



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2026 – 12:27 PM EDT

PDB ID : 39AC / pdb_000039ac
Title : Crystal structure of a Nucleoside diphosphate kinase from *Treponema pallidum* (ADP complex)
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2026-09-25
Resolution : 2.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

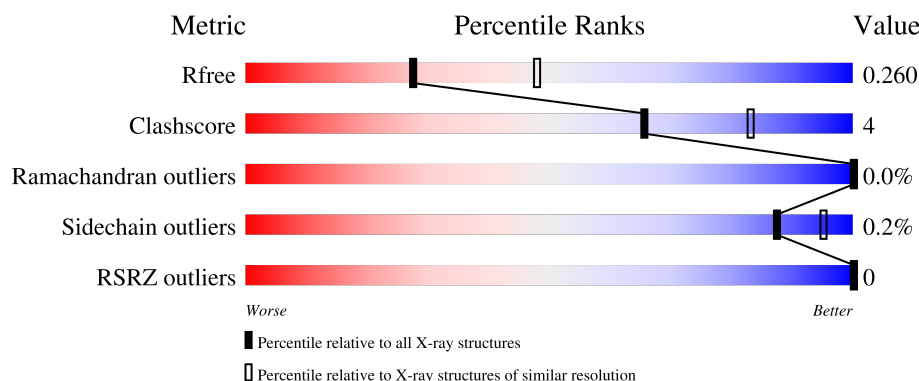
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

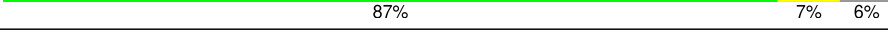
The reported resolution of this entry is 2.49 Å.

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.



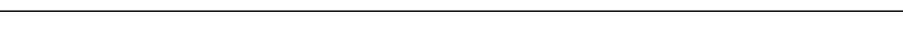
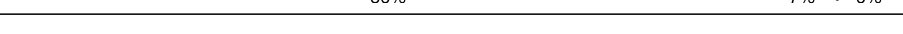
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	157	 91% 7% 2% 2%
1	B	157	 87% 7% 6% 2%
1	C	157	 83% 11% 6% 2%
1	D	157	 87% 7% 6% 2%
1	E	157	 87% 6% 6% 2%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	157	
1	G	157	
1	H	157	
1	I	157	
1	J	157	
1	K	157	
1	L	157	
1	M	157	
1	N	157	
1	O	157	
1	P	157	
1	Q	157	
1	R	157	
1	S	157	
1	T	157	
1	U	157	
1	V	157	
1	W	157	
1	X	157	
1	Y	157	
1	Z	157	
1	a	157	
1	b	157	
1	c	157	
1	d	157	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	e	157	83% 10% • 6%
1	f	157	80% 13% • 6%
1	g	157	84% 10% 6%
1	h	157	82% 10% • 8%
1	i	157	82% 11% • 6%
1	j	157	83% 10% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42596 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1176	753	204	215	4			
1	B	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	C	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	D	147	Total	C	N	O	S	0	0	0
			1147	736	196	212	3			
1	E	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	F	148	Total	C	N	O	S	0	0	0
			1154	740	200	211	3			
1	G	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	H	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	I	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	J	149	Total	C	N	O	S	0	0	0
			1159	743	201	212	3			
1	K	147	Total	C	N	O	S	0	0	0
			1149	736	198	212	3			
1	L	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	M	149	Total	C	N	O	S	0	0	0
			1163	745	201	214	3			
1	N	147	Total	C	N	O	S	0	0	0
			1145	734	198	210	3			
1	O	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	P	147	Total	C	N	O	S	0	0	0
			1144	735	196	210	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	145	Total	C	N	O	S	0	0	0
			1120	714	197	206	3			
1	R	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	S	149	Total	C	N	O	S	0	0	0
			1166	747	201	214	4			
1	T	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	U	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	V	147	Total	C	N	O	S	0	0	0
			1143	734	196	210	3			
1	W	145	Total	C	N	O	S	0	0	0
			1130	721	197	209	3			
1	X	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	Y	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	Z	148	Total	C	N	O	S	0	0	0
			1154	740	200	211	3			
1	a	147	Total	C	N	O	S	0	0	0
			1147	733	199	212	3			
1	b	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	c	147	Total	C	N	O	S	0	0	0
			1147	733	199	212	3			
1	d	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	e	148	Total	C	N	O	S	0	0	0
			1158	742	200	213	3			
1	f	147	Total	C	N	O	S	0	0	0
			1149	737	199	210	3			
1	g	147	Total	C	N	O	S	0	0	0
			1153	739	199	212	3			
1	h	145	Total	C	N	O	S	0	0	0
			1116	710	195	207	4			
1	i	147	Total	C	N	O	S	0	0	0
			1147	733	199	212	3			
1	j	146	Total	C	N	O	S	0	0	0
			1120	716	192	209	3			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP O83974
A	-6	ALA	-	expression tag	UNP O83974
A	-5	HIS	-	expression tag	UNP O83974
A	-4	HIS	-	expression tag	UNP O83974
A	-3	HIS	-	expression tag	UNP O83974
A	-2	HIS	-	expression tag	UNP O83974
A	-1	HIS	-	expression tag	UNP O83974
A	0	HIS	-	expression tag	UNP O83974
B	-7	MET	-	initiating methionine	UNP O83974
B	-6	ALA	-	expression tag	UNP O83974
B	-5	HIS	-	expression tag	UNP O83974
B	-4	HIS	-	expression tag	UNP O83974
B	-3	HIS	-	expression tag	UNP O83974
B	-2	HIS	-	expression tag	UNP O83974
B	-1	HIS	-	expression tag	UNP O83974
B	0	HIS	-	expression tag	UNP O83974
C	-7	MET	-	initiating methionine	UNP O83974
C	-6	ALA	-	expression tag	UNP O83974
C	-5	HIS	-	expression tag	UNP O83974
C	-4	HIS	-	expression tag	UNP O83974
C	-3	HIS	-	expression tag	UNP O83974
C	-2	HIS	-	expression tag	UNP O83974
C	-1	HIS	-	expression tag	UNP O83974
C	0	HIS	-	expression tag	UNP O83974
D	-7	MET	-	initiating methionine	UNP O83974
D	-6	ALA	-	expression tag	UNP O83974
D	-5	HIS	-	expression tag	UNP O83974
D	-4	HIS	-	expression tag	UNP O83974
D	-3	HIS	-	expression tag	UNP O83974
D	-2	HIS	-	expression tag	UNP O83974
D	-1	HIS	-	expression tag	UNP O83974
D	0	HIS	-	expression tag	UNP O83974
E	-7	MET	-	initiating methionine	UNP O83974
E	-6	ALA	-	expression tag	UNP O83974
E	-5	HIS	-	expression tag	UNP O83974
E	-4	HIS	-	expression tag	UNP O83974
E	-3	HIS	-	expression tag	UNP O83974
E	-2	HIS	-	expression tag	UNP O83974
E	-1	HIS	-	expression tag	UNP O83974
E	0	HIS	-	expression tag	UNP O83974
F	-7	MET	-	initiating methionine	UNP O83974
F	-6	ALA	-	expression tag	UNP O83974
F	-5	HIS	-	expression tag	UNP O83974

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	HIS	-	expression tag	UNP O83974
F	-3	HIS	-	expression tag	UNP O83974
F	-2	HIS	-	expression tag	UNP O83974
F	-1	HIS	-	expression tag	UNP O83974
F	0	HIS	-	expression tag	UNP O83974
G	-7	MET	-	initiating methionine	UNP O83974
G	-6	ALA	-	expression tag	UNP O83974
G	-5	HIS	-	expression tag	UNP O83974
G	-4	HIS	-	expression tag	UNP O83974
G	-3	HIS	-	expression tag	UNP O83974
G	-2	HIS	-	expression tag	UNP O83974
G	-1	HIS	-	expression tag	UNP O83974
G	0	HIS	-	expression tag	UNP O83974
H	-7	MET	-	initiating methionine	UNP O83974
H	-6	ALA	-	expression tag	UNP O83974
H	-5	HIS	-	expression tag	UNP O83974
H	-4	HIS	-	expression tag	UNP O83974
H	-3	HIS	-	expression tag	UNP O83974
H	-2	HIS	-	expression tag	UNP O83974
H	-1	HIS	-	expression tag	UNP O83974
H	0	HIS	-	expression tag	UNP O83974
I	-7	MET	-	initiating methionine	UNP O83974
I	-6	ALA	-	expression tag	UNP O83974
I	-5	HIS	-	expression tag	UNP O83974
I	-4	HIS	-	expression tag	UNP O83974
I	-3	HIS	-	expression tag	UNP O83974
I	-2	HIS	-	expression tag	UNP O83974
I	-1	HIS	-	expression tag	UNP O83974
I	0	HIS	-	expression tag	UNP O83974
J	-7	MET	-	initiating methionine	UNP O83974
J	-6	ALA	-	expression tag	UNP O83974
J	-5	HIS	-	expression tag	UNP O83974
J	-4	HIS	-	expression tag	UNP O83974
J	-3	HIS	-	expression tag	UNP O83974
J	-2	HIS	-	expression tag	UNP O83974
J	-1	HIS	-	expression tag	UNP O83974
J	0	HIS	-	expression tag	UNP O83974
K	-7	MET	-	initiating methionine	UNP O83974
K	-6	ALA	-	expression tag	UNP O83974
K	-5	HIS	-	expression tag	UNP O83974
K	-4	HIS	-	expression tag	UNP O83974
K	-3	HIS	-	expression tag	UNP O83974

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	HIS	-	expression tag	UNP O83974
K	-1	HIS	-	expression tag	UNP O83974
K	0	HIS	-	expression tag	UNP O83974
L	-7	MET	-	initiating methionine	UNP O83974
L	-6	ALA	-	expression tag	UNP O83974
L	-5	HIS	-	expression tag	UNP O83974
L	-4	HIS	-	expression tag	UNP O83974
L	-3	HIS	-	expression tag	UNP O83974
L	-2	HIS	-	expression tag	UNP O83974
L	-1	HIS	-	expression tag	UNP O83974
L	0	HIS	-	expression tag	UNP O83974
M	-7	MET	-	initiating methionine	UNP O83974
M	-6	ALA	-	expression tag	UNP O83974
M	-5	HIS	-	expression tag	UNP O83974
M	-4	HIS	-	expression tag	UNP O83974
M	-3	HIS	-	expression tag	UNP O83974
M	-2	HIS	-	expression tag	UNP O83974
M	-1	HIS	-	expression tag	UNP O83974
M	0	HIS	-	expression tag	UNP O83974
N	-7	MET	-	initiating methionine	UNP O83974
N	-6	ALA	-	expression tag	UNP O83974
N	-5	HIS	-	expression tag	UNP O83974
N	-4	HIS	-	expression tag	UNP O83974
N	-3	HIS	-	expression tag	UNP O83974
N	-2	HIS	-	expression tag	UNP O83974
N	-1	HIS	-	expression tag	UNP O83974
N	0	HIS	-	expression tag	UNP O83974
O	-7	MET	-	initiating methionine	UNP O83974
O	-6	ALA	-	expression tag	UNP O83974
O	-5	HIS	-	expression tag	UNP O83974
O	-4	HIS	-	expression tag	UNP O83974
O	-3	HIS	-	expression tag	UNP O83974
O	-2	HIS	-	expression tag	UNP O83974
O	-1	HIS	-	expression tag	UNP O83974
O	0	HIS	-	expression tag	UNP O83974
P	-7	MET	-	initiating methionine	UNP O83974
P	-6	ALA	-	expression tag	UNP O83974
P	-5	HIS	-	expression tag	UNP O83974
P	-4	HIS	-	expression tag	UNP O83974
P	-3	HIS	-	expression tag	UNP O83974
P	-2	HIS	-	expression tag	UNP O83974
P	-1	HIS	-	expression tag	UNP O83974

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	0	HIS	-	expression tag	UNP O83974
Q	-7	MET	-	initiating methionine	UNP O83974
Q	-6	ALA	-	expression tag	UNP O83974
Q	-5	HIS	-	expression tag	UNP O83974
Q	-4	HIS	-	expression tag	UNP O83974
Q	-3	HIS	-	expression tag	UNP O83974
Q	-2	HIS	-	expression tag	UNP O83974
Q	-1	HIS	-	expression tag	UNP O83974
Q	0	HIS	-	expression tag	UNP O83974
R	-7	MET	-	initiating methionine	UNP O83974
R	-6	ALA	-	expression tag	UNP O83974
R	-5	HIS	-	expression tag	UNP O83974
R	-4	HIS	-	expression tag	UNP O83974
R	-3	HIS	-	expression tag	UNP O83974
R	-2	HIS	-	expression tag	UNP O83974
R	-1	HIS	-	expression tag	UNP O83974
R	0	HIS	-	expression tag	UNP O83974
S	-7	MET	-	initiating methionine	UNP O83974
S	-6	ALA	-	expression tag	UNP O83974
S	-5	HIS	-	expression tag	UNP O83974
S	-4	HIS	-	expression tag	UNP O83974
S	-3	HIS	-	expression tag	UNP O83974
S	-2	HIS	-	expression tag	UNP O83974
S	-1	HIS	-	expression tag	UNP O83974
S	0	HIS	-	expression tag	UNP O83974
T	-7	MET	-	initiating methionine	UNP O83974
T	-6	ALA	-	expression tag	UNP O83974
T	-5	HIS	-	expression tag	UNP O83974
T	-4	HIS	-	expression tag	UNP O83974
T	-3	HIS	-	expression tag	UNP O83974
T	-2	HIS	-	expression tag	UNP O83974
T	-1	HIS	-	expression tag	UNP O83974
T	0	HIS	-	expression tag	UNP O83974
U	-7	MET	-	initiating methionine	UNP O83974
U	-6	ALA	-	expression tag	UNP O83974
U	-5	HIS	-	expression tag	UNP O83974
U	-4	HIS	-	expression tag	UNP O83974
U	-3	HIS	-	expression tag	UNP O83974
U	-2	HIS	-	expression tag	UNP O83974
U	-1	HIS	-	expression tag	UNP O83974
U	0	HIS	-	expression tag	UNP O83974
V	-7	MET	-	initiating methionine	UNP O83974

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
V	-6	ALA	-	expression tag	UNP O83974
V	-5	HIS	-	expression tag	UNP O83974
V	-4	HIS	-	expression tag	UNP O83974
V	-3	HIS	-	expression tag	UNP O83974
V	-2	HIS	-	expression tag	UNP O83974
V	-1	HIS	-	expression tag	UNP O83974
V	0	HIS	-	expression tag	UNP O83974
W	-7	MET	-	initiating methionine	UNP O83974
W	-6	ALA	-	expression tag	UNP O83974
W	-5	HIS	-	expression tag	UNP O83974
W	-4	HIS	-	expression tag	UNP O83974
W	-3	HIS	-	expression tag	UNP O83974
W	-2	HIS	-	expression tag	UNP O83974
W	-1	HIS	-	expression tag	UNP O83974
W	0	HIS	-	expression tag	UNP O83974
X	-7	MET	-	initiating methionine	UNP O83974
X	-6	ALA	-	expression tag	UNP O83974
X	-5	HIS	-	expression tag	UNP O83974
X	-4	HIS	-	expression tag	UNP O83974
X	-3	HIS	-	expression tag	UNP O83974
X	-2	HIS	-	expression tag	UNP O83974
X	-1	HIS	-	expression tag	UNP O83974
X	0	HIS	-	expression tag	UNP O83974
Y	-7	MET	-	initiating methionine	UNP O83974
Y	-6	ALA	-	expression tag	UNP O83974
Y	-5	HIS	-	expression tag	UNP O83974
Y	-4	HIS	-	expression tag	UNP O83974
Y	-3	HIS	-	expression tag	UNP O83974
Y	-2	HIS	-	expression tag	UNP O83974
Y	-1	HIS	-	expression tag	UNP O83974
Y	0	HIS	-	expression tag	UNP O83974
Z	-7	MET	-	initiating methionine	UNP O83974
Z	-6	ALA	-	expression tag	UNP O83974
Z	-5	HIS	-	expression tag	UNP O83974
Z	-4	HIS	-	expression tag	UNP O83974
Z	-3	HIS	-	expression tag	UNP O83974
Z	-2	HIS	-	expression tag	UNP O83974
Z	-1	HIS	-	expression tag	UNP O83974
Z	0	HIS	-	expression tag	UNP O83974
a	-7	MET	-	initiating methionine	UNP O83974
a	-6	ALA	-	expression tag	UNP O83974
a	-5	HIS	-	expression tag	UNP O83974

Continued on next page...

Continued from previous page...

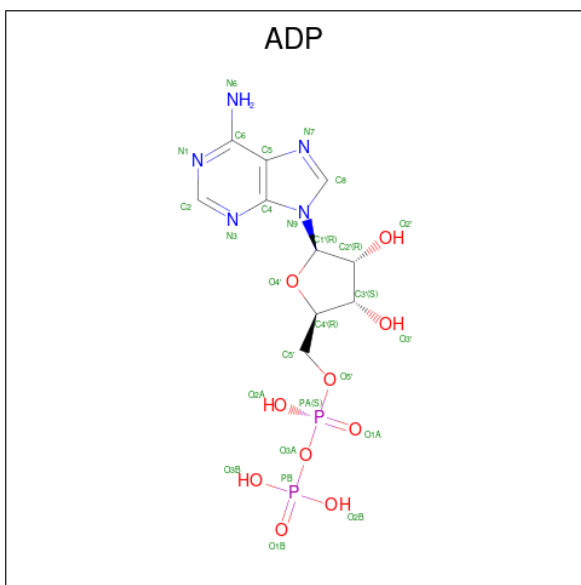
Chain	Residue	Modelled	Actual	Comment	Reference
a	-4	HIS	-	expression tag	UNP O83974
a	-3	HIS	-	expression tag	UNP O83974
a	-2	HIS	-	expression tag	UNP O83974
a	-1	HIS	-	expression tag	UNP O83974
a	0	HIS	-	expression tag	UNP O83974
b	-7	MET	-	initiating methionine	UNP O83974
b	-6	ALA	-	expression tag	UNP O83974
b	-5	HIS	-	expression tag	UNP O83974
b	-4	HIS	-	expression tag	UNP O83974
b	-3	HIS	-	expression tag	UNP O83974
b	-2	HIS	-	expression tag	UNP O83974
b	-1	HIS	-	expression tag	UNP O83974
b	0	HIS	-	expression tag	UNP O83974
c	-7	MET	-	initiating methionine	UNP O83974
c	-6	ALA	-	expression tag	UNP O83974
c	-5	HIS	-	expression tag	UNP O83974
c	-4	HIS	-	expression tag	UNP O83974
c	-3	HIS	-	expression tag	UNP O83974
c	-2	HIS	-	expression tag	UNP O83974
c	-1	HIS	-	expression tag	UNP O83974
c	0	HIS	-	expression tag	UNP O83974
d	-7	MET	-	initiating methionine	UNP O83974
d	-6	ALA	-	expression tag	UNP O83974
d	-5	HIS	-	expression tag	UNP O83974
d	-4	HIS	-	expression tag	UNP O83974
d	-3	HIS	-	expression tag	UNP O83974
d	-2	HIS	-	expression tag	UNP O83974
d	-1	HIS	-	expression tag	UNP O83974
d	0	HIS	-	expression tag	UNP O83974
e	-7	MET	-	initiating methionine	UNP O83974
e	-6	ALA	-	expression tag	UNP O83974
e	-5	HIS	-	expression tag	UNP O83974
e	-4	HIS	-	expression tag	UNP O83974
e	-3	HIS	-	expression tag	UNP O83974
e	-2	HIS	-	expression tag	UNP O83974
e	-1	HIS	-	expression tag	UNP O83974
e	0	HIS	-	expression tag	UNP O83974
f	-7	MET	-	initiating methionine	UNP O83974
f	-6	ALA	-	expression tag	UNP O83974
f	-5	HIS	-	expression tag	UNP O83974
f	-4	HIS	-	expression tag	UNP O83974
f	-3	HIS	-	expression tag	UNP O83974

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
f	-2	HIS	-	expression tag	UNP O83974
f	-1	HIS	-	expression tag	UNP O83974
f	0	HIS	-	expression tag	UNP O83974
g	-7	MET	-	initiating methionine	UNP O83974
g	-6	ALA	-	expression tag	UNP O83974
g	-5	HIS	-	expression tag	UNP O83974
g	-4	HIS	-	expression tag	UNP O83974
g	-3	HIS	-	expression tag	UNP O83974
g	-2	HIS	-	expression tag	UNP O83974
g	-1	HIS	-	expression tag	UNP O83974
g	0	HIS	-	expression tag	UNP O83974
h	-7	MET	-	initiating methionine	UNP O83974
h	-6	ALA	-	expression tag	UNP O83974
h	-5	HIS	-	expression tag	UNP O83974
h	-4	HIS	-	expression tag	UNP O83974
h	-3	HIS	-	expression tag	UNP O83974
h	-2	HIS	-	expression tag	UNP O83974
h	-1	HIS	-	expression tag	UNP O83974
h	0	HIS	-	expression tag	UNP O83974
i	-7	MET	-	initiating methionine	UNP O83974
i	-6	ALA	-	expression tag	UNP O83974
i	-5	HIS	-	expression tag	UNP O83974
i	-4	HIS	-	expression tag	UNP O83974
i	-3	HIS	-	expression tag	UNP O83974
i	-2	HIS	-	expression tag	UNP O83974
i	-1	HIS	-	expression tag	UNP O83974
i	0	HIS	-	expression tag	UNP O83974
j	-7	MET	-	initiating methionine	UNP O83974
j	-6	ALA	-	expression tag	UNP O83974
j	-5	HIS	-	expression tag	UNP O83974
j	-4	HIS	-	expression tag	UNP O83974
j	-3	HIS	-	expression tag	UNP O83974
j	-2	HIS	-	expression tag	UNP O83974
j	-1	HIS	-	expression tag	UNP O83974
j	0	HIS	-	expression tag	UNP O83974

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	L	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	M	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	N	1	Total 27	C 10	N 5	O 10	P 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	P	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	Q	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	R	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	S	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	T	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	U	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	V	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	W	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	X	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	Y	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	Z	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	a	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	b	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	c	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	d	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	e	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	f	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	g	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	h	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	i	1	Total 27	C 10	N 5	O 10	P 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	j	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	M	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		
3	P	1	Total	Mg	0	0
			1	1		
3	Q	1	Total	Mg	0	0
			1	1		
3	W	1	Total	Mg	0	0
			1	1		
3	X	1	Total	Mg	0	0
			1	1		
3	Z	1	Total	Mg	0	0
			1	1		
3	b	1	Total	Mg	0	0
			1	1		
3	c	1	Total	Mg	0	0
			1	1		
3	d	1	Total	Mg	0	0
			1	1		
3	f	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	h	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	7	Total 7	O 7	0	0
4	C	5	Total 5	O 5	0	0
4	D	12	Total 12	O 12	0	0
4	E	16	Total 16	O 16	0	0
4	F	13	Total 13	O 13	0	0
4	G	10	Total 10	O 10	0	0
4	H	16	Total 16	O 16	0	0
4	I	15	Total 15	O 15	0	0
4	J	8	Total 8	O 8	0	0
4	K	12	Total 12	O 12	0	0
4	L	8	Total 8	O 8	0	0
4	M	6	Total 6	O 6	0	0
4	N	6	Total 6	O 6	0	0
4	O	4	Total 4	O 4	0	0
4	P	4	Total 4	O 4	0	0
4	Q	5	Total 5	O 5	0	0
4	R	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	4	Total O 4 4	0	0
4	T	5	Total O 5 5	0	0
4	U	5	Total O 5 5	0	0
4	V	6	Total O 6 6	0	0
4	W	6	Total O 6 6	0	0
4	X	13	Total O 13 13	0	0
4	Y	1	Total O 1 1	0	0
4	Z	2	Total O 2 2	0	0
4	a	4	Total O 4 4	0	0
4	b	2	Total O 2 2	0	0
4	c	4	Total O 4 4	0	0
4	d	6	Total O 6 6	0	0
4	e	2	Total O 2 2	0	0
4	f	4	Total O 4 4	0	0
4	h	1	Total O 1 1	0	0
4	i	1	Total O 1 1	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: Nucleoside diphosphate kinase

Chain A:  91% 7% 2%



- Molecule 1: Nucleoside diphosphate kinase

Chain B:  87% 7% 6%



- Molecule 1: Nucleoside diphosphate kinase

Chain C:  83% 11% 6%



- Molecule 1: Nucleoside diphosphate kinase

Chain D:  87% 7% 6%



- Molecule 1: Nucleoside diphosphate kinase

Chain E:  87% 6% 6%

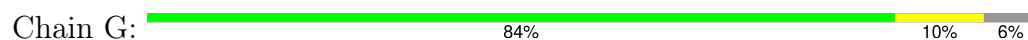


- Molecule 1: Nucleoside diphosphate kinase

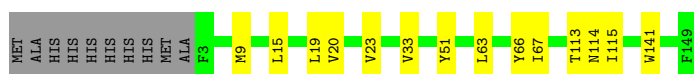
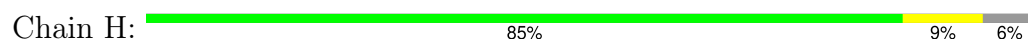
Chain F:  89% 6% 6%



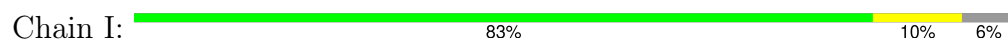
- Molecule 1: Nucleoside diphosphate kinase



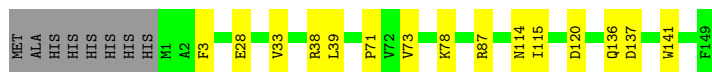
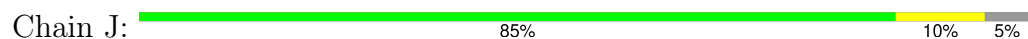
- Molecule 1: Nucleoside diphosphate kinase



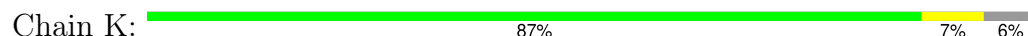
- Molecule 1: Nucleoside diphosphate kinase



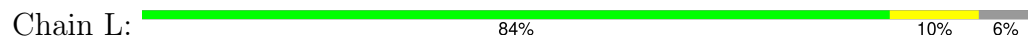
- Molecule 1: Nucleoside diphosphate kinase



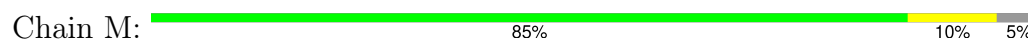
- Molecule 1: Nucleoside diphosphate kinase

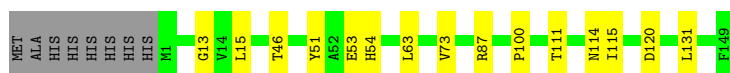


- Molecule 1: Nucleoside diphosphate kinase

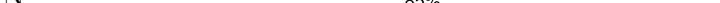


- Molecule 1: Nucleoside diphosphate kinase





- Molecule 1: Nucleoside diphosphate kinase

Chain N:  85% 9% 6%

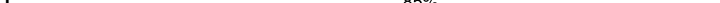


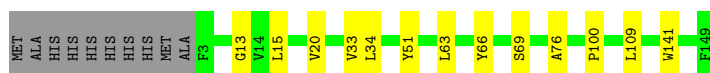
- Molecule 1: Nucleoside diphosphate kinase

Chain 0: 85% 8% • 6%

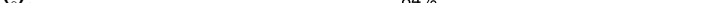


- Molecule 1: Nucleoside diphosphate kinase

Chain P:  85% 8% 6%



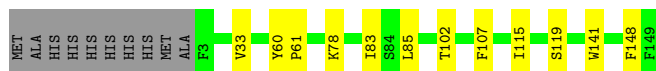
- Molecule 1: Nucleoside diphosphate kinase

Chain Q:  84% 8% 8%



- Molecule 1: Nucleoside diphosphate kinase

Chain R:  86% 8% 6%



- Molecule 1: Nucleoside diphosphate kinase

Chain S: 89% 6% 5%



- Molecule 1: Nucleoside diphosphate kinase

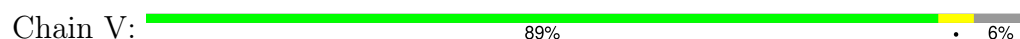
Chain T:  86% 7% • 6%



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



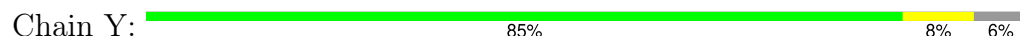
- Molecule 1: Nucleoside diphosphate kinase



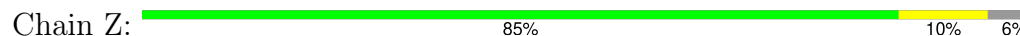
- Molecule 1: Nucleoside diphosphate kinase



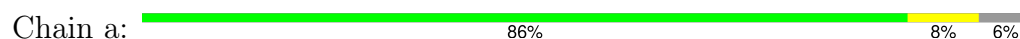
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase





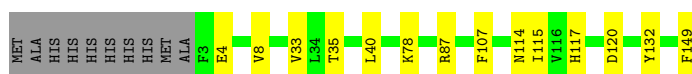
- Molecule 1: Nucleoside diphosphate kinase

Chain b: 85% 8% 6%



- Molecule 1: Nucleoside diphosphate kinase

Chain c: 85% 9% 6%



- Molecule 1: Nucleoside diphosphate kinase

Chain d:  87% 7% 6%

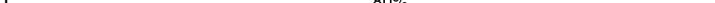


- Molecule 1: Nucleoside diphosphate kinase

Chain e: 83% 10% • 6%

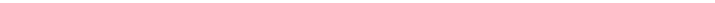


- Molecule 1: Nucleoside diphosphate kinase

Chain f:  80% 13% • 6%



- Molecule 1: Nucleoside diphosphate kinase

Chain g:  84% 10% 6%

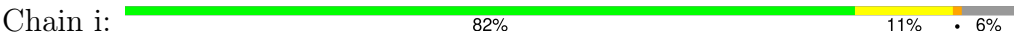


- Molecule 1: Nucleoside diphosphate kinase

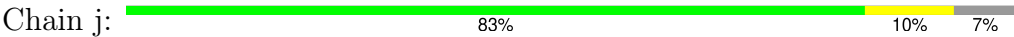
Chain h: 82% 10% 8%



• Molecule 1: Nucleoside diphosphate kinase



• Molecule 1: Nucleoside diphosphate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	115.78Å 115.86Å 128.60Å 90.08° 106.37° 119.90°	Depositor
Resolution (Å)	48.83 – 2.49 48.83 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.83-2.49) 96.4 (48.83-2.49)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.48Å)	Xtriage
Refinement program	PHENIX (2.0_5936: ???)	Depositor
R, R_{free}	0.209 , 0.257 0.220 , 0.260	Depositor DCC
R_{free} test set	9238 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 10.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.400 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42596	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	0.15	0/1203	0.33	0/1633
1	B	0.15	0/1179	0.34	0/1601
1	C	0.15	0/1179	0.36	0/1601
1	D	0.15	0/1173	0.37	0/1594
1	E	0.15	0/1179	0.36	0/1601
1	F	0.14	0/1180	0.35	0/1603
1	G	0.14	0/1179	0.36	0/1601
1	H	0.14	0/1179	0.36	0/1601
1	I	0.14	0/1179	0.36	0/1601
1	J	0.16	0/1185	0.37	0/1610
1	K	0.16	0/1175	0.37	0/1597
1	L	0.20	0/1179	0.40	0/1601
1	M	0.14	0/1189	0.34	0/1615
1	N	0.14	0/1171	0.35	0/1592
1	O	0.13	0/1179	0.35	0/1601
1	P	0.12	0/1170	0.31	0/1590
1	Q	0.14	0/1143	0.34	0/1554
1	R	0.12	0/1179	0.32	0/1601
1	S	0.14	0/1192	0.33	0/1618
1	T	0.14	0/1179	0.36	0/1601
1	U	0.13	0/1179	0.33	0/1601
1	V	0.14	0/1169	0.33	0/1589
1	W	0.13	0/1154	0.33	0/1569
1	X	0.15	0/1179	0.33	0/1601
1	Y	0.15	0/1179	0.32	0/1601
1	Z	0.13	0/1180	0.33	0/1603
1	a	0.12	0/1172	0.31	0/1592
1	b	0.13	0/1179	0.33	0/1601
1	c	0.13	0/1172	0.32	0/1592
1	d	0.13	0/1179	0.32	0/1601
1	e	0.13	0/1184	0.32	0/1608
1	f	0.13	0/1175	0.35	0/1596

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	0.15	0/1179	0.33	0/1601
1	h	0.17	0/1138	0.36	0/1545
1	i	0.17	0/1172	0.33	0/1592
1	j	0.16	0/1144	0.36	0/1557
All	All	0.14	0/42305	0.34	0/57465

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	1176	0	1165	4	0
1	B	1153	0	1141	7	0
1	C	1153	0	1141	12	0
1	D	1147	0	1130	9	0
1	E	1153	0	1141	7	0
1	F	1154	0	1142	6	0
1	G	1153	0	1141	11	0
1	H	1153	0	1141	9	0
1	I	1153	0	1141	11	0
1	J	1159	0	1147	11	0
1	K	1149	0	1130	8	0
1	L	1153	0	1141	9	0
1	M	1163	0	1151	10	0
1	N	1145	0	1126	9	0
1	O	1153	0	1141	11	0
1	P	1144	0	1128	9	0
1	Q	1120	0	1114	11	0
1	R	1153	0	1141	11	0
1	S	1166	0	1158	7	0
1	T	1153	0	1141	10	0
1	U	1153	0	1141	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	1143	0	1126	5	0
1	W	1130	0	1123	5	0
1	X	1153	0	1141	4	0
1	Y	1153	0	1141	9	0
1	Z	1154	0	1142	10	0
1	a	1147	0	1134	6	0
1	b	1153	0	1141	8	0
1	c	1147	0	1134	13	0
1	d	1153	0	1141	8	0
1	e	1158	0	1146	18	0
1	f	1149	0	1137	18	0
1	g	1153	0	1141	12	0
1	h	1116	0	1102	13	0
1	i	1147	0	1134	18	0
1	j	1120	0	1092	11	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	0	0
2	K	27	0	12	0	0
2	L	27	0	12	0	0
2	M	27	0	12	0	0
2	N	27	0	12	0	0
2	O	27	0	12	0	0
2	P	27	0	12	0	0
2	Q	27	0	12	1	0
2	R	27	0	12	0	0
2	S	27	0	12	0	0
2	T	27	0	12	0	0
2	U	27	0	12	0	0
2	V	27	0	12	0	0
2	W	27	0	12	0	0
2	X	27	0	12	0	0
2	Y	27	0	12	0	0
2	Z	27	0	12	0	0
2	a	27	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	27	0	12	0	0
2	c	27	0	12	0	0
2	d	27	0	12	0	0
2	e	27	0	12	0	0
2	f	27	0	12	1	0
2	g	27	0	12	1	0
2	h	27	0	12	0	0
2	i	27	0	12	0	0
2	j	27	0	12	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
3	Z	1	0	0	0	0
3	b	1	0	0	0	0
3	c	1	0	0	0	0
3	d	1	0	0	0	0
3	f	1	0	0	0	0
3	h	1	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	5	0	0	0	0
4	D	12	0	0	0	0
4	E	16	0	0	0	0
4	F	13	0	0	0	0
4	G	10	0	0	0	0
4	H	16	0	0	0	0
4	I	15	0	0	0	0
4	J	8	0	0	0	0
4	K	12	0	0	0	0
4	L	8	0	0	0	0
4	M	6	0	0	0	0
4	N	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	4	0	0	0	0
4	P	4	0	0	0	0
4	Q	5	0	0	0	0
4	R	3	0	0	0	0
4	S	4	0	0	0	0
4	T	5	0	0	0	0
4	U	5	0	0	0	0
4	V	6	0	0	0	0
4	W	6	0	0	0	0
4	X	13	0	0	0	0
4	Y	1	0	0	0	0
4	Z	2	0	0	0	0
4	a	4	0	0	0	0
4	b	2	0	0	0	0
4	c	4	0	0	0	0
4	d	6	0	0	0	0
4	e	2	0	0	0	0
4	f	4	0	0	0	0
4	h	1	0	0	0	0
4	i	1	0	0	0	0
All	All	42596	0	41349	316	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 4.

All (316) 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:g:49:LEU:HD12	1:g:131:LEU:HD11	1.48	0.92
1:O:46:THR:HG23	1:O:131:LEU:HD13	1.60	0.81
1:h:46:THR:HG23	1:h:131:LEU:HD13	1.65	0.78
1:L:64:ILE:HA	1:L:67:ILE:HD12	1.67	0.77
1:L:63:LEU:HG	1:L:67:ILE:HD11	1.66	0.77
1:i:46:THR:CG2	1:i:131:LEU:HD13	2.18	0.74
1:T:63:LEU:O	1:T:67:ILE:HD12	1.88	0.73
1:e:46:THR:HG23	1:e:131:LEU:HD13	1.71	0.72
1:S:33:VAL:HG13	1:S:141:TRP:CZ2	2.26	0.70
1:O:46:THR:CG2	1:O:131:LEU:HD13	2.24	0.66
1:c:35:THR:CG2	1:c:78:LYS:HE3	2.26	0.66
1:g:49:LEU:HD13	1:g:49:LEU:O	1.96	0.66
1:H:51:TYR:CD1	1:H:63:LEU:HD21	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:33:VAL:HG13	1:I:141:TRP:CZ2	2.31	0.65
1:e:33:VAL:HG13	1:e:141:TRP:CZ2	2.30	0.65
1:j:49:LEU:HD12	1:j:131:LEU:HD11	1.78	0.65
1:f:9:MET:SD	1:f:67:ILE:HD11	2.37	0.64
2:E:201:ADP:O1A	2:E:201:ADP:O1B	2.16	0.64
1:I:35:THR:HG21	1:I:78:LYS:HE2	1.80	0.64
1:f:131:LEU:HD11	1:f:132:TYR:CE2	2.33	0.64
1:i:46:THR:HG23	1:i:131:LEU:HD13	1.80	0.62
1:W:52:ALA:O	1:W:55:ARG:HG2	1.99	0.62
1:G:40:LEU:HD11	1:G:132:TYR:HD1	1.63	0.62
2:f:201:ADP:O1A	2:f:201:ADP:O1B	2.18	0.62
1:K:33:VAL:HG13	1:K:141:TRP:CZ2	2.35	0.61
1:I:62:SER:HA	1:T:44:THR:HG21	1.84	0.60
1:g:49:LEU:HD13	1:g:49:LEU:C	2.26	0.60
1:N:135:ALA:HB2	1:Z:46:THR:HG21	1.83	0.60
1:h:80:GLU:O	1:h:81:ASN:OD1	2.19	0.60
1:d:3:PHE:HZ	1:d:78:LYS:HD3	1.67	0.59
1:K:33:VAL:HG13	1:K:141:TRP:CE2	2.38	0.59
1:f:33:VAL:HG13	1:f:141:TRP:CZ2	2.38	0.59
1:C:39:LEU:CD2	1:C:73:VAL:HG22	2.33	0.59
1:P:33:VAL:HG13	1:P:141:TRP:CZ2	2.38	0.59
1:e:131:LEU:C	1:e:131:LEU:HD12	2.29	0.58
1:c:35:THR:HG23	1:c:78:LYS:HE3	1.85	0.58
1:M:51:TYR:CD1	1:M:63:LEU:HD21	2.40	0.57
1:i:131:LEU:C	1:i:131:LEU:HD12	2.28	0.57
1:i:131:LEU:HD11	1:i:132:TYR:CE2	2.39	0.57
1:h:33:VAL:HG13	1:h:141:TRP:CZ2	2.40	0.57
1:H:15:LEU:HD23	1:H:20:VAL:HG21	1.86	0.57
1:Q:33:VAL:HG13	1:Q:141:TRP:CZ2	2.40	0.57
1:Q:49:LEU:HD12	1:Q:131:LEU:HD11	1.86	0.57
1:e:33:VAL:HG13	1:e:141:TRP:CE2	2.40	0.57
1:P:33:VAL:HG13	1:P:141:TRP:CE2	2.39	0.57
1:P:34:LEU:HD12	1:P:76:ALA:O	2.05	0.57
1:e:46:THR:CG2	1:e:131:LEU:HD13	2.35	0.56
1:Z:33:VAL:HG13	1:Z:141:TRP:CZ2	2.41	0.56
1:O:131:LEU:HD11	1:O:132:TYR:CE2	2.40	0.56
1:A:39:LEU:CD2	1:A:73:VAL:HG22	2.36	0.56
1:B:100:PRO:HG2	1:C:102:THR:HG22	1.87	0.56
1:O:131:LEU:C	1:O:131:LEU:HD12	2.30	0.56
1:a:54:HIS:HA	1:a:57:LYS:HD3	1.88	0.55
1:D:87:ARG:HD2	1:D:120:ASP:HA	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:LEU:HD11	1:G:132:TYR:CD1	2.40	0.55
1:H:33:VAL:HG13	1:H:141:TRP:CZ2	2.41	0.55
1:b:38:ARG:HD2	1:b:137:ASP:CG	2.31	0.55
1:f:46:THR:CG2	1:f:131:LEU:HD13	2.37	0.55
1:A:83:ILE:HG22	1:A:87:ARG:NH1	2.22	0.55
1:I:33:VAL:HG13	1:I:141:TRP:CE2	2.41	0.55
1:K:87:ARG:HD2	1:K:120:ASP:HA	1.89	0.55
1:J:33:VAL:HG13	1:J:141:TRP:CZ2	2.41	0.54
1:T:107:PHE:HB2	1:T:115:ILE:HD13	1.90	0.54
1:h:131:LEU:HD11	1:h:132:TYR:CE2	2.42	0.54
1:G:87:ARG:HD2	1:G:120:ASP:HA	1.90	0.54
1:M:87:ARG:HD2	1:M:120:ASP:HA	1.89	0.53
1:R:107:PHE:HB2	1:R:115:ILE:HD13	1.89	0.53
1:h:33:VAL:HG13	1:h:141:TRP:CE2	2.43	0.53
1:P:51:TYR:CD1	1:P:63:LEU:HD21	2.44	0.53
1:Q:136:GLN:HG3	1:Q:137:ASP:OD1	2.07	0.53
1:J:33:VAL:HG13	1:J:141:TRP:CE2	2.43	0.53
1:j:49:LEU:HD11	1:j:127:ARG:HD2	1.89	0.53
1:F:33:VAL:HG13	1:F:141:TRP:CZ2	2.44	0.53
1:e:107:PHE:HB2	1:e:115:ILE:HD13	1.91	0.52
1:L:38:ARG:HH21	1:L:137:ASP:CG	2.17	0.52
1:Q:33:VAL:HG13	1:Q:141:TRP:CE2	2.44	0.52
1:T:87:ARG:HD2	1:T:120:ASP:HA	1.92	0.52
1:i:131:LEU:HD11	1:i:132:TYR:CZ	2.44	0.52
1:L:38:ARG:NH2	1:L:137:ASP:OD1	2.39	0.52
1:Q:49:LEU:HD13	1:Q:49:LEU:O	2.09	0.52
1:S:51:TYR:CG	1:S:63:LEU:HD21	2.44	0.52
1:W:87:ARG:HD2	1:W:120:ASP:HA	1.92	0.52
1:i:87:ARG:HG2	1:i:118:ALA:HB3	1.91	0.51
1:O:131:LEU:HD11	1:O:132:TYR:CZ	2.45	0.51
1:Y:134:SER:OG	1:Y:136:GLN:HG2	2.11	0.51
1:Z:87:ARG:HD2	1:Z:120:ASP:HA	1.92	0.51
1:e:131:LEU:HD11	1:e:132:TYR:CZ	2.46	0.51
1:C:87:ARG:HD2	1:C:120:ASP:HA	1.93	0.51
1:d:87:ARG:HD2	1:d:120:ASP:HA	1.93	0.51
1:B:9:MET:SD	1:B:67:ILE:HD11	2.51	0.50
1:c:33:VAL:HB	1:c:78:LYS:CG	2.41	0.50
1:J:3:PHE:CE2	1:J:78:LYS:HE2	2.46	0.50
2:Q:201:ADP:O1A	2:Q:201:ADP:O1B	2.29	0.50
1:S:15:LEU:HD11	1:S:73:VAL:HG23	1.93	0.50
1:b:61:PRO:HB2	1:g:55:ARG:HE	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:33:VAL:HG13	1:Z:141:TRP:CE2	2.47	0.50
1:N:44:THR:HG23	1:N:64:ILE:CG2	2.42	0.50
1:Q:136:GLN:HG3	1:Q:137:ASP:N	2.27	0.50
1:J:136:GLN:NE2	1:J:137:ASP:OD1	2.45	0.50
1:L:39:LEU:CD2	1:L:73:VAL:HG22	2.42	0.50
1:T:107:PHE:HB2	1:T:115:ILE:CD1	2.41	0.50
1:a:10:LEU:HD12	1:a:20:VAL:HG13	1.94	0.50
1:d:39:LEU:CD2	1:d:73:VAL:HG22	2.42	0.50
1:G:104:ARG:HG2	1:G:114:ASN:O	2.12	0.50
2:F:201:ADP:O1B	2:F:201:ADP:O1A	2.30	0.50
1:a:12:PRO:HB3	1:a:70:ALA:HB3	1.95	0.49
1:h:81:ASN:OD1	1:h:85:LEU:HG	2.12	0.49
1:f:46:THR:HG23	1:f:131:LEU:HD13	1.94	0.49
1:E:33:VAL:HG13	1:E:141:TRP:CZ2	2.47	0.49
1:M:111:THR:O	1:M:114:ASN:OD1	2.31	0.49
1:Q:44:THR:O	1:Q:48:GLU:HG3	2.13	0.49
1:c:107:PHE:HB2	1:c:115:ILE:HD13	1.93	0.49
1:O:33:VAL:HG13	1:O:141:TRP:CZ2	2.48	0.49
1:e:131:LEU:HD11	1:e:132:TYR:CE2	2.48	0.49
1:Y:94:ARG:HD3	1:Y:96:GLU:OE1	2.13	0.49
1:j:15:LEU:HD11	1:j:73:VAL:HG23	1.94	0.49
1:U:104:ARG:HG2	1:U:114:ASN:O	2.13	0.49
1:h:1:MET:C	1:h:80:GLU:OE2	2.56	0.49
1:I:87:ARG:HD2	1:I:120:ASP:HA	1.94	0.48
1:b:107:PHE:HB2	1:b:115:ILE:HD13	1.95	0.48
1:f:51:TYR:CG	1:f:63:LEU:HD21	2.48	0.48
1:C:9:MET:SD	1:C:67:ILE:HD11	2.53	0.48
1:P:66:TYR:HA	1:P:69:SER:OG	2.13	0.48
1:Y:136:GLN:HG3	1:Y:137:ASP:N	2.28	0.48
1:i:51:TYR:CD1	1:i:63:LEU:HD21	2.48	0.48
1:C:3:PHE:CZ	1:C:78:LYS:HD2	2.49	0.48
1:C:33:VAL:HG13	1:C:141:TRP:CZ2	2.48	0.48
1:Q:49:LEU:CD1	1:Q:127:ARG:HD2	2.44	0.48
1:D:33:VAL:HB	1:D:78:LYS:HG3	1.94	0.48
1:i:46:THR:HG21	1:i:131:LEU:HD13	1.92	0.48
1:B:40:LEU:HD11	1:B:132:TYR:HD1	1.79	0.48
1:H:9:MET:SD	1:H:67:ILE:HD11	2.54	0.48
1:Y:35:THR:HG23	1:Y:76:ALA:HB3	1.96	0.48
1:F:2:ALA:HB3	1:F:80:GLU:HG3	1.95	0.47
1:f:33:VAL:HB	1:f:78:LYS:HG3	1.96	0.47
1:X:12:PRO:HB3	1:X:70:ALA:HB3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HD23	1:C:149:PHE:O	2.14	0.47
1:L:10:LEU:HG	1:L:75:LEU:HD11	1.97	0.47
1:h:22:GLU:O	1:h:26:ARG:HG2	2.15	0.47
1:f:40:LEU:HD11	1:f:132:TYR:CD1	2.50	0.47
1:g:50:HIS:HE2	1:g:117:HIS:CE1	2.32	0.47
1:F:33:VAL:HG13	1:F:141:TRP:CE2	2.50	0.46
1:U:33:VAL:HG13	1:U:141:TRP:CZ2	2.50	0.46
1:W:55:ARG:HD2	1:W:60:TYR:CZ	2.50	0.46
1:T:6:THR:HG21	1:T:86:VAL:HG21	1.96	0.46
1:V:51:TYR:CD1	1:V:63:LEU:HD21	2.49	0.46
1:G:33:VAL:HG13	1:G:141:TRP:CZ2	2.51	0.46
1:O:87:ARG:HD3	1:O:120:ASP:HA	1.97	0.46
1:h:102:THR:HG22	1:i:100:PRO:HG2	1.98	0.46
1:C:104:ARG:HG2	1:C:114:ASN:O	2.16	0.46
1:c:35:THR:HG21	1:c:78:LYS:HE3	1.98	0.46
1:i:145:ASN:O	1:i:149:PHE:HD1	1.99	0.46
1:G:33:VAL:HG13	1:G:141:TRP:CE2	2.51	0.46
1:G:35:THR:HG23	1:G:76:ALA:HB3	1.98	0.46
1:P:15:LEU:HD23	1:P:20:VAL:HG21	1.97	0.46
1:f:51:TYR:CD1	1:f:63:LEU:HD21	2.51	0.46
1:M:46:THR:HG23	1:M:131:LEU:HD22	1.98	0.46
1:R:83:ILE:HG23	1:R:119:SER:O	2.15	0.46
1:c:33:VAL:HB	1:c:78:LYS:HG3	1.98	0.46
1:f:26:ARG:NH2	1:f:101:GLY:O	2.49	0.45
1:Y:100:PRO:HD3	1:Z:88:THR:HG22	1.99	0.45
1:C:33:VAL:HG13	1:C:141:TRP:CE2	2.51	0.45
1:M:15:LEU:HD11	1:M:73:VAL:CG2	2.46	0.45
1:P:100:PRO:HG2	1:R:102:THR:HG22	1.99	0.45
1:e:18:ARG:NE	1:i:149:PHE:CE2	2.85	0.45
1:i:36:ALA:HB1	1:i:133:PHE:CE1	2.52	0.45
1:V:51:TYR:CG	1:V:63:LEU:HD21	2.52	0.45
1:c:4:GLU:O	1:c:78:LYS:HA	2.17	0.45
1:h:46:THR:CG2	1:h:131:LEU:HD13	2.41	0.45
1:I:51:TYR:CD1	1:I:63:LEU:HD21	2.52	0.45
1:J:38:ARG:HG3	1:J:39:LEU:N	2.32	0.45
1:J:39:LEU:CD2	1:J:73:VAL:HG22	2.47	0.45
1:Z:12:PRO:HB3	1:Z:70:ALA:HB3	1.98	0.45
1:D:138:PHE:CG	1:K:43:ASP:OD2	2.70	0.45
1:I:34:LEU:HG	1:J:39:LEU:HD11	1.98	0.45
1:A:104:ARG:HG2	1:A:114:ASN:O	2.17	0.45
1:H:15:LEU:CD2	1:H:20:VAL:HG21	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:114:ASN:O	1:T:115:ILE:HB	2.17	0.45
1:O:131:LEU:HD11	1:O:132:TYR:CD2	2.51	0.45
1:Z:114:ASN:O	1:Z:115:ILE:HB	2.17	0.44
1:i:131:LEU:HD11	1:i:132:TYR:CD2	2.52	0.44
1:L:46:THR:HG23	1:L:131:LEU:HD22	1.98	0.44
1:C:28:GLU:OE2	1:D:20:VAL:HB	2.18	0.44
1:S:33:VAL:HG13	1:S:141:TRP:CE2	2.53	0.44
1:e:12:PRO:HB3	1:e:70:ALA:HB3	2.00	0.44
1:Z:38:ARG:HE	1:Z:137:ASP:CG	2.25	0.44
1:e:114:ASN:O	1:e:115:ILE:HB	2.18	0.44
1:g:35:THR:HG23	1:g:76:ALA:HB3	1.99	0.44
1:H:19:LEU:O	1:H:23:VAL:HG23	2.17	0.44
1:M:100:PRO:HG2	1:N:102:THR:HG22	2.00	0.44
1:T:107:PHE:C	1:T:115:ILE:HD11	2.43	0.44
1:N:87:ARG:HD2	1:N:120:ASP:HA	2.00	0.44
1:a:114:ASN:O	1:a:115:ILE:HB	2.18	0.44
1:g:60:TYR:HB3	1:g:61:PRO:HD3	2.00	0.44
1:g:87:ARG:HD2	1:g:120:ASP:HA	2.00	0.44
1:h:12:PRO:HB3	1:h:70:ALA:HB3	2.00	0.44
1:j:108:ALA:HB1	1:j:114:ASN:HA	2.00	0.44
1:A:28:GLU:OE2	1:E:20:VAL:HB	2.18	0.43
1:H:66:TYR:CE1	1:H:113:THR:HG22	2.53	0.43
1:J:87:ARG:HD2	1:J:120:ASP:HA	2.00	0.43
1:I:104:ARG:HG2	1:I:114:ASN:O	2.18	0.43
1:D:14:VAL:HG13	1:D:19:LEU:HB2	2.00	0.43
1:S:51:TYR:CD1	1:S:63:LEU:HD21	2.53	0.43
1:V:35:THR:O	1:V:139:VAL:HG22	2.19	0.43
1:d:35:THR:OG1	1:d:78:LYS:HG2	2.18	0.43
1:f:33:VAL:HG13	1:f:141:TRP:CE2	2.53	0.43
1:B:104:ARG:HG2	1:B:114:ASN:O	2.19	0.43
1:K:19:LEU:O	1:K:23:VAL:HG23	2.18	0.43
1:a:63:LEU:O	1:a:67:ILE:HD12	2.18	0.43
1:b:35:THR:HG23	1:b:139:VAL:O	2.18	0.43
1:E:33:VAL:HG13	1:E:141:TRP:CE2	2.53	0.43
1:Q:49:LEU:HD11	1:Q:127:ARG:HD2	1.99	0.43
1:S:12:PRO:HB3	1:S:70:ALA:HB3	2.00	0.43
1:N:33:VAL:HG13	1:N:141:TRP:CE2	2.54	0.43
1:P:109:LEU:HD12	1:R:85:LEU:HD13	2.01	0.43
1:T:109:LEU:HD23	1:U:149:PHE:O	2.18	0.43
1:i:12:PRO:HB3	1:i:70:ALA:HB3	2.01	0.43
1:d:104:ARG:HG2	1:d:114:ASN:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:VAL:HB	1:J:28:GLU:OE2	2.19	0.43
1:R:33:VAL:HB	1:R:78:LYS:HB3	1.99	0.43
1:c:87:ARG:HD2	1:c:120:ASP:HA	2.01	0.43
1:i:104:ARG:HG2	1:i:114:ASN:O	2.19	0.43
1:M:100:PRO:HD3	1:N:88:THR:HG22	2.01	0.43
1:M:114:ASN:O	1:M:115:ILE:HB	2.18	0.43
1:N:42:VAL:O	1:N:68:THR:HG22	2.19	0.43
1:f:114:ASN:O	1:f:115:ILE:HB	2.19	0.43
1:F:87:ARG:HD2	1:F:120:ASP:HA	2.00	0.42
1:b:87:ARG:HD2	1:b:120:ASP:HA	2.00	0.42
1:c:40:LEU:HD11	1:c:132:TYR:CD1	2.54	0.42
1:G:33:VAL:HB	1:G:78:LYS:HG3	2.00	0.42
1:R:107:PHE:C	1:R:115:ILE:HD11	2.44	0.42
1:O:63:LEU:O	1:O:67:ILE:HG12	2.19	0.42
1:W:48:GLU:HG2	1:W:60:TYR:OH	2.20	0.42
1:a:93:THR:HB	1:a:94:ARG:HH11	1.85	0.42
1:f:87:ARG:HD2	1:f:120:ASP:HA	2.02	0.42
1:E:87:ARG:HD2	1:E:120:ASP:HA	2.01	0.42
1:e:131:LEU:HD11	1:e:132:TYR:CE1	2.54	0.42
1:d:35:THR:OG1	1:d:78:LYS:HE3	2.19	0.42
1:B:28:GLU:OE2	1:F:20:VAL:HB	2.20	0.42
1:D:102:THR:HG22	1:E:100:PRO:HG2	2.02	0.42
1:Z:95:VAL:HG21	1:Z:110:ARG:HA	2.01	0.42
1:f:131:LEU:HD11	1:f:132:TYR:CZ	2.55	0.42
1:i:102:THR:HG22	1:j:100:PRO:HG2	2.02	0.42
1:C:71:PRO:HG2	1:D:141:TRP:HB3	2.01	0.42
1:G:102:THR:HG22	1:I:100:PRO:HG2	2.02	0.42
1:W:19:LEU:O	1:W:23:VAL:HG23	2.20	0.42
1:h:131:LEU:HD12	1:h:131:LEU:C	2.45	0.42
1:j:15:LEU:HD11	1:j:73:VAL:CG2	2.49	0.42
1:j:54:HIS:O	1:j:60:TYR:HB2	2.19	0.42
1:K:54:HIS:O	1:K:60:TYR:HB2	2.20	0.42
1:N:34:LEU:HD21	1:N:37:LEU:HD22	2.01	0.42
1:Q:60:TYR:HB3	1:Q:61:PRO:HD3	2.02	0.42
1:Y:40:LEU:HD11	1:Y:132:TYR:HD1	1.85	0.42
1:e:141:TRP:HB3	1:i:71:PRO:HD2	2.01	0.42
1:K:40:LEU:HD11	1:K:42:VAL:HG22	2.01	0.42
1:O:143:ASP:HB3	1:O:146:TYR:HB2	2.02	0.42
1:e:106:ASP:O	1:f:29:ARG:HG3	2.19	0.42
1:i:12:PRO:HG2	1:i:66:TYR:O	2.20	0.42
1:Q:38:ARG:HG2	1:Q:39:LEU:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:54:HIS:O	1:V:60:TYR:HB2	2.20	0.42
1:Y:104:ARG:HG2	1:Y:114:ASN:O	2.20	0.42
1:f:131:LEU:HD11	1:f:132:TYR:CD2	2.55	0.42
1:g:33:VAL:HG13	1:g:141:TRP:CZ2	2.55	0.42
1:j:104:ARG:HG2	1:j:114:ASN:O	2.20	0.42
1:L:40:LEU:HD11	1:L:132:TYR:HD1	1.85	0.41
1:M:13:GLY:HA3	1:N:148:PHE:HB3	2.02	0.41
1:U:33:VAL:HG13	1:U:141:TRP:CE2	2.54	0.41
1:b:114:ASN:O	1:b:115:ILE:HB	2.19	0.41
1:j:33:VAL:HG13	1:j:141:TRP:CZ2	2.55	0.41
1:E:54:HIS:O	1:E:60:TYR:HB2	2.20	0.41
1:L:55:ARG:HA	1:L:60:TYR:CG	2.55	0.41
1:M:53:GLU:HG2	1:M:54:HIS:CD2	2.54	0.41
1:O:34:LEU:HD12	1:O:76:ALA:O	2.20	0.41
1:R:60:TYR:HB3	1:R:61:PRO:HD3	2.01	0.41
1:X:104:ARG:HG2	1:X:114:ASN:O	2.20	0.41
1:J:114:ASN:O	1:J:115:ILE:HB	2.21	0.41
1:P:13:GLY:HA3	1:R:148:PHE:HB3	2.01	0.41
1:j:114:ASN:O	1:j:115:ILE:HB	2.20	0.41
1:G:12:PRO:HB3	1:G:70:ALA:HB3	2.02	0.41
1:U:9:MET:HA	1:U:73:VAL:O	2.20	0.41
1:c:114:ASN:O	1:c:115:ILE:HB	2.21	0.41
1:e:111:THR:O	1:e:114:ASN:OD1	2.39	0.41
1:E:12:PRO:HG2	1:E:66:TYR:O	2.21	0.41
1:T:28:GLU:OE2	1:X:20:VAL:HB	2.20	0.41
1:U:12:PRO:HB3	1:U:70:ALA:HB3	2.03	0.41
1:I:141:TRP:HB3	1:J:71:PRO:HG2	2.01	0.41
1:R:33:VAL:HG13	1:R:141:TRP:CZ2	2.55	0.41
1:f:38:ARG:HD3	1:f:40:LEU:HB3	2.03	0.41
1:B:60:TYR:HB3	1:B:61:PRO:HD3	2.03	0.41
1:C:20:VAL:HB	1:D:28:GLU:OE2	2.21	0.41
1:b:87:ARG:HG2	1:b:118:ALA:HB3	2.02	0.41
1:c:8:VAL:HA	1:c:117:HIS:O	2.21	0.41
1:e:13:GLY:HA3	1:f:148:PHE:HB3	2.03	0.41
1:g:49:LEU:C	1:g:49:LEU:CD1	2.93	0.41
1:g:54:HIS:O	1:g:60:TYR:HB2	2.21	0.41
1:h:114:ASN:O	1:h:115:ILE:HB	2.21	0.41
1:j:63:LEU:HD22	2:j:201:ADP:O4'	2.21	0.41
1:G:40:LEU:HD21	1:G:74:ALA:HB2	2.03	0.41
1:R:33:VAL:HG13	1:R:141:TRP:CE2	2.57	0.41
1:X:114:ASN:O	1:X:115:ILE:HB	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:42:VAL:O	1:e:68:THR:HG22	2.21	0.41
1:R:107:PHE:CB	1:R:115:ILE:HD13	2.51	0.40
1:c:149:PHE:OXT	1:d:109:LEU:HB3	2.21	0.40
1:V:60:TYR:HB3	1:V:61:PRO:HD3	2.03	0.40
1:b:15:LEU:HD11	1:b:73:VAL:CG2	2.52	0.40
1:c:40:LEU:HD11	1:c:132:TYR:HD1	1.86	0.40
1:F:114:ASN:O	1:F:115:ILE:HB	2.22	0.40
1:H:51:TYR:CG	1:H:63:LEU:HD21	2.56	0.40
1:H:114:ASN:O	1:H:115:ILE:HB	2.22	0.40
1:Y:114:ASN:O	1:Y:115:ILE:HB	2.21	0.40
1:Z:18:ARG:HD3	1:d:28:GLU:O	2.21	0.40
1:S:149:PHE:OXT	1:U:109:LEU:HB3	2.21	0.40
1:e:107:PHE:C	1:e:115:ILE:HD11	2.47	0.40
1:D:138:PHE:CB	1:K:43:ASP:OD2	2.70	0.40
1:Y:40:LEU:HD11	1:Y:132:TYR:CD1	2.55	0.40
1:g:11:LYS:NZ	2:g:201:ADP:O3'	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/157 (94%)	147 (99%)	1 (1%)	0	100	100
1	B	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	C	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	D	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	E	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	F	146/157 (93%)	145 (99%)	1 (1%)	0	100	100
1	G	145/157 (92%)	143 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	I	145/157 (92%)	143 (99%)	1 (1%)	1 (1%)	18	34
1	J	147/157 (94%)	145 (99%)	2 (1%)	0	100	100
1	K	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	L	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	M	147/157 (94%)	146 (99%)	1 (1%)	0	100	100
1	N	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	O	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	P	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	Q	143/157 (91%)	142 (99%)	1 (1%)	0	100	100
1	R	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	S	147/157 (94%)	145 (99%)	2 (1%)	0	100	100
1	T	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	U	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	V	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	W	143/157 (91%)	142 (99%)	1 (1%)	0	100	100
1	X	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	Y	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	Z	146/157 (93%)	144 (99%)	2 (1%)	0	100	100
1	a	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	b	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	c	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	d	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	e	146/157 (93%)	145 (99%)	1 (1%)	0	100	100
1	f	145/157 (92%)	143 (99%)	1 (1%)	1 (1%)	18	34
1	g	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	h	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
1	i	145/157 (92%)	144 (99%)	1 (1%)	0	100	100
1	j	144/157 (92%)	143 (99%)	1 (1%)	0	100	100
All	All	5223/5652 (92%)	5170 (99%)	51 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	115	ILE
1	f	115	ILE

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	123/131 (94%)	123 (100%)	0	100	100
1	B	121/131 (92%)	121 (100%)	0	100	100
1	C	121/131 (92%)	121 (100%)	0	100	100
1	D	120/131 (92%)	120 (100%)	0	100	100
1	E	121/131 (92%)	121 (100%)	0	100	100
1	F	120/131 (92%)	120 (100%)	0	100	100
1	G	121/131 (92%)	121 (100%)	0	100	100
1	H	121/131 (92%)	121 (100%)	0	100	100
1	I	121/131 (92%)	120 (99%)	1 (1%)	73	88
1	J	120/131 (92%)	120 (100%)	0	100	100
1	K	120/131 (92%)	120 (100%)	0	100	100
1	L	121/131 (92%)	121 (100%)	0	100	100
1	M	121/131 (92%)	121 (100%)	0	100	100
1	N	119/131 (91%)	119 (100%)	0	100	100
1	O	121/131 (92%)	119 (98%)	2 (2%)	53	78
1	P	119/131 (91%)	119 (100%)	0	100	100
1	Q	117/131 (89%)	117 (100%)	0	100	100
1	R	121/131 (92%)	121 (100%)	0	100	100
1	S	122/131 (93%)	122 (100%)	0	100	100
1	T	121/131 (92%)	120 (99%)	1 (1%)	73	88
1	U	121/131 (92%)	121 (100%)	0	100	100
1	V	119/131 (91%)	119 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	119/131 (91%)	119 (100%)	0	100	100
1	X	121/131 (92%)	121 (100%)	0	100	100
1	Y	121/131 (92%)	121 (100%)	0	100	100
1	Z	120/131 (92%)	120 (100%)	0	100	100
1	a	120/131 (92%)	120 (100%)	0	100	100
1	b	121/131 (92%)	121 (100%)	0	100	100
1	c	120/131 (92%)	120 (100%)	0	100	100
1	d	121/131 (92%)	121 (100%)	0	100	100
1	e	121/131 (92%)	119 (98%)	2 (2%)	53	78
1	f	120/131 (92%)	119 (99%)	1 (1%)	73	88
1	g	121/131 (92%)	121 (100%)	0	100	100
1	h	116/131 (88%)	115 (99%)	1 (1%)	70	87
1	i	120/131 (92%)	119 (99%)	1 (1%)	73	88
1	j	115/131 (88%)	115 (100%)	0	100	100
All	All	4327/4716 (92%)	4318 (100%)	9 (0%)	87	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	22	GLU
1	O	56	GLU
1	O	131	LEU
1	T	67	ILE
1	e	38	ARG
1	e	131	LEU
1	f	110	ARG
1	h	1	MET
1	i	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	54	HIS
1	D	97	HIS
1	E	97	HIS
1	H	97	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	136	GLN
1	R	145	ASN
1	Y	99	GLN
1	a	54	HIS
1	d	97	HIS
1	f	54	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 55 ligands modelled in this entry, 19 are monoatomic - leaving 36 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	ADP	R	201	-	28,29,29	1.44	5 (17%)	43,45,45	1.89	11 (25%)
2	ADP	h	201	3	28,29,29	1.42	4 (14%)	43,45,45	1.86	10 (23%)
2	ADP	C	201	3	28,29,29	1.42	5 (17%)	43,45,45	1.91	11 (25%)
2	ADP	M	201	3	28,29,29	1.43	4 (14%)	43,45,45	1.86	11 (25%)
2	ADP	L	201	-	28,29,29	1.45	5 (17%)	43,45,45	1.86	11 (25%)
2	ADP	G	201	3	28,29,29	1.39	4 (14%)	43,45,45	1.86	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	O	201	3	28,29,29	1.44	5 (17%)	43,45,45	1.87	10 (23%)
2	ADP	N	201	-	28,29,29	1.44	5 (17%)	43,45,45	1.89	11 (25%)
2	ADP	Y	201	-	28,29,29	1.43	4 (14%)	43,45,45	1.87	11 (25%)
2	ADP	f	201	3	28,29,29	1.41	5 (17%)	43,45,45	1.86	11 (25%)
2	ADP	Q	201	3	28,29,29	1.43	5 (17%)	43,45,45	1.90	11 (25%)
2	ADP	K	201	-	28,29,29	1.47	5 (17%)	43,45,45	1.89	10 (23%)
2	ADP	S	201	-	28,29,29	1.42	5 (17%)	43,45,45	1.84	11 (25%)
2	ADP	X	201	3	28,29,29	1.37	5 (17%)	43,45,45	1.90	10 (23%)
2	ADP	b	201	3	28,29,29	1.40	5 (17%)	43,45,45	1.91	10 (23%)
2	ADP	i	201	-	28,29,29	1.41	5 (17%)	43,45,45	1.85	10 (23%)
2	ADP	I	201	3	28,29,29	1.43	4 (14%)	43,45,45	1.87	9 (20%)
2	ADP	D	201	3	28,29,29	1.41	5 (17%)	43,45,45	1.89	11 (25%)
2	ADP	B	201	3	28,29,29	1.43	5 (17%)	43,45,45	1.87	10 (23%)
2	ADP	T	201	-	28,29,29	1.39	4 (14%)	43,45,45	1.86	9 (20%)
2	ADP	c	201	3	28,29,29	1.37	4 (14%)	43,45,45	1.90	11 (25%)
2	ADP	F	201	3	28,29,29	1.38	5 (17%)	43,45,45	1.86	10 (23%)
2	ADP	W	201	3	28,29,29	1.39	4 (14%)	43,45,45	1.87	9 (20%)
2	ADP	d	201	3	28,29,29	1.39	4 (14%)	43,45,45	1.88	10 (23%)
2	ADP	j	201	-	28,29,29	1.44	5 (17%)	43,45,45	1.87	11 (25%)
2	ADP	Z	201	3	28,29,29	1.44	5 (17%)	43,45,45	1.87	11 (25%)
2	ADP	A	201	-	28,29,29	1.43	5 (17%)	43,45,45	1.87	10 (23%)
2	ADP	E	201	3	28,29,29	1.39	6 (21%)	43,45,45	1.86	10 (23%)
2	ADP	J	201	-	28,29,29	1.45	5 (17%)	43,45,45	1.86	10 (23%)
2	ADP	g	201	-	28,29,29	1.43	5 (17%)	43,45,45	1.87	9 (20%)
2	ADP	H	201	-	28,29,29	1.42	5 (17%)	43,45,45	1.88	11 (25%)
2	ADP	e	201	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	10 (23%)
2	ADP	U	201	-	28,29,29	1.41	3 (10%)	43,45,45	1.85	11 (25%)
2	ADP	V	201	-	28,29,29	1.41	5 (17%)	43,45,45	1.85	10 (23%)
2	ADP	P	201	3	28,29,29	1.43	5 (17%)	43,45,45	1.87	11 (25%)
2	ADP	a	201	-	28,29,29	1.42	4 (14%)	43,45,45	1.88	11 (25%)

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
2	ADP	R	201	-	-	1/16/32/32	0/3/3/3
2	ADP	h	201	3	-	1/16/32/32	0/3/3/3
2	ADP	C	201	3	-	5/16/32/32	0/3/3/3
2	ADP	M	201	3	-	3/16/32/32	0/3/3/3
2	ADP	L	201	-	-	1/16/32/32	0/3/3/3
2	ADP	G	201	3	-	4/16/32/32	0/3/3/3
2	ADP	O	201	3	-	6/16/32/32	0/3/3/3
2	ADP	N	201	-	-	0/16/32/32	0/3/3/3
2	ADP	Y	201	-	-	5/16/32/32	0/3/3/3
2	ADP	f	201	3	-	4/16/32/32	0/3/3/3
2	ADP	Q	201	3	-	3/16/32/32	0/3/3/3
2	ADP	K	201	-	-	2/16/32/32	0/3/3/3
2	ADP	S	201	-	-	2/16/32/32	0/3/3/3
2	ADP	X	201	3	-	1/16/32/32	0/3/3/3
2	ADP	b	201	3	-	1/16/32/32	0/3/3/3
2	ADP	i	201	-	-	8/16/32/32	0/3/3/3
2	ADP	I	201	3	-	4/16/32/32	0/3/3/3
2	ADP	D	201	3	-	3/16/32/32	0/3/3/3
2	ADP	B	201	3	-	0/16/32/32	0/3/3/3
2	ADP	T	201	-	-	6/16/32/32	0/3/3/3
2	ADP	c	201	3	-	2/16/32/32	0/3/3/3
2	ADP	F	201	3	-	3/16/32/32	0/3/3/3
2	ADP	W	201	3	-	2/16/32/32	0/3/3/3
2	ADP	d	201	3	-	0/16/32/32	0/3/3/3
2	ADP	j	201	-	-	5/16/32/32	0/3/3/3
2	ADP	Z	201	3	-	0/16/32/32	0/3/3/3
2	ADP	A	201	-	-	0/16/32/32	0/3/3/3
2	ADP	E	201	3	-	4/16/32/32	0/3/3/3
2	ADP	J	201	-	-	0/16/32/32	0/3/3/3
2	ADP	g	201	-	-	4/16/32/32	0/3/3/3
2	ADP	H	201	-	-	4/16/32/32	0/3/3/3
2	ADP	e	201	-	-	5/16/32/32	0/3/3/3
2	ADP	U	201	-	-	4/16/32/32	0/3/3/3
2	ADP	V	201	-	-	0/16/32/32	0/3/3/3
2	ADP	P	201	3	-	0/16/32/32	0/3/3/3
2	ADP	a	201	-	-	1/16/32/32	0/3/3/3

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	201	ADP	C5-C4	4.79	1.47	1.39
2	L	201	ADP	C5-C4	4.78	1.47	1.39
2	N	201	ADP	C5-C4	4.76	1.47	1.39
2	j	201	ADP	C5-C4	4.75	1.47	1.39
2	Z	201	ADP	C5-C4	4.74	1.47	1.39
2	I	201	ADP	C5-C4	4.72	1.47	1.39
2	K	201	ADP	C5-C4	4.72	1.47	1.39
2	U	201	ADP	C5-C4	4.71	1.47	1.39
2	J	201	ADP	C5-C4	4.71	1.47	1.39
2	A	201	ADP	C5-C4	4.70	1.47	1.39
2	a	201	ADP	C5-C4	4.69	1.47	1.39
2	h	201	ADP	C5-C4	4.69	1.47	1.39
2	T	201	ADP	C5-C4	4.66	1.47	1.39
2	G	201	ADP	C5-C4	4.66	1.47	1.39
2	Q	201	ADP	C5-C4	4.64	1.47	1.39
2	B	201	ADP	C5-C4	4.64	1.47	1.39
2	R	201	ADP	C5-C4	4.64	1.47	1.39
2	O	201	ADP	C5-C4	4.63	1.47	1.39
2	H	201	ADP	C5-C4	4.63	1.47	1.39
2	M	201	ADP	C5-C4	4.62	1.47	1.39
2	P	201	ADP	C5-C4	4.61	1.47	1.39
2	c	201	ADP	C5-C4	4.57	1.47	1.39
2	S	201	ADP	C5-C4	4.57	1.47	1.39
2	D	201	ADP	C5-C4	4.57	1.47	1.39
2	C	201	ADP	C5-C4	4.56	1.47	1.39
2	e	201	ADP	C5-C4	4.56	1.47	1.39
2	W	201	ADP	C5-C4	4.55	1.47	1.39
2	i	201	ADP	C5-C4	4.54	1.47	1.39
2	g	201	ADP	C5-C4	4.54	1.47	1.39
2	f	201	ADP	C5-C4	4.54	1.47	1.39
2	V	201	ADP	C5-C4	4.51	1.47	1.39
2	b	201	ADP	C5-C4	4.50	1.47	1.39
2	E	201	ADP	C5-C4	4.49	1.47	1.39
2	d	201	ADP	C5-C4	4.48	1.47	1.39
2	F	201	ADP	C5-C4	4.48	1.47	1.39
2	X	201	ADP	C5-C4	4.39	1.46	1.39
2	K	201	ADP	PA-O3A	2.88	1.62	1.59
2	h	201	ADP	C5-C6	2.79	1.48	1.41
2	a	201	ADP	C5-C6	2.76	1.48	1.41
2	A	201	ADP	C5-C6	2.76	1.48	1.41
2	j	201	ADP	C5-C6	2.74	1.48	1.41
2	N	201	ADP	C5-C6	2.74	1.48	1.41
2	O	201	ADP	C5-C6	2.74	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	201	ADP	C5-C6	2.73	1.48	1.41
2	K	201	ADP	C5-C6	2.73	1.48	1.41
2	R	201	ADP	C5-C6	2.73	1.48	1.41
2	J	201	ADP	C5-C6	2.72	1.48	1.41
2	C	201	ADP	C5-C6	2.71	1.48	1.41
2	L	201	ADP	C5-C6	2.71	1.48	1.41
2	B	201	ADP	C5-C6	2.70	1.48	1.41
2	Z	201	ADP	C5-C6	2.70	1.48	1.41
2	g	201	ADP	C5-C6	2.69	1.48	1.41
2	i	201	ADP	C5-C6	2.68	1.48	1.41
2	Q	201	ADP	C5-C6	2.67	1.48	1.41
2	M	201	ADP	C5-C6	2.66	1.48	1.41
2	X	201	ADP	C5-C6	2.65	1.48	1.41
2	H	201	ADP	C5-C6	2.65	1.48	1.41
2	d	201	ADP	C5-C6	2.64	1.48	1.41
2	P	201	ADP	C5-C6	2.64	1.48	1.41
2	U	201	ADP	C5-C6	2.63	1.48	1.41
2	c	201	ADP	C5-C6	2.63	1.48	1.41
2	f	201	ADP	C5-C6	2.61	1.48	1.41
2	D	201	ADP	C5-C6	2.61	1.48	1.41
2	G	201	ADP	C5-C6	2.60	1.48	1.41
2	V	201	ADP	C5-C6	2.59	1.48	1.41
2	W	201	ADP	C5-C6	2.59	1.48	1.41
2	b	201	ADP	C5-C6	2.58	1.48	1.41
2	T	201	ADP	C5-C6	2.58	1.48	1.41
2	e	201	ADP	C5-C6	2.57	1.48	1.41
2	I	201	ADP	C5-C6	2.54	1.48	1.41
2	S	201	ADP	C5-C6	2.53	1.48	1.41
2	R	201	ADP	PA-O3A	2.53	1.62	1.59
2	V	201	ADP	PA-O3A	2.52	1.62	1.59
2	F	201	ADP	C5-C6	2.50	1.47	1.41
2	E	201	ADP	C5-C6	2.49	1.47	1.41
2	I	201	ADP	C8-N7	2.48	1.36	1.31
2	G	201	ADP	C8-N7	2.48	1.36	1.31
2	b	201	ADP	C8-N7	2.47	1.36	1.31
2	W	201	ADP	C8-N7	2.46	1.36	1.31
2	J	201	ADP	PA-O3A	2.45	1.62	1.59
2	J	201	ADP	C8-N7	2.45	1.36	1.31
2	Q	201	ADP	PA-O3A	2.44	1.62	1.59
2	c	201	ADP	C8-N7	2.43	1.36	1.31
2	L	201	ADP	C8-N7	2.42	1.36	1.31
2	S	201	ADP	C8-N7	2.41	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	ADP	C8-N7	2.40	1.36	1.31
2	e	201	ADP	C8-N7	2.39	1.36	1.31
2	P	201	ADP	PA-O3A	2.39	1.62	1.59
2	g	201	ADP	PA-O3A	2.39	1.62	1.59
2	N	201	ADP	C8-N7	2.39	1.36	1.31
2	B	201	ADP	C8-N7	2.37	1.36	1.31
2	A	201	ADP	C8-N7	2.37	1.36	1.31
2	U	201	ADP	C8-N7	2.36	1.36	1.31
2	a	201	ADP	C8-N7	2.36	1.36	1.31
2	d	201	ADP	C8-N7	2.36	1.36	1.31
2	e	201	ADP	C5-N7	-2.35	1.34	1.39
2	R	201	ADP	C8-N7	2.35	1.36	1.31
2	f	201	ADP	C8-N7	2.35	1.36	1.31
2	Q	201	ADP	C8-N7	2.35	1.36	1.31
2	Z	201	ADP	C8-N7	2.34	1.36	1.31
2	E	201	ADP	C8-N7	2.34	1.36	1.31
2	T	201	ADP	C8-N7	2.33	1.36	1.31
2	P	201	ADP	C8-N7	2.33	1.36	1.31
2	h	201	ADP	C8-N7	2.32	1.36	1.31
2	F	201	ADP	C8-N7	2.32	1.36	1.31
2	C	201	ADP	PA-O3A	2.32	1.62	1.59
2	D	201	ADP	C8-N7	2.32	1.36	1.31
2	S	201	ADP	C5-N7	-2.32	1.34	1.39
2	D	201	ADP	PA-O3A	2.32	1.62	1.59
2	O	201	ADP	PA-O3A	2.31	1.62	1.59
2	P	201	ADP	C5-N7	-2.31	1.34	1.39
2	L	201	ADP	PA-O3A	2.31	1.62	1.59
2	K	201	ADP	C8-N7	2.30	1.36	1.31
2	f	201	ADP	PA-O3A	2.30	1.62	1.59
2	j	201	ADP	C5-N7	-2.30	1.34	1.39
2	O	201	ADP	C8-N7	2.30	1.36	1.31
2	j	201	ADP	C8-N7	2.29	1.36	1.31
2	M	201	ADP	C8-N7	2.29	1.36	1.31
2	i	201	ADP	C8-N7	2.28	1.36	1.31
2	d	201	ADP	C5-N7	-2.28	1.34	1.39
2	Y	201	ADP	C8-N7	2.27	1.36	1.31
2	X	201	ADP	C8-N7	2.26	1.36	1.31
2	C	201	ADP	C8-N7	2.25	1.36	1.31
2	Z	201	ADP	C5-N7	-2.25	1.35	1.39
2	i	201	ADP	C5-N7	-2.25	1.35	1.39
2	g	201	ADP	C8-N7	2.24	1.36	1.31
2	I	201	ADP	C5-N7	-2.24	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	201	ADP	C8-N7	2.24	1.36	1.31
2	M	201	ADP	C5-N7	-2.24	1.35	1.39
2	i	201	ADP	PA-O3A	2.24	1.61	1.59
2	f	201	ADP	C5-N7	-2.23	1.35	1.39
2	g	201	ADP	C5-N7	-2.23	1.35	1.39
2	B	201	ADP	PA-O3A	2.22	1.61	1.59
2	W	201	ADP	C5-N7	-2.22	1.35	1.39
2	b	201	ADP	PA-O3A	2.22	1.61	1.59
2	O	201	ADP	C5-N7	-2.22	1.35	1.39
2	b	201	ADP	C5-N7	-2.21	1.35	1.39
2	E	201	ADP	C5-N7	-2.20	1.35	1.39
2	D	201	ADP	C5-N7	-2.20	1.35	1.39
2	N	201	ADP	PA-O3A	2.20	1.61	1.59
2	H	201	ADP	PA-O3A	2.20	1.61	1.59
2	Z	201	ADP	PA-O3A	2.19	1.61	1.59
2	h	201	ADP	C5-N7	-2.19	1.35	1.39
2	Q	201	ADP	C5-N7	-2.18	1.35	1.39
2	C	201	ADP	C5-N7	-2.18	1.35	1.39
2	N	201	ADP	C5-N7	-2.18	1.35	1.39
2	E	201	ADP	PA-O3A	2.17	1.61	1.59
2	R	201	ADP	C5-N7	-2.16	1.35	1.39
2	G	201	ADP	C5-N7	-2.16	1.35	1.39
2	L	201	ADP	C5-N7	-2.15	1.35	1.39
2	a	201	ADP	C5-N7	-2.15	1.35	1.39
2	S	201	ADP	PA-O3A	2.15	1.61	1.59
2	j	201	ADP	PA-O3A	2.15	1.61	1.59
2	F	201	ADP	PA-O3A	2.14	1.61	1.59
2	Y	201	ADP	C5-N7	-2.14	1.35	1.39
2	K	201	ADP	C5-N7	-2.14	1.35	1.39
2	J	201	ADP	C5-N7	-2.14	1.35	1.39
2	B	201	ADP	C5-N7	-2.14	1.35	1.39
2	A	201	ADP	PA-O3A	2.13	1.61	1.59
2	V	201	ADP	C5-N7	-2.12	1.35	1.39
2	A	201	ADP	C5-N7	-2.10	1.35	1.39
2	c	201	ADP	C5-N7	-2.09	1.35	1.39
2	X	201	ADP	C5-N7	-2.09	1.35	1.39
2	F	201	ADP	C5-N7	-2.08	1.35	1.39
2	H	201	ADP	C5-N7	-2.07	1.35	1.39
2	T	201	ADP	C5-N7	-2.06	1.35	1.39
2	X	201	ADP	PA-O3A	2.01	1.61	1.59
2	E	201	ADP	C4-N9	-2.00	1.33	1.37

All (373) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	201	ADP	C5-C4-N3	-5.91	118.59	126.72
2	H	201	ADP	C5-C4-N3	-5.89	118.61	126.72
2	d	201	ADP	C5-C4-N3	-5.82	118.70	126.72
2	I	201	ADP	C5-C4-N3	-5.82	118.70	126.72
2	N	201	ADP	C5-C4-N3	-5.82	118.70	126.72
2	O	201	ADP	C5-C4-N3	-5.81	118.71	126.72
2	j	201	ADP	C5-C4-N3	-5.80	118.73	126.72
2	W	201	ADP	C5-C4-N3	-5.78	118.75	126.72
2	g	201	ADP	C5-C4-N3	-5.78	118.75	126.72
2	b	201	ADP	C5-C4-N3	-5.77	118.78	126.72
2	Q	201	ADP	C5-C4-N3	-5.76	118.79	126.72
2	Y	201	ADP	C5-C4-N3	-5.74	118.81	126.72
2	T	201	ADP	C5-C4-N3	-5.74	118.82	126.72
2	L	201	ADP	C5-C4-N3	-5.71	118.86	126.72
2	e	201	ADP	C5-C4-N3	-5.71	118.86	126.72
2	P	201	ADP	C5-C4-N3	-5.70	118.87	126.72
2	C	201	ADP	C5-C4-N3	-5.69	118.88	126.72
2	R	201	ADP	C5-C4-N3	-5.69	118.88	126.72
2	G	201	ADP	C5-C4-N3	-5.69	118.89	126.72
2	Z	201	ADP	C5-C4-N3	-5.69	118.89	126.72
2	a	201	ADP	C5-C4-N3	-5.67	118.91	126.72
2	D	201	ADP	C5-C4-N3	-5.66	118.92	126.72
2	B	201	ADP	C5-C4-N3	-5.64	118.94	126.72
2	f	201	ADP	C5-C4-N3	-5.64	118.94	126.72
2	A	201	ADP	C5-C4-N3	-5.64	118.96	126.72
2	h	201	ADP	C5-C4-N3	-5.57	119.05	126.72
2	M	201	ADP	C5-C4-N3	-5.57	119.05	126.72
2	E	201	ADP	C5-C4-N3	-5.56	119.07	126.72
2	J	201	ADP	C5-C4-N3	-5.55	119.07	126.72
2	c	201	ADP	C5-C4-N3	-5.53	119.10	126.72
2	X	201	ADP	C5-C4-N3	-5.52	119.11	126.72
2	F	201	ADP	C5-C4-N3	-5.51	119.13	126.72
2	S	201	ADP	C5-C4-N3	-5.46	119.20	126.72
2	i	201	ADP	C5-C4-N3	-5.44	119.22	126.72
2	V	201	ADP	C5-C4-N3	-5.32	119.39	126.72
2	U	201	ADP	C5-C4-N3	-5.31	119.41	126.72
2	I	201	ADP	N3-C4-N9	4.97	135.62	127.17
2	j	201	ADP	N3-C4-N9	4.89	135.49	127.17
2	T	201	ADP	N3-C4-N9	4.89	135.49	127.17
2	H	201	ADP	N3-C4-N9	4.89	135.49	127.17
2	K	201	ADP	N3-C4-N9	4.88	135.47	127.17
2	Y	201	ADP	N3-C4-N9	4.87	135.45	127.17
2	W	201	ADP	N3-C4-N9	4.86	135.43	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	201	ADP	N3-C4-N9	4.85	135.41	127.17
2	N	201	ADP	N3-C4-N9	4.83	135.39	127.17
2	g	201	ADP	N3-C4-N9	4.82	135.37	127.17
2	Z	201	ADP	N3-C4-N9	4.81	135.34	127.17
2	E	201	ADP	N3-C4-N9	4.81	135.34	127.17
2	d	201	ADP	N3-C4-N9	4.80	135.34	127.17
2	R	201	ADP	N3-C4-N9	4.80	135.33	127.17
2	B	201	ADP	N3-C4-N9	4.80	135.33	127.17
2	O	201	ADP	N3-C4-N9	4.79	135.32	127.17
2	D	201	ADP	N3-C4-N9	4.79	135.31	127.17
2	e	201	ADP	N3-C4-N9	4.78	135.29	127.17
2	M	201	ADP	N3-C4-N9	4.76	135.27	127.17
2	P	201	ADP	N3-C4-N9	4.76	135.26	127.17
2	L	201	ADP	N3-C4-N9	4.75	135.25	127.17
2	f	201	ADP	N3-C4-N9	4.73	135.21	127.17
2	F	201	ADP	N3-C4-N9	4.72	135.19	127.17
2	b	201	ADP	N3-C4-N9	4.71	135.18	127.17
2	a	201	ADP	N3-C4-N9	4.71	135.18	127.17
2	C	201	ADP	N3-C4-N9	4.71	135.17	127.17
2	G	201	ADP	N3-C4-N9	4.71	135.17	127.17
2	A	201	ADP	N3-C4-N9	4.71	135.17	127.17
2	c	201	ADP	N3-C4-N9	4.66	135.10	127.17
2	S	201	ADP	N3-C4-N9	4.65	135.08	127.17
2	h	201	ADP	N3-C4-N9	4.65	135.07	127.17
2	X	201	ADP	N3-C4-N9	4.62	135.02	127.17
2	J	201	ADP	N3-C4-N9	4.60	135.00	127.17
2	i	201	ADP	N3-C4-N9	4.57	134.93	127.17
2	V	201	ADP	N3-C4-N9	4.56	134.92	127.17
2	U	201	ADP	N3-C4-N9	4.52	134.85	127.17
2	d	201	ADP	C2-N3-C4	3.95	121.48	111.83
2	H	201	ADP	C2-N3-C4	3.94	121.46	111.83
2	O	201	ADP	C2-N3-C4	3.94	121.45	111.83
2	M	201	ADP	N3-C2-N1	-3.94	122.62	128.58
2	i	201	ADP	N3-C2-N1	-3.91	122.66	128.58
2	K	201	ADP	C2-N3-C4	3.90	121.35	111.83
2	b	201	ADP	C2-N3-C4	3.90	121.34	111.83
2	R	201	ADP	C2-N3-C4	3.88	121.32	111.83
2	g	201	ADP	C2-N3-C4	3.88	121.31	111.83
2	G	201	ADP	N3-C2-N1	-3.88	122.71	128.58
2	G	201	ADP	C2-N3-C4	3.87	121.28	111.83
2	I	201	ADP	C2-N3-C4	3.87	121.28	111.83
2	C	201	ADP	C2-N3-C4	3.87	121.27	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	201	ADP	C2-N3-C4	3.86	121.27	111.83
2	D	201	ADP	C2-N3-C4	3.86	121.26	111.83
2	V	201	ADP	N3-C2-N1	-3.85	122.75	128.58
2	M	201	ADP	C2-N3-C4	3.85	121.23	111.83
2	U	201	ADP	N3-C2-N1	-3.85	122.75	128.58
2	X	201	ADP	N3-C2-N1	-3.85	122.76	128.58
2	f	201	ADP	C2-N3-C4	3.85	121.22	111.83
2	L	201	ADP	C2-N3-C4	3.84	121.20	111.83
2	c	201	ADP	C2-N3-C4	3.84	121.20	111.83
2	d	201	ADP	N3-C2-N1	-3.84	122.78	128.58
2	B	201	ADP	C2-N3-C4	3.83	121.19	111.83
2	H	201	ADP	N3-C2-N1	-3.83	122.79	128.58
2	P	201	ADP	C2-N3-C4	3.83	121.18	111.83
2	a	201	ADP	C2-N3-C4	3.83	121.18	111.83
2	i	201	ADP	C2-N3-C4	3.83	121.18	111.83
2	Q	201	ADP	C2-N3-C4	3.83	121.17	111.83
2	S	201	ADP	N3-C2-N1	-3.83	122.79	128.58
2	c	201	ADP	N3-C2-N1	-3.82	122.80	128.58
2	j	201	ADP	C2-N3-C4	3.82	121.16	111.83
2	D	201	ADP	N3-C2-N1	-3.82	122.80	128.58
2	C	201	ADP	N3-C2-N1	-3.81	122.81	128.58
2	O	201	ADP	N3-C2-N1	-3.81	122.82	128.58
2	T	201	ADP	C2-N3-C4	3.81	121.13	111.83
2	X	201	ADP	C2-N3-C4	3.81	121.13	111.83
2	e	201	ADP	C2-N3-C4	3.81	121.13	111.83
2	L	201	ADP	N3-C2-N1	-3.81	122.82	128.58
2	W	201	ADP	C2-N3-C4	3.80	121.10	111.83
2	A	201	ADP	C2-N3-C4	3.80	121.10	111.83
2	R	201	ADP	N3-C2-N1	-3.80	122.84	128.58
2	I	201	ADP	N3-C2-N1	-3.79	122.84	128.58
2	F	201	ADP	N3-C2-N1	-3.79	122.84	128.58
2	E	201	ADP	N3-C2-N1	-3.79	122.85	128.58
2	f	201	ADP	N3-C2-N1	-3.79	122.85	128.58
2	Z	201	ADP	C2-N3-C4	3.78	121.06	111.83
2	b	201	ADP	N3-C2-N1	-3.77	122.87	128.58
2	Y	201	ADP	C2-N3-C4	3.77	121.04	111.83
2	E	201	ADP	C2-N3-C4	3.77	121.04	111.83
2	J	201	ADP	C2-N3-C4	3.77	121.04	111.83
2	h	201	ADP	C2-N3-C4	3.77	121.03	111.83
2	e	201	ADP	N3-C2-N1	-3.76	122.88	128.58
2	S	201	ADP	C2-N3-C4	3.76	121.01	111.83
2	F	201	ADP	C2-N3-C4	3.75	120.99	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	201	ADP	N3-C2-N1	-3.75	122.91	128.58
2	P	201	ADP	N3-C2-N1	-3.75	122.91	128.58
2	B	201	ADP	N3-C2-N1	-3.74	122.92	128.58
2	a	201	ADP	N3-C2-N1	-3.74	122.93	128.58
2	J	201	ADP	N3-C2-N1	-3.73	122.93	128.58
2	A	201	ADP	N3-C2-N1	-3.72	122.95	128.58
2	V	201	ADP	C2-N3-C4	3.71	120.90	111.83
2	Z	201	ADP	N3-C2-N1	-3.70	122.99	128.58
2	Q	201	ADP	N3-C2-N1	-3.69	122.99	128.58
2	K	201	ADP	N3-C2-N1	-3.68	123.02	128.58
2	g	201	ADP	N3-C2-N1	-3.68	123.02	128.58
2	h	201	ADP	N3-C2-N1	-3.68	123.02	128.58
2	N	201	ADP	N3-C2-N1	-3.67	123.02	128.58
2	W	201	ADP	N3-C2-N1	-3.67	123.03	128.58
2	U	201	ADP	C2-N3-C4	3.66	120.78	111.83
2	Y	201	ADP	N3-C2-N1	-3.65	123.06	128.58
2	j	201	ADP	N3-C2-N1	-3.64	123.08	128.58
2	X	201	ADP	C4-N9-C8	3.59	109.50	105.74
2	V	201	ADP	C4-N9-C8	3.57	109.48	105.74
2	U	201	ADP	C4-N9-C8	3.54	109.46	105.74
2	X	201	ADP	C4-C5-N7	-3.51	106.57	110.58
2	C	201	ADP	C4-C5-N7	-3.50	106.58	110.58
2	K	201	ADP	C4-C5-N7	-3.49	106.59	110.58
2	A	201	ADP	C4-C5-N7	-3.49	106.59	110.58
2	F	201	ADP	C4-N9-C8	3.46	109.37	105.74
2	E	201	ADP	C4-N9-C8	3.45	109.36	105.74
2	c	201	ADP	C4-N9-C8	3.45	109.36	105.74
2	a	201	ADP	C4-C5-N7	-3.45	106.64	110.58
2	D	201	ADP	C4-N9-C8	3.41	109.32	105.74
2	Q	201	ADP	C4-C5-N7	-3.41	106.69	110.58
2	g	201	ADP	C4-C5-N7	-3.39	106.70	110.58
2	W	201	ADP	C4-N9-C8	3.39	109.29	105.74
2	Q	201	ADP	C4-N9-C8	3.38	109.29	105.74
2	A	201	ADP	C4-N9-C8	3.38	109.28	105.74
2	N	201	ADP	C4-C5-N7	-3.37	106.73	110.58
2	M	201	ADP	C4-N9-C8	3.36	109.27	105.74
2	h	201	ADP	C4-C5-N7	-3.36	106.75	110.58
2	T	201	ADP	C4-N9-C8	3.34	109.24	105.74
2	R	201	ADP	C4-C5-N7	-3.34	106.77	110.58
2	L	201	ADP	C4-C5-N7	-3.33	106.77	110.58
2	O	201	ADP	C4-C5-N7	-3.33	106.78	110.58
2	D	201	ADP	C4-C5-N7	-3.33	106.78	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	201	ADP	C4-C5-N7	-3.32	106.79	110.58
2	b	201	ADP	C4-C5-N7	-3.32	106.79	110.58
2	d	201	ADP	C4-C5-N7	-3.31	106.80	110.58
2	J	201	ADP	C4-C5-N7	-3.31	106.80	110.58
2	i	201	ADP	C4-N9-C8	3.31	109.21	105.74
2	R	201	ADP	C4-N9-C8	3.30	109.20	105.74
2	W	201	ADP	C4-C5-N7	-3.30	106.81	110.58
2	B	201	ADP	C4-N9-C8	3.29	109.20	105.74
2	Z	201	ADP	C4-C5-N7	-3.29	106.82	110.58
2	g	201	ADP	C4-N9-C8	3.29	109.20	105.74
2	U	201	ADP	C4-C5-N7	-3.29	106.82	110.58
2	C	201	ADP	C4-N9-C8	3.29	109.19	105.74
2	h	201	ADP	C4-N9-C8	3.29	109.19	105.74
2	S	201	ADP	C4-N9-C8	3.28	109.18	105.74
2	V	201	ADP	C4-C5-N7	-3.28	106.83	110.58
2	f	201	ADP	C4-N9-C8	3.28	109.18	105.74
2	j	201	ADP	C4-C5-N7	-3.28	106.84	110.58
2	e	201	ADP	C4-N9-C8	3.27	109.17	105.74
2	Y	201	ADP	C4-C5-N7	-3.27	106.84	110.58
2	e	201	ADP	C4-C5-N7	-3.27	106.85	110.58
2	H	201	ADP	C4-C5-N7	-3.26	106.85	110.58
2	Z	201	ADP	C4-N9-C8	3.25	109.15	105.74
2	i	201	ADP	C4-C5-N7	-3.25	106.86	110.58
2	I	201	ADP	C4-N9-C8	3.24	109.14	105.74
2	H	201	ADP	C4-N9-C8	3.24	109.14	105.74
2	J	201	ADP	C4-N9-C8	3.24	109.14	105.74
2	Y	201	ADP	C4-N9-C8	3.24	109.14	105.74
2	B	201	ADP	C4-C5-N7	-3.24	106.88	110.58
2	f	201	ADP	C4-C5-N7	-3.23	106.89	110.58
2	a	201	ADP	C4-N9-C8	3.21	109.11	105.74
2	c	201	ADP	C4-C5-N7	-3.21	106.91	110.58
2	b	201	ADP	C4-N9-C8	3.20	109.10	105.74
2	P	201	ADP	C4-N9-C8	3.20	109.10	105.74
2	L	201	ADP	C4-N9-C8	3.19	109.08	105.74
2	G	201	ADP	C4-C5-N7	-3.17	106.96	110.58
2	M	201	ADP	C4-C5-N7	-3.16	106.97	110.58
2	K	201	ADP	C4-N9-C8	3.16	109.06	105.74
2	T	201	ADP	C4-C5-N7	-3.15	106.98	110.58
2	j	201	ADP	C4-N9-C8	3.15	109.04	105.74
2	d	201	ADP	C4-N9-C8	3.13	109.02	105.74
2	O	201	ADP	C4-N9-C8	3.13	109.02	105.74
2	F	201	ADP	C4-C5-N7	-3.10	107.03	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	201	ADP	C4-N9-C8	3.10	108.99	105.74
2	G	201	ADP	C4-N9-C8	3.08	108.98	105.74
2	I	201	ADP	C4-C5-N7	-3.04	107.11	110.58
2	S	201	ADP	C4-C5-N7	-2.99	107.16	110.58
2	E	201	ADP	C4-C5-N7	-2.90	107.27	110.58
2	X	201	ADP	C5-N7-C8	2.85	107.93	103.45
2	Q	201	ADP	C5-N7-C8	2.81	107.86	103.45
2	C	201	ADP	C5-N7-C8	2.78	107.83	103.45
2	A	201	ADP	C5-N7-C8	2.77	107.80	103.45
2	R	201	ADP	C5-N7-C8	2.75	107.77	103.45
2	K	201	ADP	C5-N7-C8	2.74	107.76	103.45
2	a	201	ADP	C5-N7-C8	2.73	107.74	103.45
2	D	201	ADP	C5-N7-C8	2.72	107.72	103.45
2	g	201	ADP	C5-N7-C8	2.71	107.71	103.45
2	W	201	ADP	C5-N7-C8	2.71	107.71	103.45
2	N	201	ADP	C5-N7-C8	2.69	107.68	103.45
2	V	201	ADP	C5-N7-C8	2.69	107.68	103.45
2	e	201	ADP	C5-N7-C8	2.69	107.67	103.45
2	X	201	ADP	N9-C8-N7	-2.69	110.13	113.94
2	h	201	ADP	C5-N7-C8	2.67	107.65	103.45
2	B	201	ADP	C5-N7-C8	2.67	107.65	103.45
2	Z	201	ADP	C5-N7-C8	2.67	107.65	103.45
2	d	201	ADP	C5-N7-C8	2.67	107.64	103.45
2	P	201	ADP	C5-N7-C8	2.67	107.64	103.45
2	j	201	ADP	C5-N7-C8	2.64	107.60	103.45
2	L	201	ADP	C5-N7-C8	2.63	107.58	103.45
2	J	201	ADP	C5-N7-C8	2.63	107.58	103.45
2	f	201	ADP	C5-N7-C8	2.62	107.57	103.45
2	Y	201	ADP	C5-N7-C8	2.61	107.56	103.45
2	i	201	ADP	C5-N7-C8	2.60	107.54	103.45
2	b	201	ADP	C5-N7-C8	2.60	107.53	103.45
2	O	201	ADP	C5-N7-C8	2.59	107.53	103.45
2	U	201	ADP	C5-N7-C8	2.59	107.52	103.45
2	H	201	ADP	C5-N7-C8	2.57	107.50	103.45
2	M	201	ADP	C5-N7-C8	2.57	107.49	103.45
2	c	201	ADP	C5-N7-C8	2.57	107.49	103.45
2	V	201	ADP	N9-C8-N7	-2.55	110.31	113.94
2	I	201	ADP	C5-N7-C8	2.54	107.45	103.45
2	T	201	ADP	C5-N7-C8	2.53	107.42	103.45
2	F	201	ADP	C5-N7-C8	2.52	107.42	103.45
2	W	201	ADP	N9-C8-N7	-2.52	110.36	113.94
2	Q	201	ADP	N9-C8-N7	-2.52	110.36	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	ADP	N9-C8-N7	-2.49	110.40	113.94
2	G	201	ADP	C5-N7-C8	2.48	107.35	103.45
2	c	201	ADP	N9-C8-N7	-2.47	110.44	113.94
2	A	201	ADP	N9-C8-N7	-2.46	110.45	113.94
2	S	201	ADP	C5-N7-C8	2.46	107.31	103.45
2	C	201	ADP	N9-C8-N7	-2.45	110.45	113.94
2	e	201	ADP	N9-C8-N7	-2.45	110.46	113.94
2	U	201	ADP	N9-C8-N7	-2.45	110.47	113.94
2	R	201	ADP	N9-C8-N7	-2.44	110.47	113.94
2	j	201	ADP	C3'-C2'-C1'	2.44	106.07	101.46
2	E	201	ADP	C5-N7-C8	2.42	107.25	103.45
2	F	201	ADP	N9-C8-N7	-2.42	110.50	113.94
2	f	201	ADP	N9-C8-N7	-2.41	110.51	113.94
2	g	201	ADP	N9-C8-N7	-2.41	110.52	113.94
2	E	201	ADP	N9-C8-N7	-2.41	110.52	113.94
2	h	201	ADP	N9-C8-N7	-2.40	110.53	113.94
2	b	201	ADP	N9-C8-N7	-2.40	110.53	113.94
2	S	201	ADP	C3'-C2'-C1'	2.40	106.00	101.46
2	U	201	ADP	C2-N1-C6	2.39	122.66	118.73
2	i	201	ADP	N9-C8-N7	-2.39	110.54	113.94
2	B	201	ADP	N9-C8-N7	-2.39	110.55	113.94
2	J	201	ADP	N9-C8-N7	-2.39	110.55	113.94
2	X	201	ADP	C6-C5-N7	2.38	136.68	132.09
2	B	201	ADP	C3'-C2'-C1'	2.37	105.95	101.46
2	d	201	ADP	N9-C8-N7	-2.37	110.57	113.94
2	a	201	ADP	N9-C8-N7	-2.36	110.59	113.94
2	M	201	ADP	N9-C8-N7	-2.36	110.59	113.94
2	P	201	ADP	N9-C8-N7	-2.34	110.61	113.94
2	Z	201	ADP	N9-C8-N7	-2.34	110.61	113.94
2	H	201	ADP	N9-C8-N7	-2.34	110.61	113.94
2	I	201	ADP	N9-C8-N7	-2.33	110.63	113.94
2	S	201	ADP	N9-C8-N7	-2.33	110.63	113.94
2	V	201	ADP	C2-N1-C6	2.33	122.55	118.73
2	A	201	ADP	C6-C5-N7	2.32	136.57	132.09
2	K	201	ADP	N9-C8-N7	-2.32	110.65	113.94
2	T	201	ADP	N9-C8-N7	-2.31	110.66	113.94
2	L	201	ADP	N9-C8-N7	-2.31	110.67	113.94
2	I	201	ADP	C3'-C2'-C1'	2.29	105.80	101.46
2	V	201	ADP	C6-C5-N7	2.29	136.51	132.09
2	N	201	ADP	N9-C8-N7	-2.29	110.69	113.94
2	O	201	ADP	N9-C8-N7	-2.28	110.71	113.94
2	Q	201	ADP	C3'-C2'-C1'	2.27	105.76	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	ADP	C6-C5-N7	2.26	136.46	132.09
2	Y	201	ADP	N9-C8-N7	-2.26	110.72	113.94
2	c	201	ADP	C6-C5-N7	2.26	136.45	132.09
2	i	201	ADP	C2-N1-C6	2.26	122.44	118.73
2	i	201	ADP	C6-C5-N7	2.26	136.44	132.09
2	U	201	ADP	C6-C5-N7	2.26	136.44	132.09
2	D	201	ADP	C3'-C2'-C1'	2.25	105.72	101.46
2	j	201	ADP	N9-C8-N7	-2.25	110.74	113.94
2	L	201	ADP	C2-N1-C6	2.25	122.43	118.73
2	G	201	ADP	N9-C8-N7	-2.23	110.77	113.94
2	M	201	ADP	C2-N1-C6	2.23	122.39	118.73
2	a	201	ADP	C6-C5-N7	2.22	136.37	132.09
2	R	201	ADP	C6-C5-N7	2.22	136.37	132.09
2	J	201	ADP	C6-C5-N7	2.21	136.36	132.09
2	h	201	ADP	C2-N1-C6	2.21	122.37	118.73
2	J	201	ADP	C2-N1-C6	2.21	122.36	118.73
2	X	201	ADP	C2-N1-C6	2.20	122.35	118.73
2	f	201	ADP	C6-C5-N7	2.20	136.33	132.09
2	G	201	ADP	C2-N1-C6	2.19	122.33	118.73
2	S	201	ADP	C2-N1-C6	2.19	122.33	118.73
2	Z	201	ADP	C3'-C2'-C1'	2.19	105.60	101.46
2	B	201	ADP	C6-C5-N7	2.18	136.30	132.09
2	N	201	ADP	C3'-C2'-C1'	2.17	105.57	101.46
2	L	201	ADP	C6-C5-N7	2.17	136.28	132.09
2	D	201	ADP	C6-C5-N7	2.17	136.27	132.09
2	P	201	ADP	C6-C5-N7	2.17	136.27	132.09
2	K	201	ADP	C6-C5-N7	2.16	136.26	132.09
2	b	201	ADP	C6-C5-N7	2.16	136.25	132.09
2	Y	201	ADP	C3'-C2'-C1'	2.15	105.54	101.46
2	d	201	ADP	C6-C5-N7	2.15	136.24	132.09
2	N	201	ADP	C6-C5-N7	2.15	136.23	132.09
2	g	201	ADP	C6-C5-N7	2.15	136.23	132.09
2	e	201	ADP	C2-N1-C6	2.14	122.25	118.73
2	h	201	ADP	C6-C5-N7	2.14	136.22	132.09
2	Q	201	ADP	C6-C5-N7	2.14	136.22	132.09
2	F	201	ADP	C6-C5-N7	2.14	136.21	132.09
2	U	201	ADP	C3'-C2'-C1'	2.14	105.50	101.46
2	A	201	ADP	C2-N1-C6	2.12	122.21	118.73
2	E	201	ADP	C2-N1-C6	2.12	122.21	118.73
2	a	201	ADP	C2-N1-C6	2.12	122.21	118.73
2	b	201	ADP	C3'-C2'-C1'	2.12	105.46	101.46
2	D	201	ADP	C2-N1-C6	2.11	122.20	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	201	ADP	C2-N1-C6	2.11	122.20	118.73
2	Z	201	ADP	C2-N1-C6	2.11	122.20	118.73
2	T	201	ADP	C2-N1-C6	2.11	122.19	118.73
2	C	201	ADP	C3'-C2'-C1'	2.11	105.45	101.46
2	M	201	ADP	C6-C5-N7	2.10	136.15	132.09
2	R	201	ADP	C2-N1-C6	2.10	122.19	118.73
2	L	201	ADP	C3'-C2'-C1'	2.10	105.44	101.46
2	O	201	ADP	C6-C5-N7	2.10	136.14	132.09
2	R	201	ADP	C3'-C2'-C1'	2.10	105.43	101.46
2	W	201	ADP	C2-N1-C6	2.10	122.17	118.73
2	Q	201	ADP	C2-N1-C6	2.09	122.17	118.73
2	a	201	ADP	C3'-C2'-C1'	2.09	105.42	101.46
2	G	201	ADP	C6-C5-N7	2.09	136.12	132.09
2	c	201	ADP	C2-N1-C6	2.09	122.16	118.73
2	H	201	ADP	C2-N1-C6	2.08	122.15	118.73
2	f	201	ADP	C2-N1-C6	2.08	122.15	118.73
2	P	201	ADP	C2-N1-C6	2.08	122.14	118.73
2	P	201	ADP	C3'-C2'-C1'	2.08	105.39	101.46
2	C	201	ADP	C2-N1-C6	2.07	122.13	118.73
2	F	201	ADP	C2-N1-C6	2.07	122.13	118.73
2	Z	201	ADP	C6-C5-N7	2.06	136.06	132.09
2	K	201	ADP	C2-N1-C6	2.05	122.10	118.73
2	e	201	ADP	C6-C5-N7	2.05	136.04	132.09
2	M	201	ADP	C3'-C2'-C1'	2.05	105.34	101.46
2	H	201	ADP	C6-C5-N7	2.05	136.04	132.09
2	E	201	ADP	C3'-C2'-C1'	2.05	105.34	101.46
2	j	201	ADP	C6-C5-N7	2.05	136.04	132.09
2	d	201	ADP	C2-N1-C6	2.04	122.08	118.73
2	N	201	ADP	C2-N1-C6	2.03	122.06	118.73
2	O	201	ADP	C2-N1-C6	2.02	122.05	118.73
2	S	201	ADP	C6-C5-N7	2.02	135.98	132.09
2	j	201	ADP	C2-N1-C6	2.02	122.05	118.73
2	f	201	ADP	C3'-C2'-C1'	2.01	105.27	101.46
2	Y	201	ADP	C6-C5-N7	2.01	135.96	132.09
2	c	201	ADP	C3'-C2'-C1'	2.01	105.26	101.46
2	H	201	ADP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	ADP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	201	ADP	C5'-O5'-PA-O3A
2	D	201	ADP	C5'-O5'-PA-O1A
2	D	201	ADP	C5'-O5'-PA-O3A
2	G	201	ADP	C5'-O5'-PA-O1A
2	H	201	ADP	C5'-O5'-PA-O1A
2	H	201	ADP	C5'-O5'-PA-O3A
2	I	201	ADP	PA-O3A-PB-O3B
2	I	201	ADP	C5'-O5'-PA-O1A
2	I	201	ADP	C5'-O5'-PA-O3A
2	K	201	ADP	PA-O3A-PB-O3B
2	M	201	ADP	C5'-O5'-PA-O1A
2	M	201	ADP	C5'-O5'-PA-O3A
2	O	201	ADP	C5'-O5'-PA-O1A
2	O	201	ADP	C5'-O5'-PA-O2A
2	O	201	ADP	C5'-O5'-PA-O3A
2	T	201	ADP	C5'-O5'-PA-O1A
2	T	201	ADP	C5'-O5'-PA-O3A
2	U	201	ADP	C5'-O5'-PA-O1A
2	U	201	ADP	C5'-O5'-PA-O3A
2	Y	201	ADP	C5'-O5'-PA-O1A
2	Y	201	ADP	C5'-O5'-PA-O3A
2	e	201	ADP	C5'-O5'-PA-O1A
2	e	201	ADP	C5'-O5'-PA-O3A
2	f	201	ADP	C5'-O5'-PA-O1A
2	i	201	ADP	C5'-O5'-PA-O1A
2	i	201	ADP	C5'-O5'-PA-O3A
2	j	201	ADP	C5'-O5'-PA-O1A
2	O	201	ADP	O4'-C4'-C5'-O5'
2	Y	201	ADP	O4'-C4'-C5'-O5'
2	i	201	ADP	O4'-C4'-C5'-O5'
2	O	201	ADP	C3'-C4'-C5'-O5'
2	E	201	ADP	PA-O3A-PB-O1B
2	T	201	ADP	PA-O3A-PB-O1B
2	i	201	ADP	PA-O3A-PB-O1B
2	j	201	ADP	PA-O3A-PB-O1B
2	F	201	ADP	PA-O3A-PB-O3B
2	Q	201	ADP	PA-O3A-PB-O3B
2	E	201	ADP	PB-O3A-PA-O1A
2	F	201	ADP	PB-O3A-PA-O1A
2	W	201	ADP	PB-O3A-PA-O1A
2	e	201	ADP	PB-O3A-PA-O1A
2	j	201	ADP	PB-O3A-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	201	ADP	C5'-O5'-PA-O2A
2	D	201	ADP	C5'-O5'-PA-O2A
2	G	201	ADP	C5'-O5'-PA-O2A
2	G	201	ADP	C5'-O5'-PA-O3A
2	H	201	ADP	C5'-O5'-PA-O2A
2	I	201	ADP	C5'-O5'-PA-O2A
2	M	201	ADP	C5'-O5'-PA-O2A
2	T	201	ADP	C5'-O5'-PA-O2A
2	U	201	ADP	C5'-O5'-PA-O2A
2	Y	201	ADP	C5'-O5'-PA-O2A
2	e	201	ADP	C5'-O5'-PA-O2A
2	i	201	ADP	C5'-O5'-PA-O2A
2	g	201	ADP	PA-O3A-PB-O1B
2	Y	201	ADP	C3'-C4'-C5'-O5'
2	i	201	ADP	C3'-C4'-C5'-O5'
2	C	201	ADP	O4'-C4'-C5'-O5'
2	Q	201	ADP	PB-O3A-PA-O1A
2	X	201	ADP	PB-O3A-PA-O1A
2	c	201	ADP	PB-O3A-PA-O1A
2	f	201	ADP	PA-O3A-PB-O1B
2	C	201	ADP	PA-O3A-PB-O3B
2	E	201	ADP	PA-O3A-PB-O2B
2	E	201	ADP	PA-O3A-PB-O3B
2	H	201	ADP	PA-O3A-PB-O3B
2	S	201	ADP	PA-O3A-PB-O3B
2	T	201	ADP	PA-O3A-PB-O2B
2	T	201	ADP	PA-O3A-PB-O3B
2	U	201	ADP	PA-O3A-PB-O3B
2	f	201	ADP	PA-O3A-PB-O2B
2	g	201	ADP	PA-O3A-PB-O2B
2	g	201	ADP	PA-O3A-PB-O3B
2	i	201	ADP	PA-O3A-PB-O2B
2	i	201	ADP	PA-O3A-PB-O3B
2	j	201	ADP	PA-O3A-PB-O2B
2	j	201	ADP	PA-O3A-PB-O3B
2	F	201	ADP	PB-O3A-PA-O2A
2	L	201	ADP	PB-O3A-PA-O2A
2	Q	201	ADP	PB-O3A-PA-O2A
2	R	201	ADP	PB-O3A-PA-O2A
2	S	201	ADP	PB-O3A-PA-O2A
2	W	201	ADP	PB-O3A-PA-O2A
2	e	201	ADP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

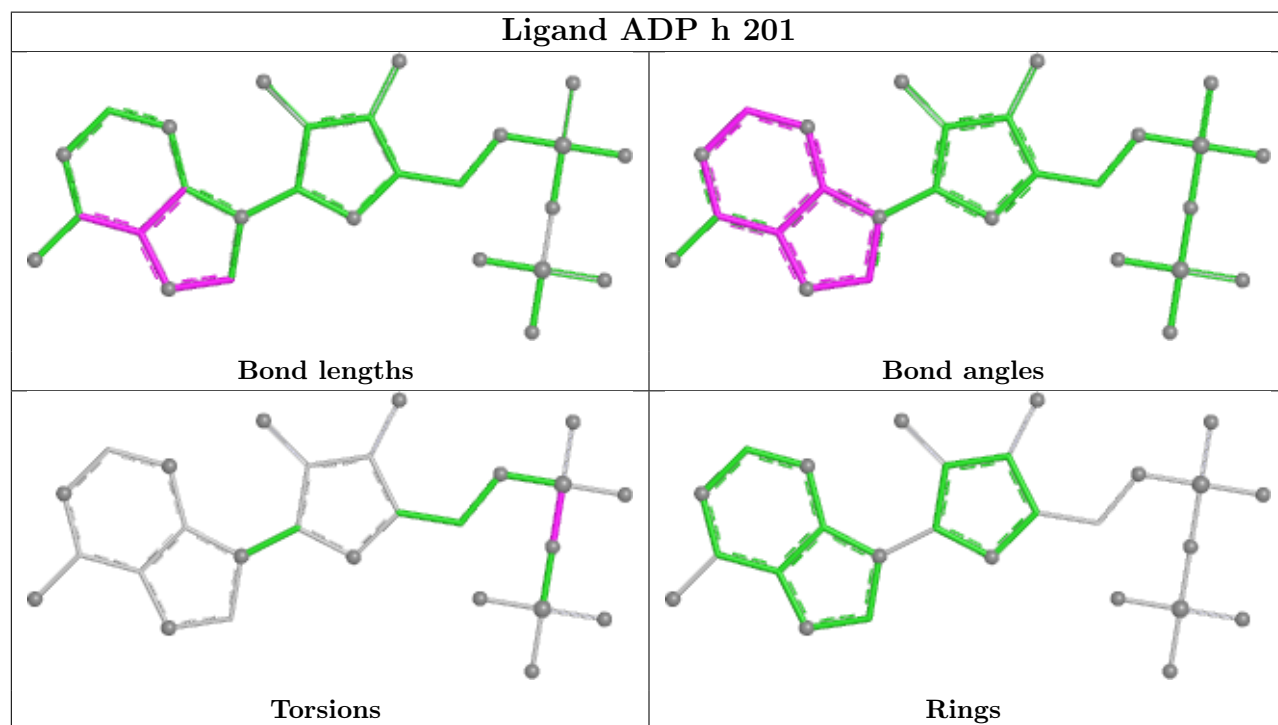
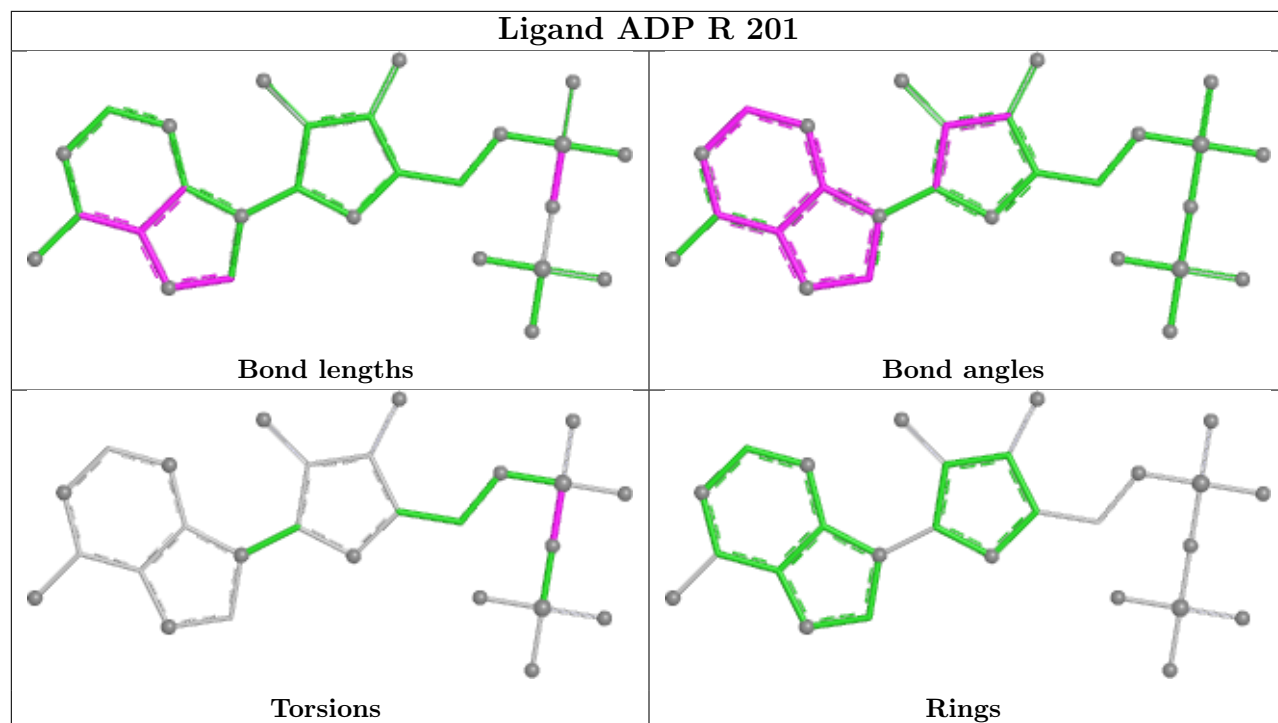
Mol	Chain	Res	Type	Atoms
2	f	201	ADP	PB-O3A-PA-O2A
2	G	201	ADP	PB-O3A-PA-O2A
2	K	201	ADP	PB-O3A-PA-O2A
2	O	201	ADP	PB-O3A-PA-O2A
2	a	201	ADP	PB-O3A-PA-O2A
2	b	201	ADP	PB-O3A-PA-O2A
2	c	201	ADP	PB-O3A-PA-O2A
2	g	201	ADP	PB-O3A-PA-O2A
2	h	201	ADP	PB-O3A-PA-O2A

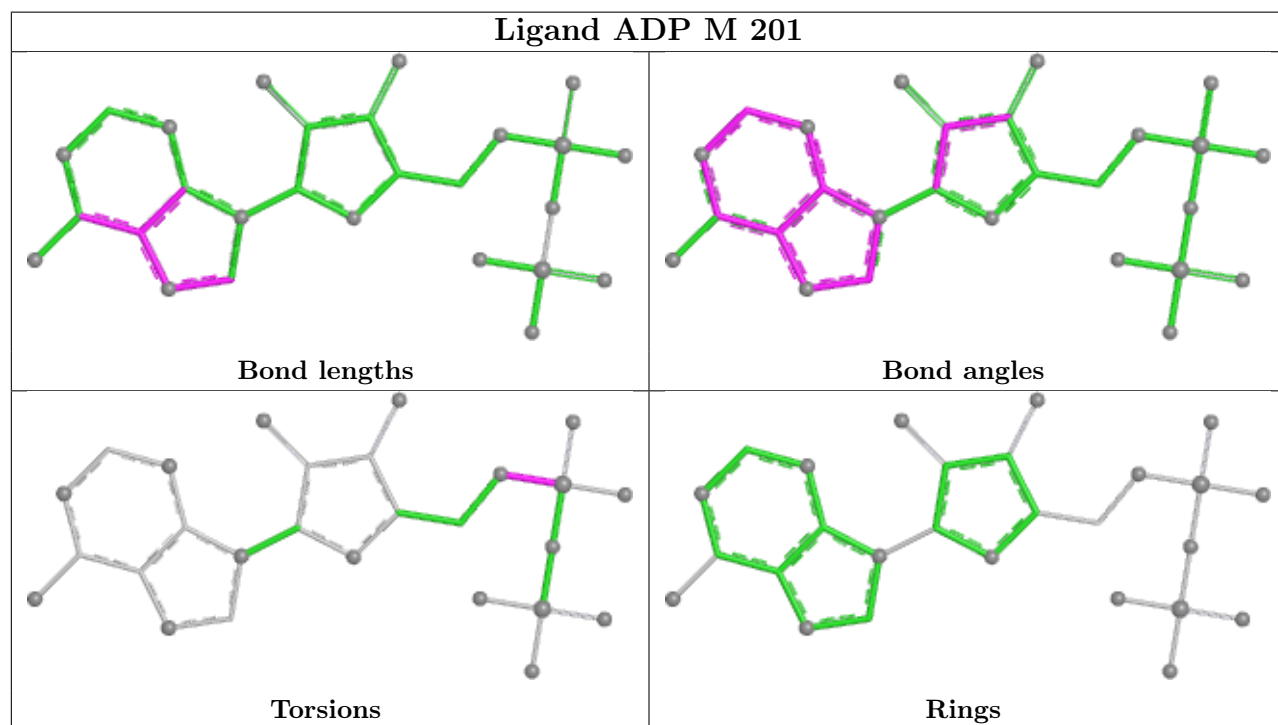
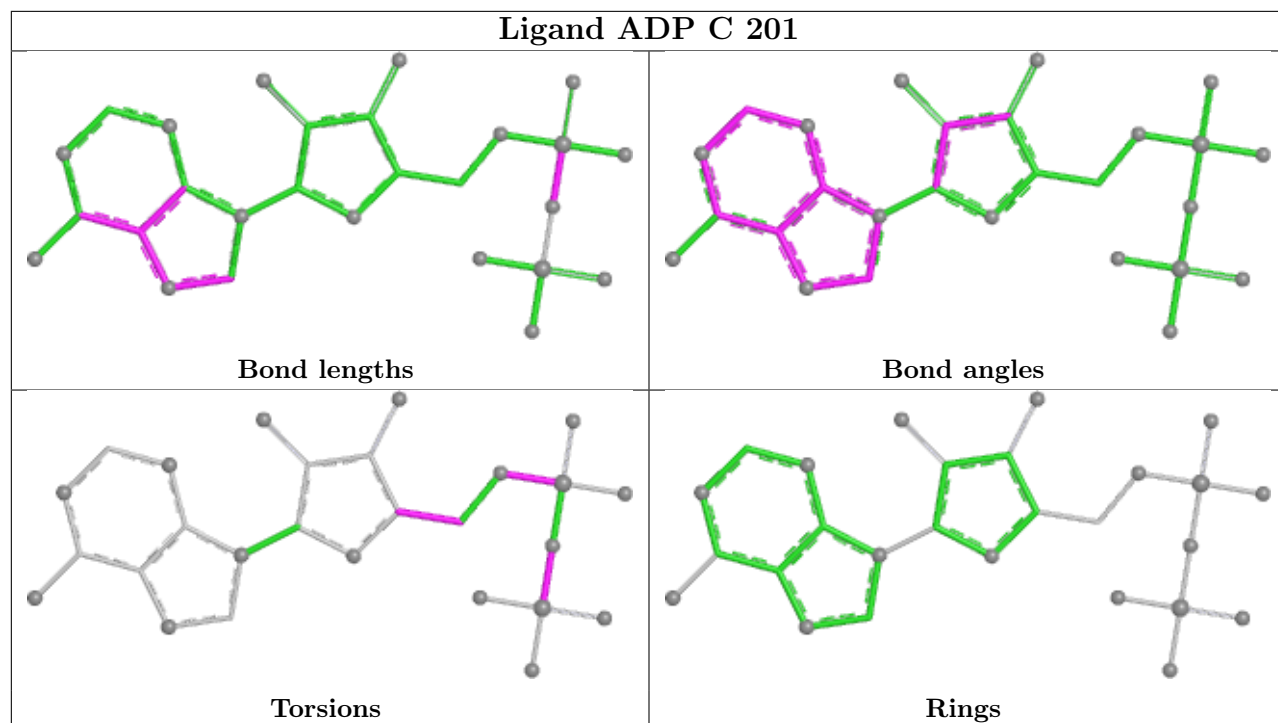
There are no ring outliers.

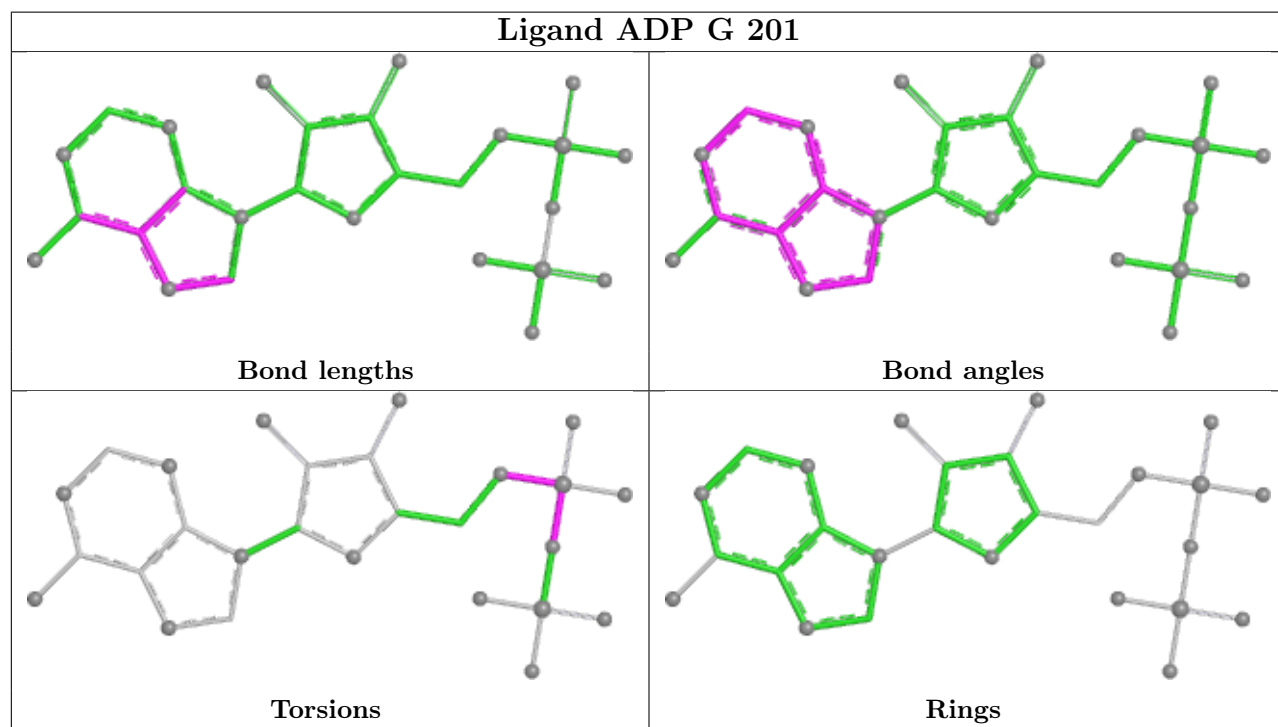
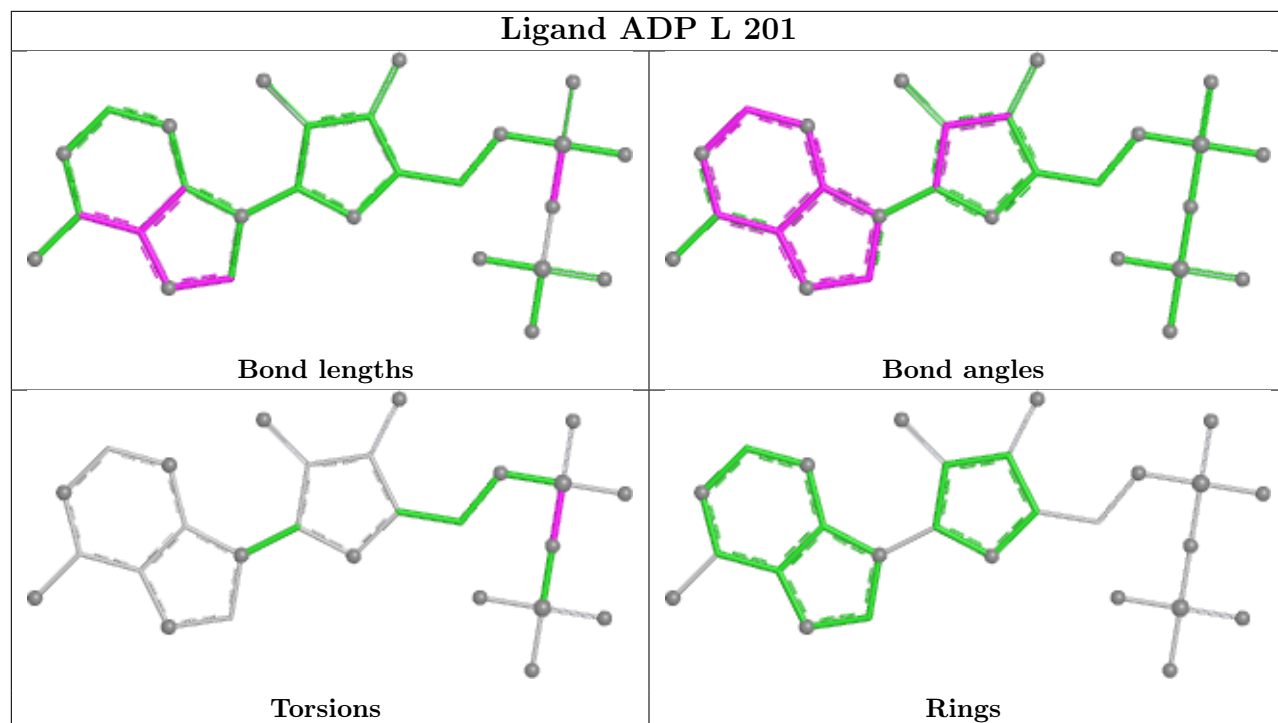
6 monomers are involved in 6 short contacts:

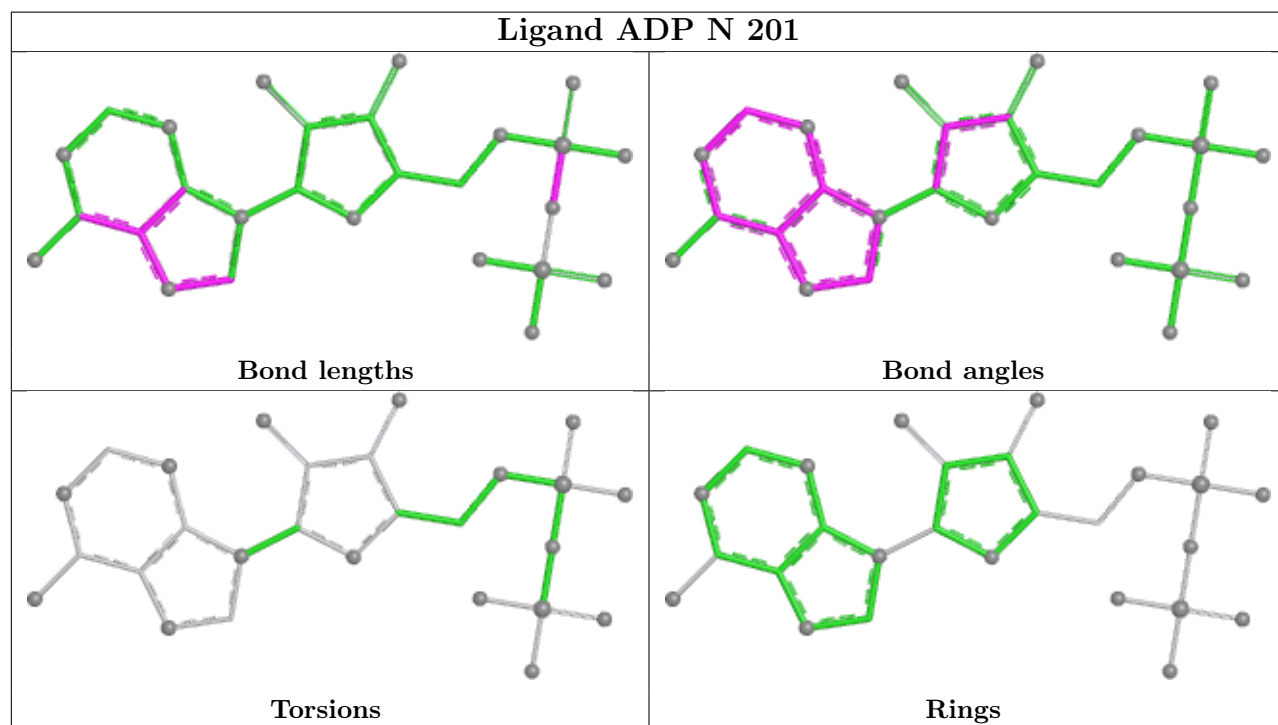
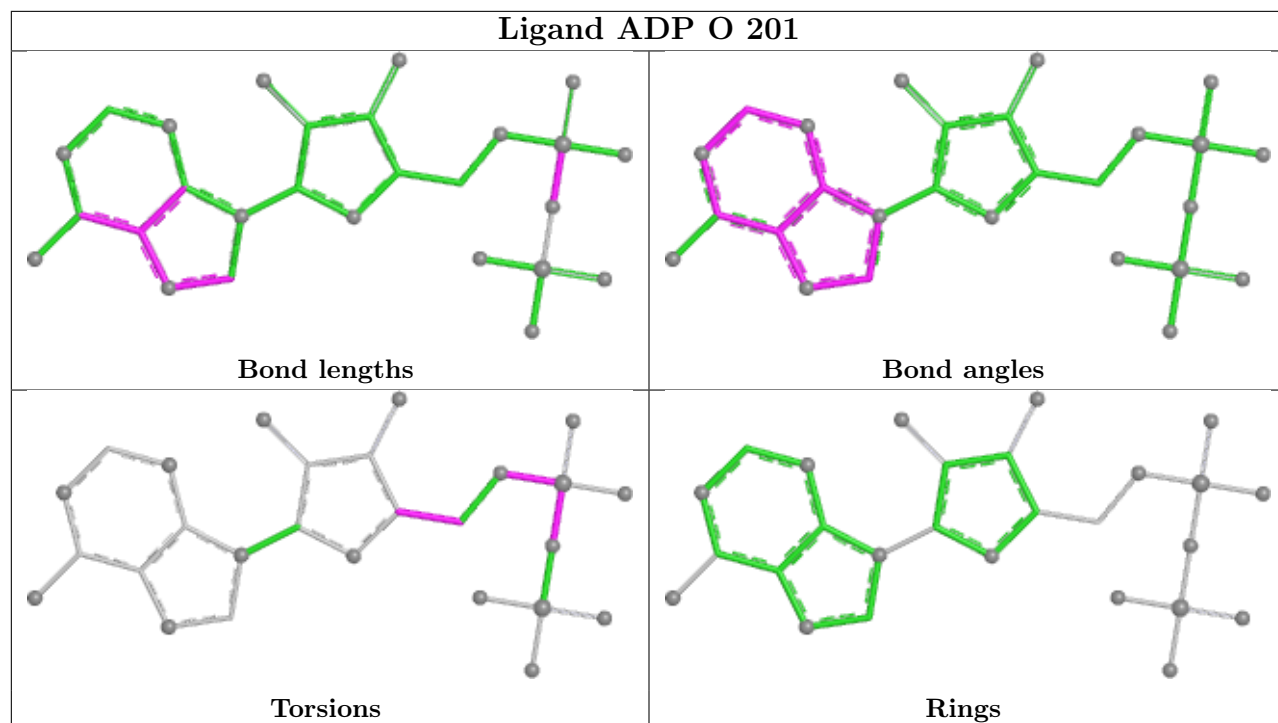
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	f	201	ADP	1	0
2	Q	201	ADP	1	0
2	F	201	ADP	1	0
2	j	201	ADP	1	0
2	E	201	ADP	1	0
2	g	201	ADP	1	0

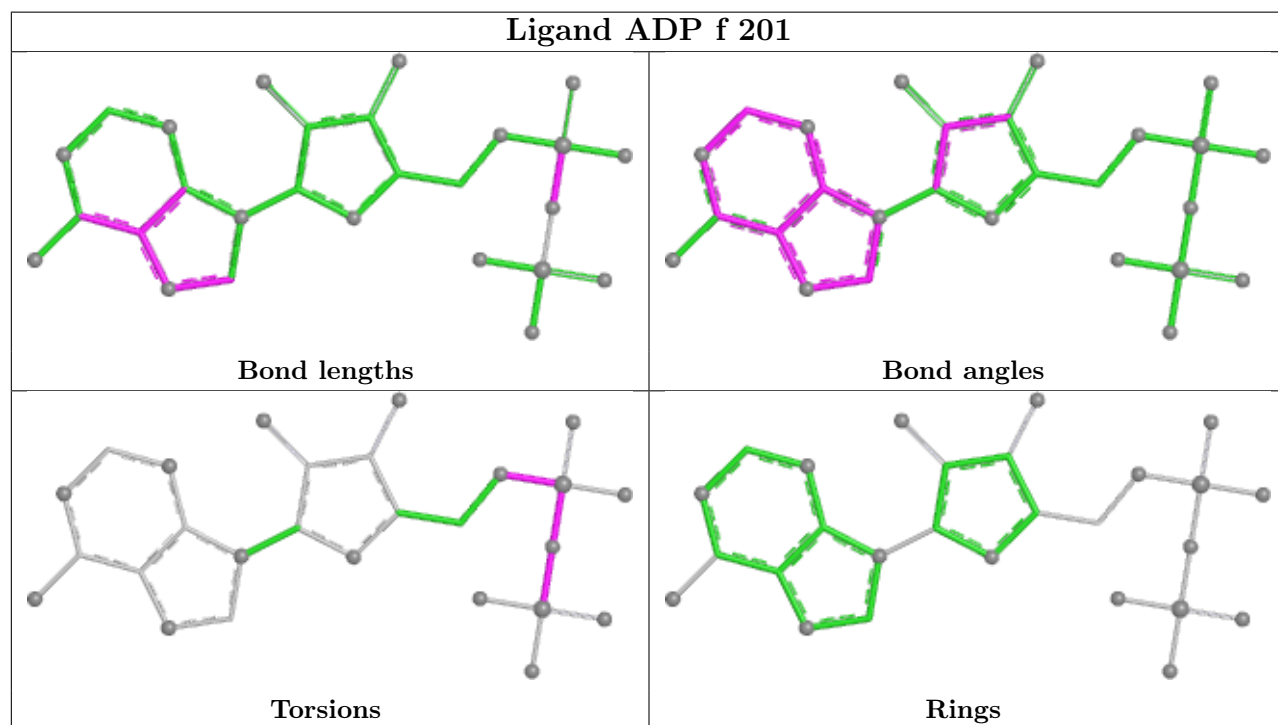
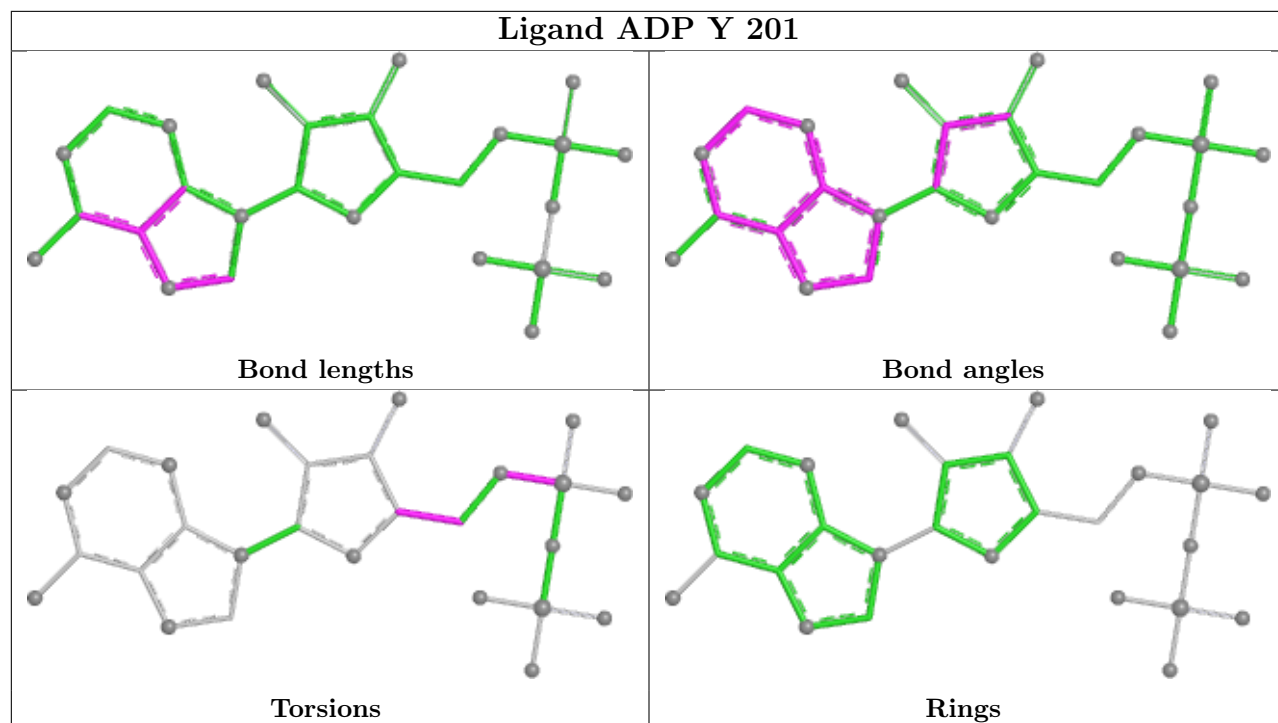
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

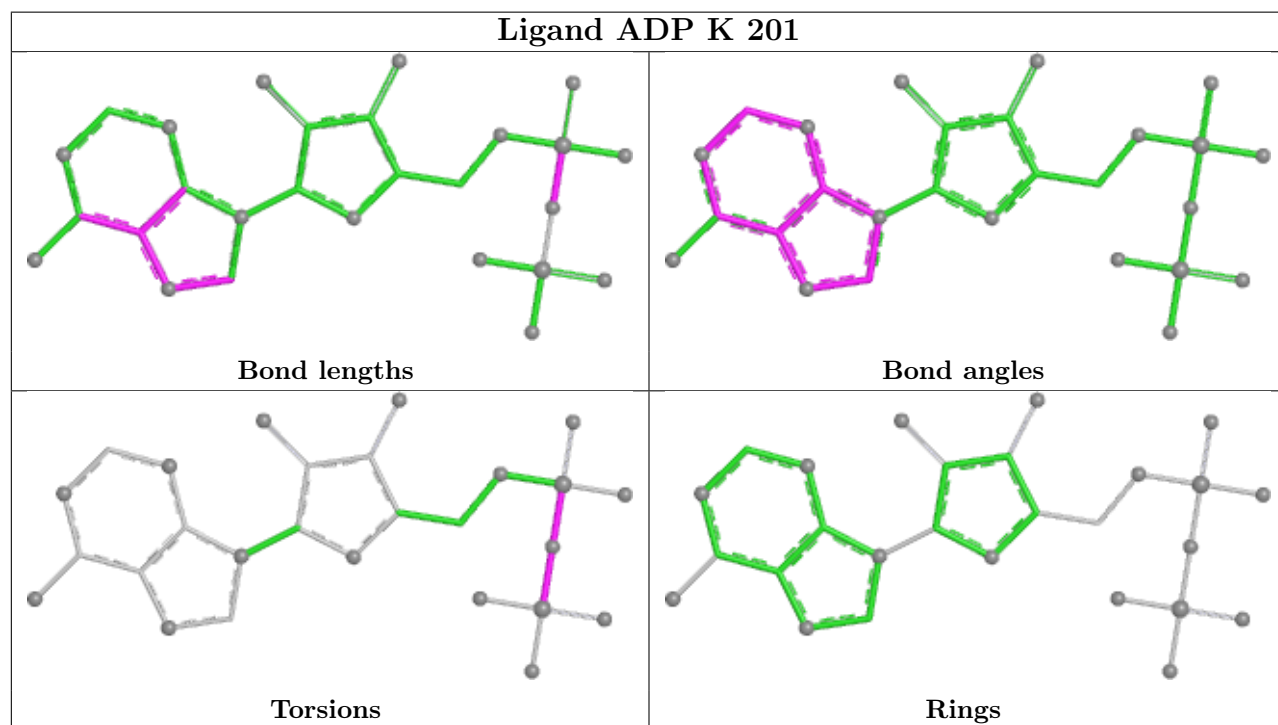
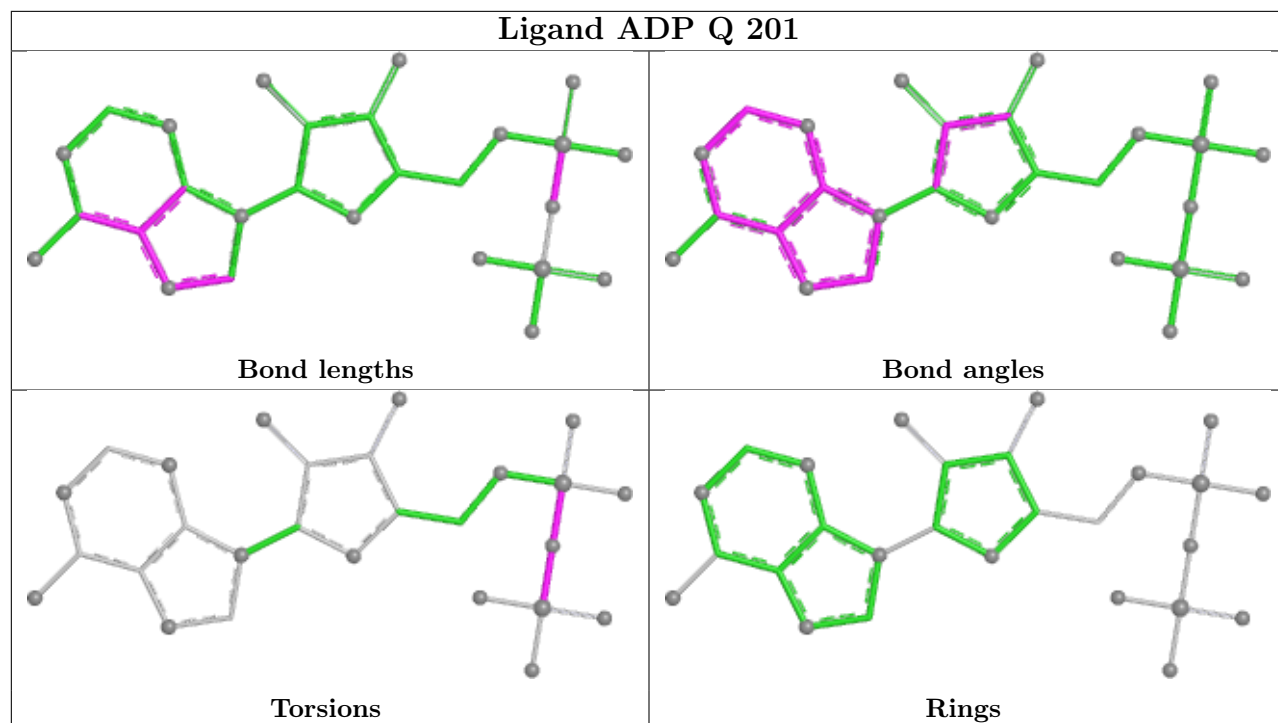


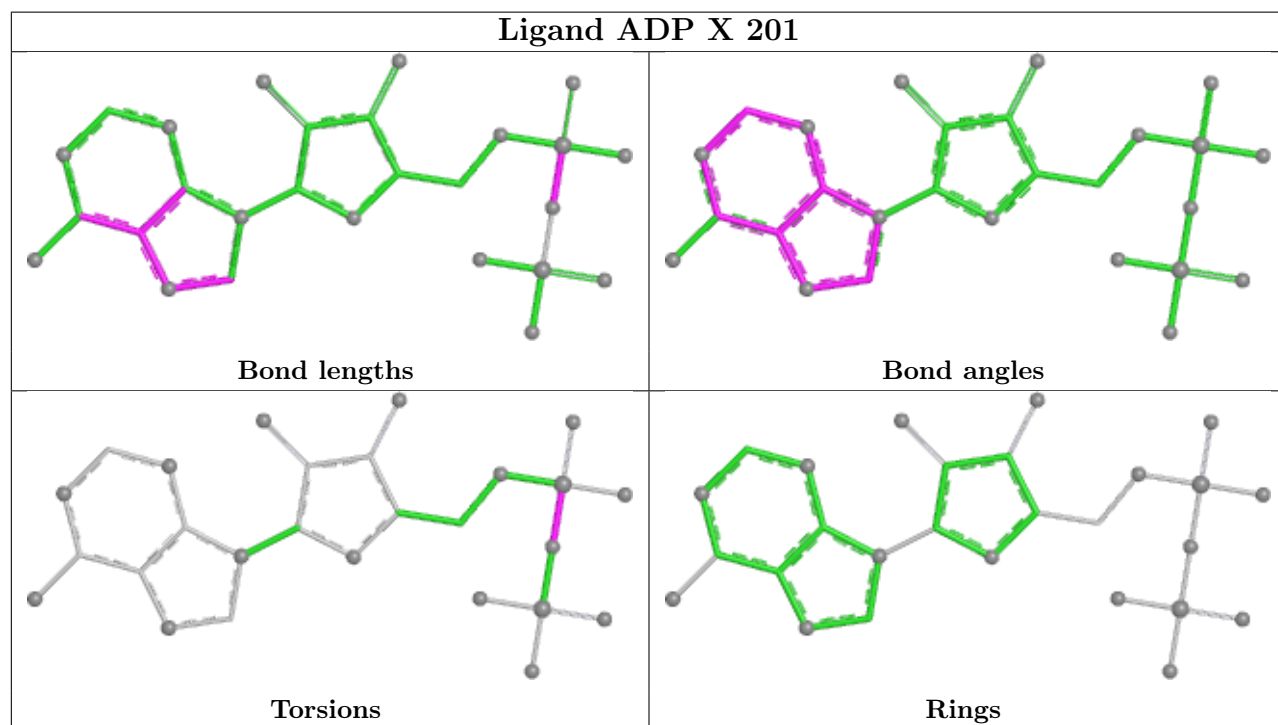
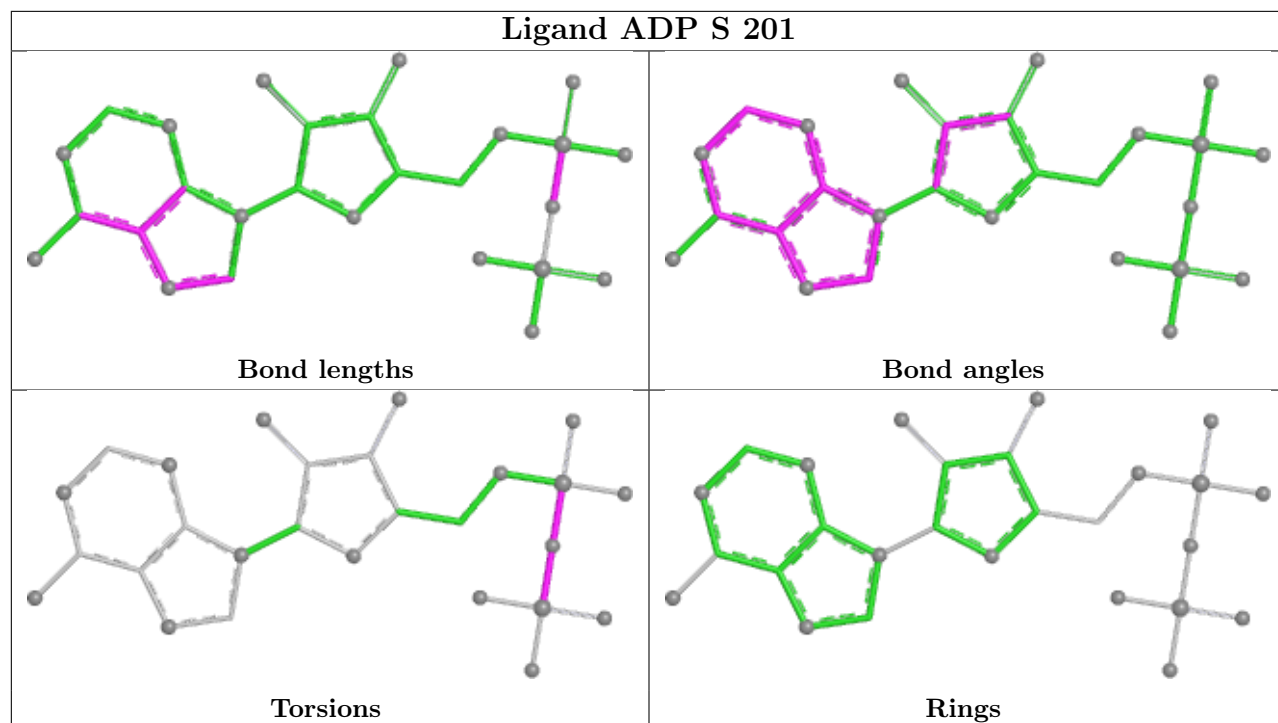


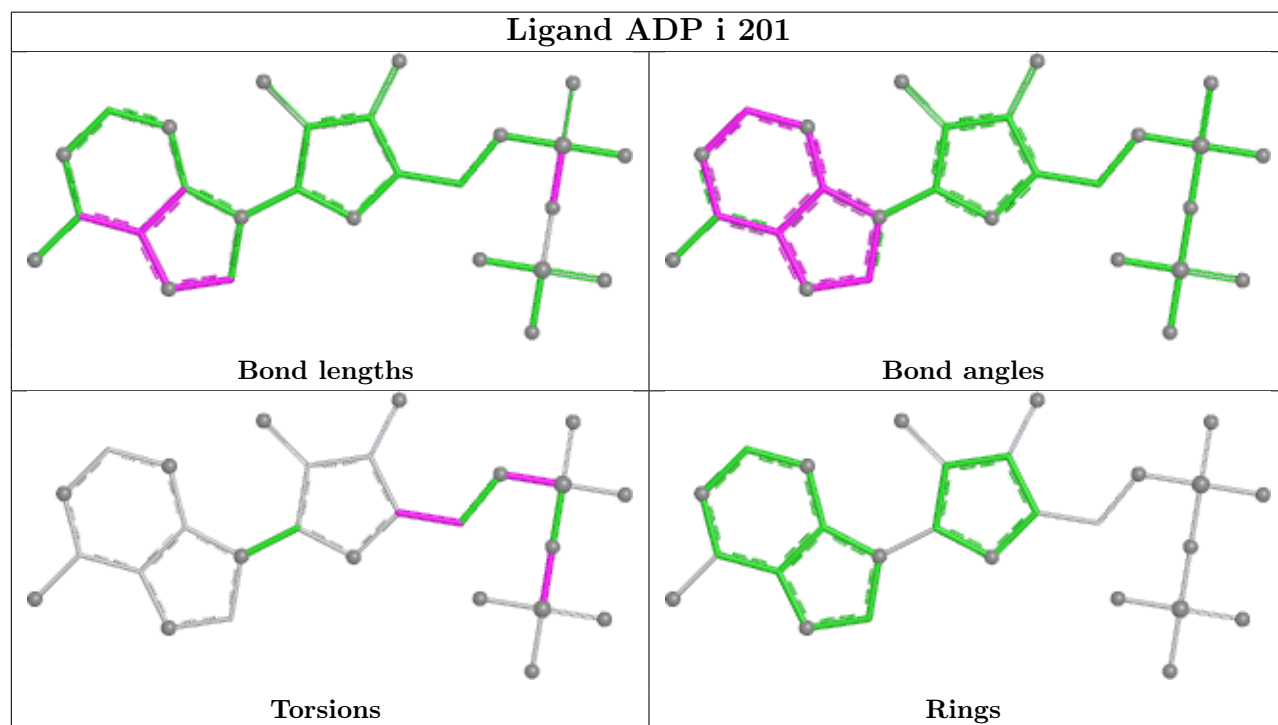
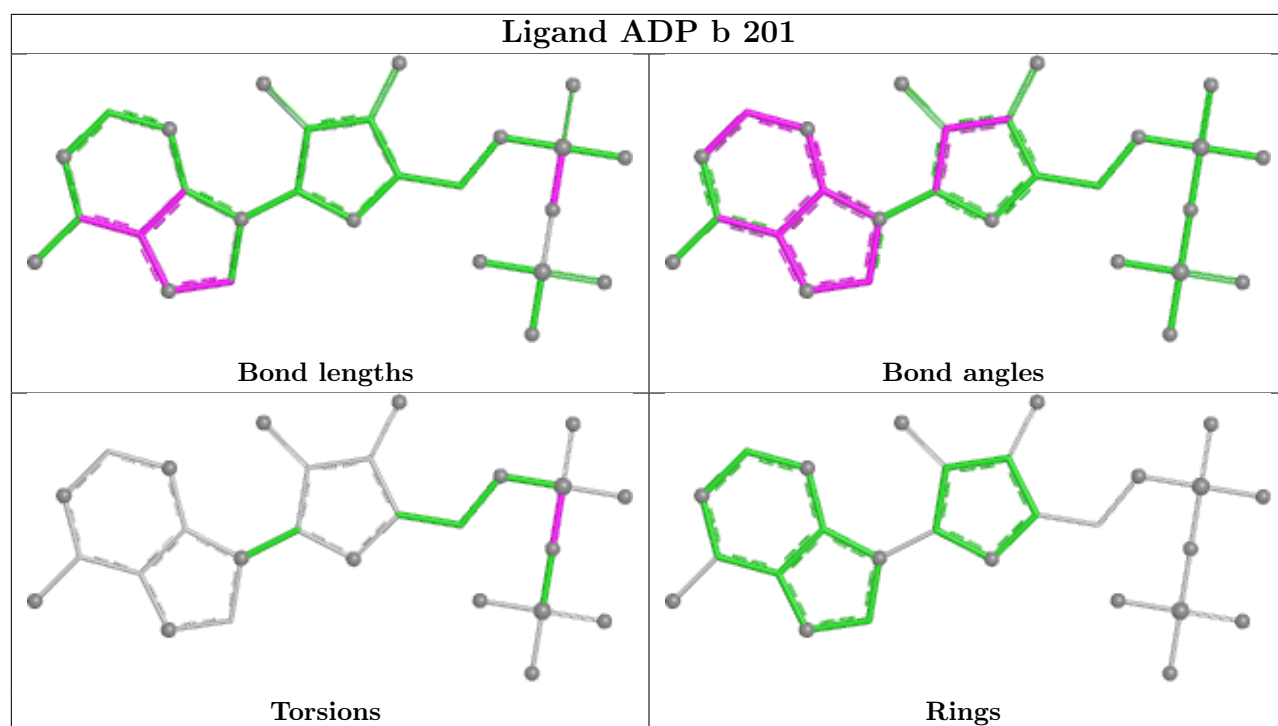




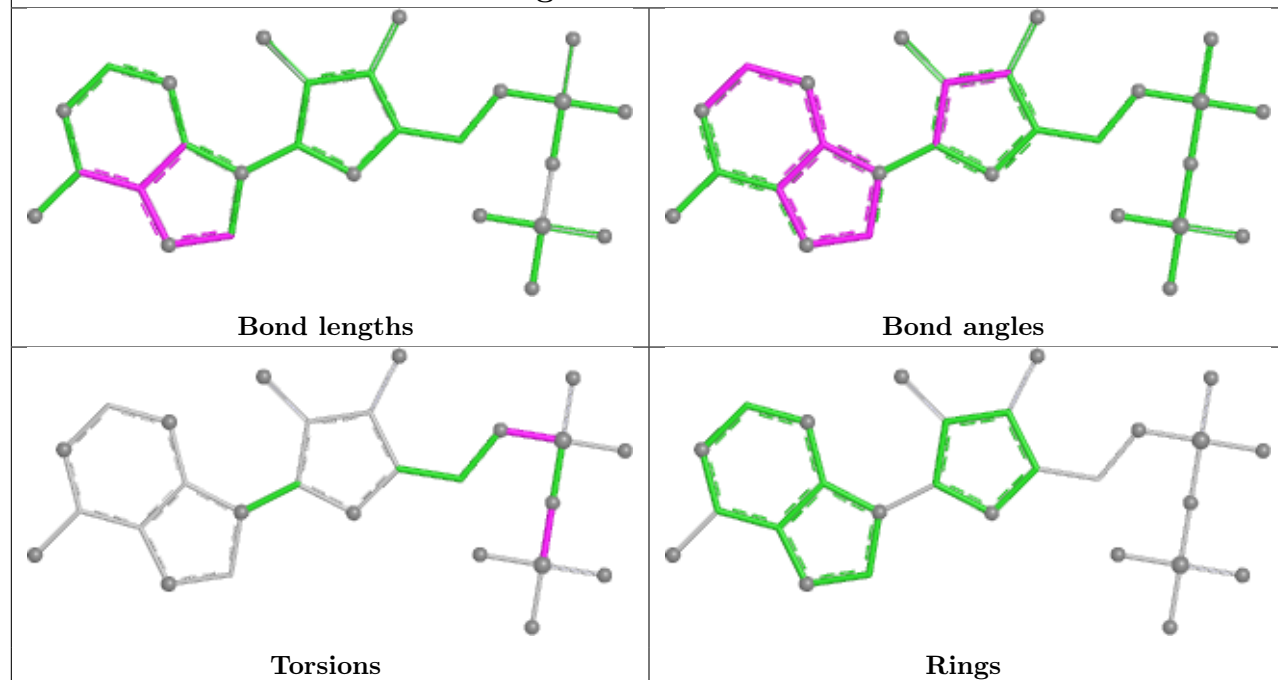




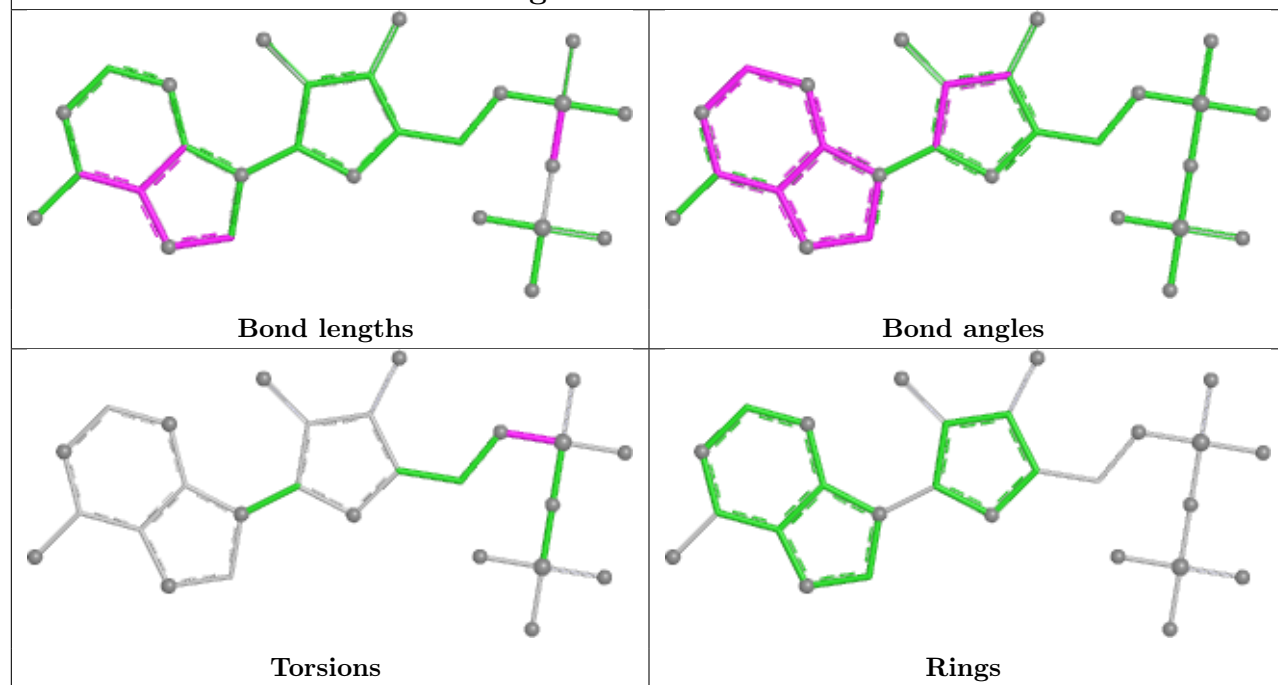


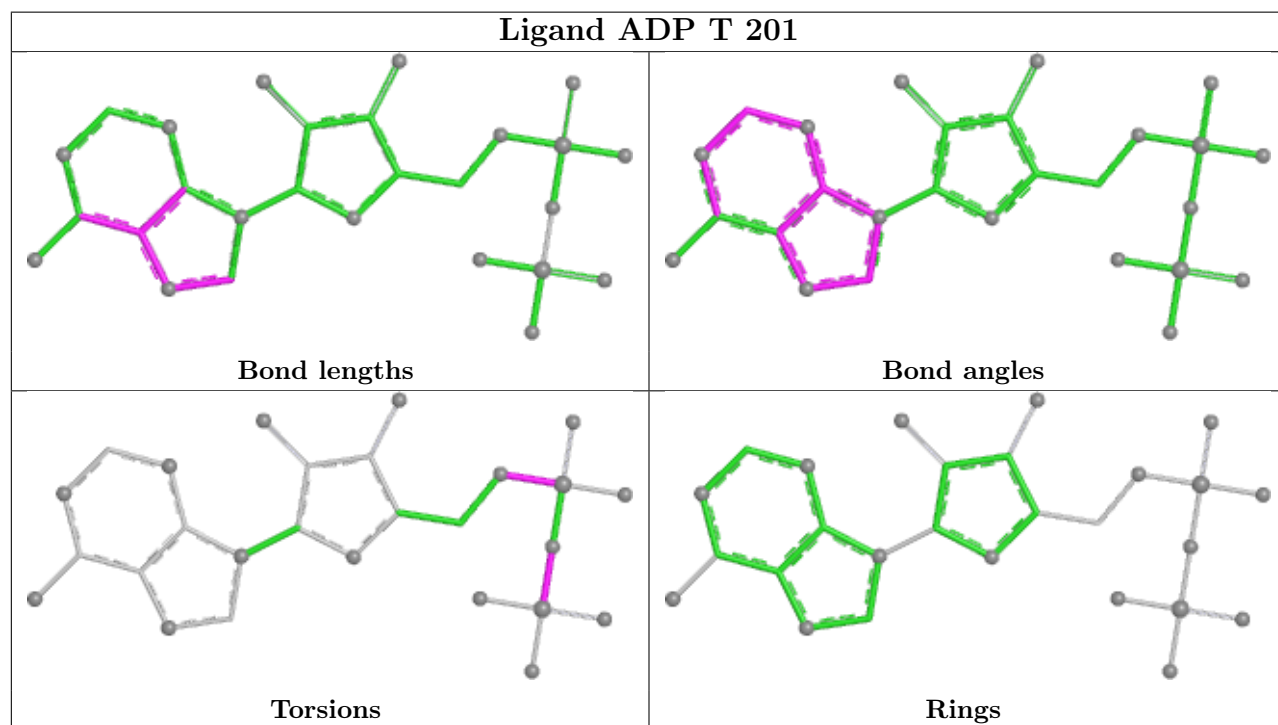
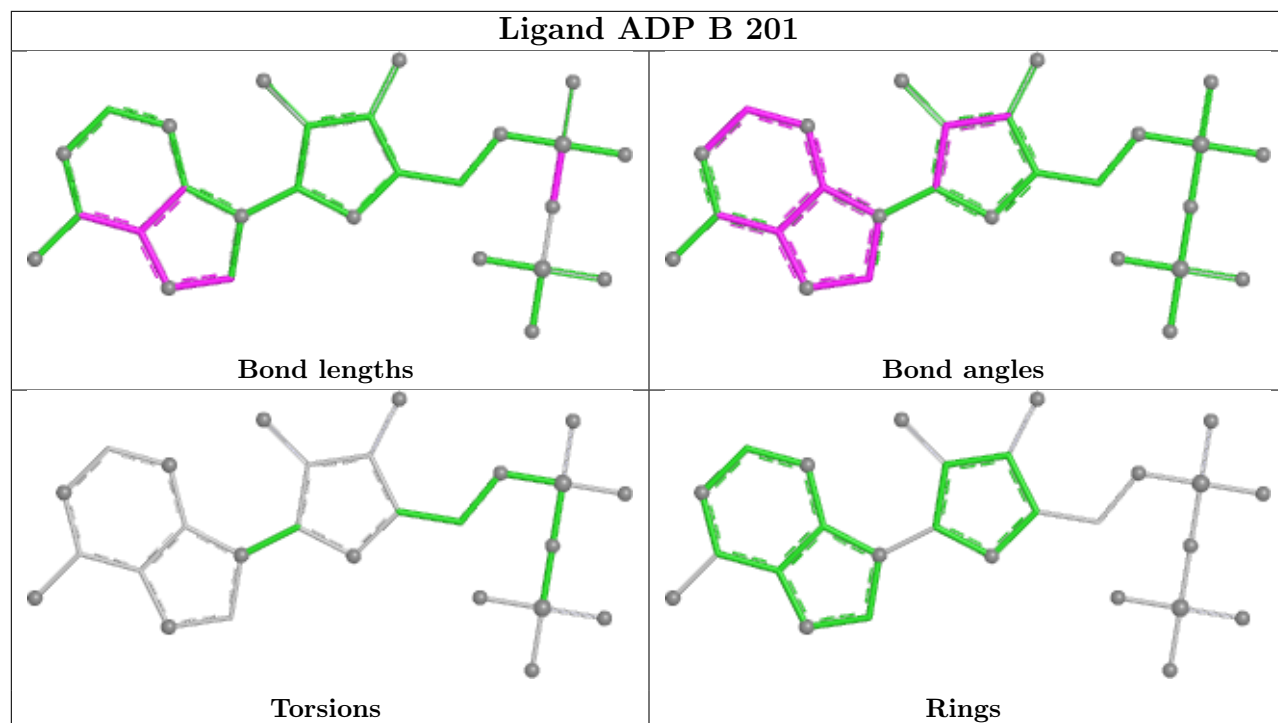


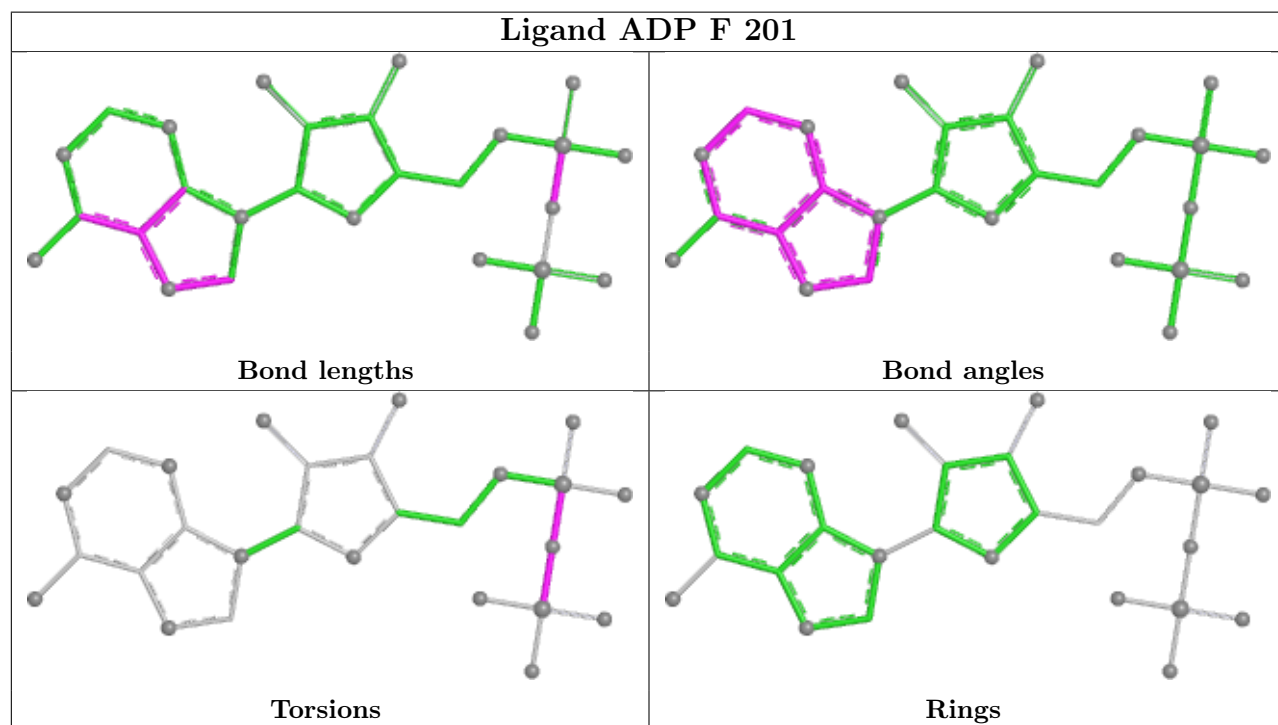
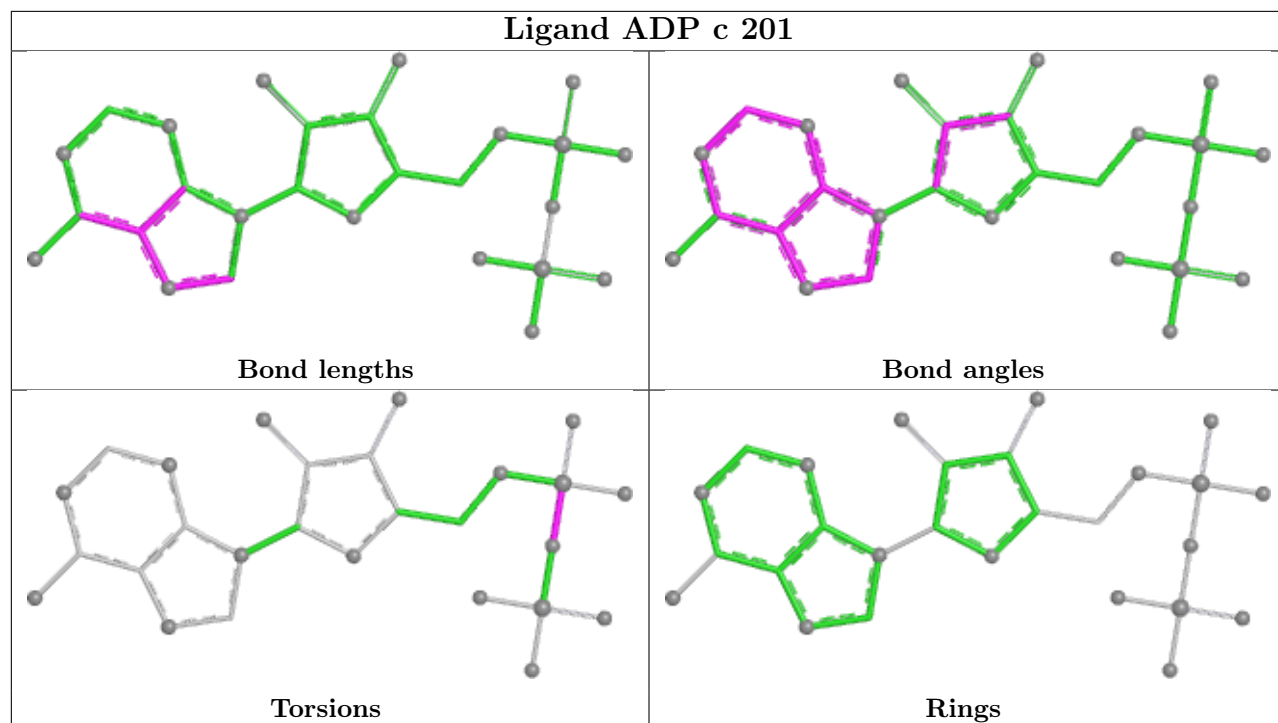
Ligand ADP I 201

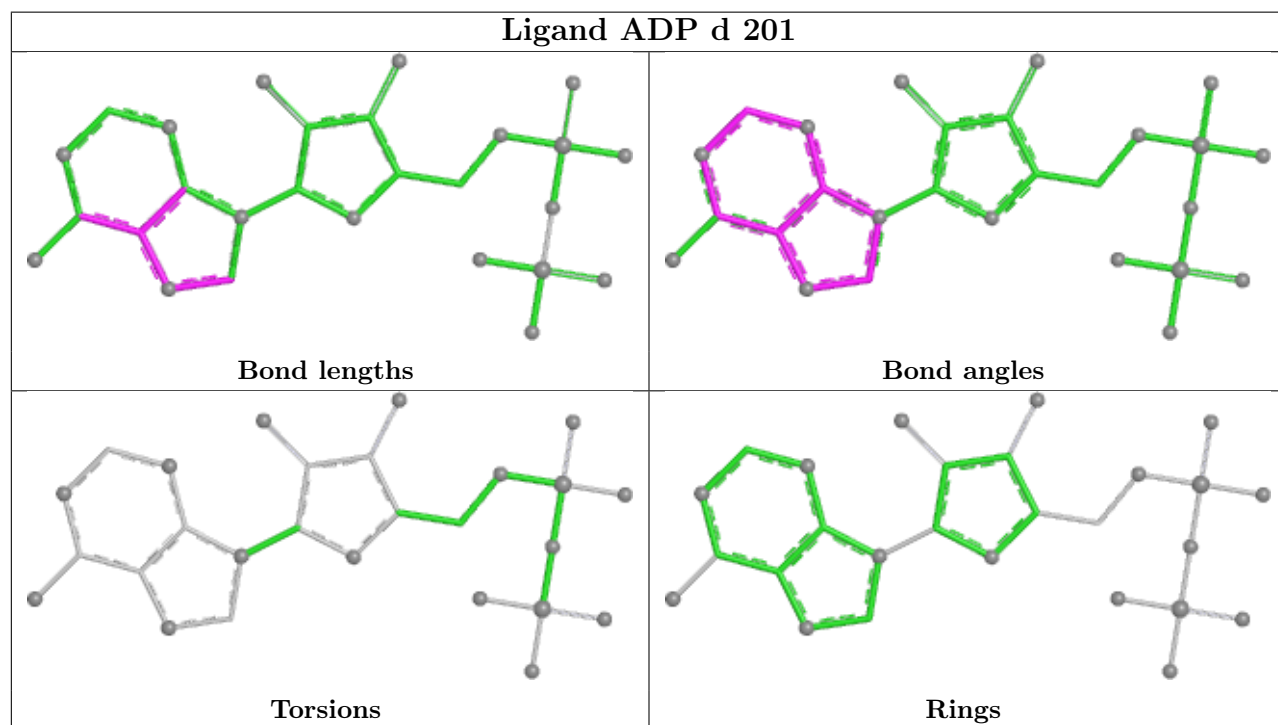
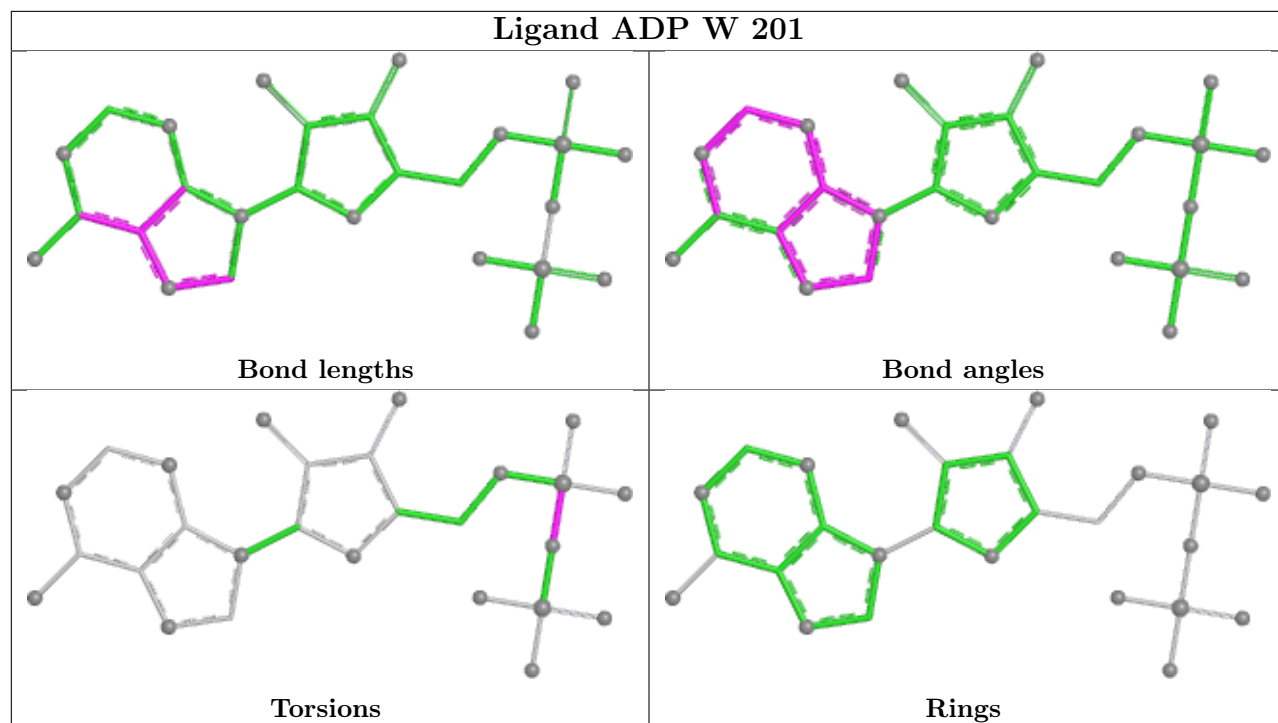


Ligand ADP D 201

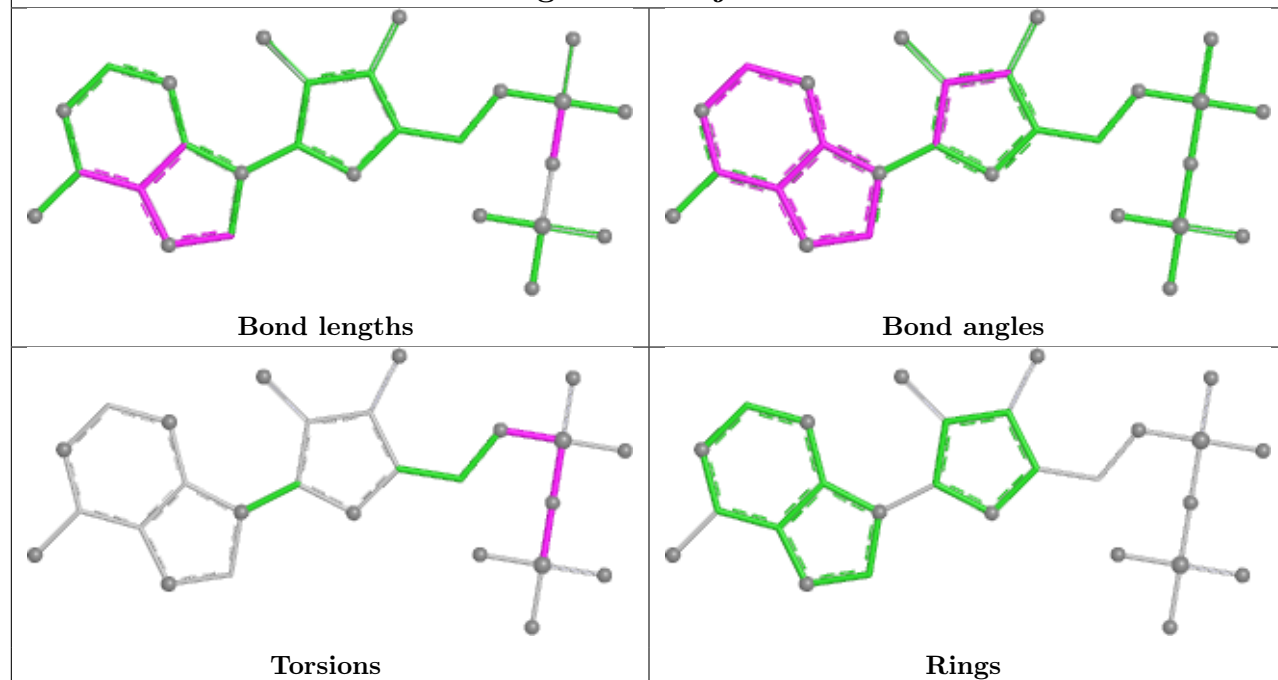




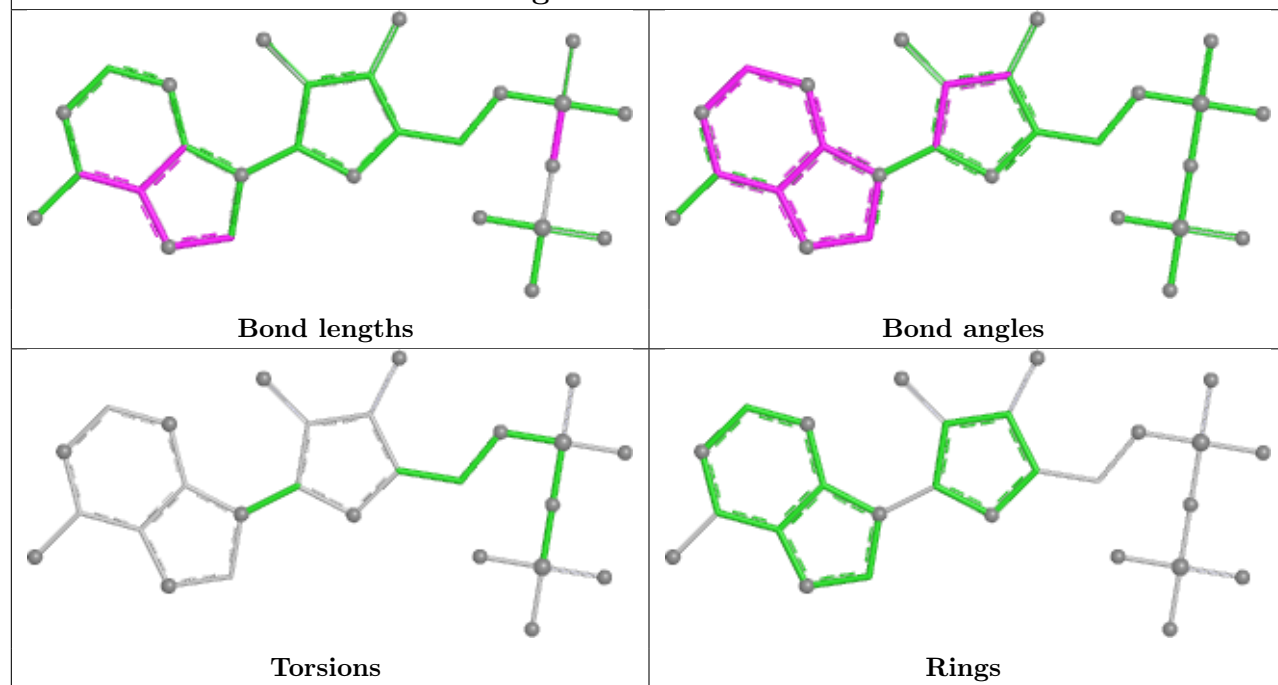


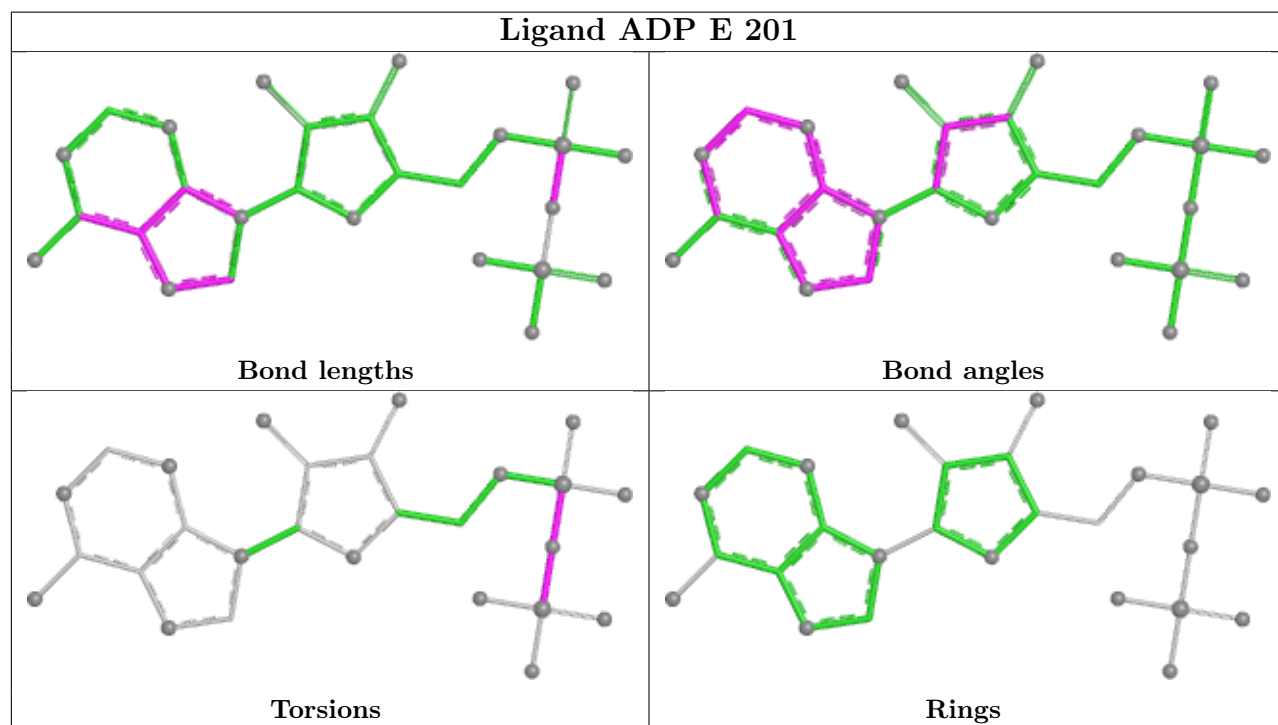
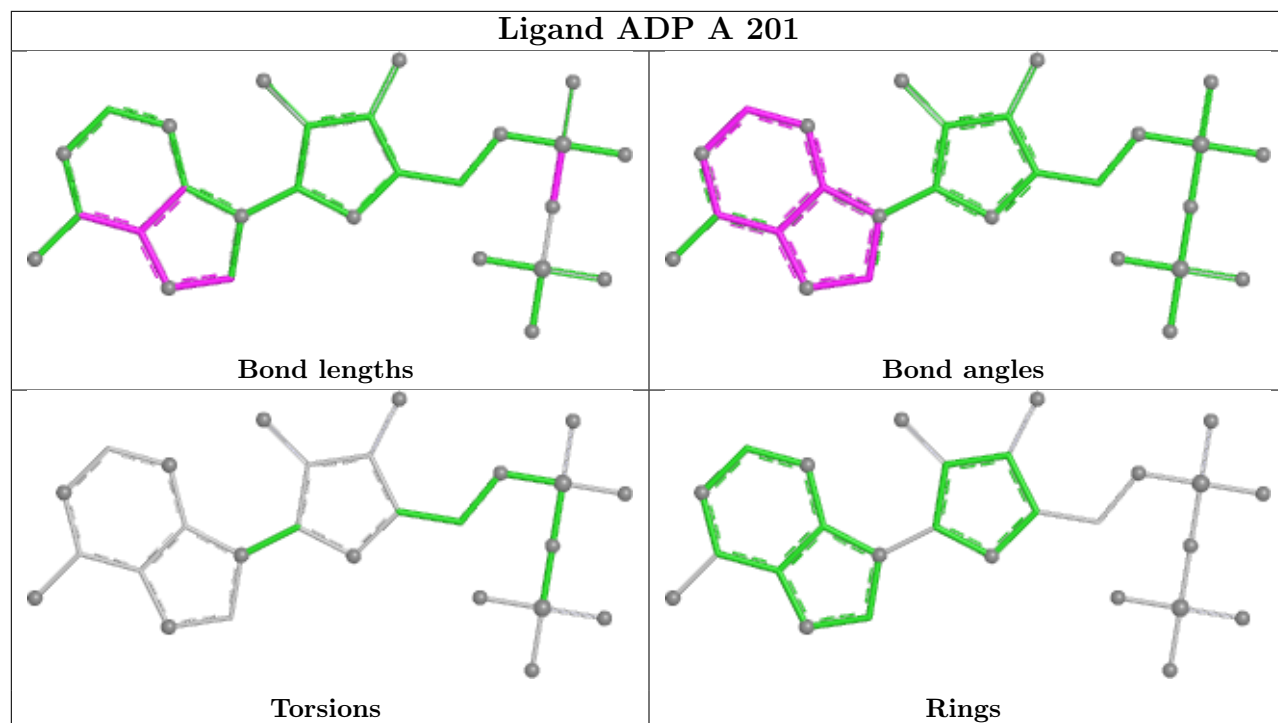


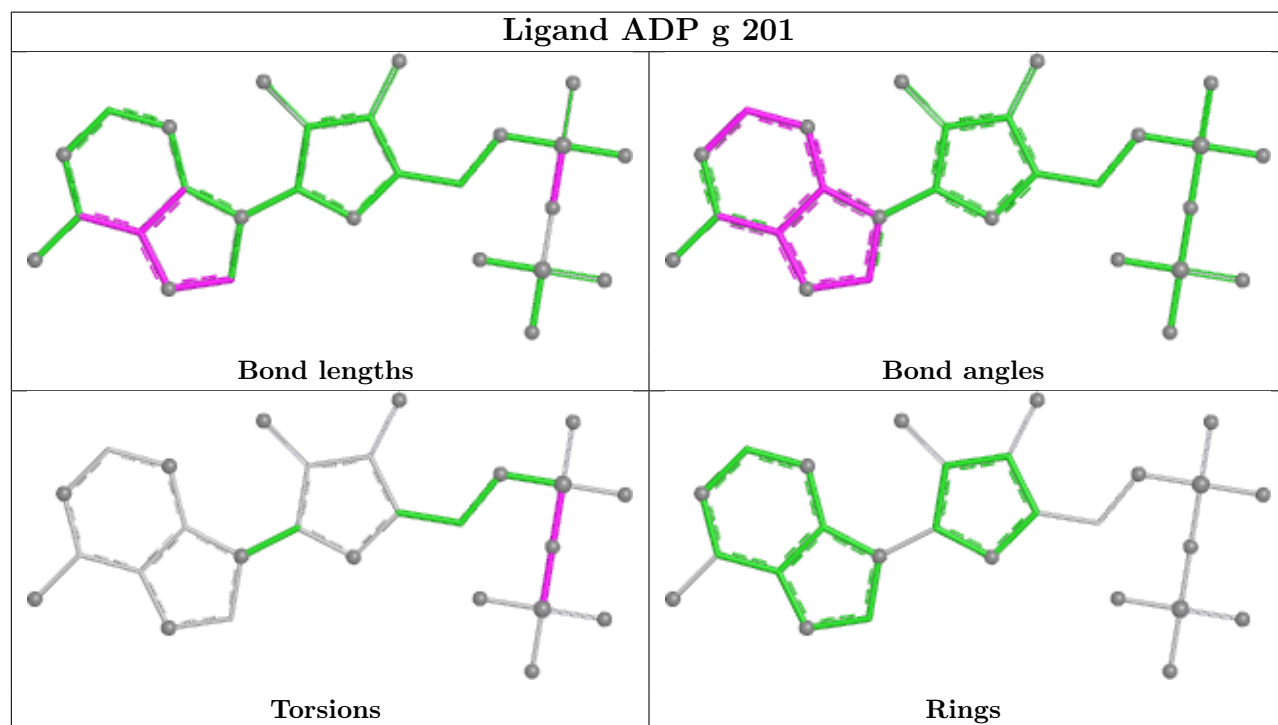
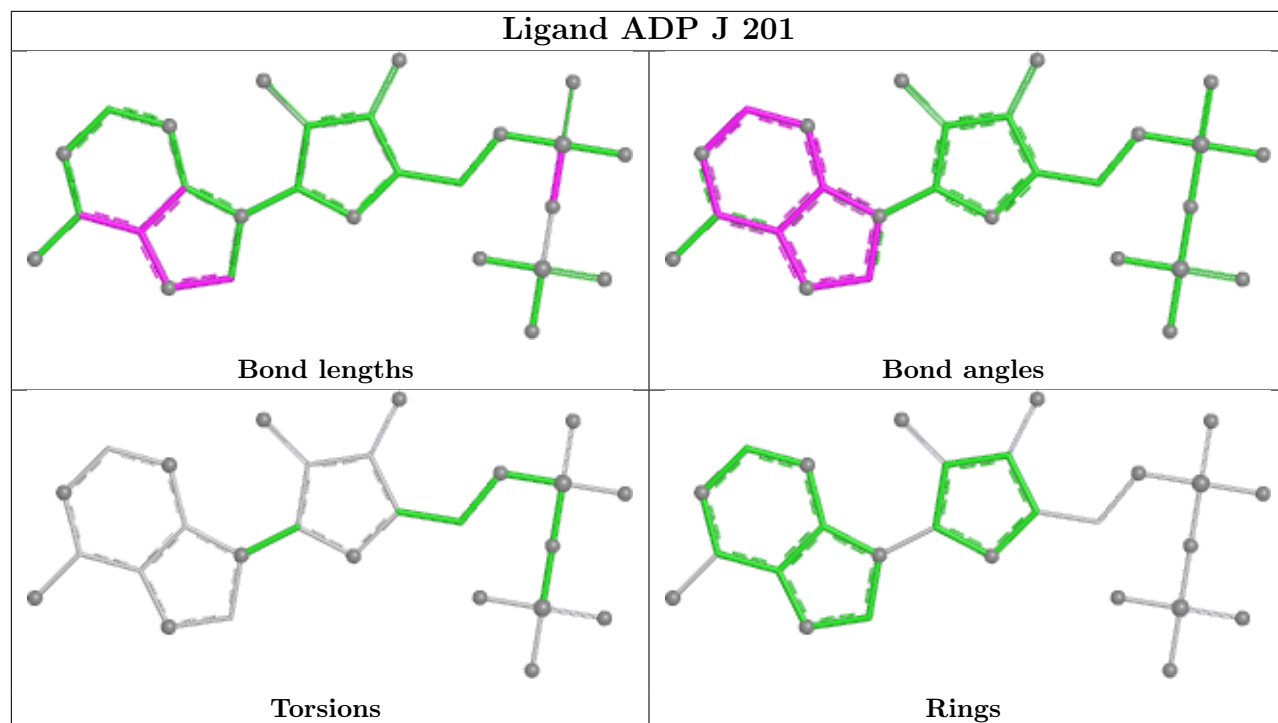
Ligand ADP j 201

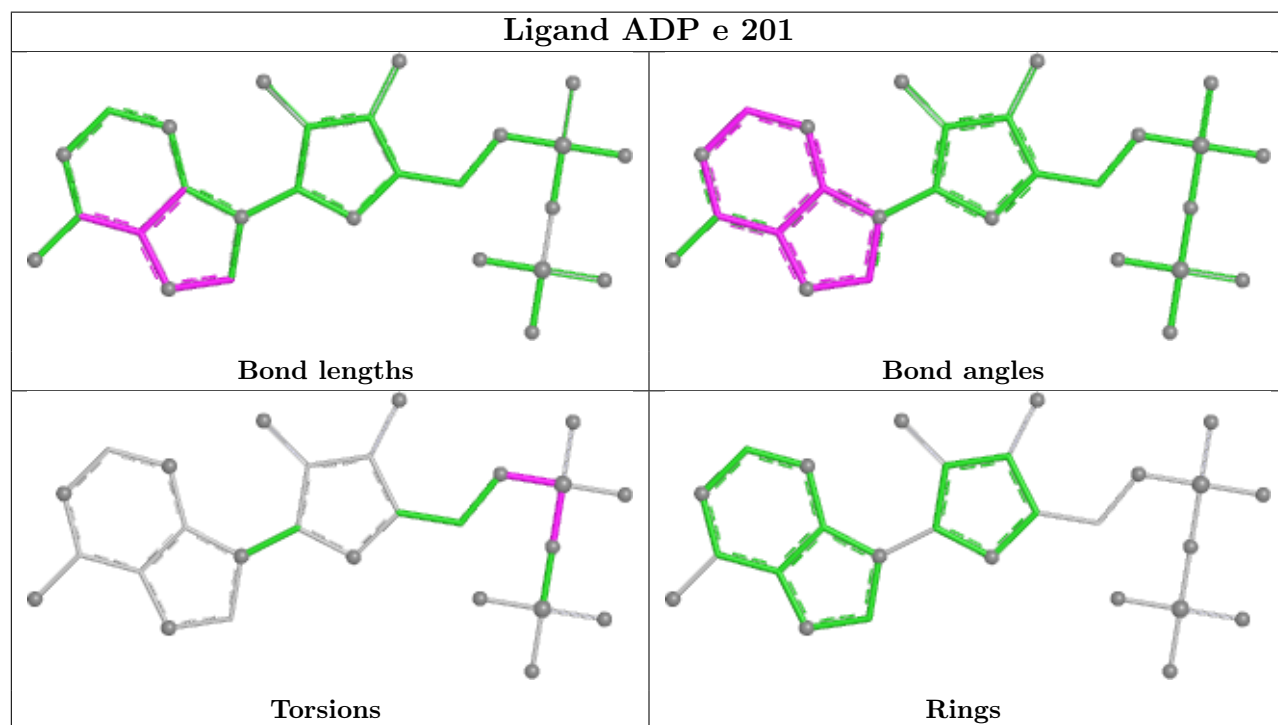
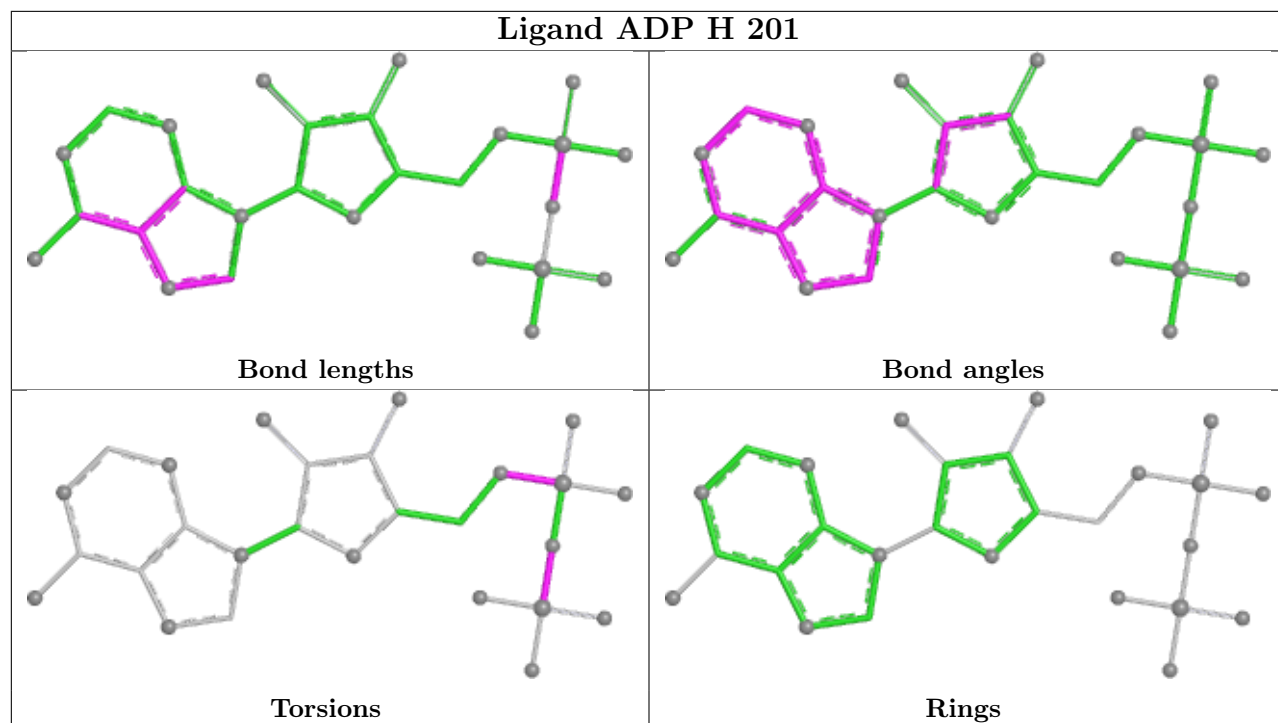


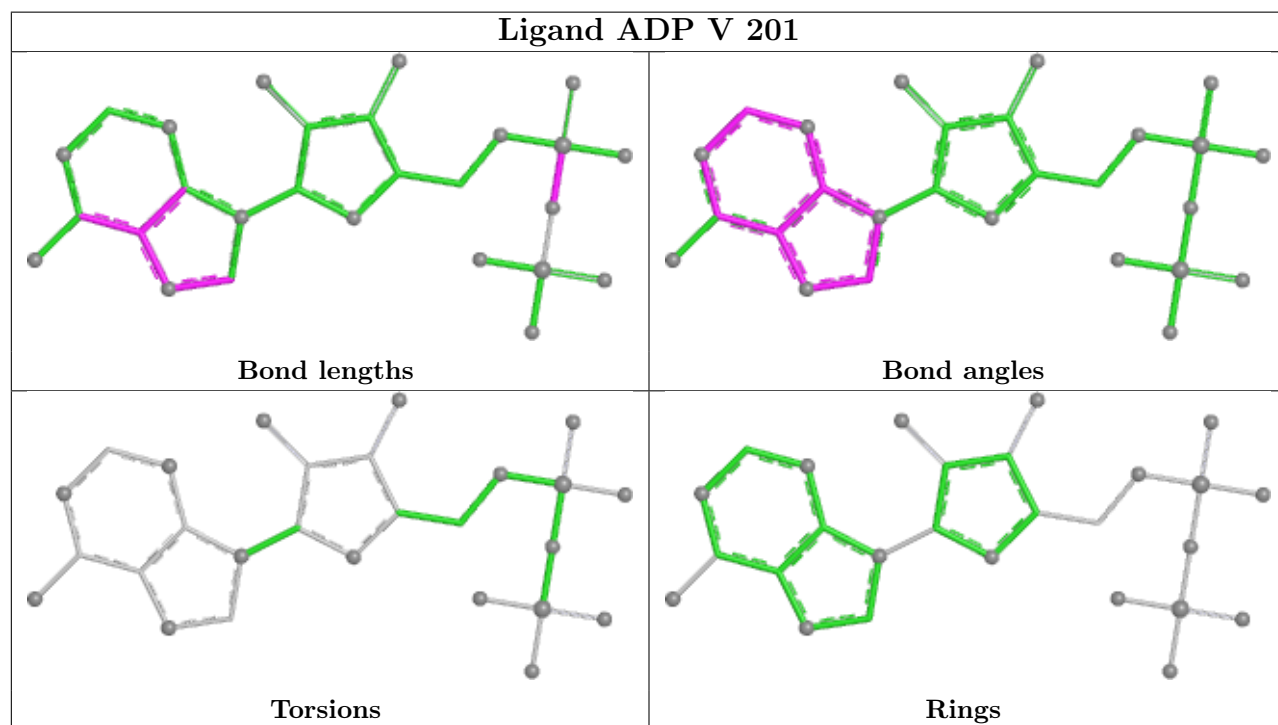
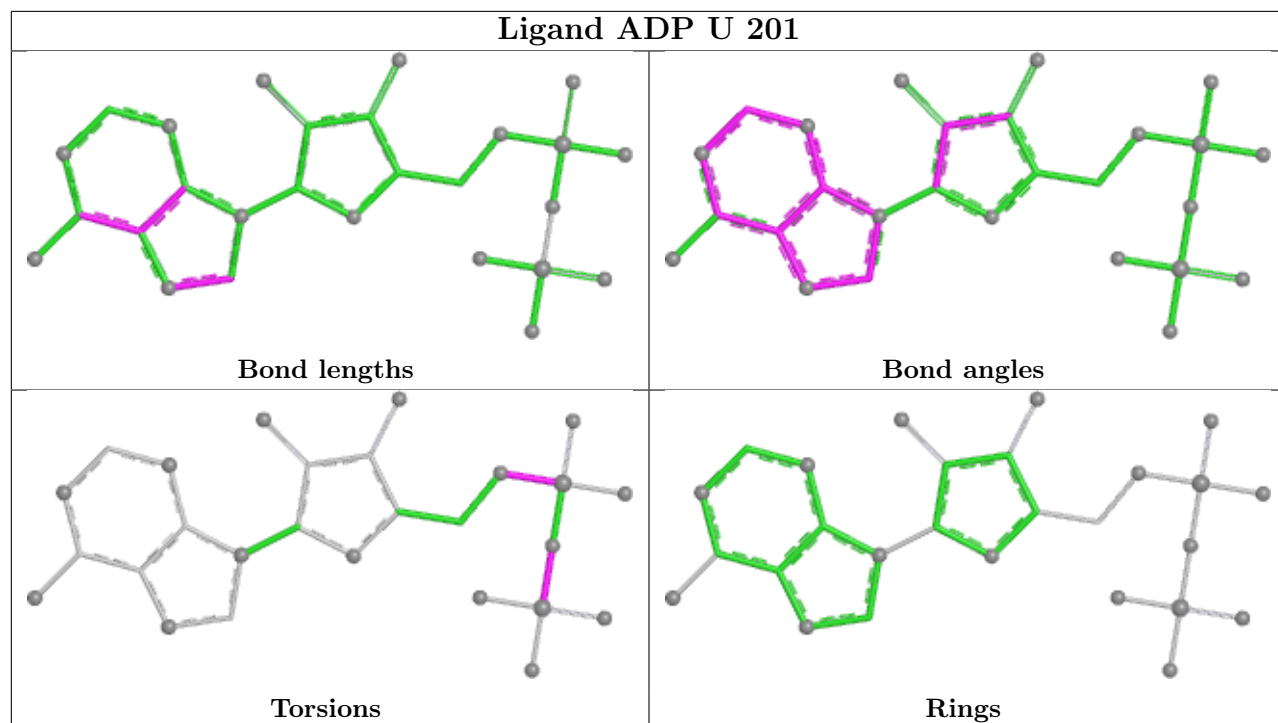
Ligand ADP Z 201

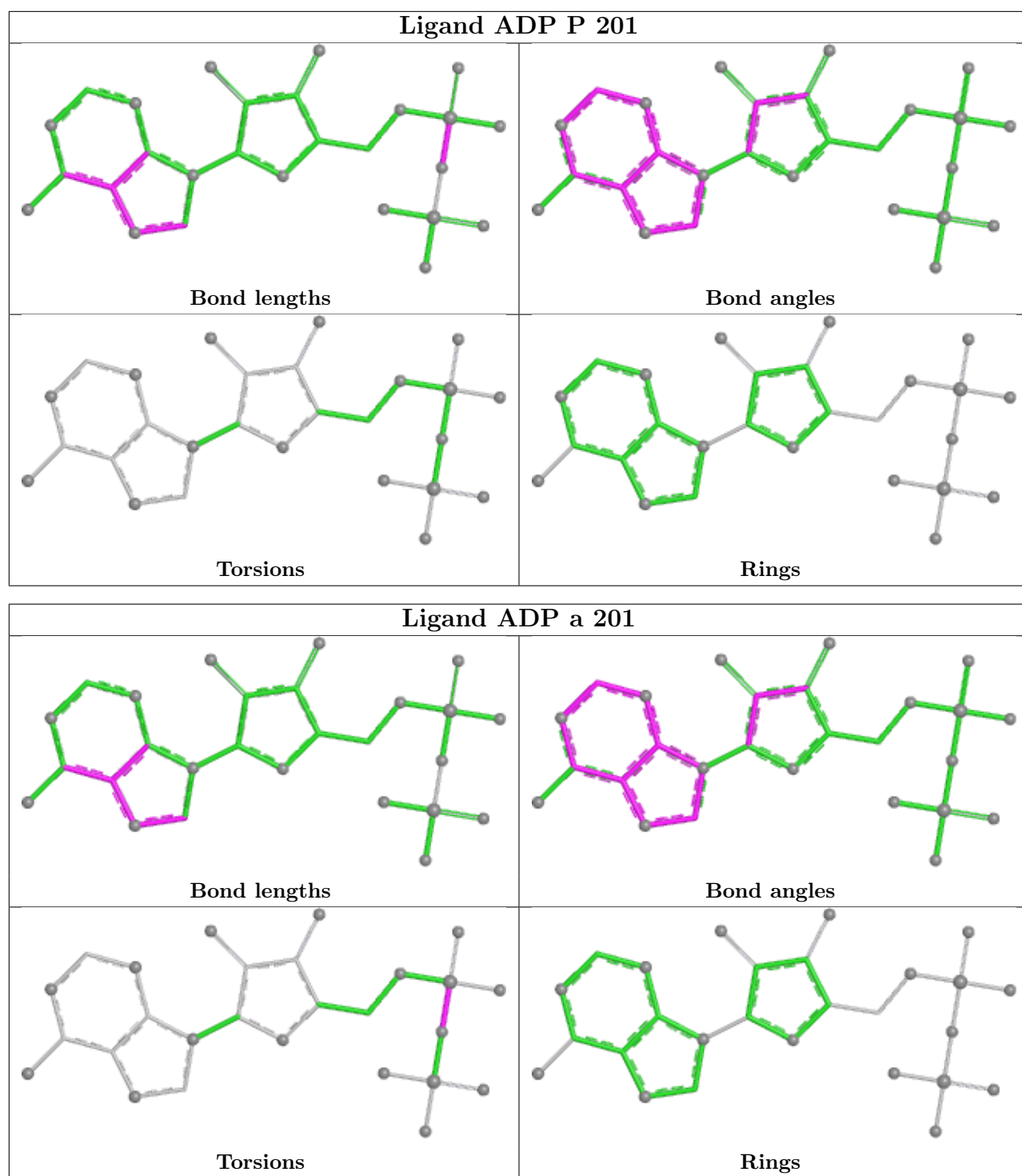












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	150/157 (95%)	-1.30	0 100 100	14, 22, 41, 85	0
1	B	147/157 (93%)	-1.29	0 100 100	15, 21, 44, 59	0
1	C	147/157 (93%)	-1.27	0 100 100	12, 21, 44, 76	0
1	D	147/157 (93%)	-1.31	0 100 100	11, 19, 35, 48	0
1	E	147/157 (93%)	-1.32	0 100 100	12, 18, 32, 39	0
1	F	148/157 (94%)	-1.31	0 100 100	12, 19, 33, 51	0
1	G	147/157 (93%)	-1.30	0 100 100	14, 23, 38, 75	0
1	H	147/157 (93%)	-1.32	0 100 100	14, 23, 36, 73	0
1	I	147/157 (93%)	-1.26	0 100 100	14, 23, 37, 69	0
1	J	149/157 (94%)	-1.25	0 100 100	15, 25, 46, 69	0
1	K	147/157 (93%)	-1.28	0 100 100	16, 24, 44, 71	0
1	L	147/157 (93%)	-1.26	0 100 100	16, 26, 45, 69	0
1	M	149/157 (94%)	-1.11	0 100 100	23, 35, 57, 76	0
1	N	147/157 (93%)	-1.16	0 100 100	25, 36, 54, 75	0
1	O	147/157 (93%)	-1.18	0 100 100	26, 36, 57, 95	0
1	P	147/157 (93%)	-1.11	0 100 100	24, 38, 61, 76	0
1	Q	145/157 (92%)	-1.15	0 100 100	26, 38, 61, 94	0
1	R	147/157 (93%)	-1.12	0 100 100	25, 39, 61, 95	0
1	S	149/157 (94%)	-1.21	0 100 100	16, 23, 40, 68	0
1	T	147/157 (93%)	-1.26	0 100 100	14, 24, 45, 71	0
1	U	147/157 (93%)	-1.24	0 100 100	15, 24, 36, 46	0
1	V	147/157 (93%)	-1.25	0 100 100	13, 22, 38, 56	0
1	W	145/157 (92%)	-1.28	0 100 100	13, 23, 36, 70	0
1	X	147/157 (93%)	-1.22	0 100 100	14, 22, 36, 71	0

Continued on next page...

Continued from previous page...

Continued from previous page.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9	
1	Y	147/157 (93%)	-1.09	0	100 100	20, 40, 59, 108	0
1	Z	148/157 (94%)	-1.13	0	100 100	25, 36, 61, 74	0
1	a	147/157 (93%)	-1.12	0	100 100	24, 39, 70, 97	0
1	b	147/157 (93%)	-1.18	0	100 100	22, 34, 54, 77	0
1	c	147/157 (93%)	-1.16	0	100 100	24, 35, 53, 74	0
1	d	147/157 (93%)	-1.14	0	100 100	23, 34, 54, 97	0
1	e	148/157 (94%)	-1.14	0	100 100	25, 35, 51, 82	0
1	f	147/157 (93%)	-1.12	0	100 100	25, 36, 53, 76	0
1	g	147/157 (93%)	-1.10	0	100 100	24, 37, 52, 66	0
1	h	145/157 (92%)	-1.04	0	100 100	25, 39, 60, 108	0
1	i	147/157 (93%)	-1.08	0	100 100	26, 41, 60, 79	0
1	j	146/157 (92%)	-1.09	0	100 100	28, 42, 61, 84	0
All	All	5297/5652 (93%)	-1.20	0	100 100	11, 31, 55, 108	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	O	202	1/1	0.95	0.05	39,39,39,39	0
3	MG	W	202	1/1	0.97	0.04	27,27,27,27	0
3	MG	f	202	1/1	0.97	0.05	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	L	201	27/27	0.98	0.04	25,32,51,65	0
2	ADP	M	201	27/27	0.98	0.04	36,44,58,68	0
2	ADP	P	201	27/27	0.98	0.05	39,55,60,62	0
2	ADP	Q	201	27/27	0.98	0.04	37,50,61,68	0
2	ADP	T	201	27/27	0.98	0.04	20,31,42,47	0
2	ADP	f	201	27/27	0.98	0.05	31,38,48,52	0
2	ADP	h	201	27/27	0.98	0.04	28,43,53,59	0
3	MG	C	202	1/1	0.98	0.04	36,36,36,36	0
3	MG	E	202	1/1	0.98	0.03	20,20,20,20	0
3	MG	G	202	1/1	0.98	0.06	35,35,35,35	0
2	ADP	B	201	27/27	0.98	0.04	29,37,41,42	0
2	ADP	H	201	27/27	0.98	0.04	21,24,36,37	0
3	MG	Z	202	1/1	0.98	0.04	42,42,42,42	0
3	MG	c	202	1/1	0.98	0.04	47,47,47,47	0
2	ADP	J	201	27/27	0.98	0.05	17,25,38,48	0
2	ADP	S	201	27/27	0.99	0.03	16,25,40,57	0
2	ADP	A	201	27/27	0.99	0.04	21,32,42,46	0
2	ADP	U	201	27/27	0.99	0.04	15,25,31,40	0
2	ADP	V	201	27/27	0.99	0.04	22,28,42,50	0
2	ADP	W	201	27/27	0.99	0.03	18,27,35,37	0
2	ADP	X	201	27/27	0.99	0.04	13,25,40,42	0
2	ADP	Y	201	27/27	0.99	0.04	42,49,53,55	0
2	ADP	Z	201	27/27	0.99	0.05	43,50,70,80	0
2	ADP	a	201	27/27	0.99	0.04	51,61,67,77	0
2	ADP	b	201	27/27	0.99	0.04	31,38,57,75	0
2	ADP	c	201	27/27	0.99	0.04	29,38,52,61	0
2	ADP	d	201	27/27	0.99	0.04	38,49,56,69	0
2	ADP	e	201	27/27	0.99	0.04	24,35,55,56	0
2	ADP	I	201	27/27	0.99	0.04	17,29,37,49	0
2	ADP	g	201	27/27	0.99	0.04	27,37,43,45	0
2	ADP	C	201	27/27	0.99	0.04	26,38,51,53	0
2	ADP	i	201	27/27	0.99	0.04	37,47,57,61	0
2	ADP	j	201	27/27	0.99	0.04	32,45,51,57	0
3	MG	B	202	1/1	0.99	0.04	28,28,28,28	0
2	ADP	K	201	27/27	0.99	0.04	28,34,45,49	0
3	MG	D	202	1/1	0.99	0.03	28,28,28,28	0
2	ADP	D	201	27/27	0.99	0.04	20,23,30,34	0
3	MG	F	202	1/1	0.99	0.02	23,23,23,23	0
2	ADP	E	201	27/27	0.99	0.03	14,22,26,34	0
3	MG	I	202	1/1	0.99	0.04	27,27,27,27	0
3	MG	M	202	1/1	0.99	0.03	26,26,26,26	0
2	ADP	N	201	27/27	0.99	0.04	34,47,62,67	0

Continued on next page...

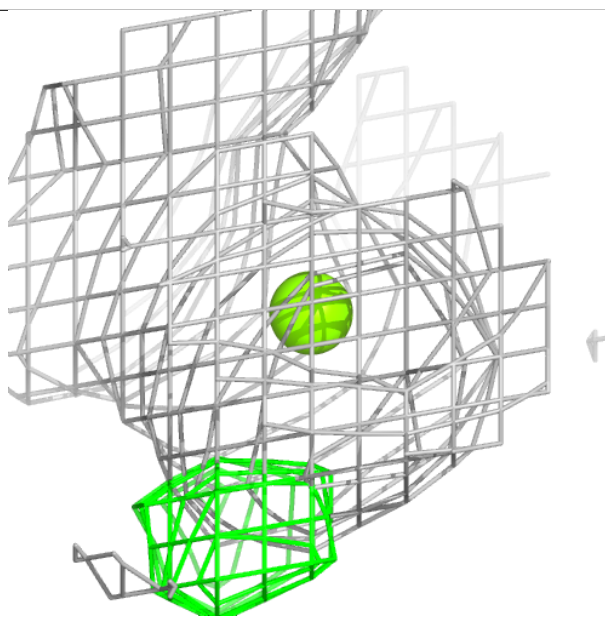
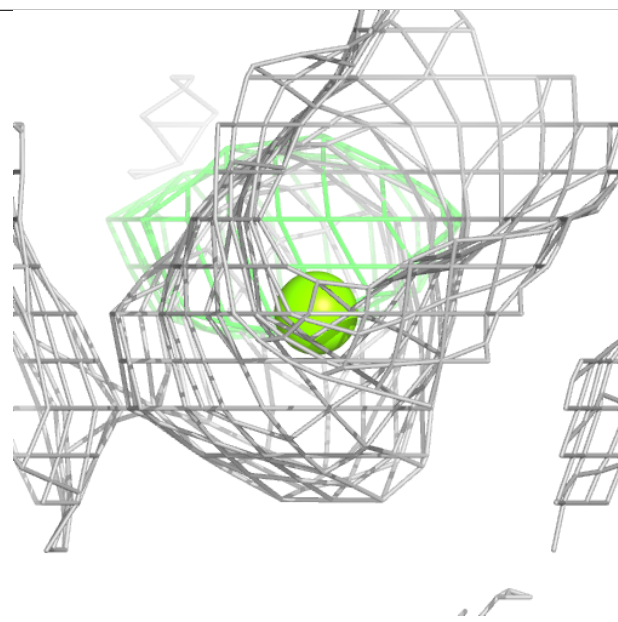
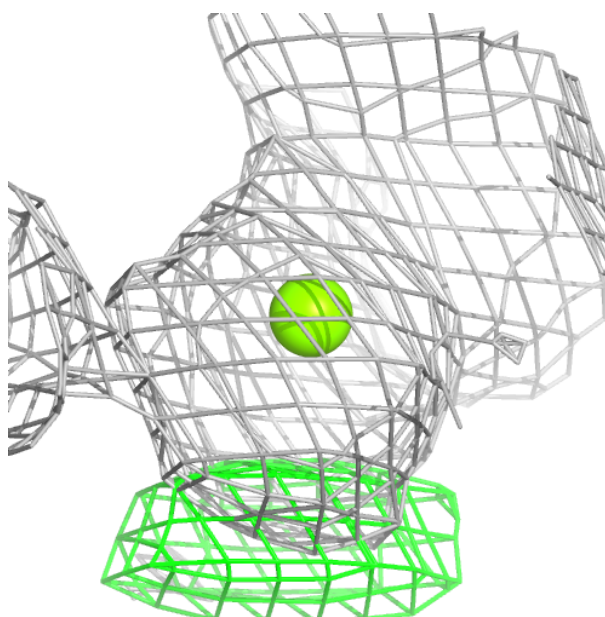
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	P	202	1/1	0.99	0.04	48,48,48,48	0
3	MG	Q	202	1/1	0.99	0.03	46,46,46,46	0
2	ADP	O	201	27/27	0.99	0.04	39,45,53,55	0
3	MG	X	202	1/1	0.99	0.04	25,25,25,25	0
2	ADP	F	201	27/27	0.99	0.03	15,21,33,44	0
3	MG	b	202	1/1	0.99	0.02	34,34,34,34	0
2	ADP	G	201	27/27	0.99	0.04	27,34,48,55	0
3	MG	d	202	1/1	0.99	0.04	43,43,43,43	0
2	ADP	R	201	27/27	0.99	0.04	33,48,60,73	0
3	MG	h	202	1/1	1.00	0.03	53,53,53,53	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.

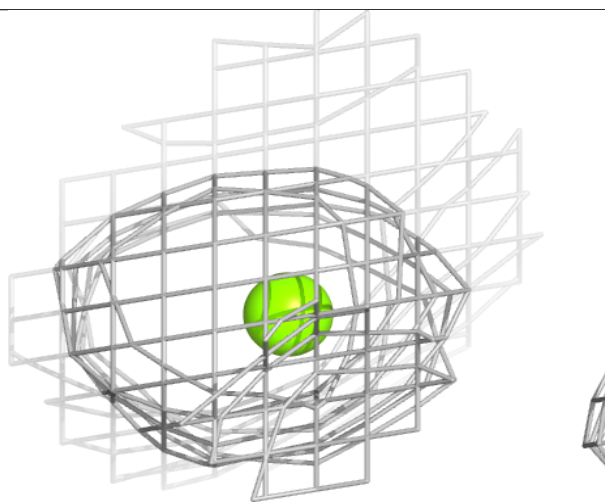
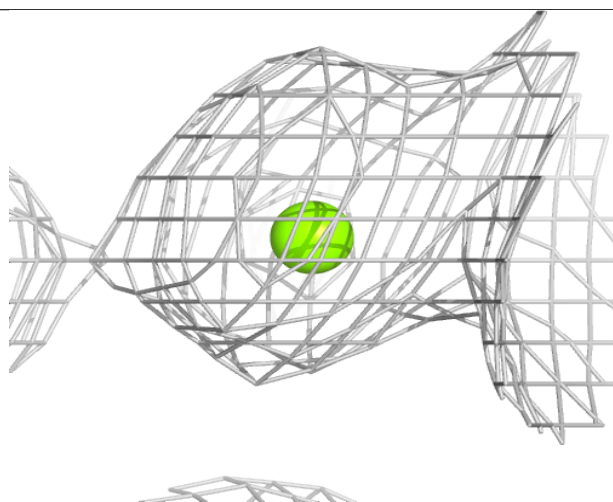
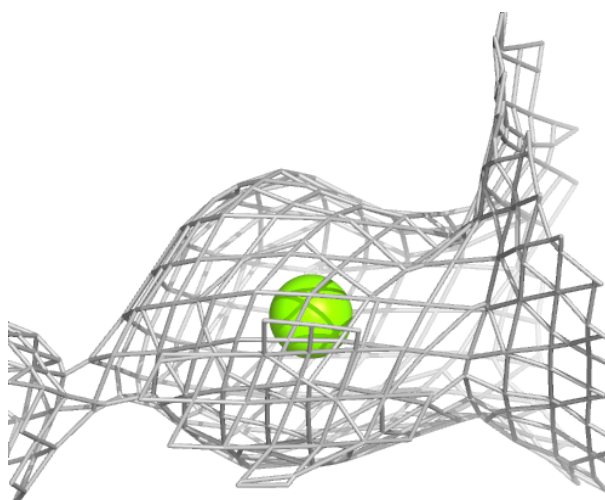
Electron density around MG O 202:

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



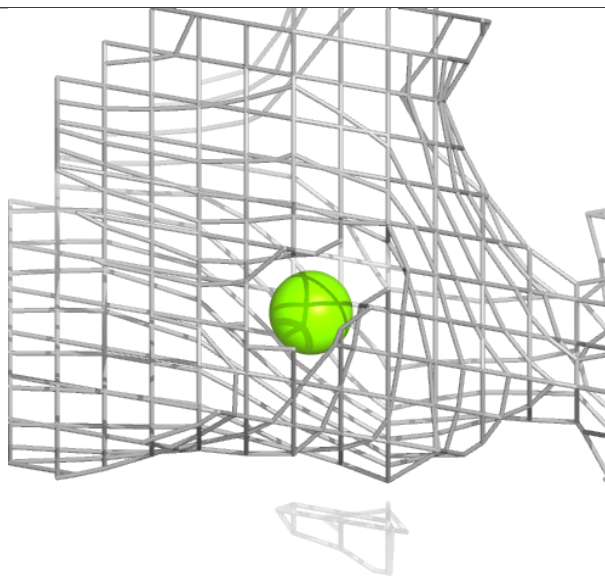
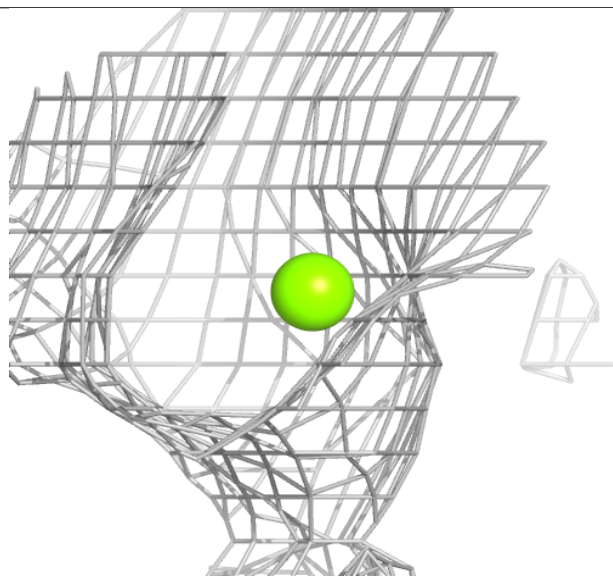
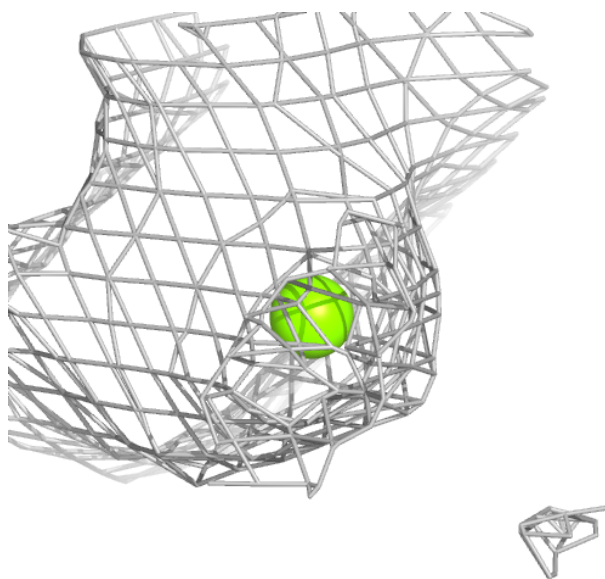
Electron density around MG W 202:

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



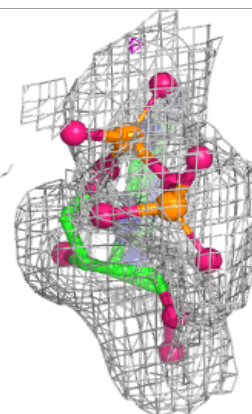
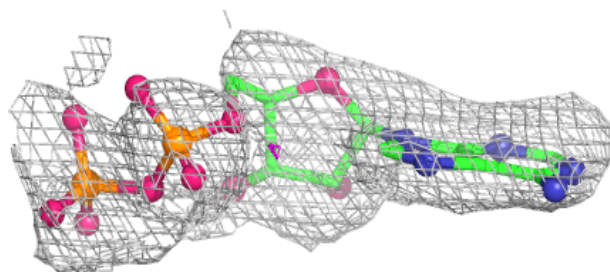
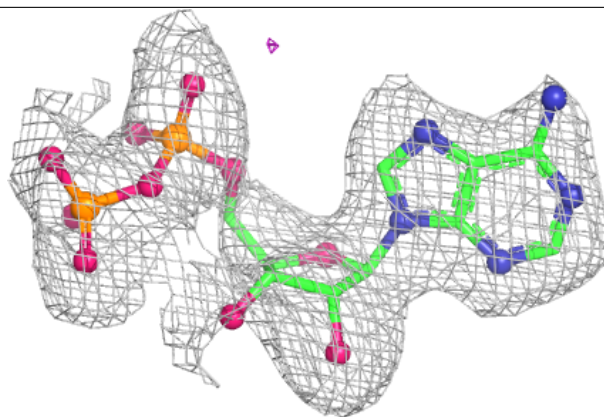
Electron density around MG f 202:

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

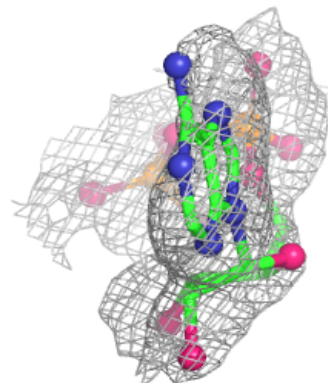
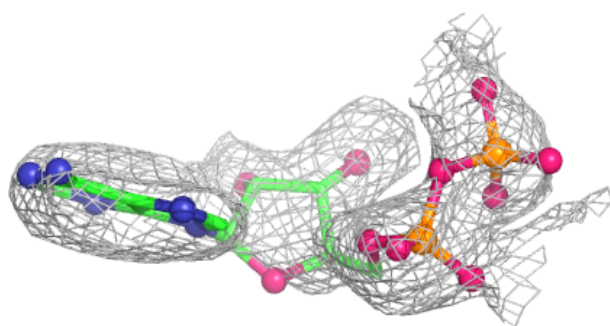
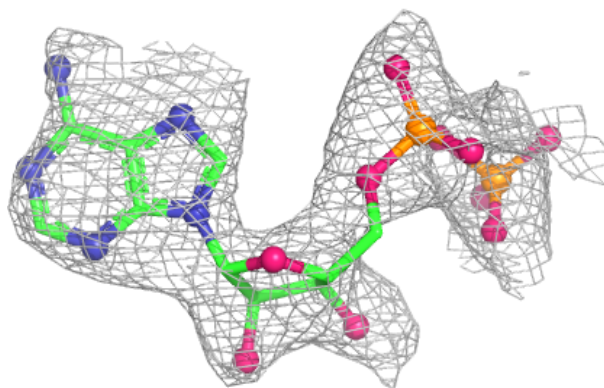


Electron density around ADP L 201:

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

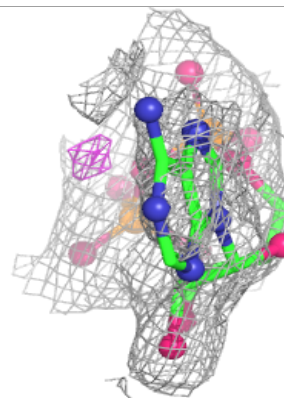
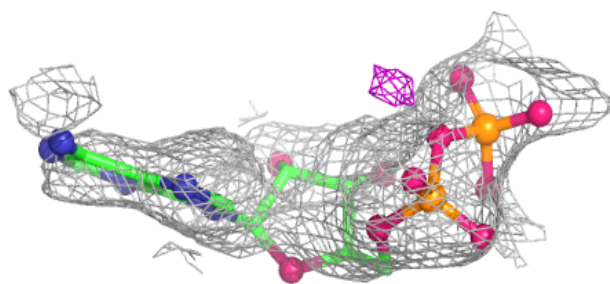
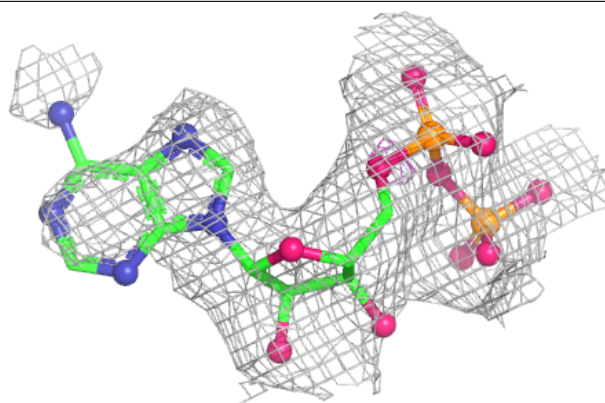
**Electron density around ADP M 201:**

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

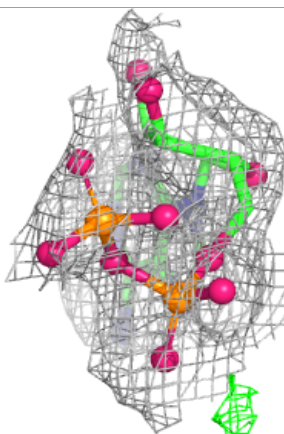
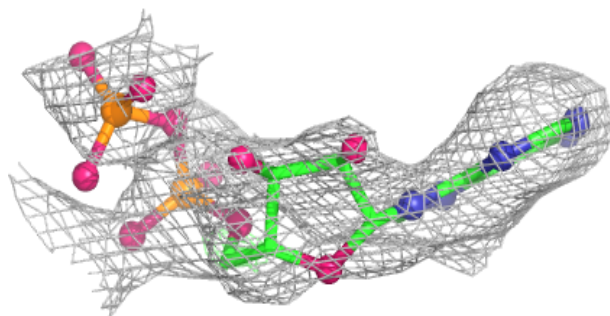
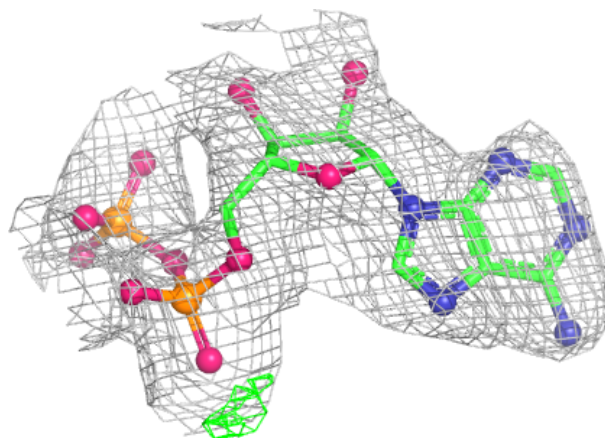


Electron density around ADP P 201:

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

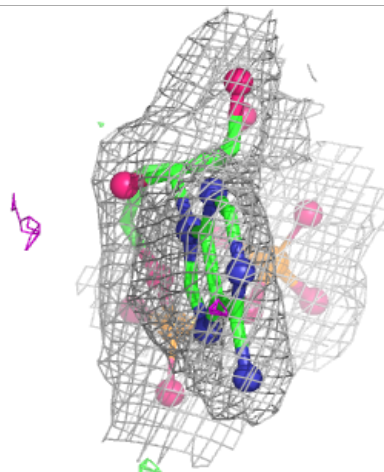
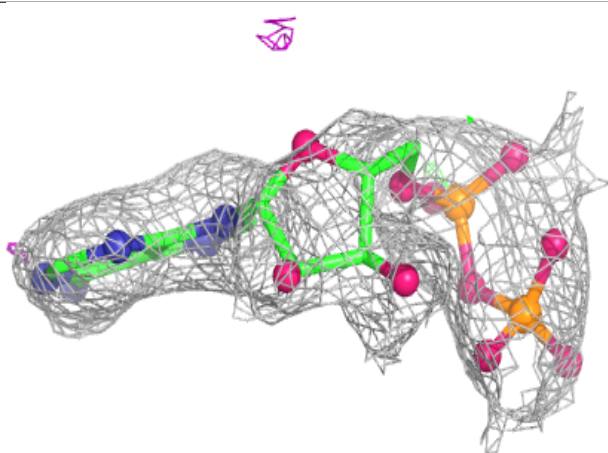
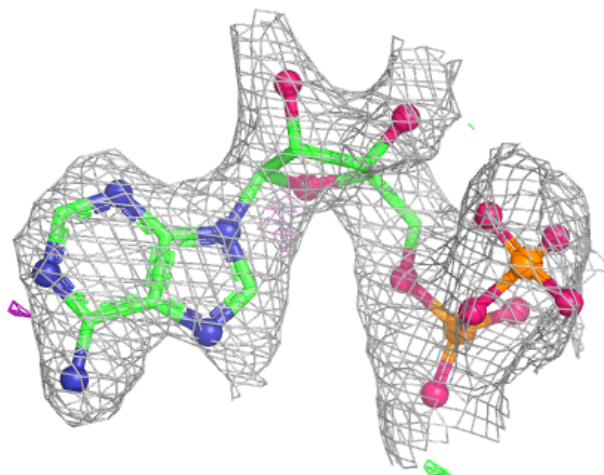
**Electron density around ADP Q 201:**

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



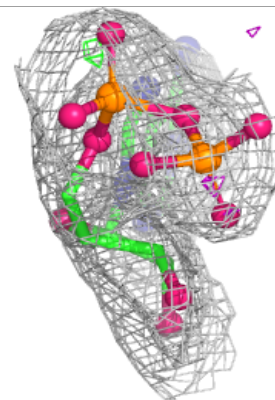
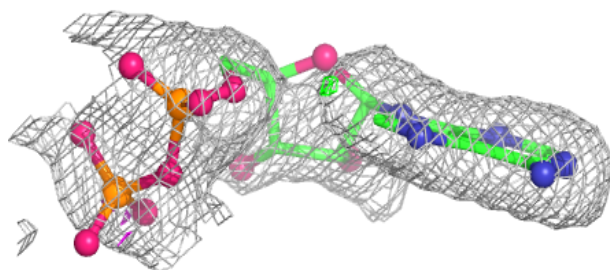
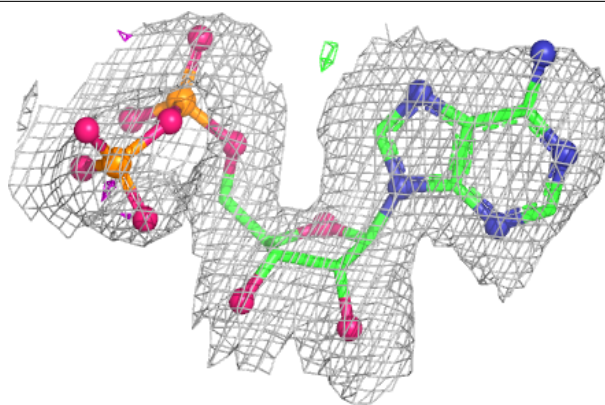
Electron density around ADP T 201:

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

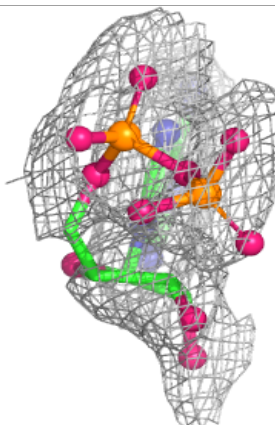
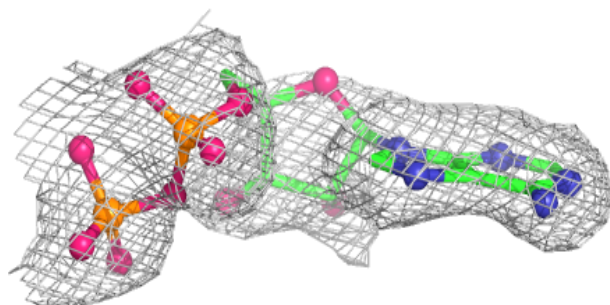
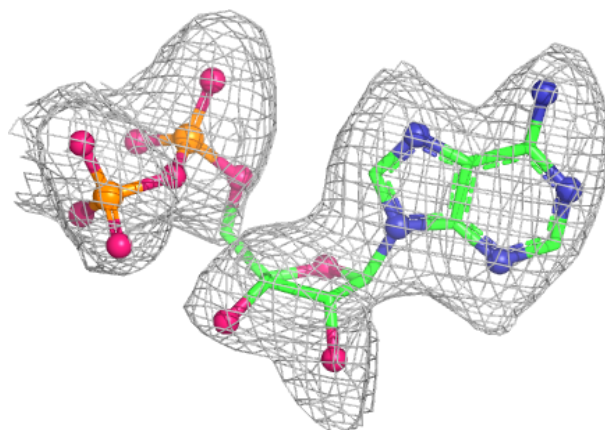


Electron density around ADP f 201:

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

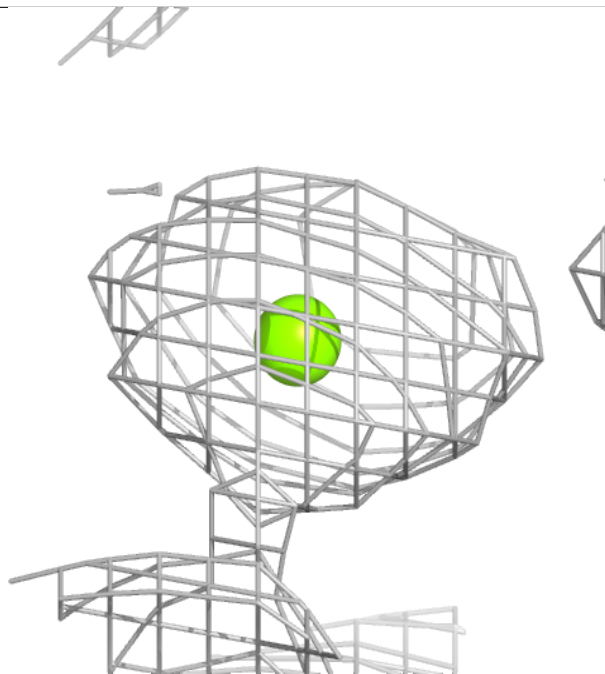
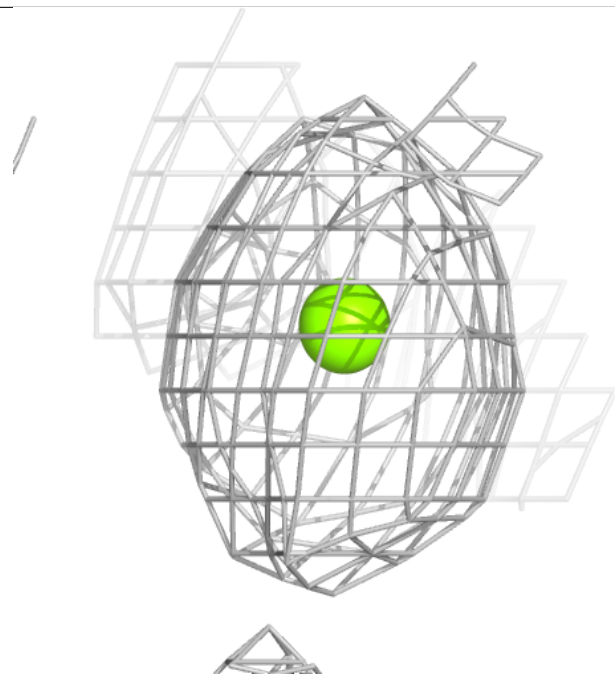
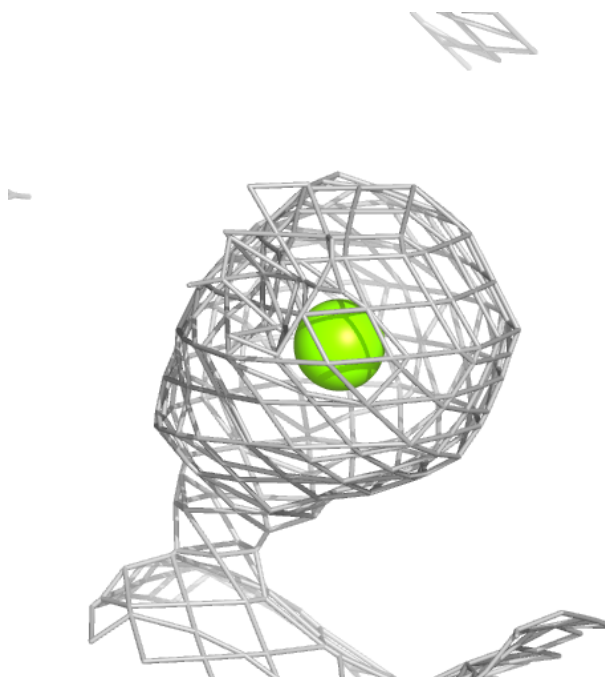
**Electron density around ADP h 201:**

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



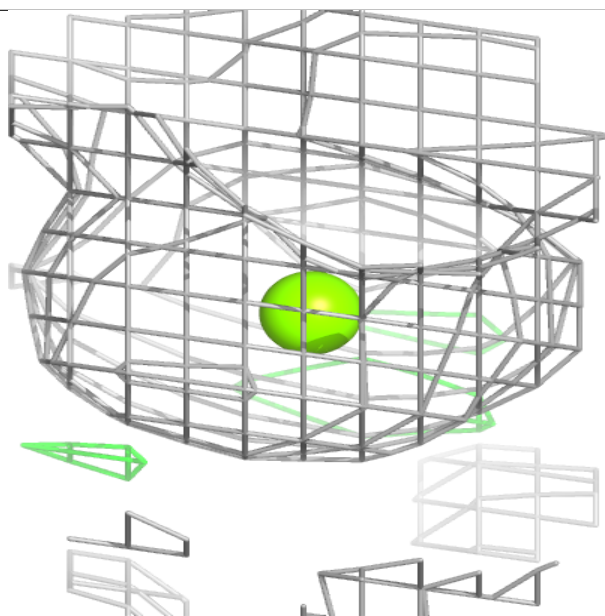
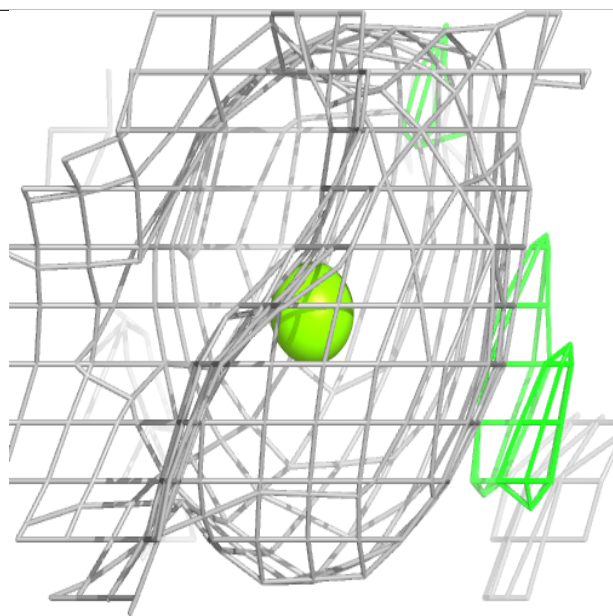
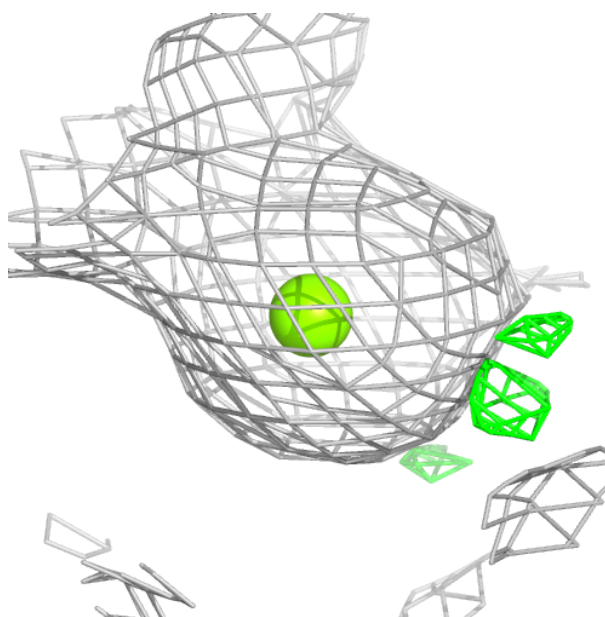
Electron density around MG C 202:

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



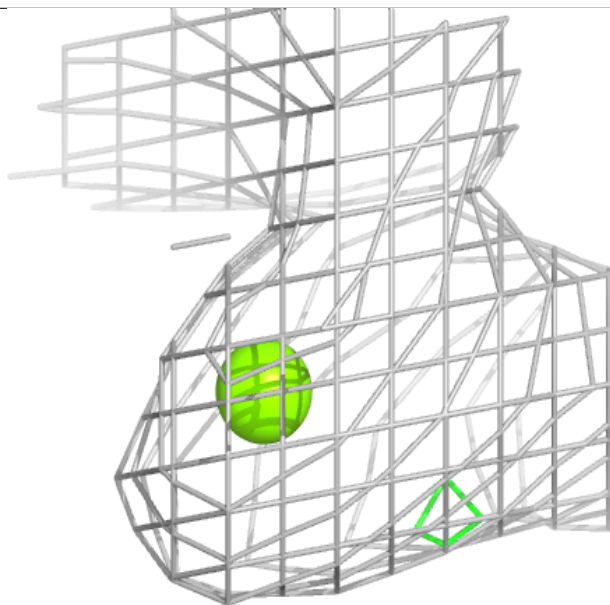
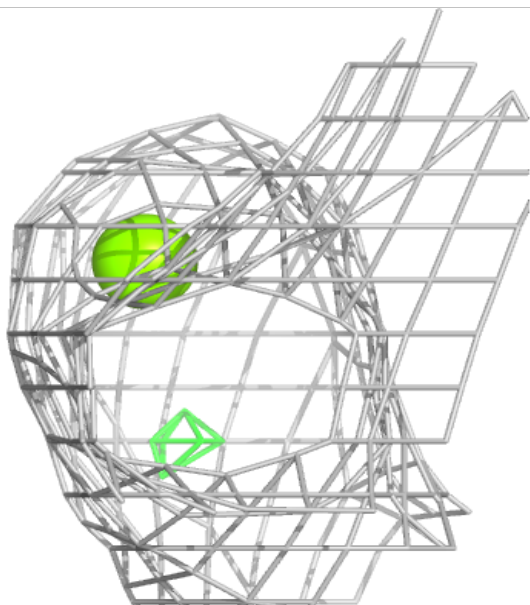
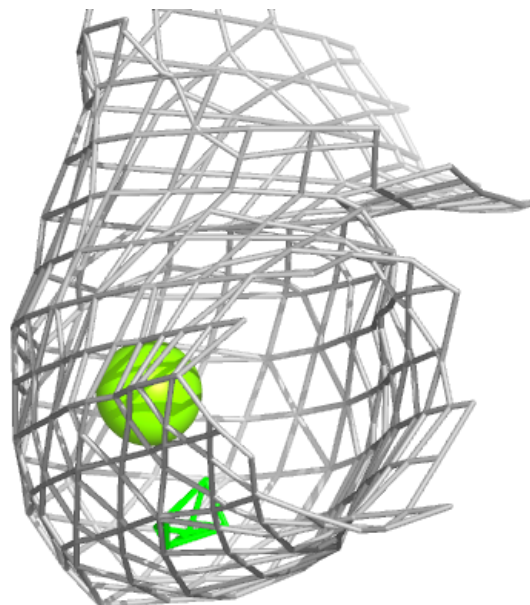
Electron density around MG E 202:

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



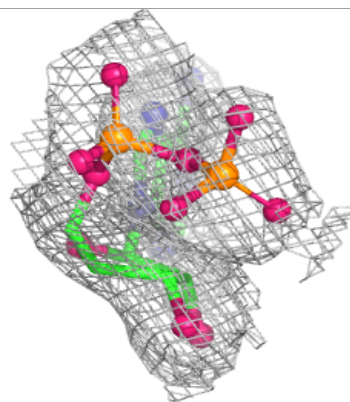
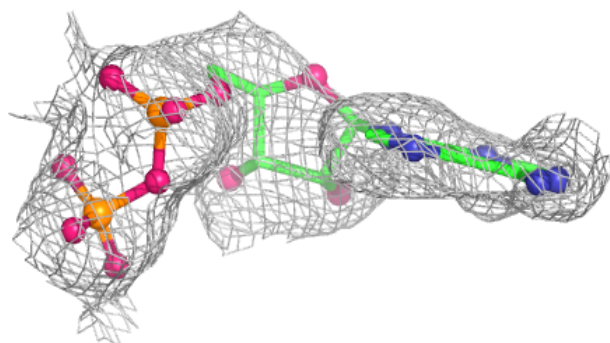
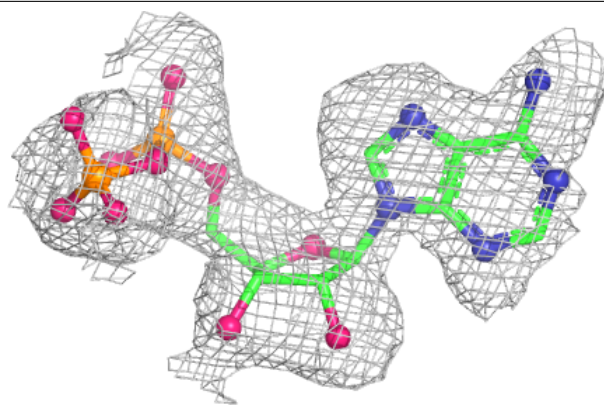
Electron density around MG G 202:

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



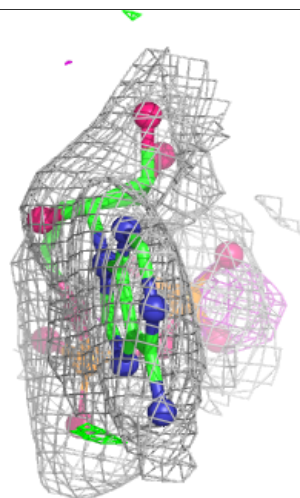
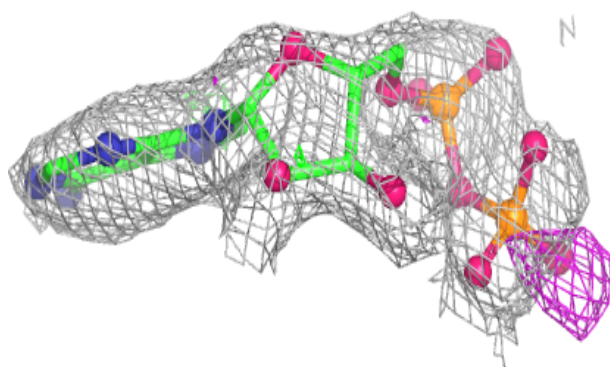
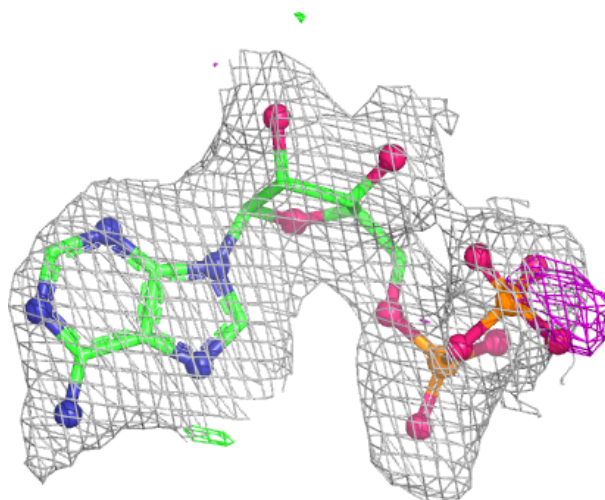
Electron density around ADP B 201:

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



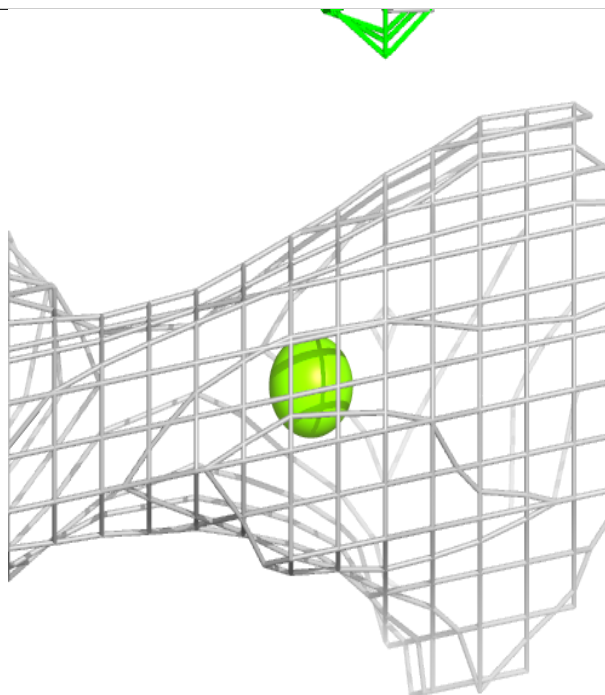
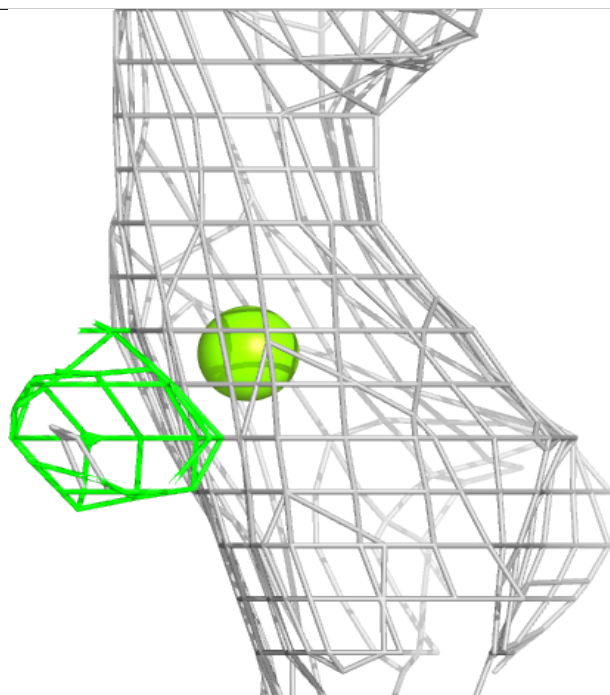
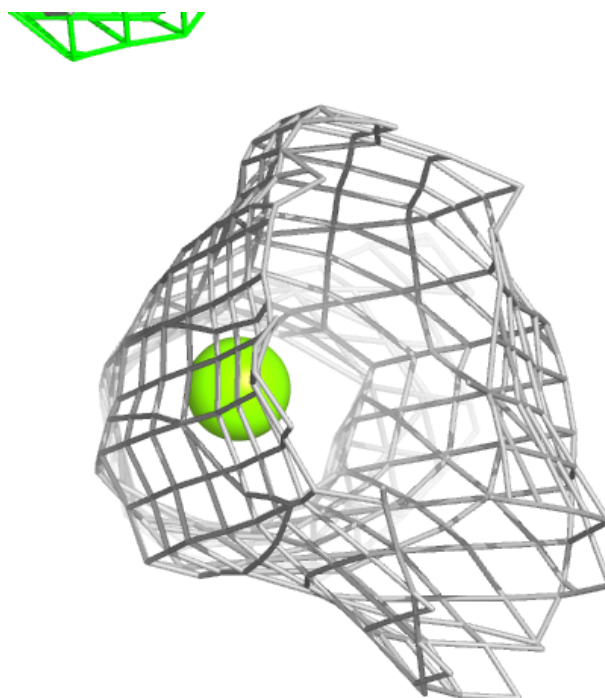
Electron density around ADP H 201:

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



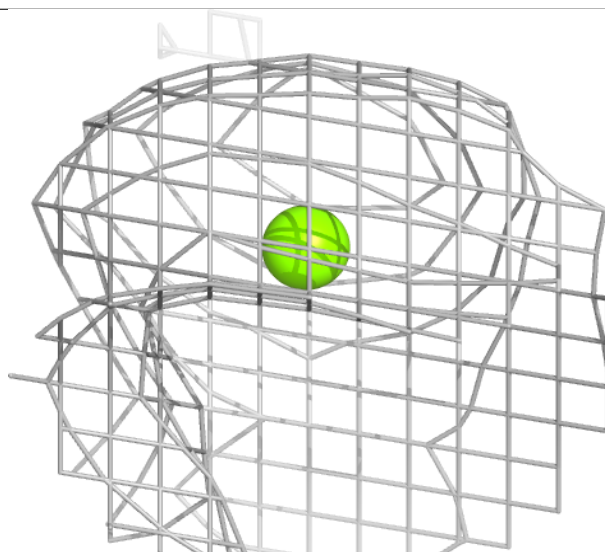
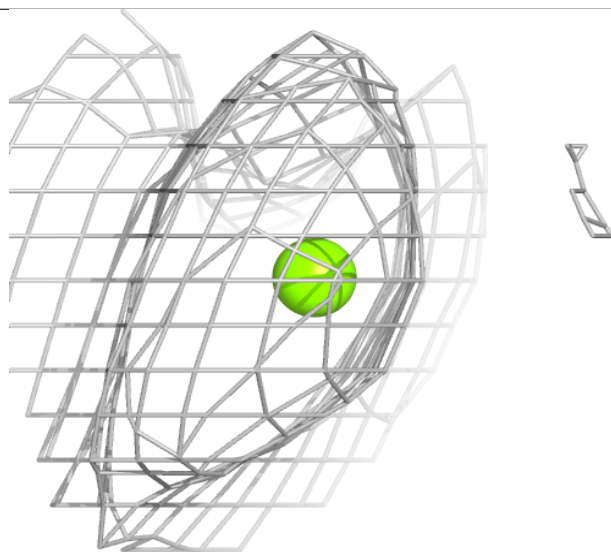
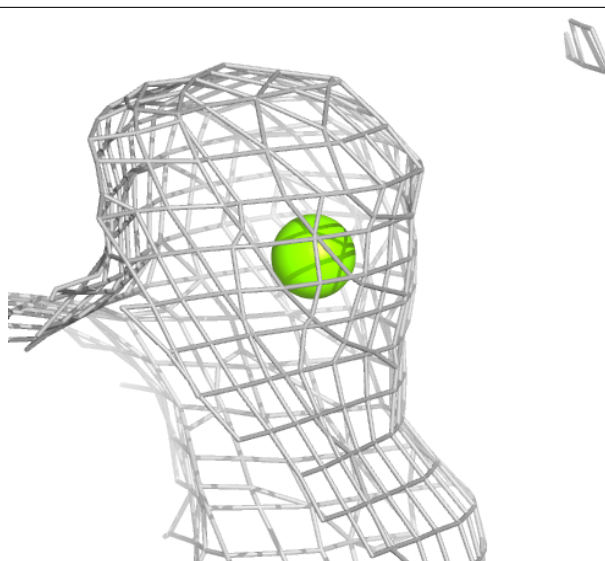
Electron density around MG Z 202:

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



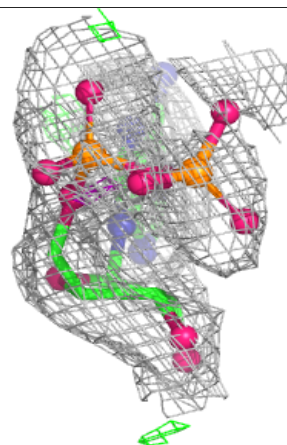
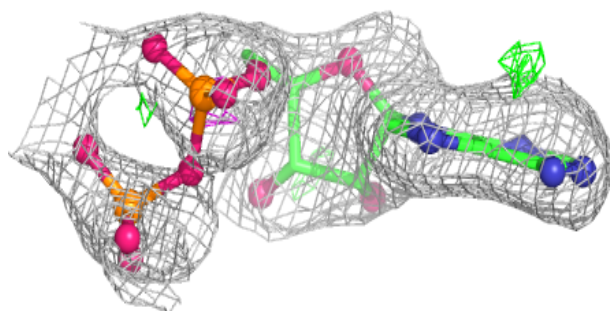
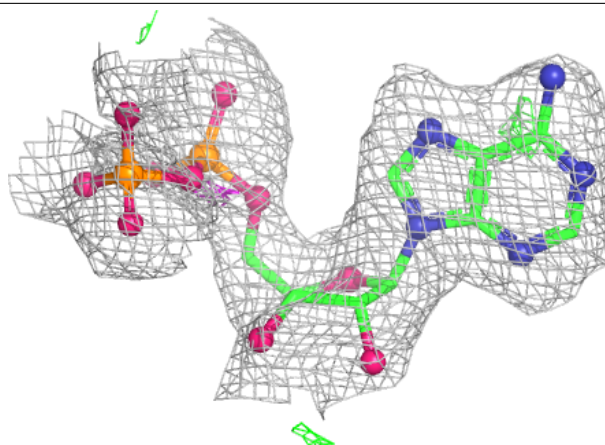
Electron density around MG c 202:

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

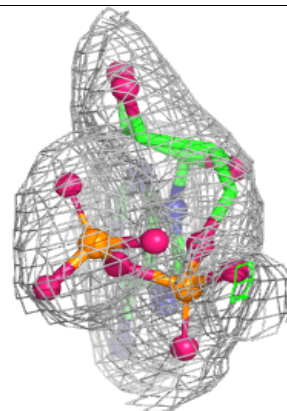
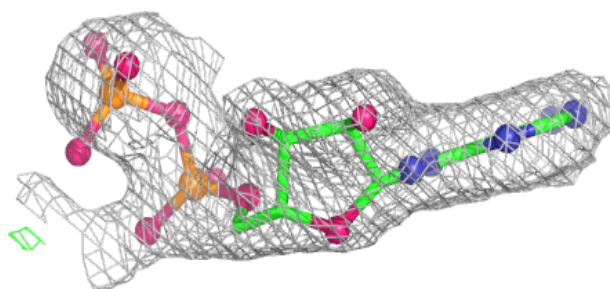
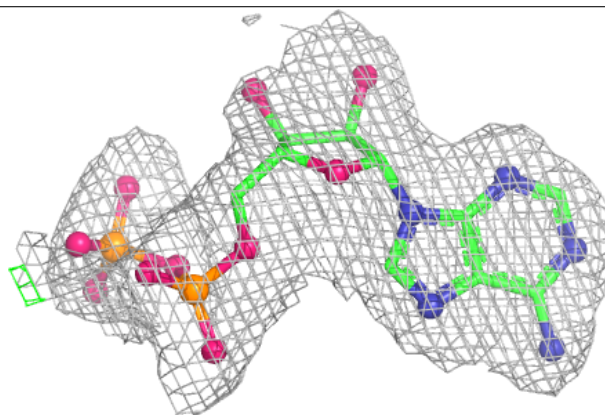


Electron density around ADP J 201:

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

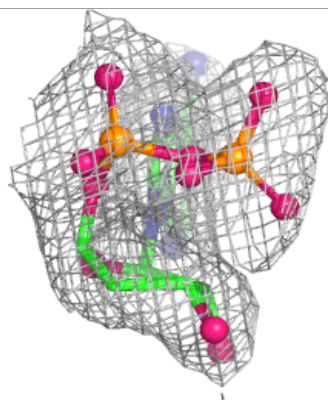
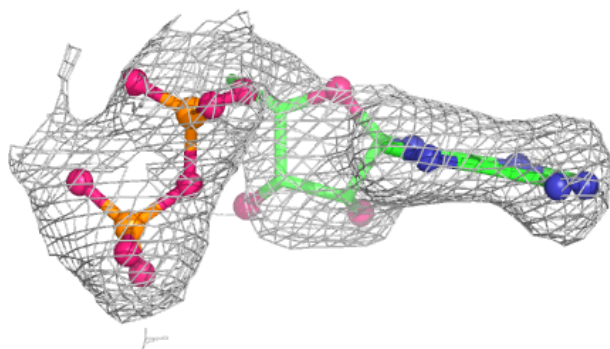
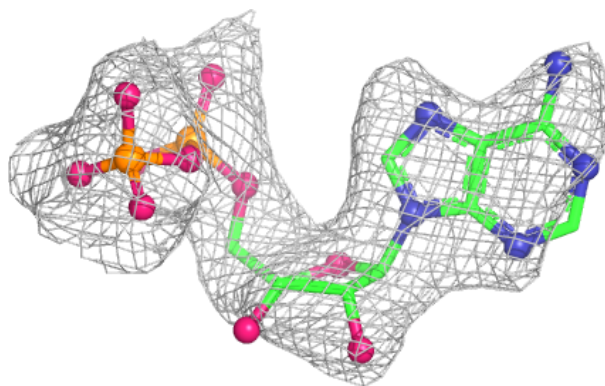
**Electron density around ADP S 201:**

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

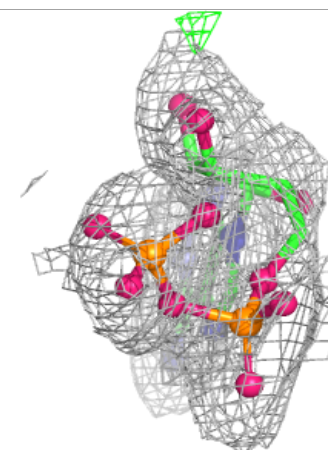
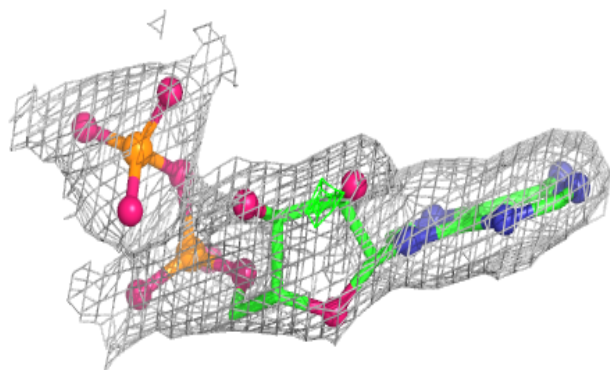
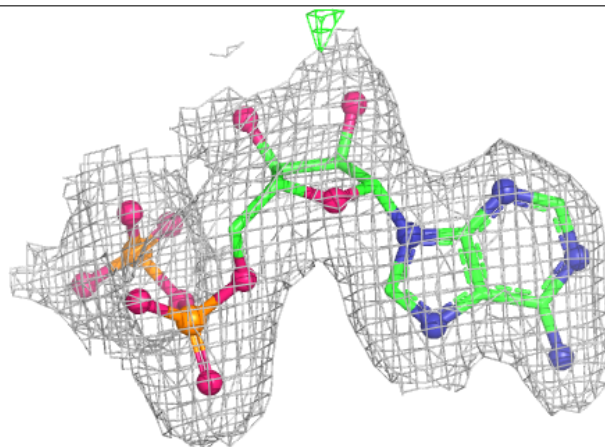


Electron density around ADP A 201:

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

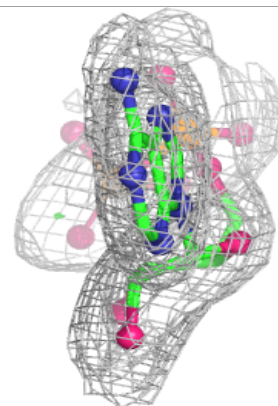
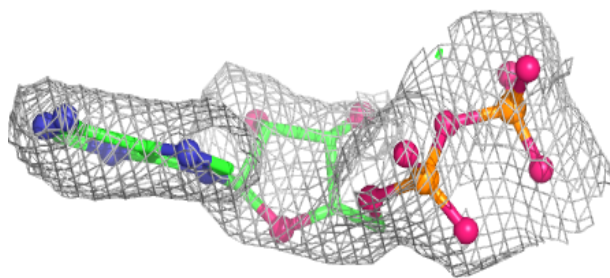
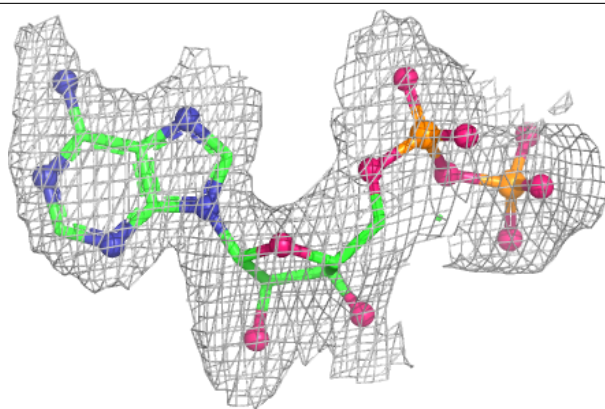
**Electron density around ADP U 201:**

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



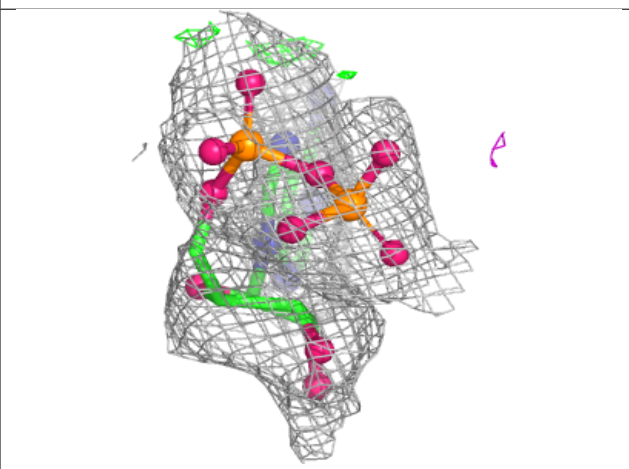
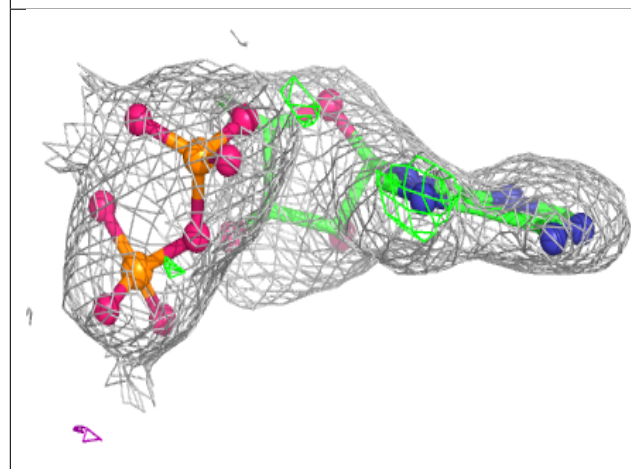
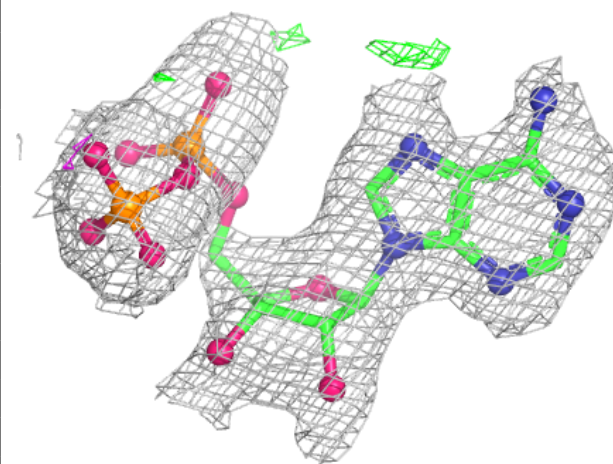
Electron density around ADP V 201:

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



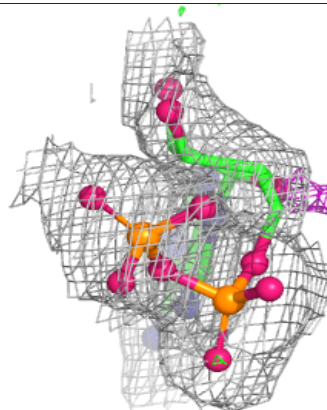
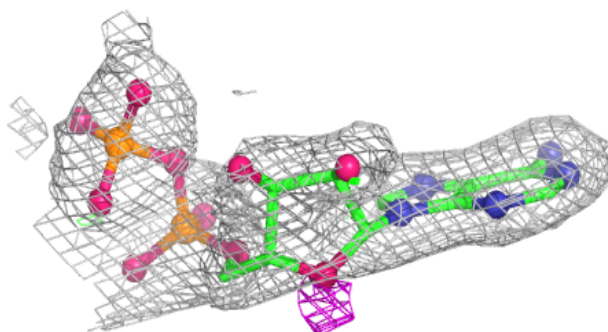
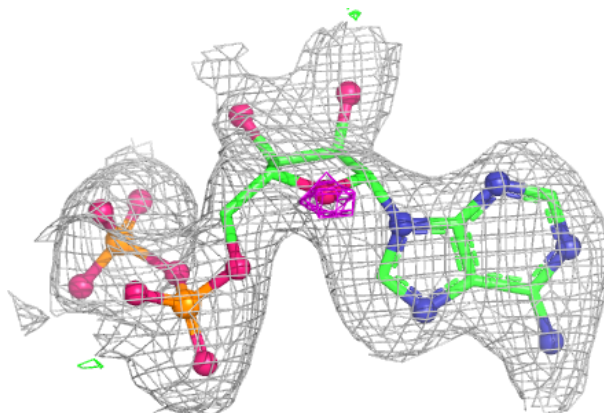
Electron density around ADP W 201:

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

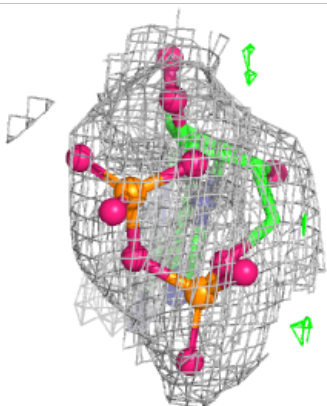
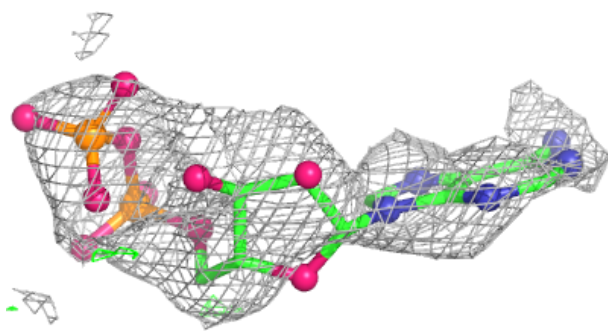
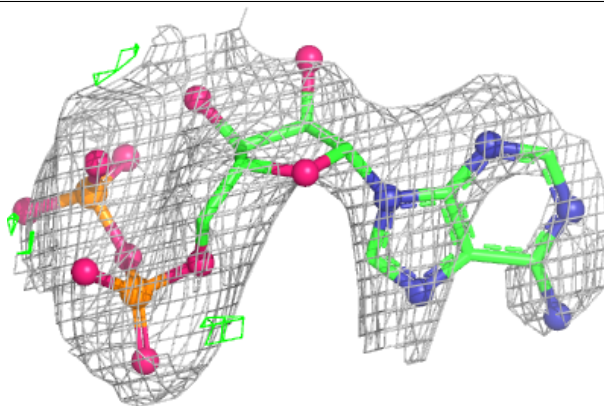


Electron density around ADP X 201:

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

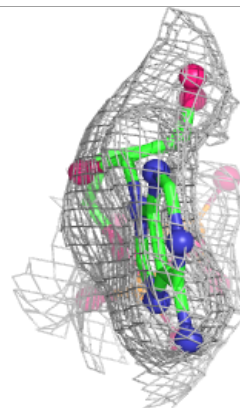
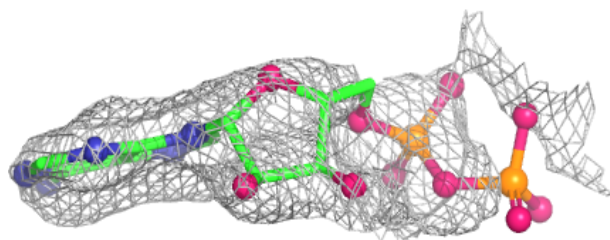
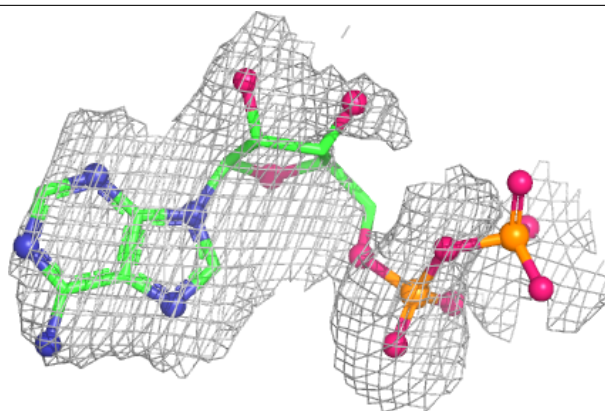
**Electron density around ADP Y 201:**

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

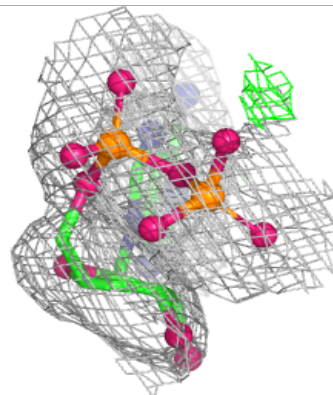
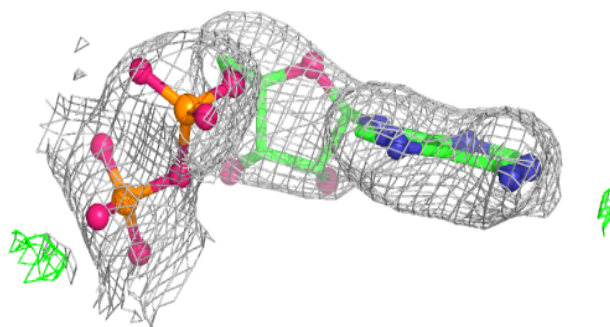
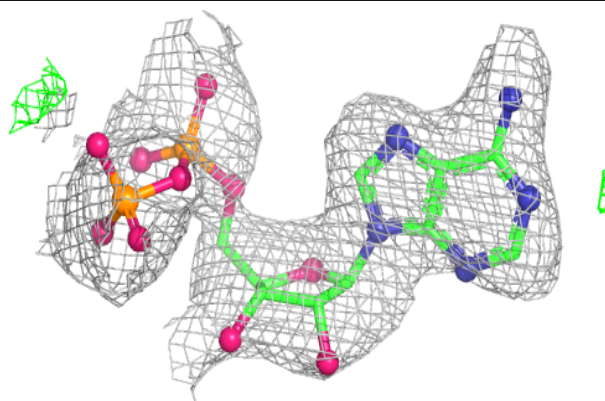


Electron density around ADP Z 201:

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

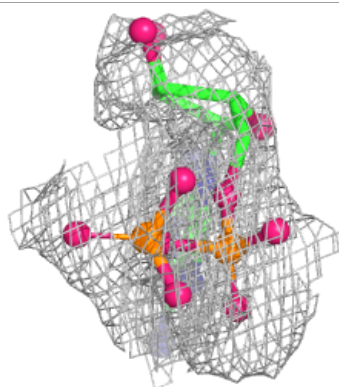
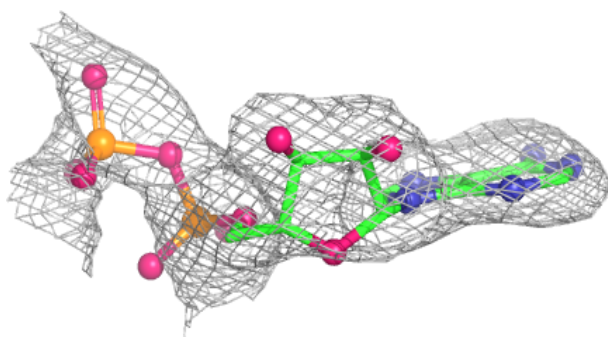
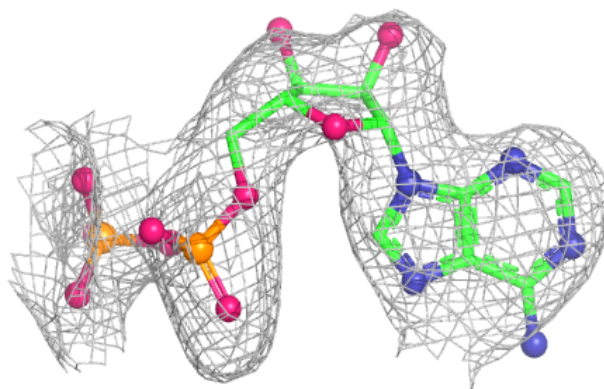
**Electron density around ADP a 201:**

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

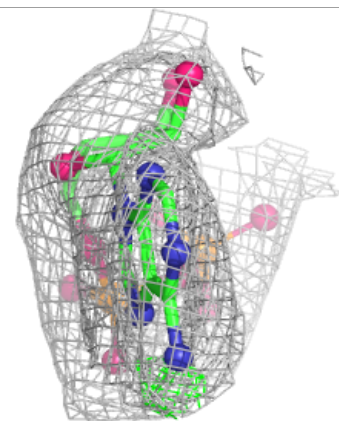
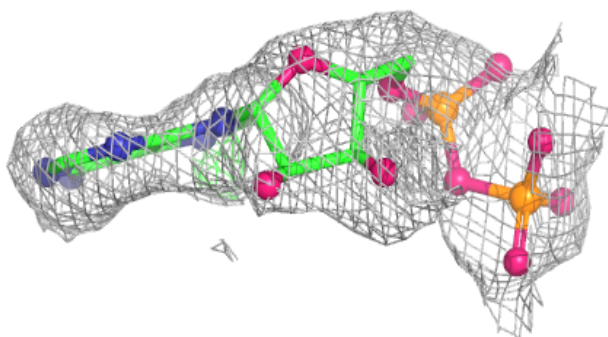
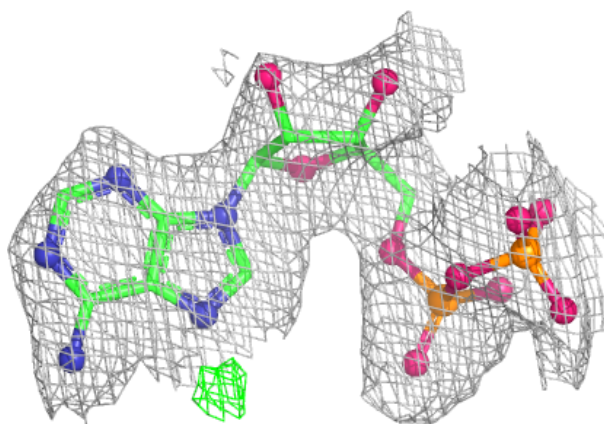


Electron density around ADP b 201:

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

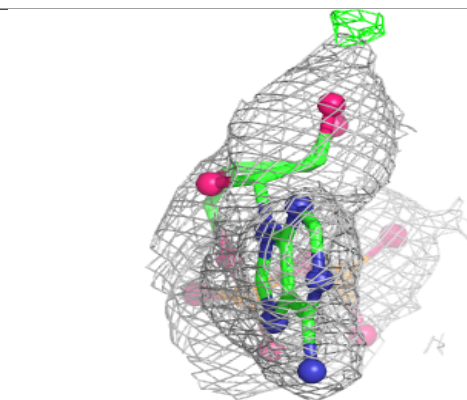
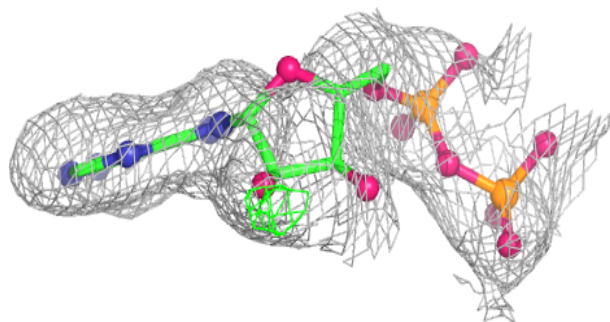
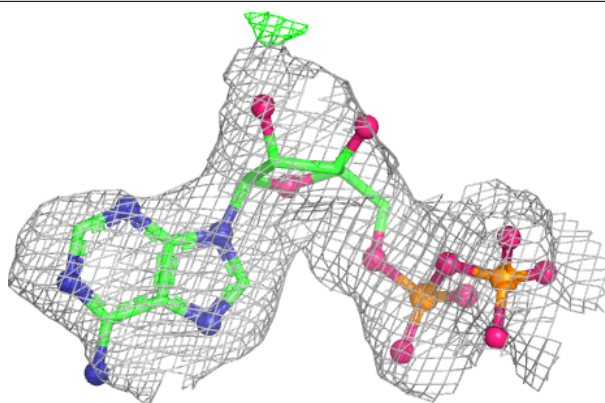
**Electron density around ADP c 201:**

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

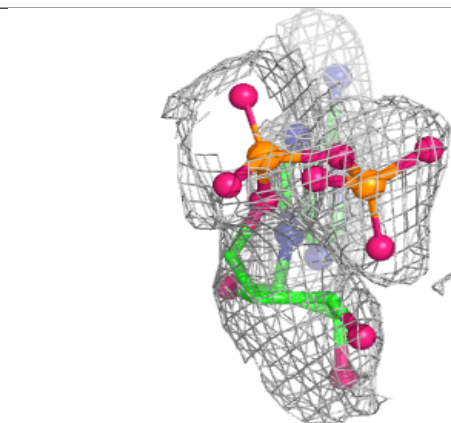
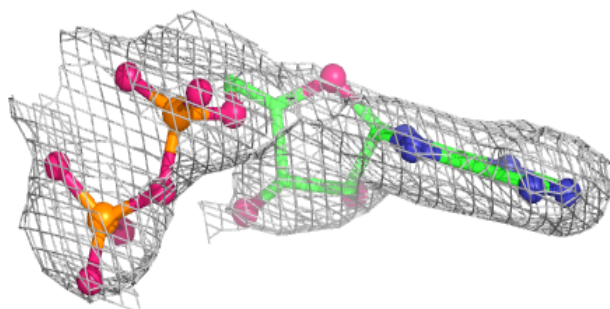
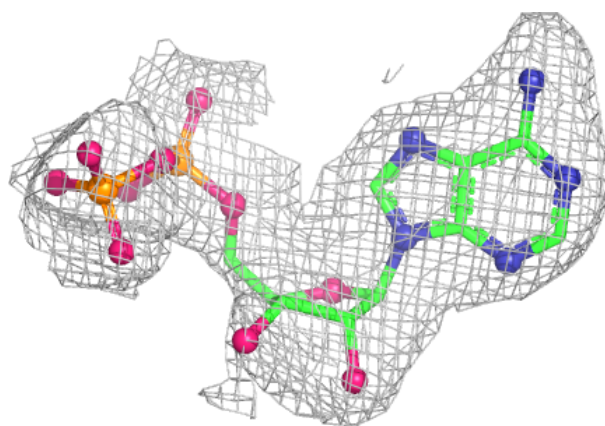


Electron density around ADP d 201:

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

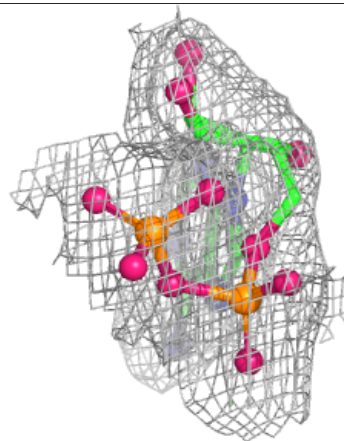
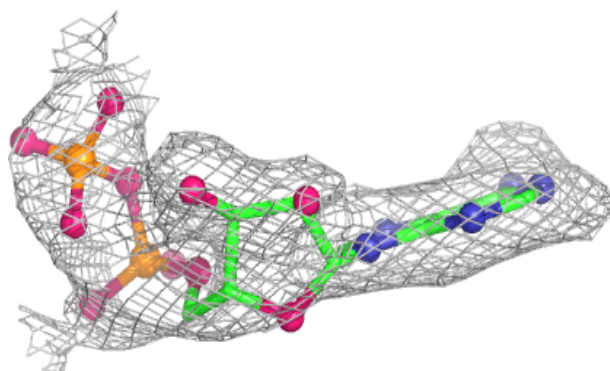
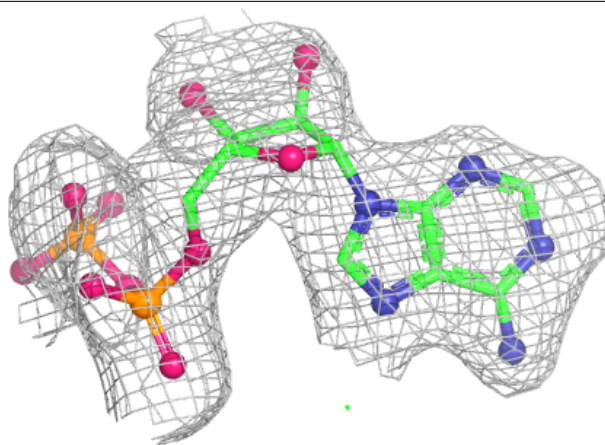
**Electron density around ADP e 201:**

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



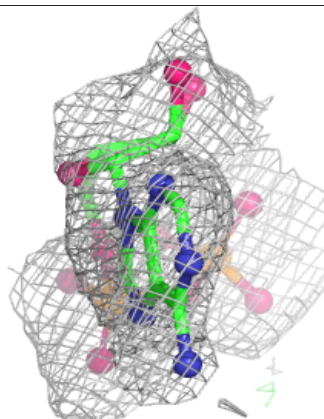
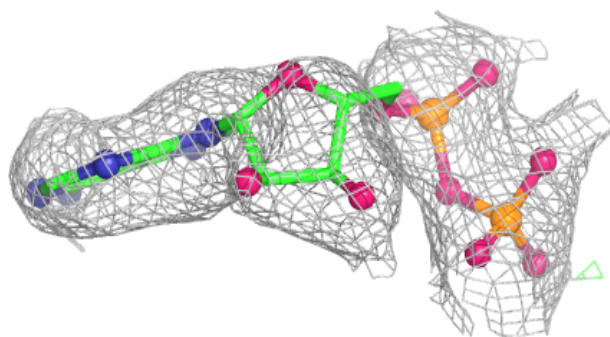
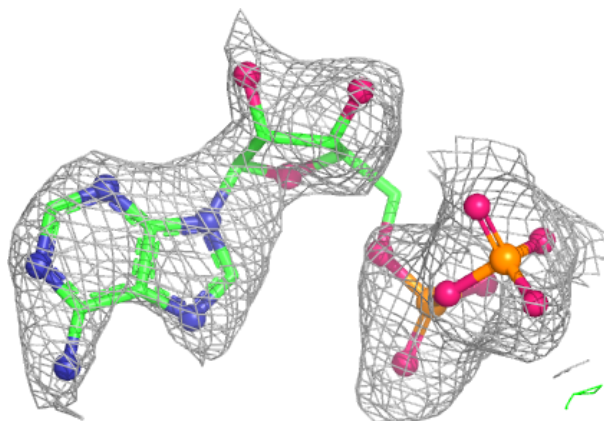
Electron density around ADP I 201:

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

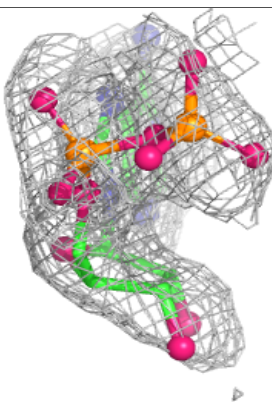
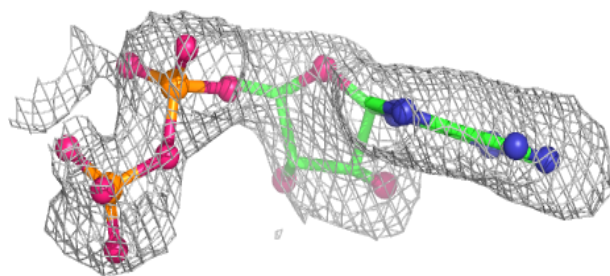
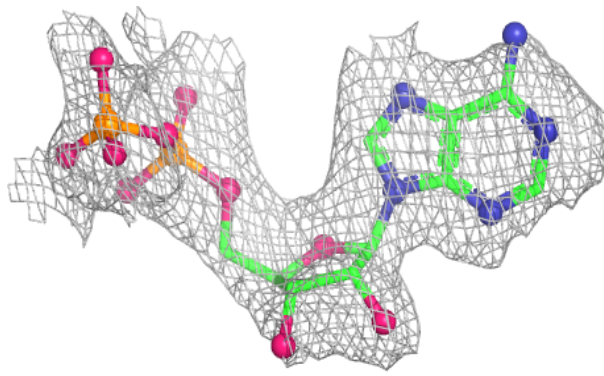


Electron density around ADP g 201:

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

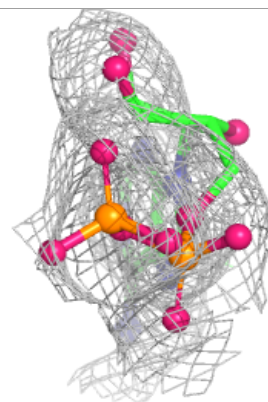
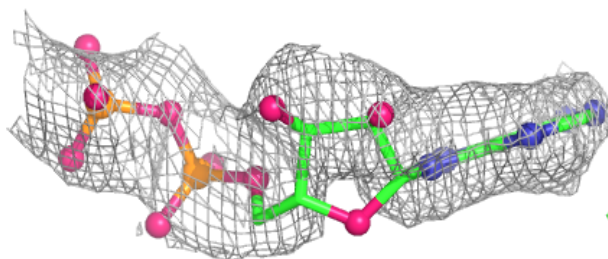
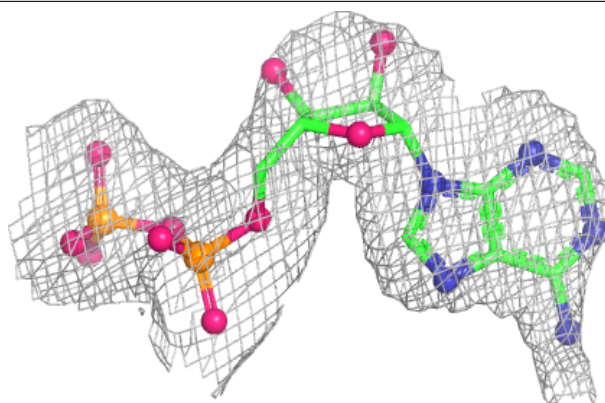
**Electron density around ADP C 201:**

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

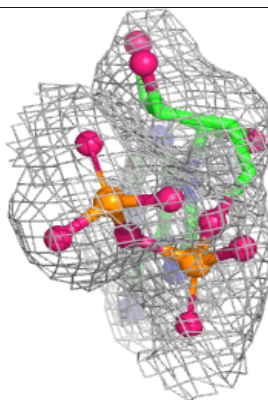
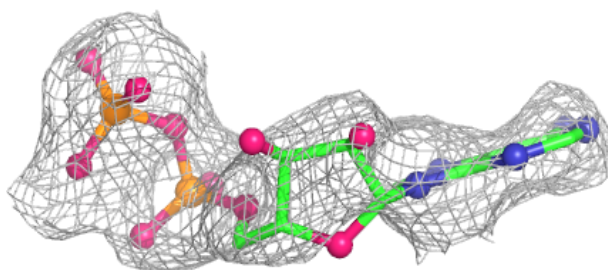
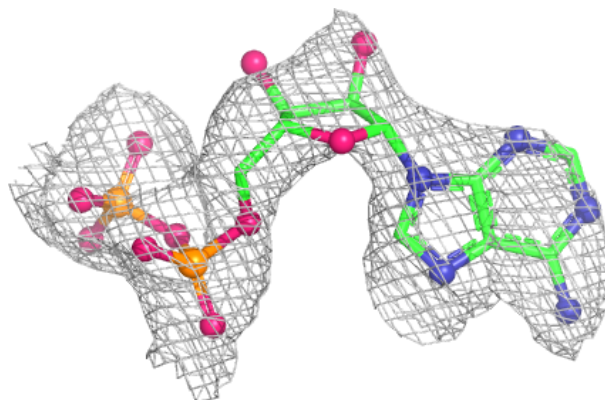


Electron density around ADP i 201:

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

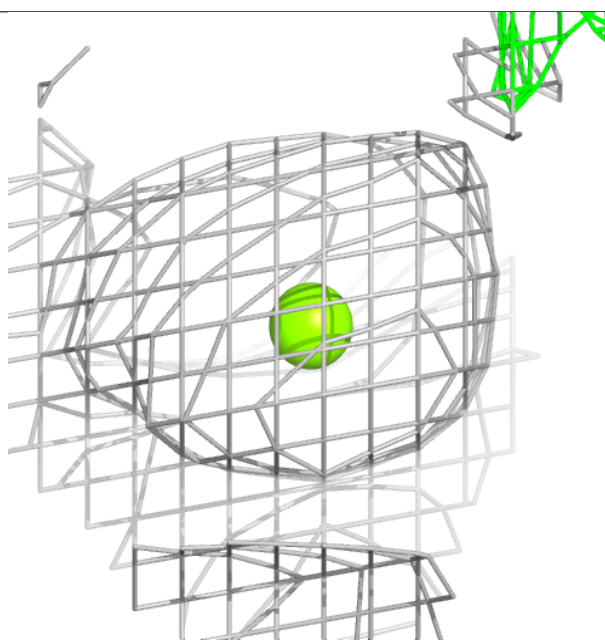
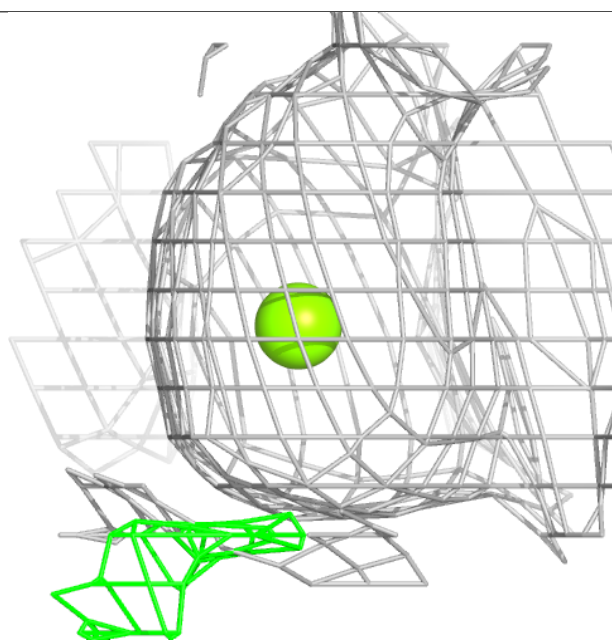
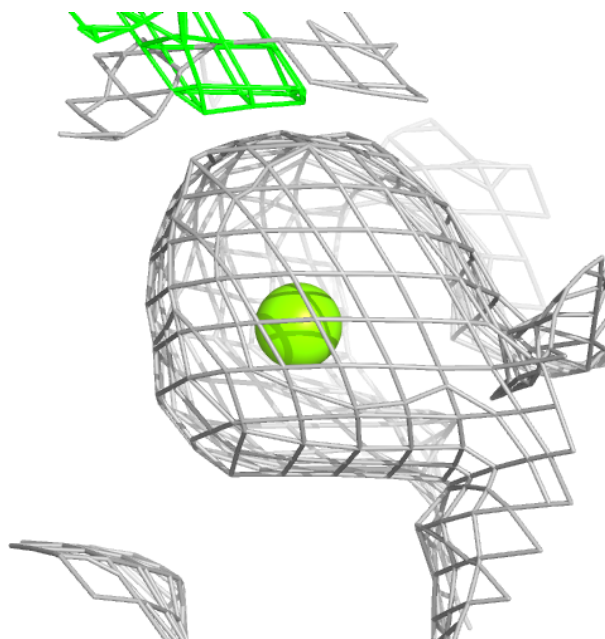
**Electron density around ADP j 201:**

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



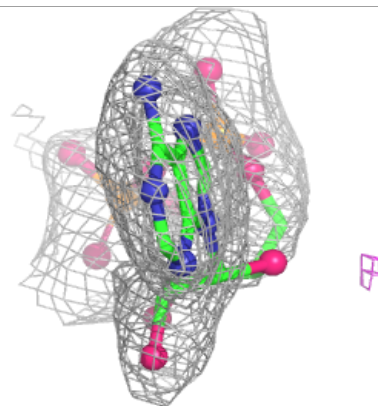
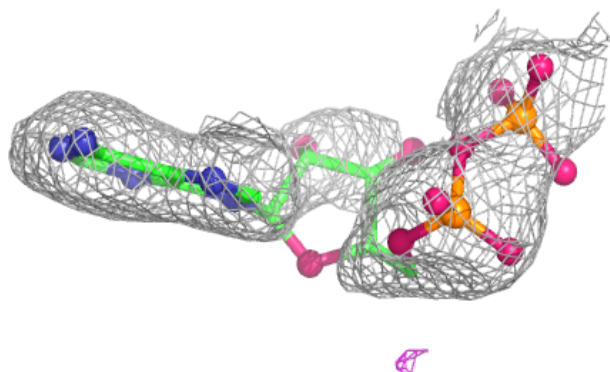
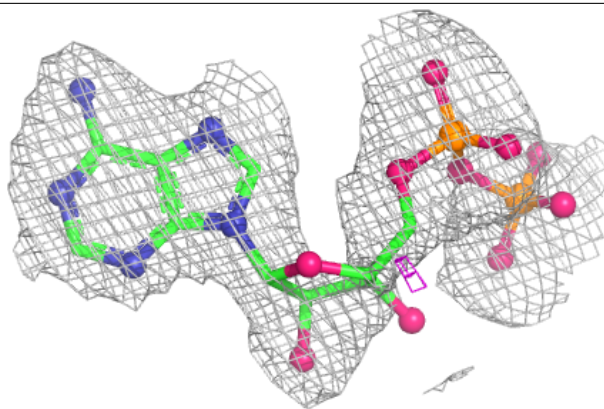
Electron density around MG B 202:

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



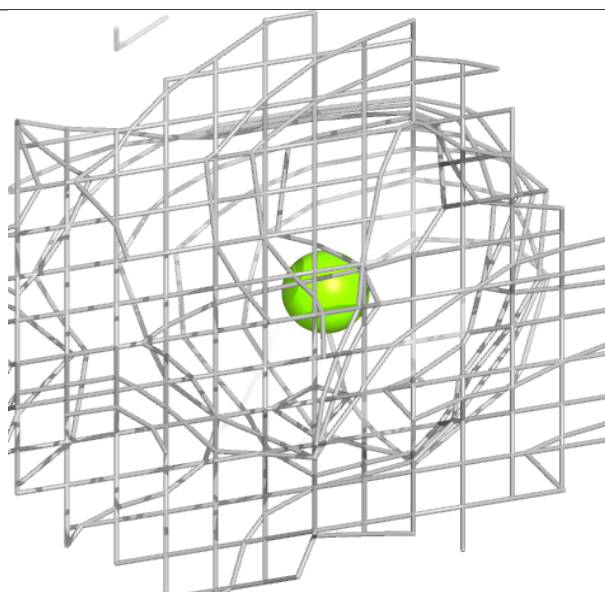
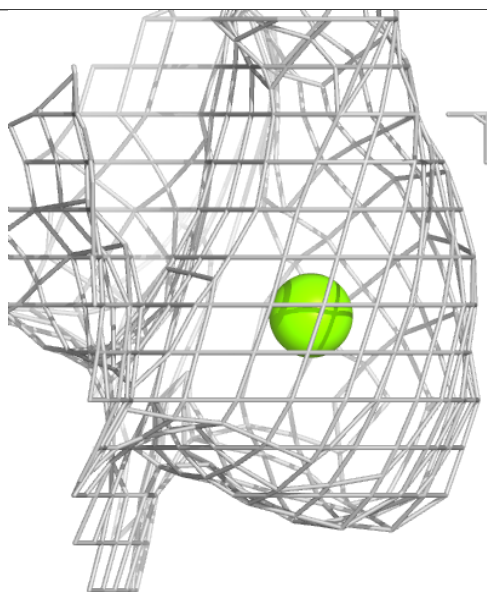
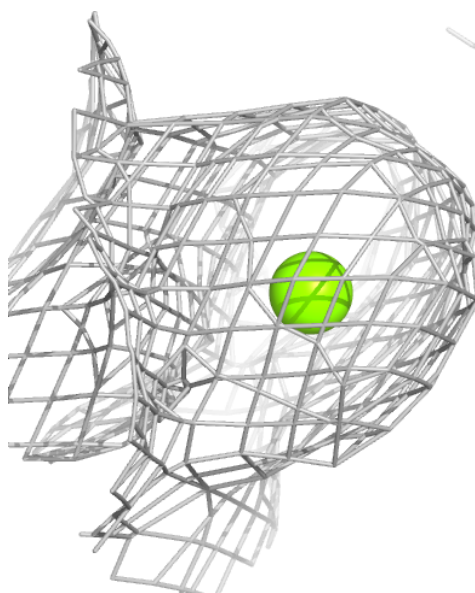
Electron density around ADP K 201:

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



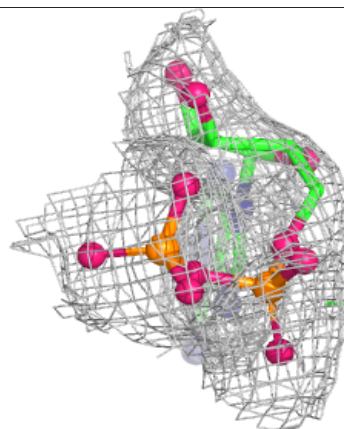
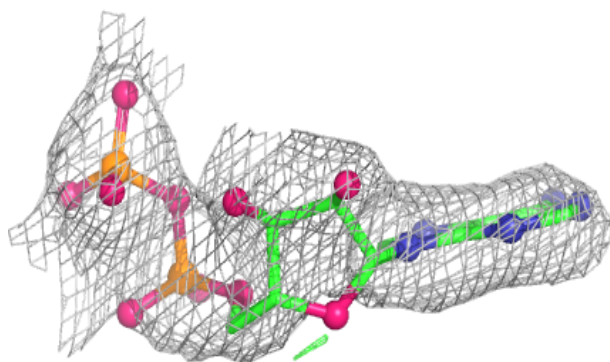
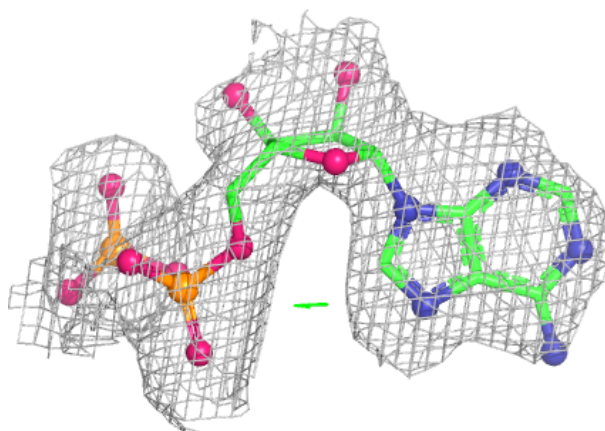
Electron density around MG D 202:

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



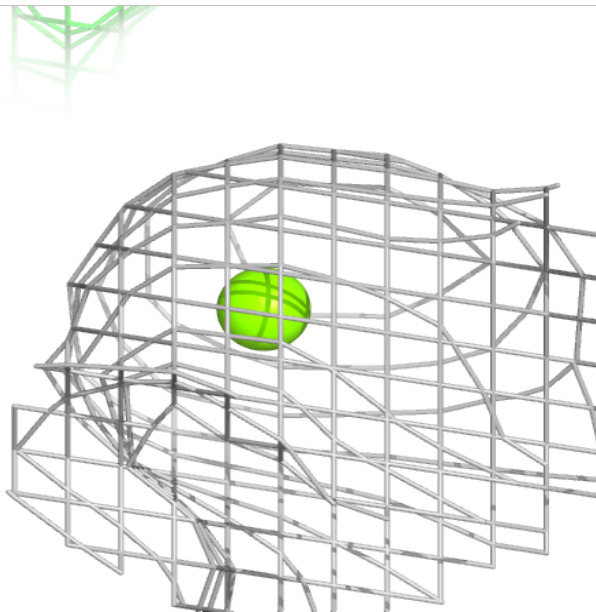
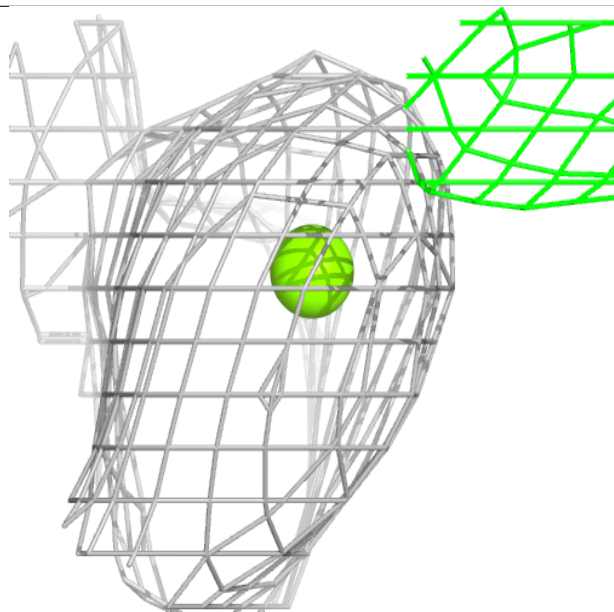
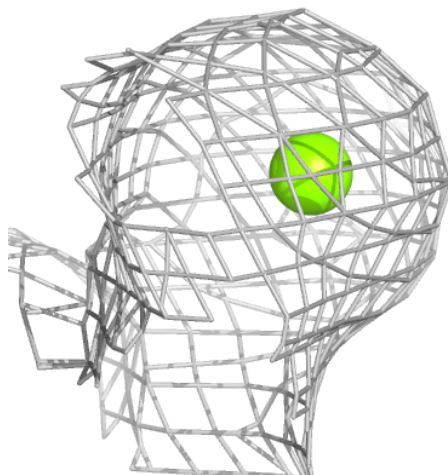
Electron density around ADP D 201:

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



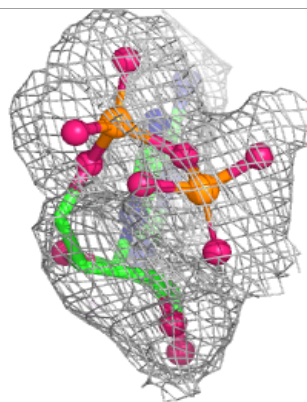
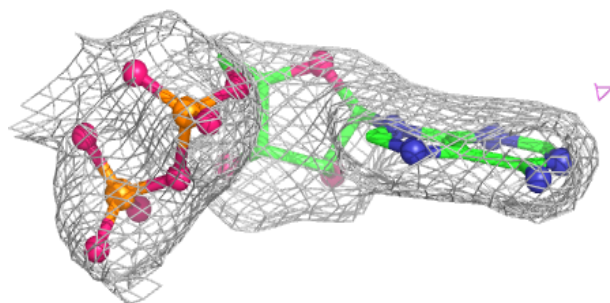
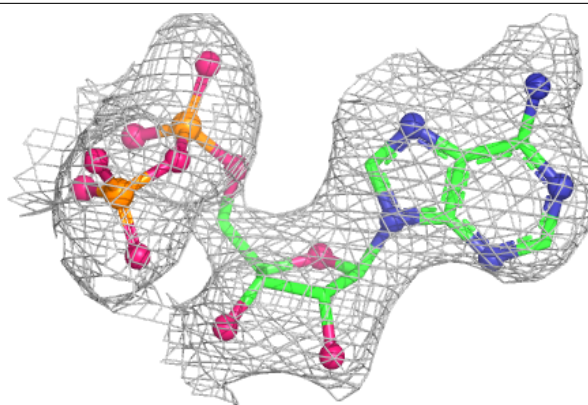
Electron density around MG F 202:

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



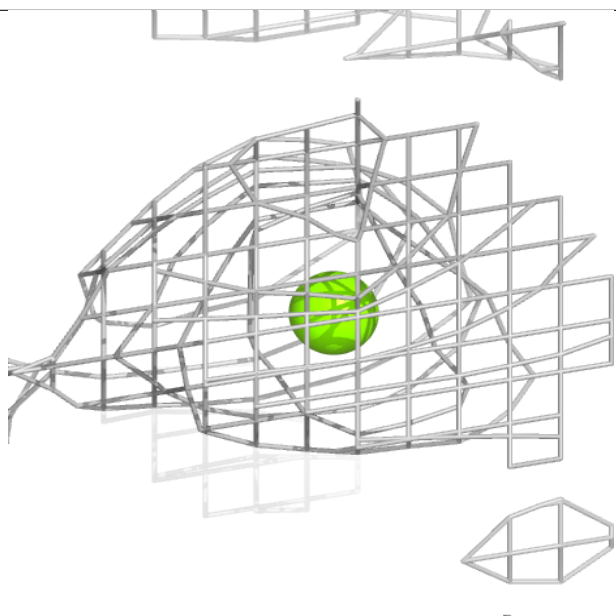
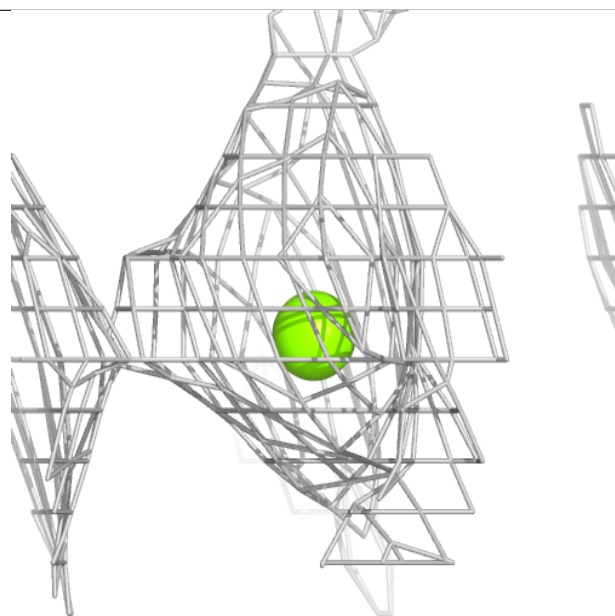
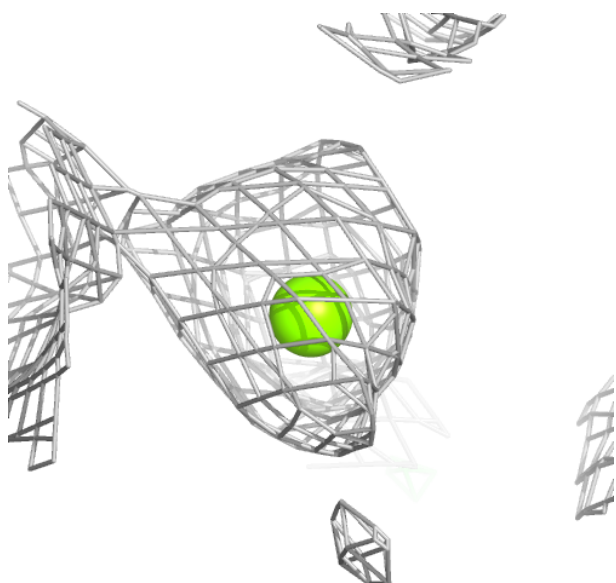
Electron density around ADP E 201:

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



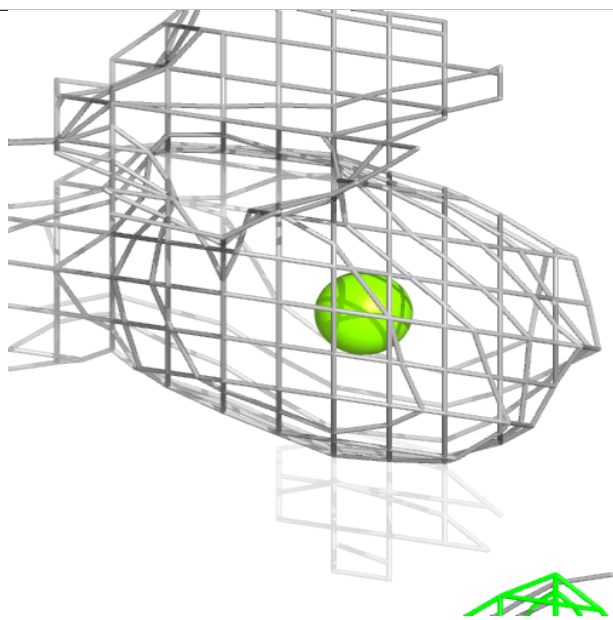
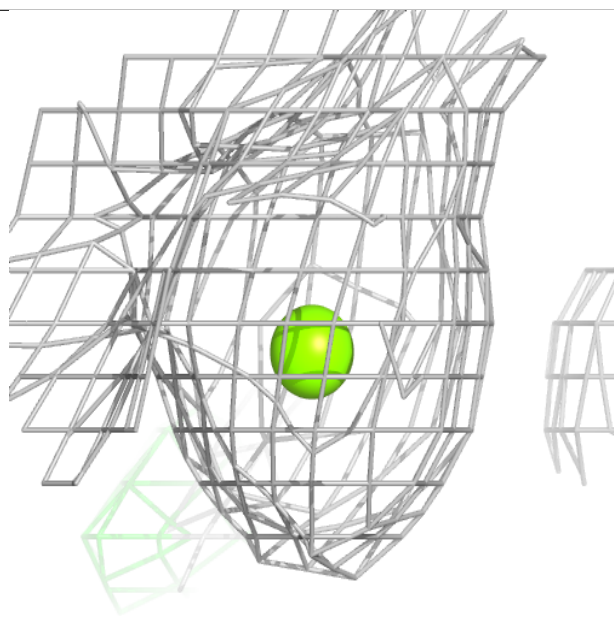
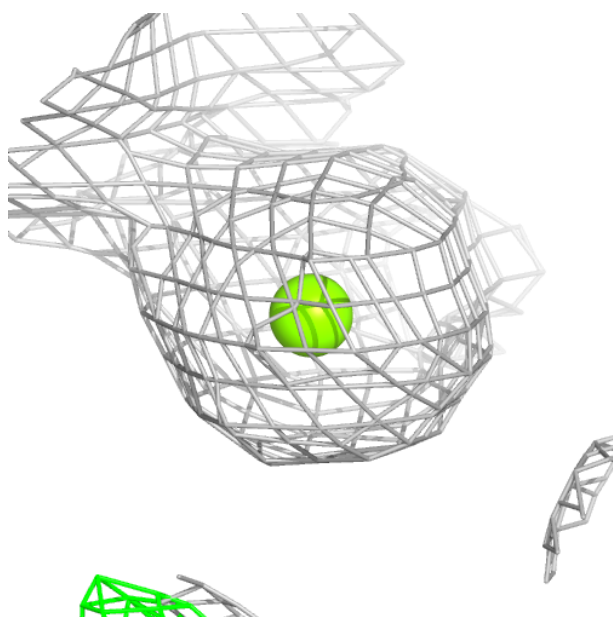
Electron density around MG I 202:

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



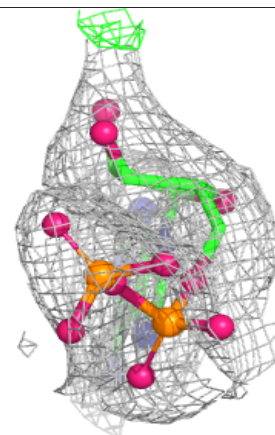
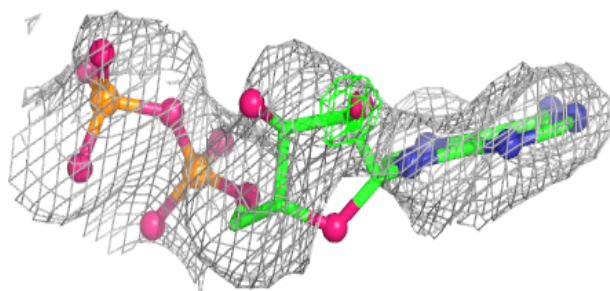
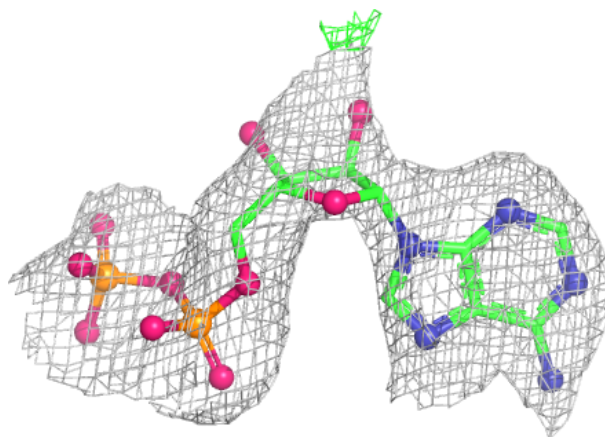
Electron density around MG M 202:

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



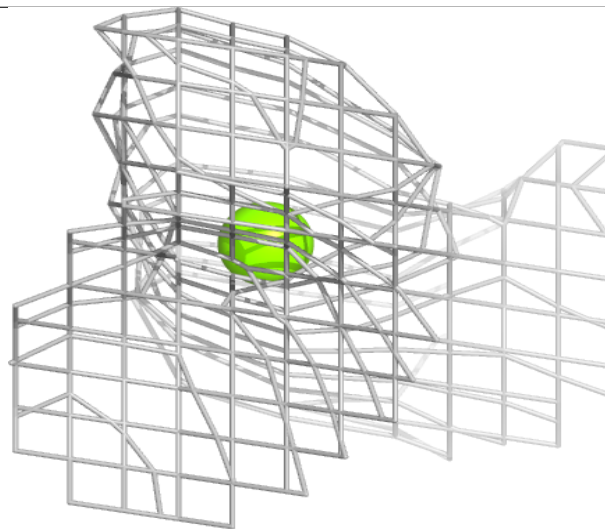
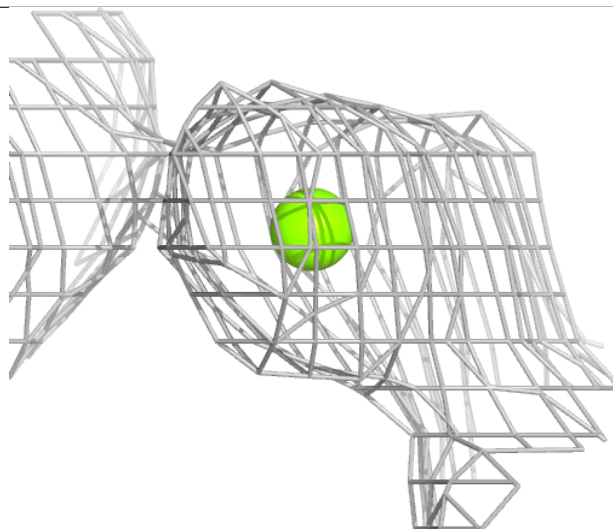
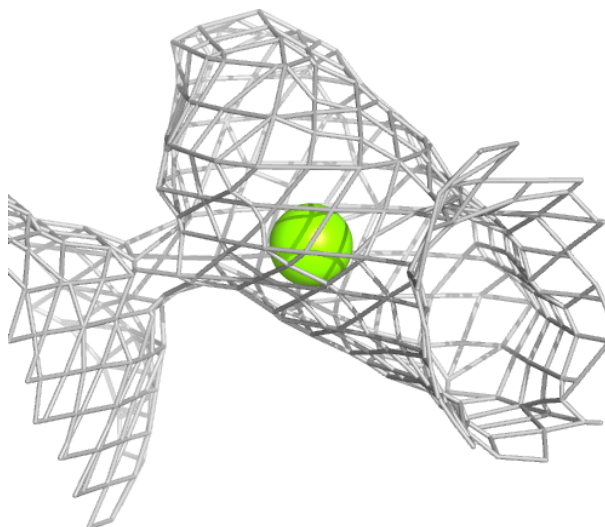
Electron density around ADP N 201:

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



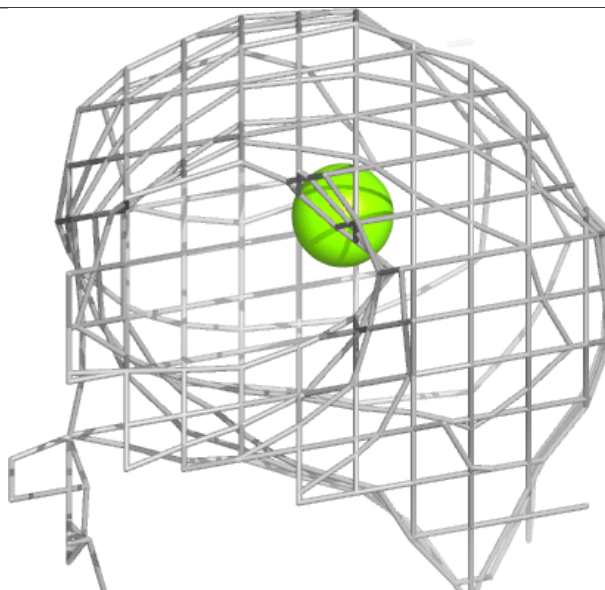
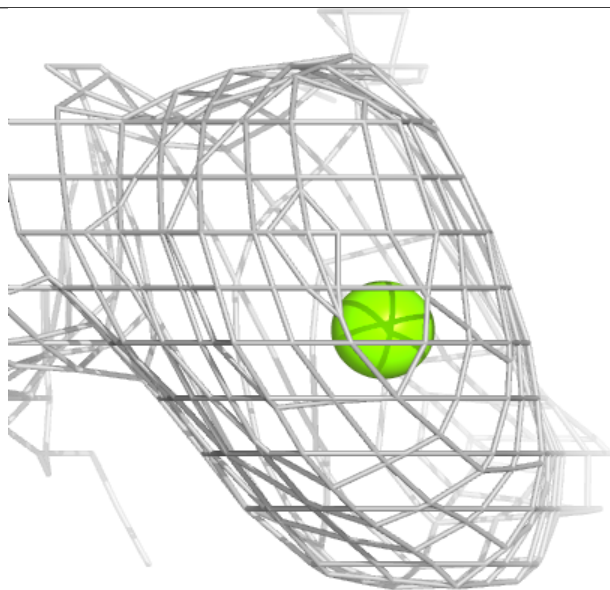
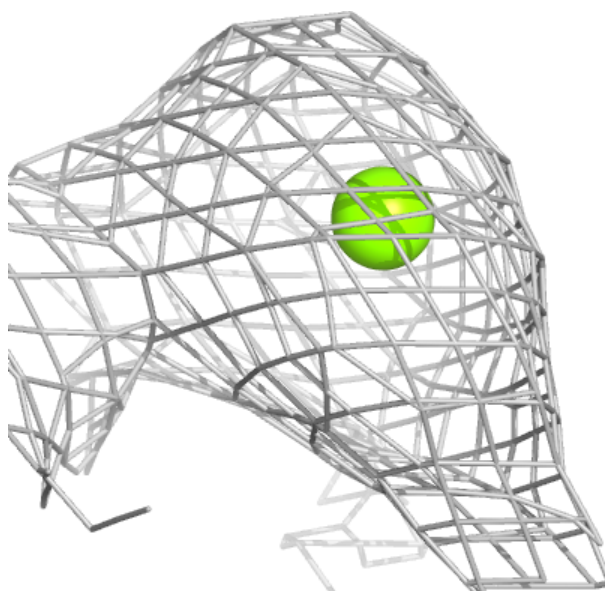
Electron density around MG P 202:

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



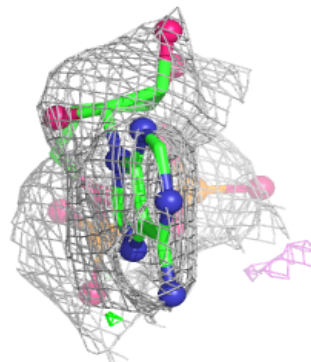
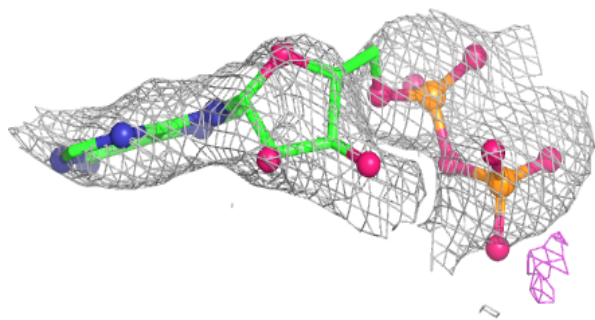
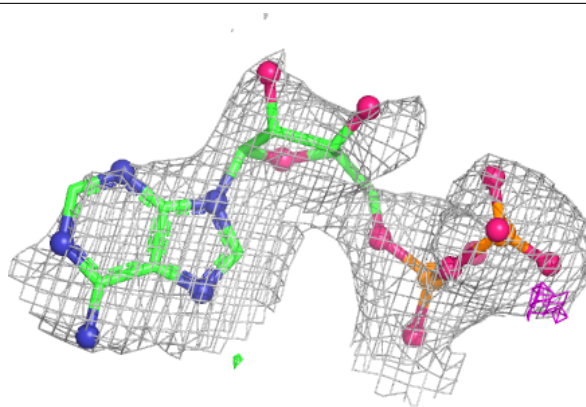
Electron density around MG Q 202:

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



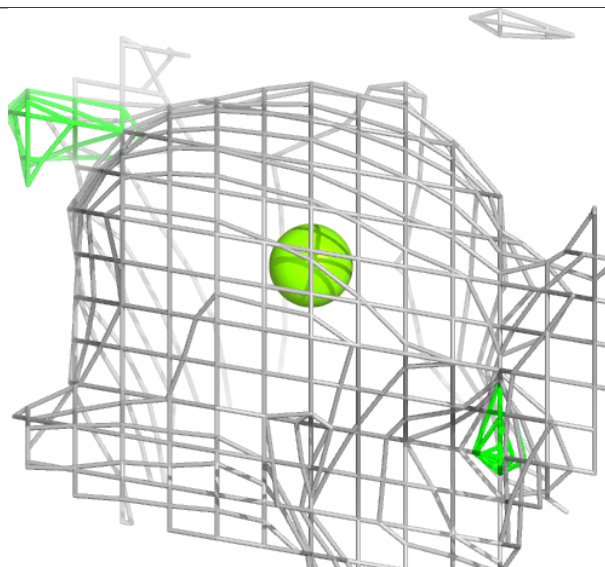
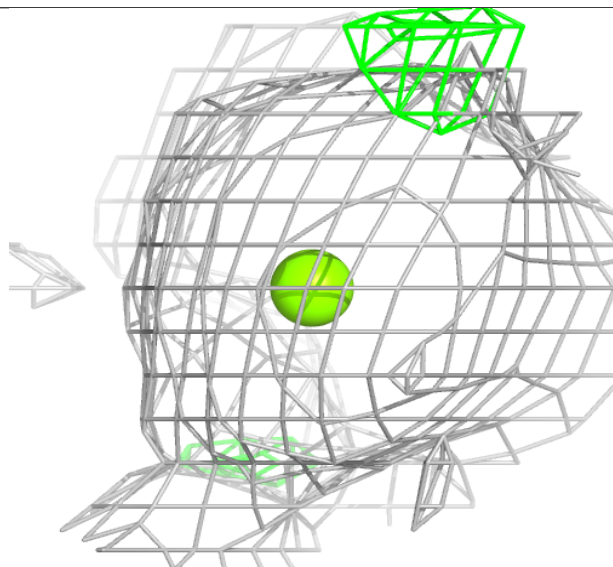
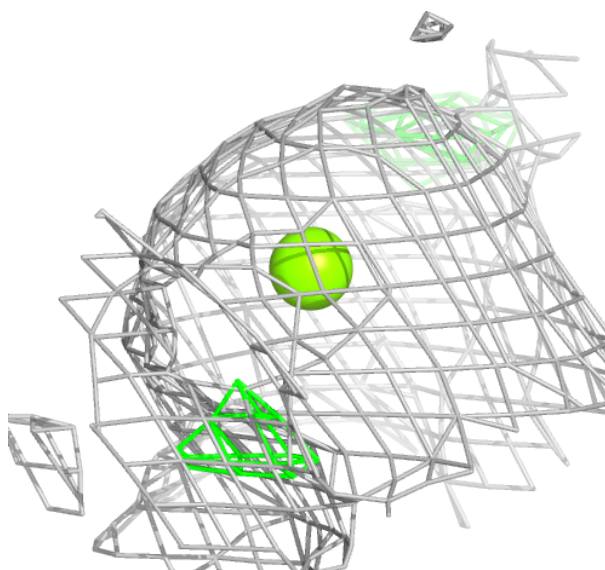
Electron density around ADP O 201:

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



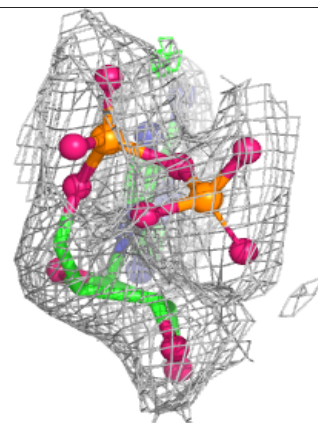
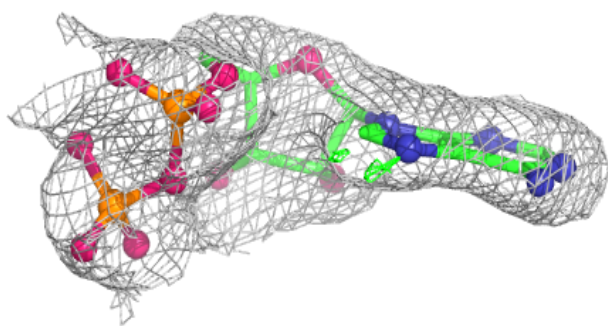
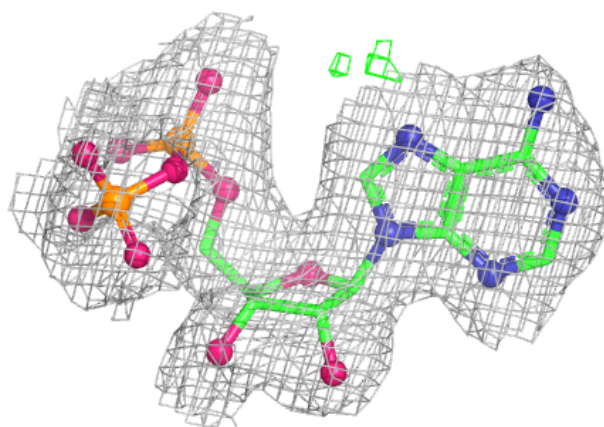
Electron density around MG X 202:

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



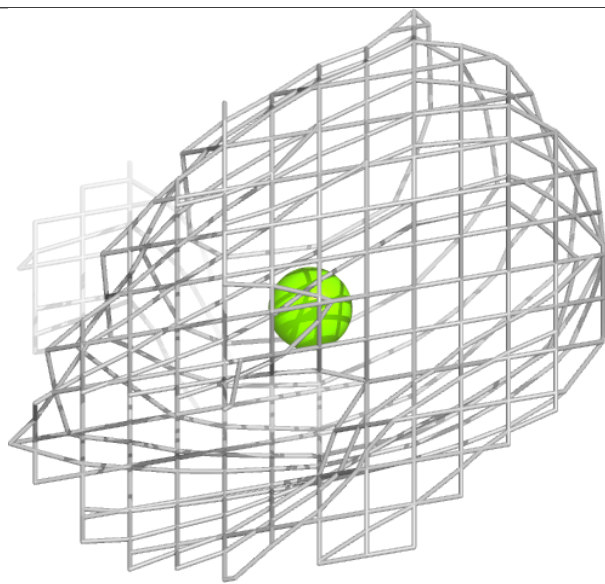
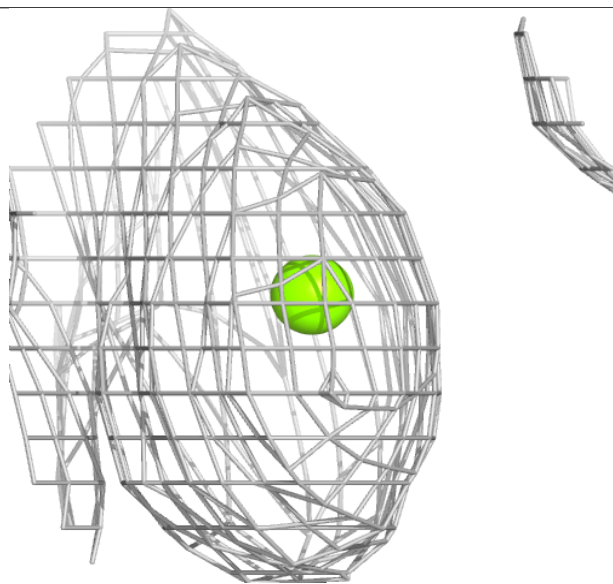
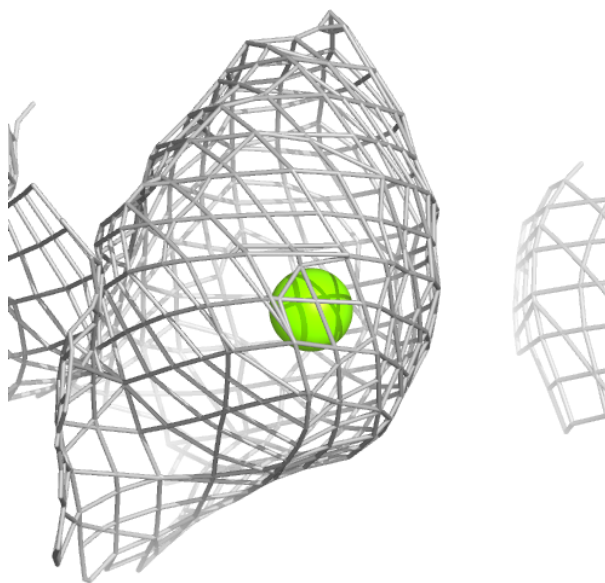
Electron density around ADP F 201:

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



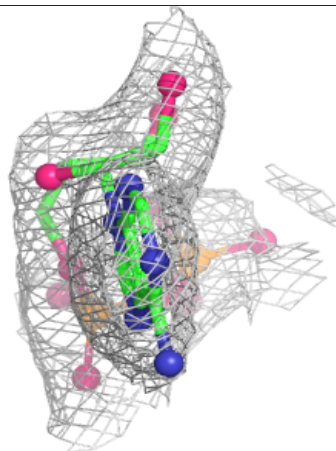
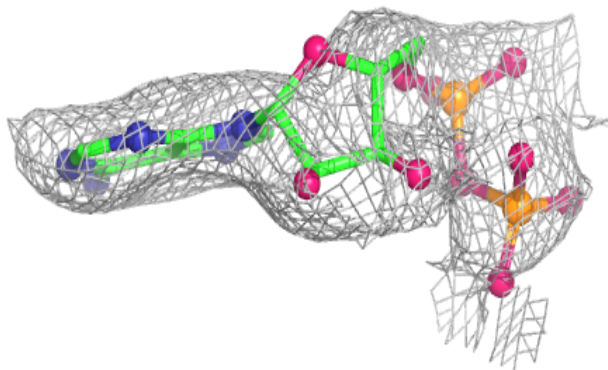
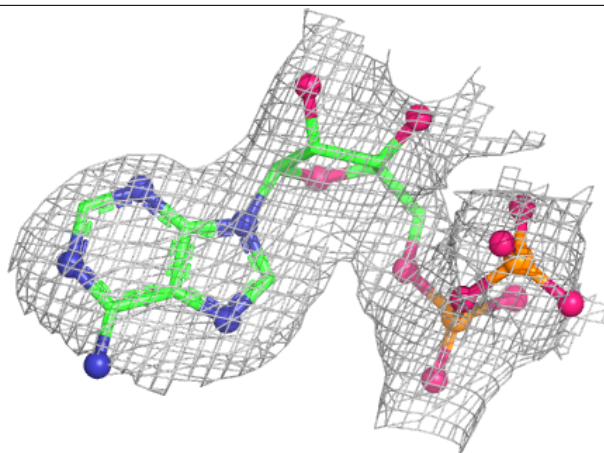
Electron density around MG b 202:

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



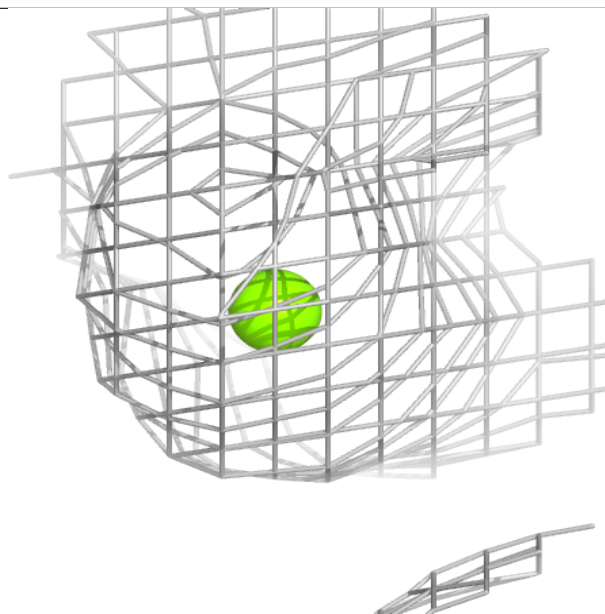
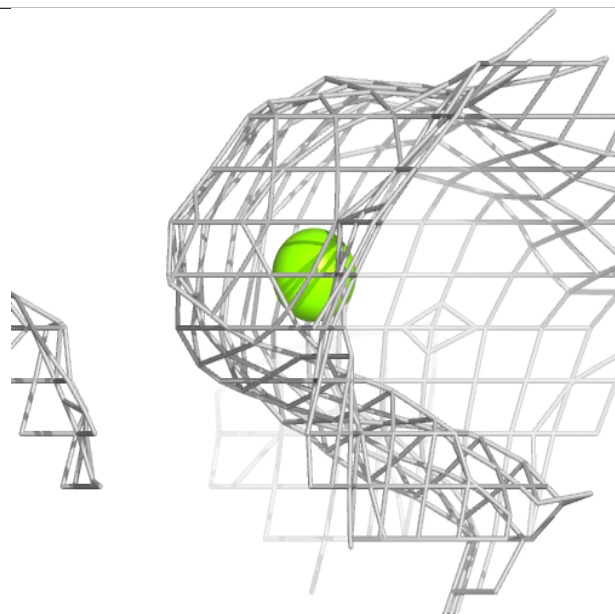
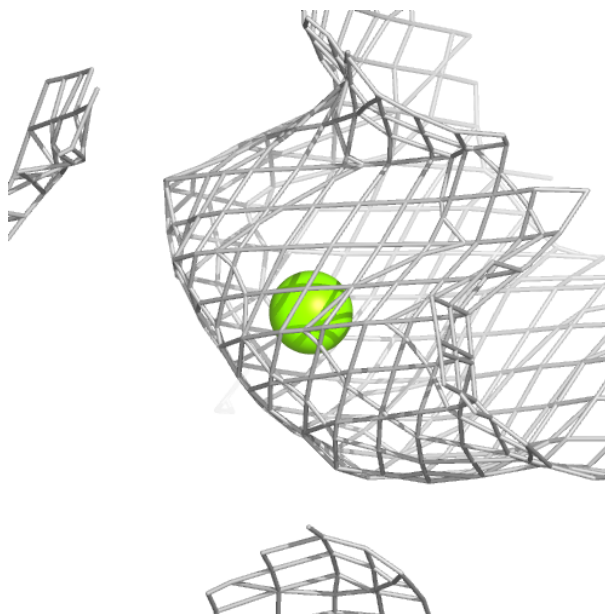
Electron density around ADP G 201:

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



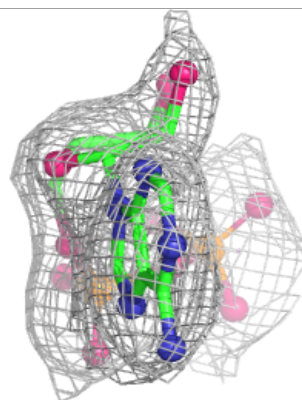
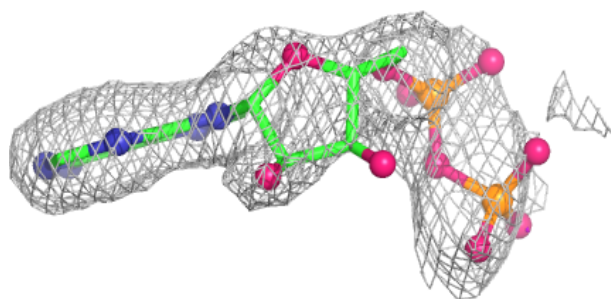
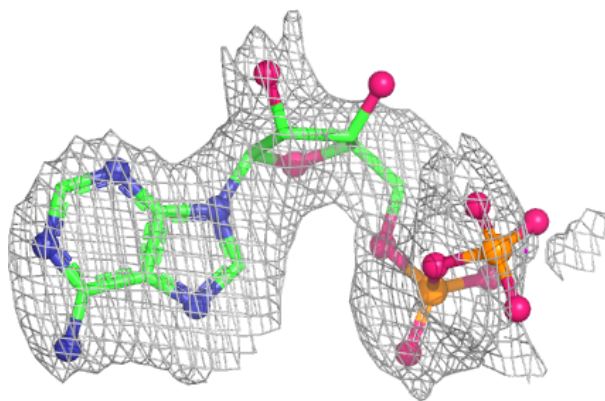
Electron density around MG d 202:

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



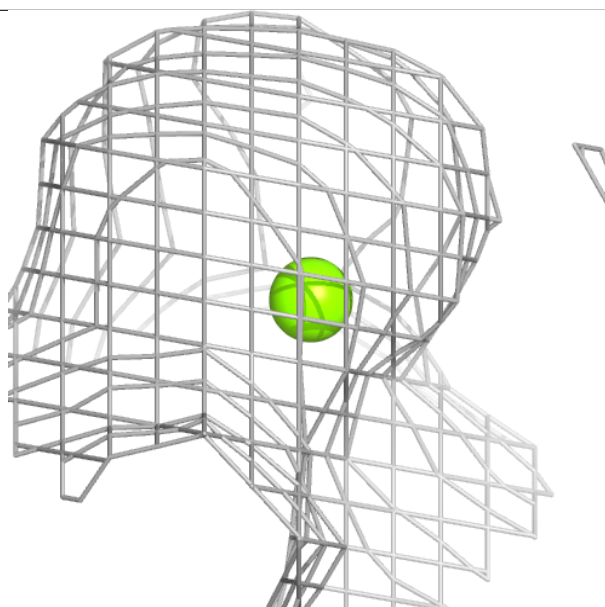
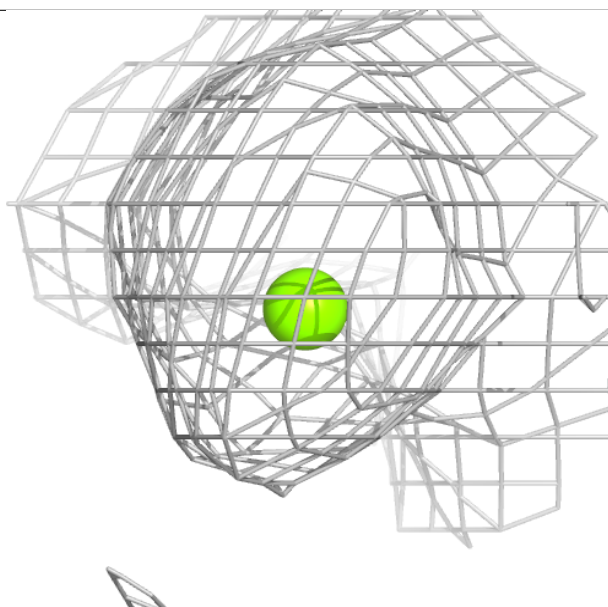
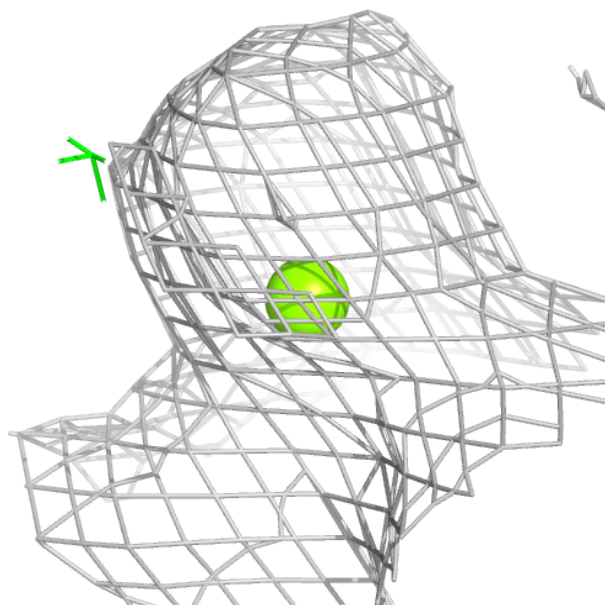
Electron density around ADP R 201:

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



Electron density around MG h 202:

$2mF_o-DF_c$ (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.