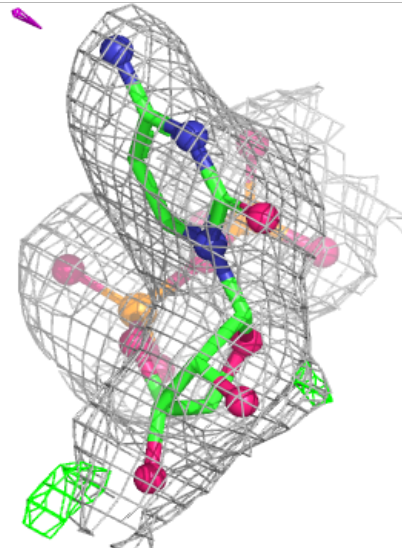
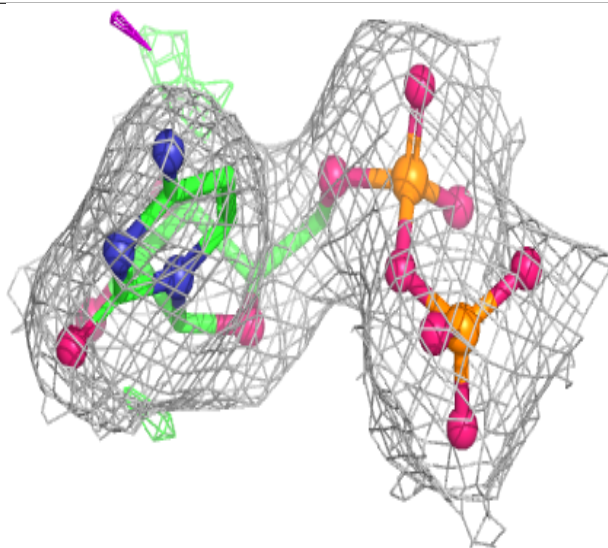
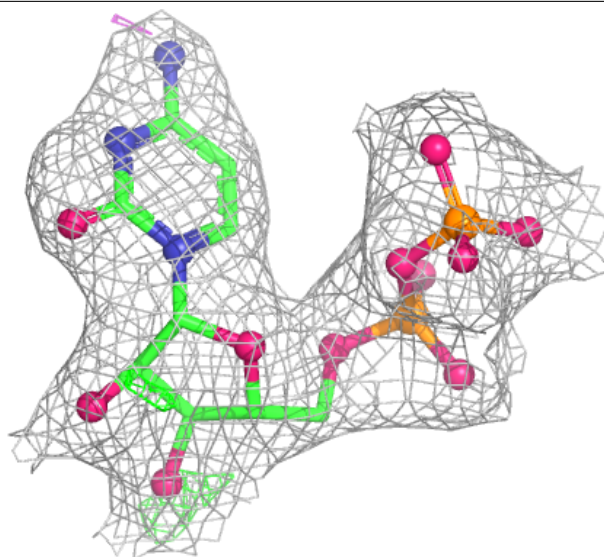
Electron density around ATP A 806:

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



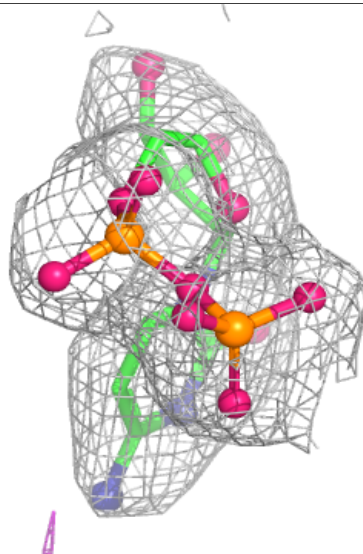
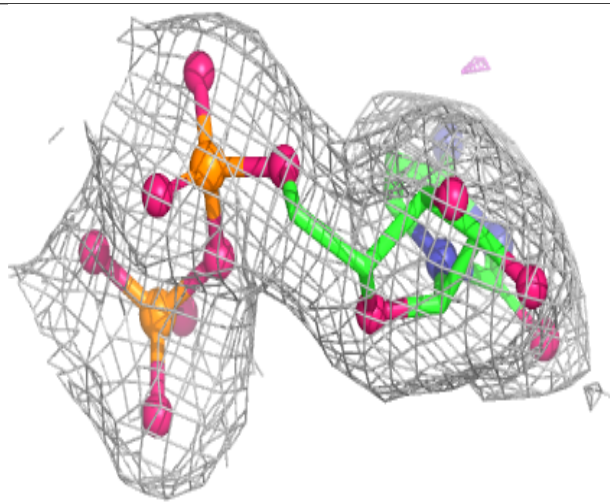
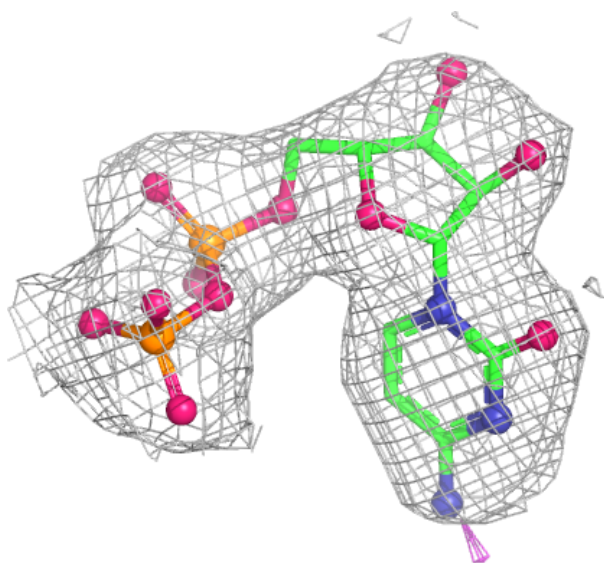
Electron density around CDP D 809:

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



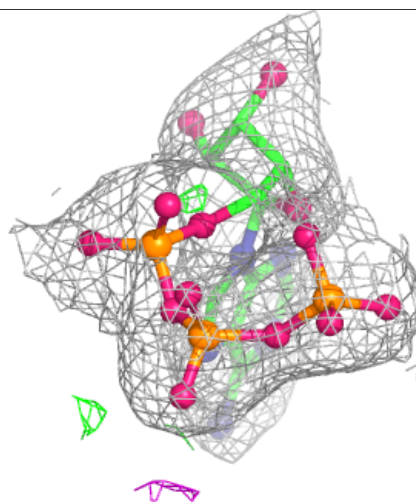
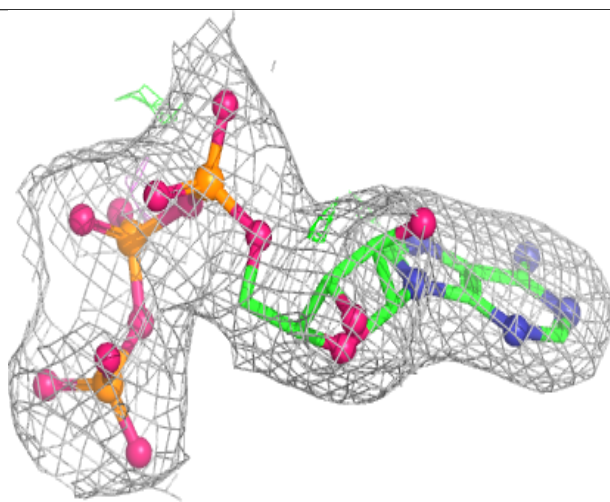
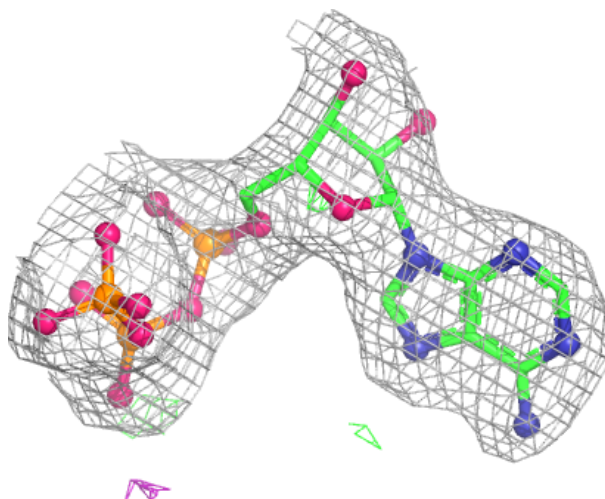
Electron density around CDP E 809:

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



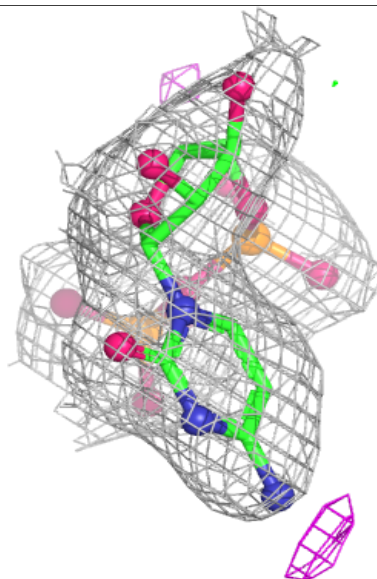
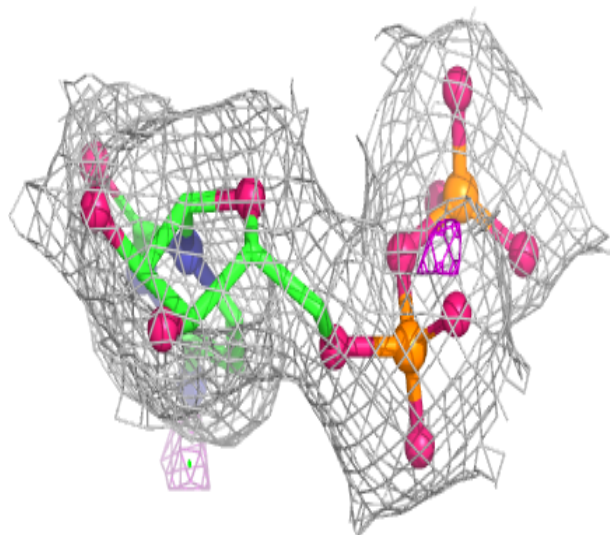
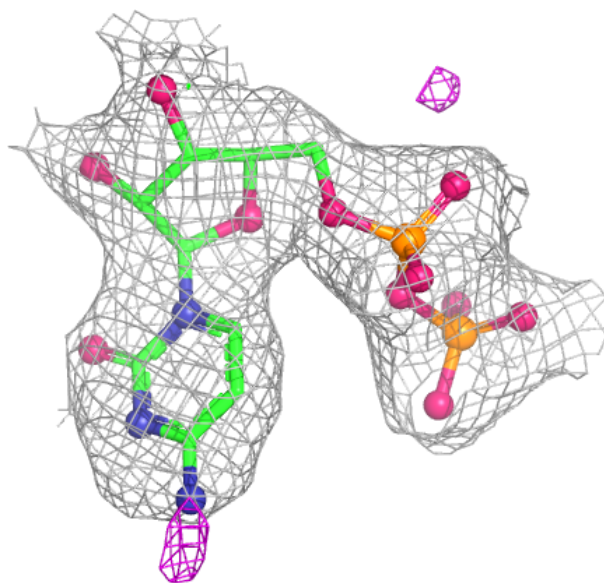
Electron density around ATP C 807:

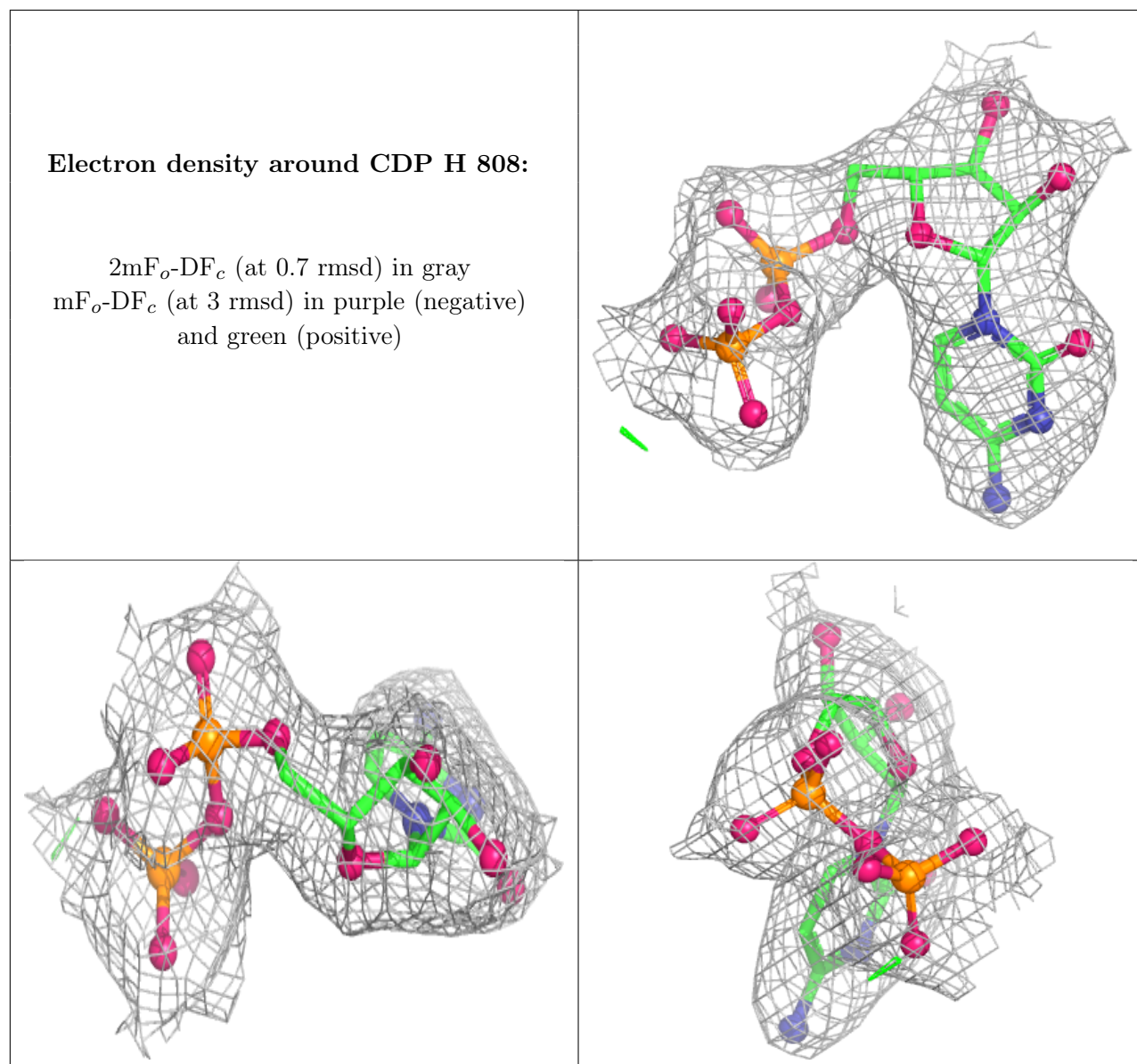
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 ⓘ

There are no such residues in this entry.