



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 07:18 AM UTC

PDB ID : 3Q2K / pdb_00003q2k
Title : Crystal structure of the WlbA dehydrogenase from Bordetella pertussis in complex with NADH and UDP-GlcNAcA
Authors : Holden, H.M.; Thoden, J.B.
Deposited on : 2010-12-20
Resolution : 2.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

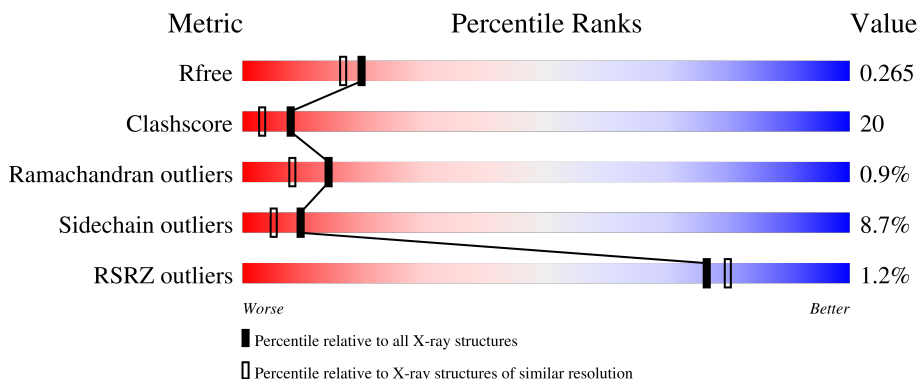
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	370	
1	B	370	
1	C	370	
1	D	370	
1	E	370	

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Mol	Chain	Length	Quality of chain
1	F	370	 % 61% 25% 5% 12%
1	G	370	 % 65% 22% 5% 8%
1	H	370	 % 60% 27% 5% 8%
1	I	370	 % 61% 27% 5% 8%
1	J	370	 % 60% 28% 5% 6%
1	K	370	 2% 54% 28% 5% 13%
1	L	370	 3% 50% 28% 8% 13%
1	M	370	 % 61% 26% 6% 6%
1	N	370	 63% 23% 6% 8%
1	O	370	 63% 22% 5% 10%
1	P	370	 2% 57% 25% 5% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43985 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 oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2707	1699	492	504	12			
1	B	329	Total	C	N	O	S	0	2	0
			2587	1625	476	474	12			
1	C	347	Total	C	N	O	S	0	0	0
			2712	1702	493	505	12			
1	D	343	Total	C	N	O	S	0	1	0
			2693	1689	492	500	12			
1	E	321	Total	C	N	O	S	0	0	0
			2501	1572	457	460	12			
1	F	327	Total	C	N	O	S	0	0	0
			2552	1600	468	472	12			
1	G	342	Total	C	N	O	S	0	0	0
			2677	1680	488	497	12			
1	H	342	Total	C	N	O	S	0	1	0
			2681	1684	488	497	12			
1	I	342	Total	C	N	O	S	0	0	0
			2677	1680	488	497	12			
1	J	346	Total	C	N	O	S	0	0	0
			2707	1699	492	504	12			
1	K	322	Total	C	N	O	S	0	0	0
			2511	1577	461	461	12			
1	L	321	Total	C	N	O	S	0	1	0
			2514	1579	463	460	12			
1	M	346	Total	C	N	O	S	0	0	0
			2707	1699	492	504	12			
1	N	342	Total	C	N	O	S	0	0	0
			2677	1680	488	497	12			
1	O	334	Total	C	N	O	S	0	0	0
			2610	1637	479	482	12			
1	P	322	Total	C	N	O	S	0	0	0
			2511	1577	461	461	12			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q79H45
A	-18	GLY	-	expression tag	UNP Q79H45
A	-17	SER	-	expression tag	UNP Q79H45
A	-16	SER	-	expression tag	UNP Q79H45
A	-15	HIS	-	expression tag	UNP Q79H45
A	-14	HIS	-	expression tag	UNP Q79H45
A	-13	HIS	-	expression tag	UNP Q79H45
A	-12	HIS	-	expression tag	UNP Q79H45
A	-11	HIS	-	expression tag	UNP Q79H45
A	-10	HIS	-	expression tag	UNP Q79H45
A	-9	SER	-	expression tag	UNP Q79H45
A	-8	SER	-	expression tag	UNP Q79H45
A	-7	GLU	-	expression tag	UNP Q79H45
A	-6	ASN	-	expression tag	UNP Q79H45
A	-5	LEU	-	expression tag	UNP Q79H45
A	-4	TYR	-	expression tag	UNP Q79H45
A	-3	PHE	-	expression tag	UNP Q79H45
A	-2	GLN	-	expression tag	UNP Q79H45
A	-1	GLY	-	expression tag	UNP Q79H45
A	0	HIS	-	expression tag	UNP Q79H45
B	-19	MET	-	expression tag	UNP Q79H45
B	-18	GLY	-	expression tag	UNP Q79H45
B	-17	SER	-	expression tag	UNP Q79H45
B	-16	SER	-	expression tag	UNP Q79H45
B	-15	HIS	-	expression tag	UNP Q79H45
B	-14	HIS	-	expression tag	UNP Q79H45
B	-13	HIS	-	expression tag	UNP Q79H45
B	-12	HIS	-	expression tag	UNP Q79H45
B	-11	HIS	-	expression tag	UNP Q79H45
B	-10	HIS	-	expression tag	UNP Q79H45
B	-9	SER	-	expression tag	UNP Q79H45
B	-8	SER	-	expression tag	UNP Q79H45
B	-7	GLU	-	expression tag	UNP Q79H45
B	-6	ASN	-	expression tag	UNP Q79H45
B	-5	LEU	-	expression tag	UNP Q79H45
B	-4	TYR	-	expression tag	UNP Q79H45
B	-3	PHE	-	expression tag	UNP Q79H45
B	-2	GLN	-	expression tag	UNP Q79H45
B	-1	GLY	-	expression tag	UNP Q79H45
B	0	HIS	-	expression tag	UNP Q79H45
C	-19	MET	-	expression tag	UNP Q79H45
C	-18	GLY	-	expression tag	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP Q79H45
C	-16	SER	-	expression tag	UNP Q79H45
C	-15	HIS	-	expression tag	UNP Q79H45
C	-14	HIS	-	expression tag	UNP Q79H45
C	-13	HIS	-	expression tag	UNP Q79H45
C	-12	HIS	-	expression tag	UNP Q79H45
C	-11	HIS	-	expression tag	UNP Q79H45
C	-10	HIS	-	expression tag	UNP Q79H45
C	-9	SER	-	expression tag	UNP Q79H45
C	-8	SER	-	expression tag	UNP Q79H45
C	-7	GLU	-	expression tag	UNP Q79H45
C	-6	ASN	-	expression tag	UNP Q79H45
C	-5	LEU	-	expression tag	UNP Q79H45
C	-4	TYR	-	expression tag	UNP Q79H45
C	-3	PHE	-	expression tag	UNP Q79H45
C	-2	GLN	-	expression tag	UNP Q79H45
C	-1	GLY	-	expression tag	UNP Q79H45
C	0	HIS	-	expression tag	UNP Q79H45
D	-19	MET	-	expression tag	UNP Q79H45
D	-18	GLY	-	expression tag	UNP Q79H45
D	-17	SER	-	expression tag	UNP Q79H45
D	-16	SER	-	expression tag	UNP Q79H45
D	-15	HIS	-	expression tag	UNP Q79H45
D	-14	HIS	-	expression tag	UNP Q79H45
D	-13	HIS	-	expression tag	UNP Q79H45
D	-12	HIS	-	expression tag	UNP Q79H45
D	-11	HIS	-	expression tag	UNP Q79H45
D	-10	HIS	-	expression tag	UNP Q79H45
D	-9	SER	-	expression tag	UNP Q79H45
D	-8	SER	-	expression tag	UNP Q79H45
D	-7	GLU	-	expression tag	UNP Q79H45
D	-6	ASN	-	expression tag	UNP Q79H45
D	-5	LEU	-	expression tag	UNP Q79H45
D	-4	TYR	-	expression tag	UNP Q79H45
D	-3	PHE	-	expression tag	UNP Q79H45
D	-2	GLN	-	expression tag	UNP Q79H45
D	-1	GLY	-	expression tag	UNP Q79H45
D	0	HIS	-	expression tag	UNP Q79H45
E	-19	MET	-	expression tag	UNP Q79H45
E	-18	GLY	-	expression tag	UNP Q79H45
E	-17	SER	-	expression tag	UNP Q79H45
E	-16	SER	-	expression tag	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP Q79H45
E	-14	HIS	-	expression tag	UNP Q79H45
E	-13	HIS	-	expression tag	UNP Q79H45
E	-12	HIS	-	expression tag	UNP Q79H45
E	-11	HIS	-	expression tag	UNP Q79H45
E	-10	HIS	-	expression tag	UNP Q79H45
E	-9	SER	-	expression tag	UNP Q79H45
E	-8	SER	-	expression tag	UNP Q79H45
E	-7	GLU	-	expression tag	UNP Q79H45
E	-6	ASN	-	expression tag	UNP Q79H45
E	-5	LEU	-	expression tag	UNP Q79H45
E	-4	TYR	-	expression tag	UNP Q79H45
E	-3	PHE	-	expression tag	UNP Q79H45
E	-2	GLN	-	expression tag	UNP Q79H45
E	-1	GLY	-	expression tag	UNP Q79H45
E	0	HIS	-	expression tag	UNP Q79H45
F	-19	MET	-	expression tag	UNP Q79H45
F	-18	GLY	-	expression tag	UNP Q79H45
F	-17	SER	-	expression tag	UNP Q79H45
F	-16	SER	-	expression tag	UNP Q79H45
F	-15	HIS	-	expression tag	UNP Q79H45
F	-14	HIS	-	expression tag	UNP Q79H45
F	-13	HIS	-	expression tag	UNP Q79H45
F	-12	HIS	-	expression tag	UNP Q79H45
F	-11	HIS	-	expression tag	UNP Q79H45
F	-10	HIS	-	expression tag	UNP Q79H45
F	-9	SER	-	expression tag	UNP Q79H45
F	-8	SER	-	expression tag	UNP Q79H45
F	-7	GLU	-	expression tag	UNP Q79H45
F	-6	ASN	-	expression tag	UNP Q79H45
F	-5	LEU	-	expression tag	UNP Q79H45
F	-4	TYR	-	expression tag	UNP Q79H45
F	-3	PHE	-	expression tag	UNP Q79H45
F	-2	GLN	-	expression tag	UNP Q79H45
F	-1	GLY	-	expression tag	UNP Q79H45
F	0	HIS	-	expression tag	UNP Q79H45
G	-19	MET	-	expression tag	UNP Q79H45
G	-18	GLY	-	expression tag	UNP Q79H45
G	-17	SER	-	expression tag	UNP Q79H45
G	-16	SER	-	expression tag	UNP Q79H45
G	-15	HIS	-	expression tag	UNP Q79H45
G	-14	HIS	-	expression tag	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	expression tag	UNP Q79H45
G	-12	HIS	-	expression tag	UNP Q79H45
G	-11	HIS	-	expression tag	UNP Q79H45
G	-10	HIS	-	expression tag	UNP Q79H45
G	-9	SER	-	expression tag	UNP Q79H45
G	-8	SER	-	expression tag	UNP Q79H45
G	-7	GLU	-	expression tag	UNP Q79H45
G	-6	ASN	-	expression tag	UNP Q79H45
G	-5	LEU	-	expression tag	UNP Q79H45
G	-4	TYR	-	expression tag	UNP Q79H45
G	-3	PHE	-	expression tag	UNP Q79H45
G	-2	GLN	-	expression tag	UNP Q79H45
G	-1	GLY	-	expression tag	UNP Q79H45
G	0	HIS	-	expression tag	UNP Q79H45
H	-19	MET	-	expression tag	UNP Q79H45
H	-18	GLY	-	expression tag	UNP Q79H45
H	-17	SER	-	expression tag	UNP Q79H45
H	-16	SER	-	expression tag	UNP Q79H45
H	-15	HIS	-	expression tag	UNP Q79H45
H	-14	HIS	-	expression tag	UNP Q79H45
H	-13	HIS	-	expression tag	UNP Q79H45
H	-12	HIS	-	expression tag	UNP Q79H45
H	-11	HIS	-	expression tag	UNP Q79H45
H	-10	HIS	-	expression tag	UNP Q79H45
H	-9	SER	-	expression tag	UNP Q79H45
H	-8	SER	-	expression tag	UNP Q79H45
H	-7	GLU	-	expression tag	UNP Q79H45
H	-6	ASN	-	expression tag	UNP Q79H45
H	-5	LEU	-	expression tag	UNP Q79H45
H	-4	TYR	-	expression tag	UNP Q79H45
H	-3	PHE	-	expression tag	UNP Q79H45
H	-2	GLN	-	expression tag	UNP Q79H45
H	-1	GLY	-	expression tag	UNP Q79H45
H	0	HIS	-	expression tag	UNP Q79H45
I	-19	MET	-	expression tag	UNP Q79H45
I	-18	GLY	-	expression tag	UNP Q79H45
I	-17	SER	-	expression tag	UNP Q79H45
I	-16	SER	-	expression tag	UNP Q79H45
I	-15	HIS	-	expression tag	UNP Q79H45
I	-14	HIS	-	expression tag	UNP Q79H45
I	-13	HIS	-	expression tag	UNP Q79H45
I	-12	HIS	-	expression tag	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	expression tag	UNP Q79H45
I	-10	HIS	-	expression tag	UNP Q79H45
I	-9	SER	-	expression tag	UNP Q79H45
I	-8	SER	-	expression tag	UNP Q79H45
I	-7	GLU	-	expression tag	UNP Q79H45
I	-6	ASN	-	expression tag	UNP Q79H45
I	-5	LEU	-	expression tag	UNP Q79H45
I	-4	TYR	-	expression tag	UNP Q79H45
I	-3	PHE	-	expression tag	UNP Q79H45
I	-2	GLN	-	expression tag	UNP Q79H45
I	-1	GLY	-	expression tag	UNP Q79H45
I	0	HIS	-	expression tag	UNP Q79H45
J	-19	MET	-	expression tag	UNP Q79H45
J	-18	GLY	-	expression tag	UNP Q79H45
J	-17	SER	-	expression tag	UNP Q79H45
J	-16	SER	-	expression tag	UNP Q79H45
J	-15	HIS	-	expression tag	UNP Q79H45
J	-14	HIS	-	expression tag	UNP Q79H45
J	-13	HIS	-	expression tag	UNP Q79H45
J	-12	HIS	-	expression tag	UNP Q79H45
J	-11	HIS	-	expression tag	UNP Q79H45
J	-10	HIS	-	expression tag	UNP Q79H45
J	-9	SER	-	expression tag	UNP Q79H45
J	-8	SER	-	expression tag	UNP Q79H45
J	-7	GLU	-	expression tag	UNP Q79H45
J	-6	ASN	-	expression tag	UNP Q79H45
J	-5	LEU	-	expression tag	UNP Q79H45
J	-4	TYR	-	expression tag	UNP Q79H45
J	-3	PHE	-	expression tag	UNP Q79H45
J	-2	GLN	-	expression tag	UNP Q79H45
J	-1	GLY	-	expression tag	UNP Q79H45
J	0	HIS	-	expression tag	UNP Q79H45
K	-19	MET	-	expression tag	UNP Q79H45
K	-18	GLY	-	expression tag	UNP Q79H45
K	-17	SER	-	expression tag	UNP Q79H45
K	-16	SER	-	expression tag	UNP Q79H45
K	-15	HIS	-	expression tag	UNP Q79H45
K	-14	HIS	-	expression tag	UNP Q79H45
K	-13	HIS	-	expression tag	UNP Q79H45
K	-12	HIS	-	expression tag	UNP Q79H45
K	-11	HIS	-	expression tag	UNP Q79H45
K	-10	HIS	-	expression tag	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	expression tag	UNP Q79H45
K	-8	SER	-	expression tag	UNP Q79H45
K	-7	GLU	-	expression tag	UNP Q79H45
K	-6	ASN	-	expression tag	UNP Q79H45
K	-5	LEU	-	expression tag	UNP Q79H45
K	-4	TYR	-	expression tag	UNP Q79H45
K	-3	PHE	-	expression tag	UNP Q79H45
K	-2	GLN	-	expression tag	UNP Q79H45
K	-1	GLY	-	expression tag	UNP Q79H45
K	0	HIS	-	expression tag	UNP Q79H45
L	-19	MET	-	expression tag	UNP Q79H45
L	-18	GLY	-	expression tag	UNP Q79H45
L	-17	SER	-	expression tag	UNP Q79H45
L	-16	SER	-	expression tag	UNP Q79H45
L	-15	HIS	-	expression tag	UNP Q79H45
L	-14	HIS	-	expression tag	UNP Q79H45
L	-13	HIS	-	expression tag	UNP Q79H45
L	-12	HIS	-	expression tag	UNP Q79H45
L	-11	HIS	-	expression tag	UNP Q79H45
L	-10	HIS	-	expression tag	UNP Q79H45
L	-9	SER	-	expression tag	UNP Q79H45
L	-8	SER	-	expression tag	UNP Q79H45
L	-7	GLU	-	expression tag	UNP Q79H45
L	-6	ASN	-	expression tag	UNP Q79H45
L	-5	LEU	-	expression tag	UNP Q79H45
L	-4	TYR	-	expression tag	UNP Q79H45
L	-3	PHE	-	expression tag	UNP Q79H45
L	-2	GLN	-	expression tag	UNP Q79H45
L	-1	GLY	-	expression tag	UNP Q79H45
L	0	HIS	-	expression tag	UNP Q79H45
M	-19	MET	-	expression tag	UNP Q79H45
M	-18	GLY	-	expression tag	UNP Q79H45
M	-17	SER	-	expression tag	UNP Q79H45
M	-16	SER	-	expression tag	UNP Q79H45
M	-15	HIS	-	expression tag	UNP Q79H45
M	-14	HIS	-	expression tag	UNP Q79H45
M	-13	HIS	-	expression tag	UNP Q79H45
M	-12	HIS	-	expression tag	UNP Q79H45
M	-11	HIS	-	expression tag	UNP Q79H45
M	-10	HIS	-	expression tag	UNP Q79H45
M	-9	SER	-	expression tag	UNP Q79H45
M	-8	SER	-	expression tag	UNP Q79H45

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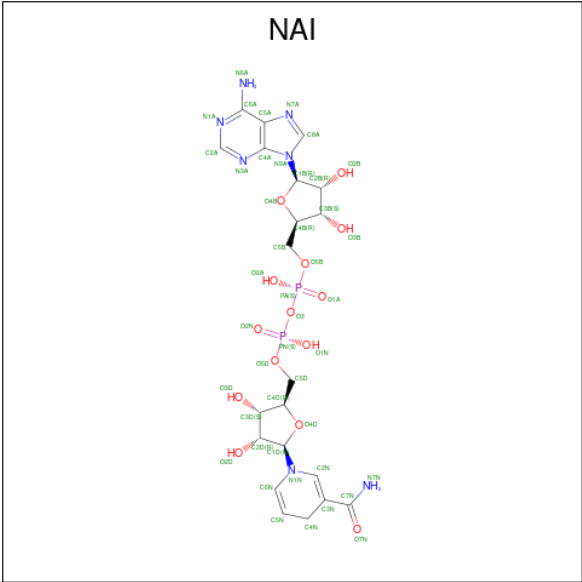
Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLU	-	expression tag	UNP Q79H45
M	-6	ASN	-	expression tag	UNP Q79H45
M	-5	LEU	-	expression tag	UNP Q79H45
M	-4	TYR	-	expression tag	UNP Q79H45
M	-3	PHE	-	expression tag	UNP Q79H45
M	-2	GLN	-	expression tag	UNP Q79H45
M	-1	GLY	-	expression tag	UNP Q79H45
M	0	HIS	-	expression tag	UNP Q79H45
N	-19	MET	-	expression tag	UNP Q79H45
N	-18	GLY	-	expression tag	UNP Q79H45
N	-17	SER	-	expression tag	UNP Q79H45
N	-16	SER	-	expression tag	UNP Q79H45
N	-15	HIS	-	expression tag	UNP Q79H45
N	-14	HIS	-	expression tag	UNP Q79H45
N	-13	HIS	-	expression tag	UNP Q79H45
N	-12	HIS	-	expression tag	UNP Q79H45
N	-11	HIS	-	expression tag	UNP Q79H45
N	-10	HIS	-	expression tag	UNP Q79H45
N	-9	SER	-	expression tag	UNP Q79H45
N	-8	SER	-	expression tag	UNP Q79H45
N	-7	GLU	-	expression tag	UNP Q79H45
N	-6	ASN	-	expression tag	UNP Q79H45
N	-5	LEU	-	expression tag	UNP Q79H45
N	-4	TYR	-	expression tag	UNP Q79H45
N	-3	PHE	-	expression tag	UNP Q79H45
N	-2	GLN	-	expression tag	UNP Q79H45
N	-1	GLY	-	expression tag	UNP Q79H45
N	0	HIS	-	expression tag	UNP Q79H45
O	-19	MET	-	expression tag	UNP Q79H45
O	-18	GLY	-	expression tag	UNP Q79H45
O	-17	SER	-	expression tag	UNP Q79H45
O	-16	SER	-	expression tag	UNP Q79H45
O	-15	HIS	-	expression tag	UNP Q79H45
O	-14	HIS	-	expression tag	UNP Q79H45
O	-13	HIS	-	expression tag	UNP Q79H45
O	-12	HIS	-	expression tag	UNP Q79H45
O	-11	HIS	-	expression tag	UNP Q79H45
O	-10	HIS	-	expression tag	UNP Q79H45
O	-9	SER	-	expression tag	UNP Q79H45
O	-8	SER	-	expression tag	UNP Q79H45
O	-7	GLU	-	expression tag	UNP Q79H45
O	-6	ASN	-	expression tag	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	LEU	-	expression tag	UNP Q79H45
O	-4	TYR	-	expression tag	UNP Q79H45
O	-3	PHE	-	expression tag	UNP Q79H45
O	-2	GLN	-	expression tag	UNP Q79H45
O	-1	GLY	-	expression tag	UNP Q79H45
O	0	HIS	-	expression tag	UNP Q79H45
P	-19	MET	-	expression tag	UNP Q79H45
P	-18	GLY	-	expression tag	UNP Q79H45
P	-17	SER	-	expression tag	UNP Q79H45
P	-16	SER	-	expression tag	UNP Q79H45
P	-15	HIS	-	expression tag	UNP Q79H45
P	-14	HIS	-	expression tag	UNP Q79H45
P	-13	HIS	-	expression tag	UNP Q79H45
P	-12	HIS	-	expression tag	UNP Q79H45
P	-11	HIS	-	expression tag	UNP Q79H45
P	-10	HIS	-	expression tag	UNP Q79H45
P	-9	SER	-	expression tag	UNP Q79H45
P	-8	SER	-	expression tag	UNP Q79H45
P	-7	GLU	-	expression tag	UNP Q79H45
P	-6	ASN	-	expression tag	UNP Q79H45
P	-5	LEU	-	expression tag	UNP Q79H45
P	-4	TYR	-	expression tag	UNP Q79H45
P	-3	PHE	-	expression tag	UNP Q79H45
P	-2	GLN	-	expression tag	UNP Q79H45
P	-1	GLY	-	expression tag	UNP Q79H45
P	0	HIS	-	expression tag	UNP Q79H45

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



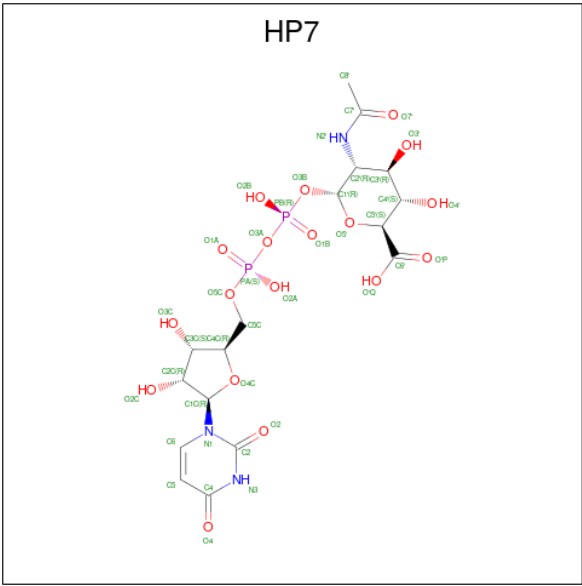
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	M	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	N	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (2S,3S,4R,5R,6R)-5-acetamido-6-[[[(2R,3S,4R,5R)-5-(2,4-dioxypyrimidin-1-yl)-3,4-dihydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl]oxy-hydroxy-phosphoryl]oxy-3,4-dihydroxy-oxane-2-carboxylic acid (CCD ID: HP7) (formula: C₁₇H₂₅N₃O₁₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	B	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	C	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	D	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	E	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	F	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	G	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	H	1	Total	C	N	O	P	0	0
			40	17	3	18	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	I	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	J	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	K	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	L	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	M	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	N	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	O	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	P	1	Total	C	N	O	P	0	0
			40	17	3	18	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	54	Total	O	0	0
			54	54		
4	C	58	Total	O	0	0
			58	58		
4	D	51	Total	O	0	0
			51	51		
4	E	21	Total	O	0	0
			21	21		
4	F	24	Total	O	0	0
			24	24		
4	G	49	Total	O	0	0
			49	49		
4	H	35	Total	O	0	0
			35	35		
4	I	36	Total	O	0	0
			36	36		
4	J	30	Total	O	0	0
			30	30		
4	K	26	Total	O	0	0
			26	26		

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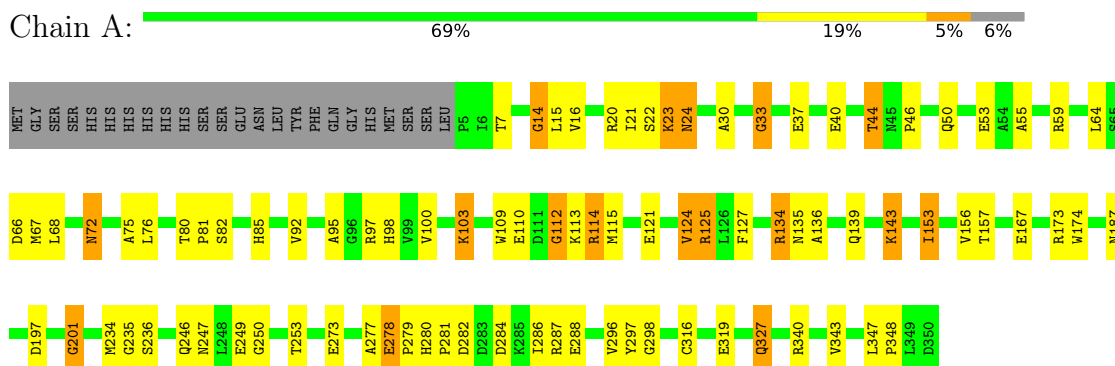
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	37	Total 37	O 37	0	0
4	M	36	Total 36	O 36	0	0
4	N	34	Total 34	O 34	0	0
4	O	17	Total 17	O 17	0	0
4	P	24	Total 24	O 24	0	0

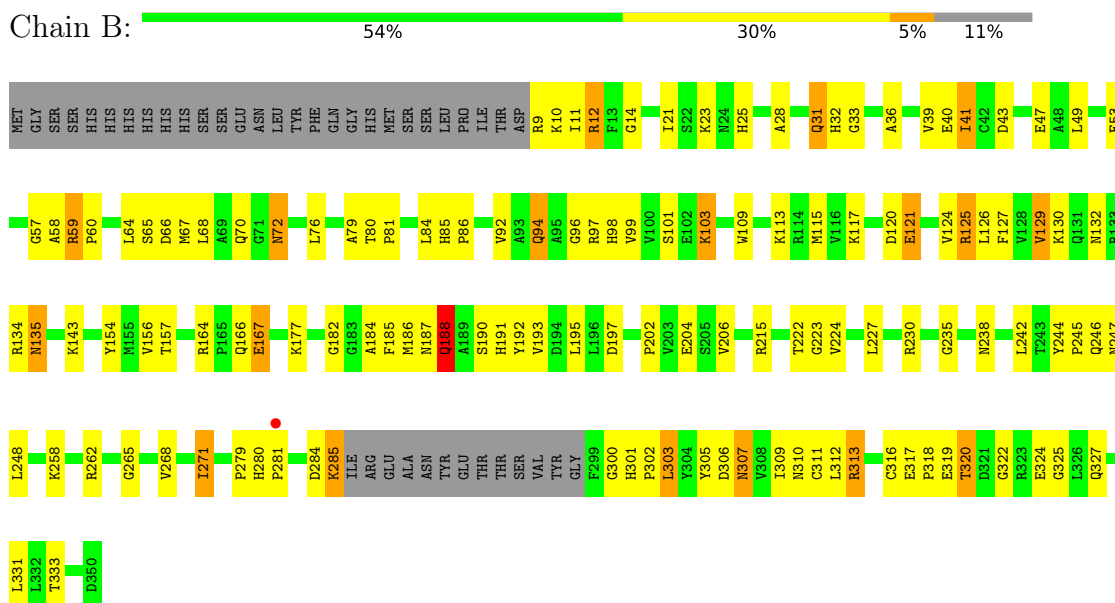
3 Residue-property plots

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: oxidoreductase

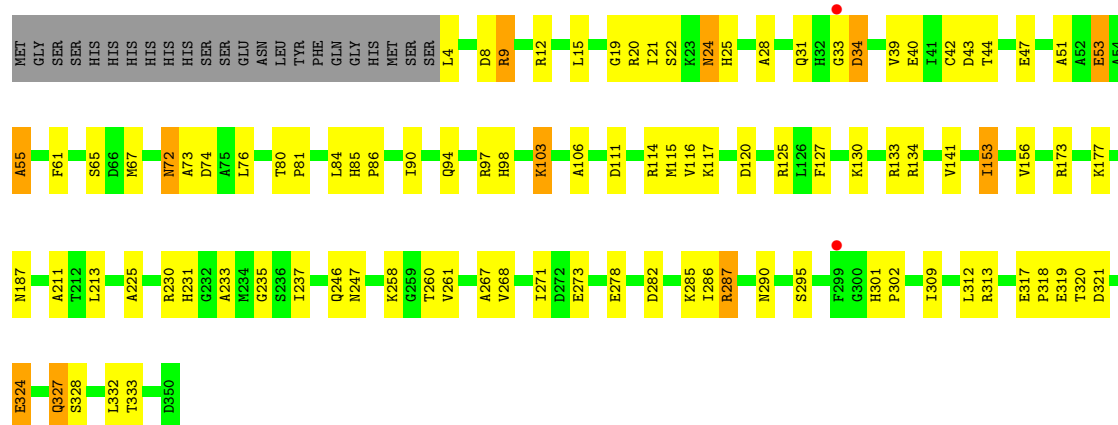


- Molecule 1: oxidoreductase

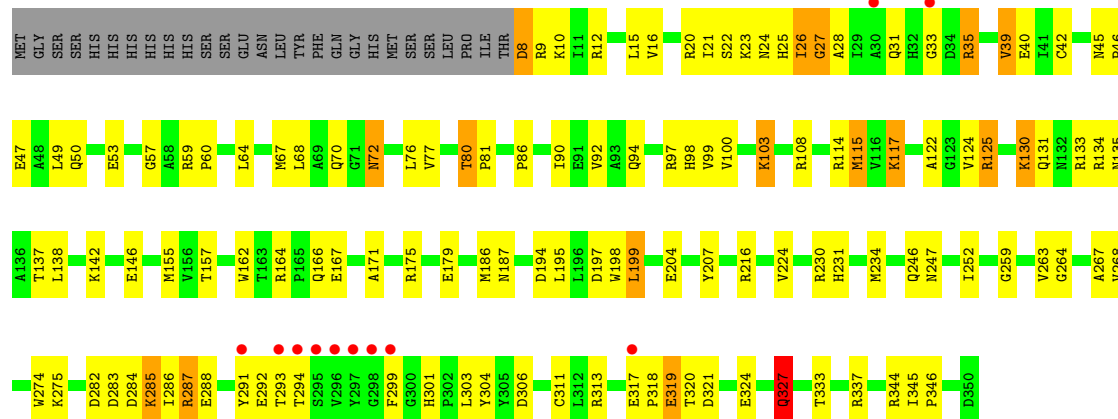


- Molecule 1: oxidoreductase

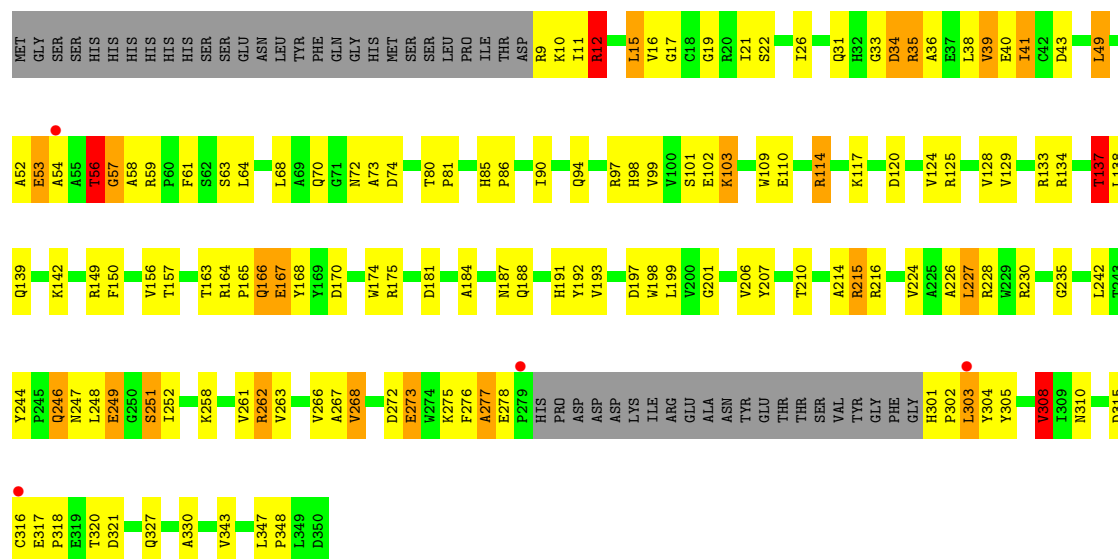




• Molecule 1: oxidoreductase



• Molecule 1: oxidoreductase



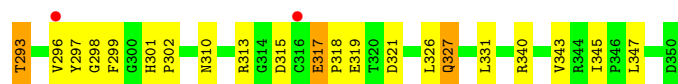
Chain F:

Chain G:

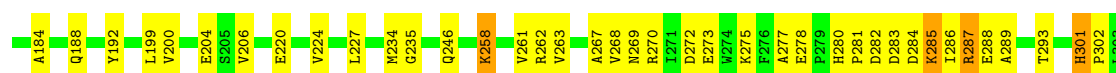
Residue	Category
Met	Grey
GLY	Grey
SER	Grey
SER	Grey
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
SER	Grey
SER	Grey
GLU	Grey
ASN	Grey
LEU	Grey
TYR	Grey
PHE	Grey
GLN	Grey
GLY	Grey
HIS	Grey
HIS	Grey
Met	Grey
SER	Grey
SER	Grey
LEU	Grey
PRO	Grey
ILE	Grey
THR	Grey
ASP	Green
R9	Green
K10	Green
I11	Yellow
R12	Yellow
V16	Yellow
I21	Green
S22	Green
K23	Yellow
I26	Orange
R32	Yellow
G33	Yellow
D34	Green
R35	Yellow
A36	Yellow
F37	Green
L38	Yellow
V39	Yellow
E40	Yellow
N45	Orange
P46	Orange
Q50	Yellow
A51	Green
A52	Yellow
F53	Orange
A54	Orange
V55	Yellow
T56	Yellow
R59	Orange
P60	Yellow
F61	Yellow
M67	Yellow
L68	Yellow
N72	Yellow
A73	Green
D74	Yellow
A75	Green
L76	Yellow
V92	Orange
A93	Green
Q94	Yellow
R97	Yellow
H98	Yellow
K103	Orange
P104	Green
M105	Yellow
D111	Yellow
G112	Yellow
M115	Yellow
V116	Green
K117	Orange
D120	Yellow
E121	Yellow
V124	Yellow
R125	Yellow
V129	Yellow
R133	Yellow
R134	Yellow
L138	Yellow
Q139	Yellow
K143	Yellow
A144	Green
I145	Yellow
R152	Orange
V156	Yellow
T157	Yellow
E167	Orange
V174	Yellow
V193	Yellow
L199	Orange
L227	Yellow
G235	Yellow
I237	Yellow
S236	Green
Y244	Yellow
P245	Yellow
G250	Yellow
K258	Yellow
R262	Yellow
V266	Yellow
A267	Green
V268	Yellow
E273	Yellow
W274	Yellow
K275	Yellow
F276	Green
A277	Yellow
E278	Orange
P279	Yellow
H280	Orange
P281	Yellow
D282	Yellow
D283	Yellow
D284	Yellow
K285	Yellow
L286	Yellow
R287	Yellow
Y297	Orange
H301	Yellow
P302	Yellow
L303	Green
Y304	Yellow
Y305	Yellow
D306	Yellow
N310	Yellow
C311	Yellow
D315	Orange
C316	Orange
E317	Yellow
P318	Green
E319	Yellow
T320	Yellow
D321	Yellow
G322	Green
R232	Yellow

Chain H:

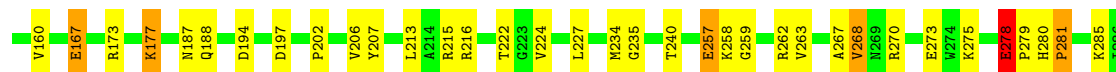
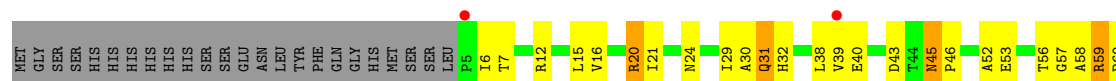
Residue	Category
MET	Grey
GLY	Grey
SER	Grey
SER	Grey
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
SER	Grey
SER	Grey
GLU	Grey
LEU	Grey
ASN	Grey
TYR	Grey
PHE	Grey
GLN	Grey
GLY	Grey
HIS	Grey
MET	Grey
SER	Grey
LEU	Grey
PRO	Grey
ILE	Grey
THR	Grey
ASP	Grey
R9	Green
K10	Yellow
V16	Yellow
G19	Yellow
I21	Yellow
S22	Yellow
K23	Yellow
R24	Red
A28	Yellow
I29	Yellow
A30	Yellow
Q31	Green
H32	Yellow
G33	Orange
D34	Yellow
R35	Yellow
A36	Yellow
V39	Yellow
E40	Orange
D43	Orange
T44	Orange
E47	Yellow
A48	Yellow
L49	Green
G50	Green
E53	Yellow
A54	Yellow
G57	Green
M67	Yellow
L68	Yellow
A69	Green
Q70	Yellow
G71	Orange
N72	Orange
L76	Yellow
V77	Yellow
L78	Yellow
A79	Orange
T80	Orange
P81	Yellow
P86	Yellow
E91	Yellow
Y92	Yellow
R97	Yellow
H98	Yellow
K103	Orange
R114	Yellow
M115	Yellow
V116	Yellow
K117	Yellow
V124	Yellow
F127	Yellow
N132	Yellow
R133	Yellow
R134	Yellow
N135	Yellow
A136	Green
T137	Yellow
L138	Green
Q139	Yellow
K142	Yellow
G151	Yellow
R152	Green
I153	Yellow
Y154	Yellow
M155	Yellow
V156	Yellow
T157	Orange
V162	Yellow
T162	Yellow
E167	Green
Y168	Yellow
A184	Yellow
F185	Yellow
M186	Yellow
N187	Yellow
Q188	Yellow
A189	Yellow
S190	Yellow
H191	Yellow
Y192	Yellow
V193	Yellow
D194	Yellow
L195	Yellow
W198	Yellow
E204	Yellow
A211	Yellow
R216	Yellow
E220	Yellow
L227	Yellow
R230	Orange
S236	Yellow
Y244	Yellow
Q245	Yellow
Q246	Yellow
N247	Yellow
L248	Yellow
E257	Yellow
K258	Yellow
A267	Yellow
V268	Yellow
A277	Yellow
E278	Yellow
E279	Yellow
H280	Yellow
P281	Yellow
D282	Yellow
D283	Yellow
D284	Green
K285	Yellow
L286	Yellow
R287	Yellow
E288	Yellow
Y291	Green
P292	Yellow



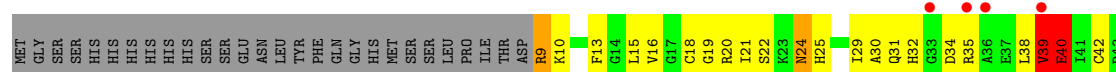
• Molecule 1: oxidoreductase



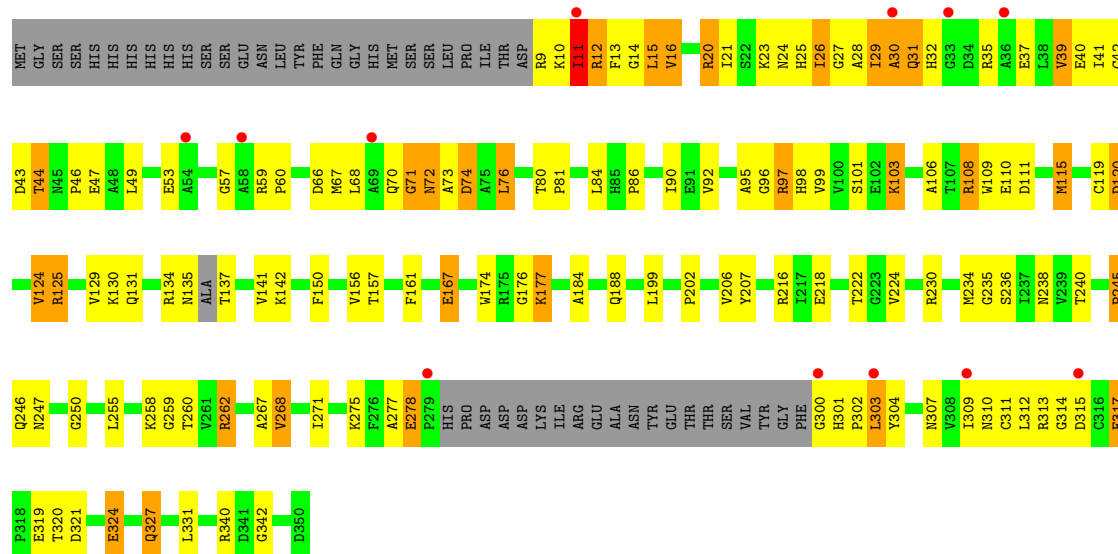
• Molecule 1: oxidoreductase



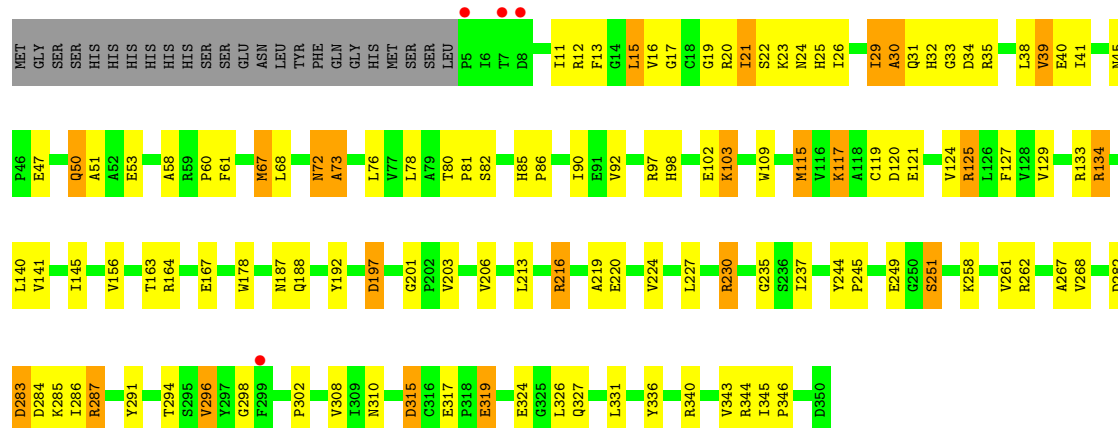
• Molecule 1: oxidoreductase



- Molecule 1: oxidoreductase

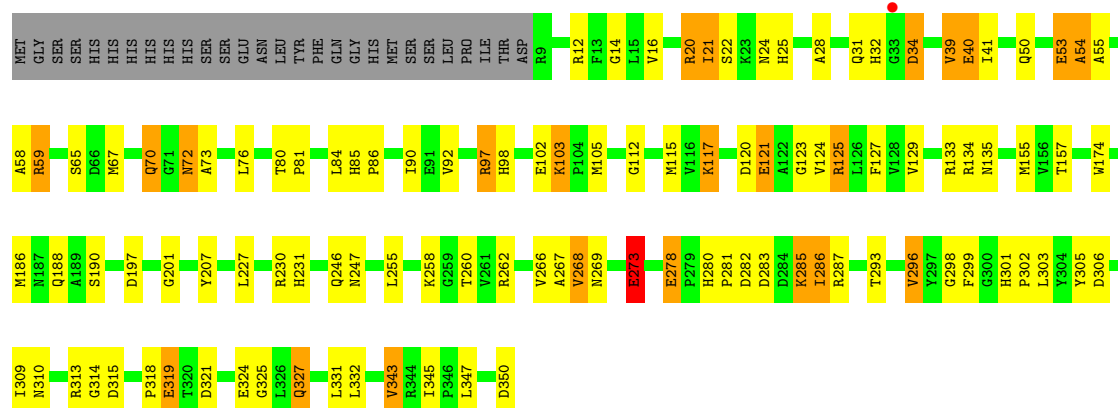


- Molecule 1: oxidoreductase



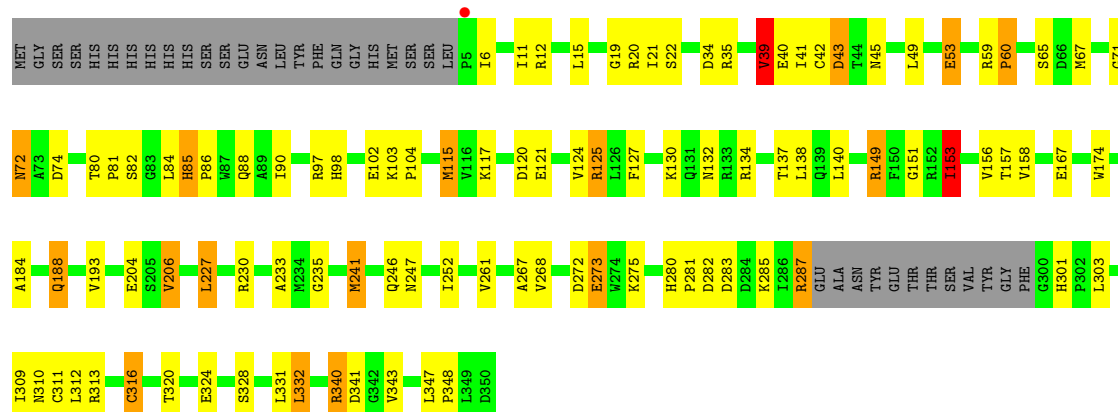
- Molecule 1: oxidoreductase





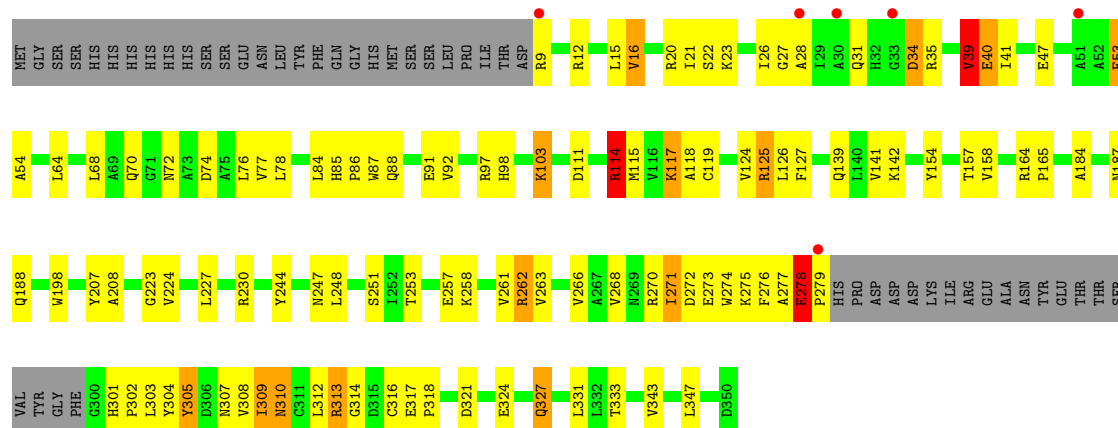
• Molecule 1: oxidoreductase

Chain O: 63% 22% 5% • 10%



• Molecule 1: oxidoreductase

Chain P: 2% 57% 25% • • 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.26Å 319.98Å 103.80Å 90.00° 119.07° 90.00°	Depositor
Resolution (Å)	30.00 – 2.13 30.00 – 2.13	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.00-2.13) 92.6 (30.00-2.13)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.183 , 0.269 0.184 , 0.265	Depositor DCC
R_{free} test set	15038 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.007 for -h-l,k,h 0.007 for l,k,-h-l 0.026 for h,-k,-h-l 0.024 for -h-l,-k,l 0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	43985	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, HP7

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	0.40	0/2767	1.44	18/3755 (0.5%)
1	B	0.37	0/2650	1.34	13/3593 (0.4%)
1	C	0.37	0/2772	1.40	19/3763 (0.5%)
1	D	0.36	0/2755	1.35	17/3737 (0.5%)
1	E	0.35	0/2554	1.37	20/3464 (0.6%)
1	F	0.37	0/2607	1.40	14/3536 (0.4%)
1	G	0.38	0/2736	1.43	20/3712 (0.5%)
1	H	0.36	0/2743	1.37	14/3722 (0.4%)
1	I	0.35	0/2736	1.37	17/3712 (0.5%)
1	J	0.35	0/2767	1.39	21/3755 (0.6%)
1	K	0.35	0/2564	1.38	16/3476 (0.5%)
1	L	0.34	0/2569	1.29	16/3480 (0.5%)
1	M	0.40	0/2767	1.42	26/3755 (0.7%)
1	N	0.39	0/2736	1.39	15/3712 (0.4%)
1	O	0.36	0/2666	1.44	22/3615 (0.6%)
1	P	0.35	0/2564	1.38	14/3476 (0.4%)
All	All	0.37	0/42953	1.39	282/58263 (0.5%)

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

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

There are no bond length outliers.

The worst 5 of 282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	230	ARG	NE-CZ-NH2	-10.07	110.14	119.20
1	J	59	ARG	CA-C-N	9.54	129.49	119.85
1	J	59	ARG	C-N-CA	9.54	129.49	119.85
1	J	278	GLU	CA-C-N	9.19	130.40	120.11
1	J	278	GLU	C-N-CA	9.19	130.40	120.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	315	ASP	Peptide

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	2707	0	2654	71	0
1	B	2587	0	2547	129	0
1	C	2712	0	2655	77	0
1	D	2693	0	2641	139	0
1	E	2501	0	2465	139	0
1	F	2552	0	2505	87	0
1	G	2677	0	2624	74	0
1	H	2681	0	2633	114	2
1	I	2677	0	2624	121	1
1	J	2707	0	2654	92	1
1	K	2511	0	2479	112	0
1	L	2514	0	2486	136	0
1	M	2707	0	2654	95	0
1	N	2677	0	2624	108	0
1	O	2610	0	2572	91	0
1	P	2511	0	2479	100	0
2	A	44	0	27	1	0
2	B	44	0	27	6	0
2	C	44	0	27	6	0
2	D	44	0	27	7	0
2	E	44	0	27	7	0
2	F	44	0	27	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	44	0	27	4	0
2	H	44	0	27	8	0
2	I	44	0	27	12	0
2	J	44	0	27	7	0
2	K	44	0	27	4	0
2	L	44	0	27	6	0
2	M	44	0	27	4	0
2	N	44	0	27	4	0
2	O	44	0	27	3	0
2	P	44	0	27	5	0
3	A	40	0	22	2	0
3	B	40	0	22	1	0
3	C	40	0	22	1	0
3	D	40	0	22	1	0
3	E	40	0	22	5	0
3	F	40	0	22	2	0
3	G	40	0	22	2	0
3	H	40	0	22	3	0
3	I	40	0	22	3	0
3	J	40	0	22	3	0
3	K	40	0	22	6	0
3	L	40	0	22	0	0
3	M	40	0	22	4	0
3	N	40	0	22	1	0
3	O	40	0	22	2	0
3	P	40	0	22	1	0
4	A	85	0	0	8	0
4	B	54	0	0	6	0
4	C	58	0	0	3	0
4	D	51	0	0	3	0
4	E	21	0	0	2	0
4	F	24	0	0	0	0
4	G	49	0	0	4	0
4	H	35	0	0	2	0
4	I	36	0	0	2	0
4	J	30	0	0	1	0
4	K	26	0	0	2	0
4	L	37	0	0	3	0
4	M	36	0	0	1	0
4	N	34	0	0	4	0
4	O	17	0	0	1	0
4	P	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	43985	0	42080	1679	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 1679 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:K:39:VAL:HG12	1:K:40:GLU:CG	1.49	1.43
1:I:64:LEU:HD23	1:I:67:MET:CE	1.59	1.31
1:B:12:ARG:HG2	1:B:39:VAL:CG2	1.61	1.28
1:B:12:ARG:CG	1:B:39:VAL:HG21	1.64	1.27
1:N:12:ARG:NH1	1:N:72:ASN:OD1	1.70	1.25

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:TYR:CE2	1:I:287:ARG:CD[2_746]	1.84	0.36
1:H:287:ARG:NH2	1:J:273:GLU:OE2[2_746]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	344/370 (93%)	323 (94%)	20 (6%)	1 (0%)	36	33
1	B	327/370 (88%)	306 (94%)	20 (6%)	1 (0%)	36	33
1	C	345/370 (93%)	322 (93%)	21 (6%)	2 (1%)	21	15
1	D	342/370 (92%)	309 (90%)	29 (8%)	4 (1%)	10	5
1	E	317/370 (86%)	278 (88%)	34 (11%)	5 (2%)	7	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	323/370 (87%)	297 (92%)	25 (8%)	1 (0%)	36	33
1	G	340/370 (92%)	317 (93%)	20 (6%)	3 (1%)	14	8
1	H	341/370 (92%)	317 (93%)	23 (7%)	1 (0%)	36	33
1	I	340/370 (92%)	306 (90%)	28 (8%)	6 (2%)	6	2
1	J	344/370 (93%)	309 (90%)	31 (9%)	4 (1%)	10	5
1	K	318/370 (86%)	287 (90%)	26 (8%)	5 (2%)	7	2
1	L	316/370 (85%)	281 (89%)	27 (8%)	8 (2%)	4	1
1	M	344/370 (93%)	321 (93%)	20 (6%)	3 (1%)	14	8
1	N	340/370 (92%)	313 (92%)	26 (8%)	1 (0%)	36	33
1	O	330/370 (89%)	299 (91%)	29 (9%)	2 (1%)	21	15
1	P	318/370 (86%)	291 (92%)	24 (8%)	3 (1%)	14	8
All	All	5329/5920 (90%)	4876 (92%)	403 (8%)	50 (1%)	14	8

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	30	ALA
1	L	26	ILE
1	L	30	ALA
1	M	30	ALA
1	M	31	GLN

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	277/299 (93%)	256 (92%)	21 (8%)	12	7
1	B	264/299 (88%)	239 (90%)	25 (10%)	8	4
1	C	277/299 (93%)	259 (94%)	18 (6%)	15	10
1	D	275/299 (92%)	253 (92%)	22 (8%)	11	7
1	E	254/299 (85%)	228 (90%)	26 (10%)	7	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	260/299 (87%)	242 (93%)	18 (7%)	14	9
1	G	273/299 (91%)	253 (93%)	20 (7%)	13	8
1	H	274/299 (92%)	247 (90%)	27 (10%)	7	3
1	I	273/299 (91%)	252 (92%)	21 (8%)	12	7
1	J	277/299 (93%)	255 (92%)	22 (8%)	11	7
1	K	255/299 (85%)	229 (90%)	26 (10%)	7	3
1	L	256/299 (86%)	223 (87%)	33 (13%)	4	1
1	M	277/299 (93%)	252 (91%)	25 (9%)	9	4
1	N	273/299 (91%)	247 (90%)	26 (10%)	8	4
1	O	267/299 (89%)	247 (92%)	20 (8%)	12	7
1	P	255/299 (85%)	234 (92%)	21 (8%)	10	6
All	All	4287/4784 (90%)	3916 (91%)	371 (9%)	9	5

5 of 371 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	72	ASN
1	M	103	LYS
1	K	204	GLU
1	L	124	VAL
1	M	319	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	88	GLN
1	L	88	GLN
1	I	246	GLN
1	K	32	HIS
1	L	301	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 ⓘ

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	HP7	B	550	-	41,42,42	1.03	3 (7%)	60,64,64	1.95	16 (26%)
2	NAI	D	500	-	47,48,48	1.28	2 (4%)	64,73,73	2.22	21 (32%)
3	HP7	K	550	-	41,42,42	1.10	5 (12%)	60,64,64	1.91	12 (20%)
3	HP7	P	550	-	41,42,42	1.05	2 (4%)	60,64,64	1.35	8 (13%)
2	NAI	H	500	-	47,48,48	1.27	3 (6%)	64,73,73	2.51	24 (37%)
2	NAI	I	500	-	47,48,48	1.24	2 (4%)	64,73,73	2.34	23 (35%)
3	HP7	O	550	-	41,42,42	1.06	2 (4%)	60,64,64	1.60	8 (13%)
2	NAI	L	500	-	47,48,48	1.30	2 (4%)	64,73,73	2.30	28 (43%)
2	NAI	E	500	-	47,48,48	1.31	3 (6%)	64,73,73	2.14	21 (32%)
3	HP7	N	550	-	41,42,42	1.07	3 (7%)	60,64,64	2.22	18 (30%)
3	HP7	J	550	-	41,42,42	1.02	3 (7%)	60,64,64	1.92	15 (25%)
2	NAI	M	500	-	47,48,48	1.31	3 (6%)	64,73,73	2.30	24 (37%)
3	HP7	E	550	-	41,42,42	1.06	3 (7%)	60,64,64	1.76	12 (20%)
2	NAI	K	500	-	47,48,48	1.27	2 (4%)	64,73,73	2.52	25 (39%)
2	NAI	P	500	-	47,48,48	1.30	2 (4%)	64,73,73	2.00	20 (31%)
3	HP7	I	550	-	41,42,42	1.08	4 (9%)	60,64,64	1.73	14 (23%)
2	NAI	O	500	-	47,48,48	1.29	2 (4%)	64,73,73	2.43	22 (34%)
2	NAI	J	500	-	47,48,48	1.29	2 (4%)	64,73,73	2.39	24 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	F	500	-	47,48,48	1.28	3 (6%)	64,73,73	2.46	31 (48%)
3	HP7	A	550	-	41,42,42	1.10	4 (9%)	60,64,64	2.15	21 (35%)
3	HP7	F	550	-	41,42,42	1.05	3 (7%)	60,64,64	1.67	12 (20%)
2	NAI	B	500	-	47,48,48	1.33	2 (4%)	64,73,73	2.22	25 (39%)
3	HP7	M	550	-	41,42,42	1.03	3 (7%)	60,64,64	2.19	21 (35%)
3	HP7	G	550	-	41,42,42	1.05	5 (12%)	60,64,64	2.01	17 (28%)
3	HP7	D	550	-	41,42,42	1.05	3 (7%)	60,64,64	1.74	12 (20%)
2	NAI	C	500	-	47,48,48	1.32	3 (6%)	64,73,73	2.37	25 (39%)
3	HP7	H	550	-	41,42,42	1.04	3 (7%)	60,64,64	2.10	17 (28%)
3	HP7	L	550	-	41,42,42	1.09	4 (9%)	60,64,64	1.82	12 (20%)
2	NAI	A	500	-	47,48,48	1.27	3 (6%)	64,73,73	2.31	25 (39%)
2	NAI	G	500	-	47,48,48	1.27	2 (4%)	64,73,73	2.30	29 (45%)
2	NAI	N	500	-	47,48,48	1.29	2 (4%)	64,73,73	2.38	25 (39%)
3	HP7	C	550	-	41,42,42	1.01	2 (4%)	60,64,64	2.10	24 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HP7	B	550	-	-	2/28/65/65	0/3/3/3
2	NAI	D	500	-	-	13/29/72/72	0/5/5/5
3	HP7	K	550	-	-	2/28/65/65	0/3/3/3
3	HP7	P	550	-	-	3/28/65/65	0/3/3/3
2	NAI	H	500	-	-	13/29/72/72	0/5/5/5
2	NAI	I	500	-	-	13/29/72/72	0/5/5/5
3	HP7	O	550	-	-	7/28/65/65	0/3/3/3
2	NAI	L	500	-	-	15/29/72/72	0/5/5/5
2	NAI	E	500	-	-	12/29/72/72	0/5/5/5
3	HP7	N	550	-	-	4/28/65/65	0/3/3/3
3	HP7	J	550	-	-	1/28/65/65	0/3/3/3
2	NAI	M	500	-	-	18/29/72/72	0/5/5/5
3	HP7	E	550	-	-	4/28/65/65	0/3/3/3
2	NAI	K	500	-	-	12/29/72/72	0/5/5/5
2	NAI	P	500	-	-	13/29/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HP7	I	550	-	-	3/28/65/65	0/3/3/3
2	NAI	O	500	-	-	16/29/72/72	0/5/5/5
2	NAI	J	500	-	-	12/29/72/72	0/5/5/5
2	NAI	F	500	-	-	13/29/72/72	0/5/5/5
3	HP7	A	550	-	-	1/28/65/65	0/3/3/3
3	HP7	F	550	-	-	2/28/65/65	0/3/3/3
2	NAI	B	500	-	-	14/29/72/72	0/5/5/5
3	HP7	M	550	-	-	6/28/65/65	0/3/3/3
3	HP7	G	550	-	-	7/28/65/65	0/3/3/3
3	HP7	D	550	-	-	6/28/65/65	0/3/3/3
2	NAI	C	500	-	-	15/29/72/72	0/5/5/5
3	HP7	H	550	-	-	0/28/65/65	0/3/3/3
3	HP7	L	550	-	-	4/28/65/65	0/3/3/3
2	NAI	A	500	-	-	11/29/72/72	0/5/5/5
2	NAI	G	500	-	-	12/29/72/72	0/5/5/5
2	NAI	N	500	-	-	15/29/72/72	0/5/5/5
3	HP7	C	550	-	-	2/28/65/65	0/3/3/3

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NAI	C4N-C3N	-5.37	1.39	1.50
2	F	500	NAI	C4N-C3N	-5.13	1.40	1.50
2	B	500	NAI	C4N-C3N	-5.04	1.40	1.50
2	E	500	NAI	C4N-C3N	-5.04	1.40	1.50
2	O	500	NAI	C4N-C3N	-4.96	1.40	1.50

The worst 5 of 631 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	500	NAI	C5B-C4B-C3B	-7.15	89.48	115.21
2	D	500	NAI	C5B-C4B-C3B	-7.05	89.82	115.21
3	N	550	HP7	C4-N3-C2	-7.05	117.86	126.61
2	O	500	NAI	C5A-C4A-N3A	-6.91	117.20	126.72
2	H	500	NAI	O4D-C4D-C5D	-6.69	87.92	109.33

There are no chirality outliers.

5 of 271 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAI	C5D-O5D-PN-O3
2	B	500	NAI	C5B-O5B-PA-O1A
2	B	500	NAI	C5B-O5B-PA-O2A
2	B	500	NAI	C5B-O5B-PA-O3
2	C	500	NAI	C5B-O5B-PA-O3

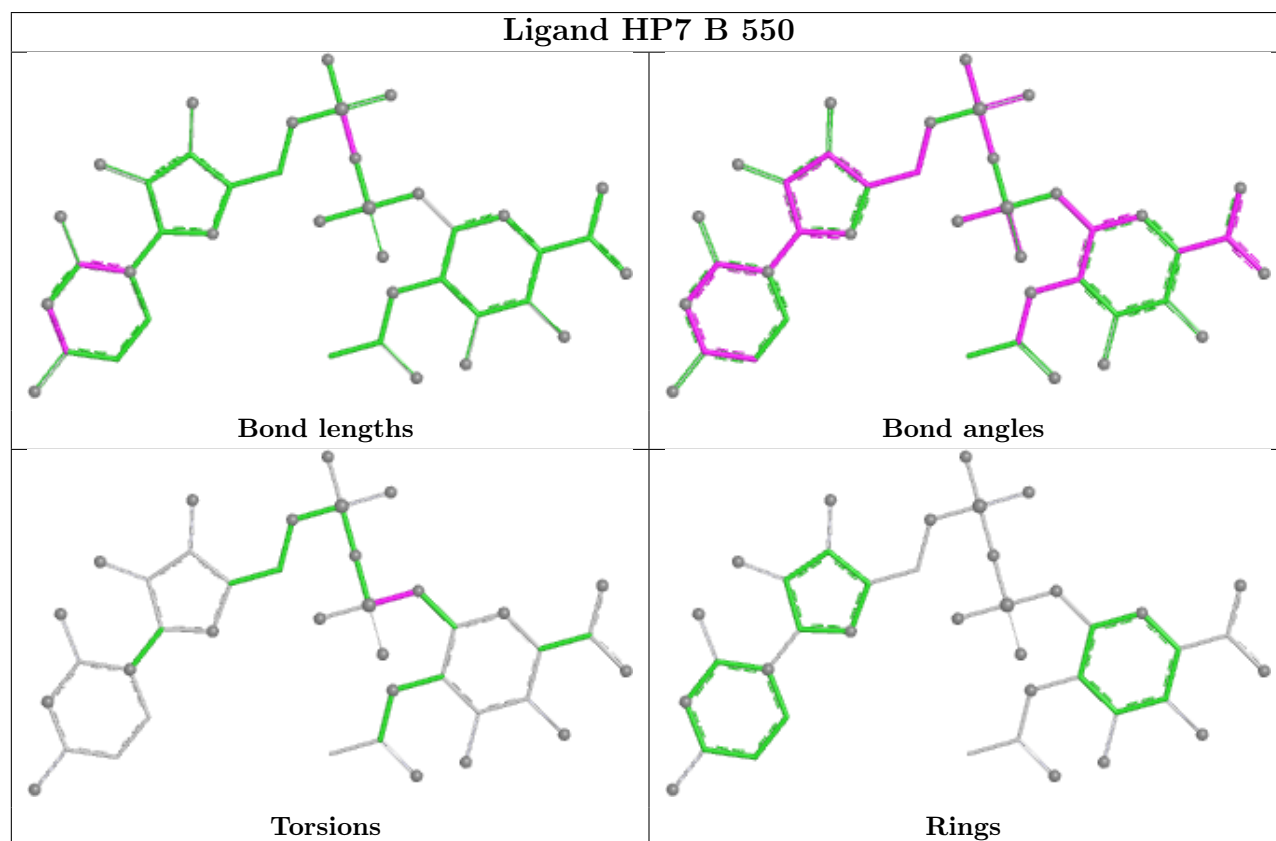
There are no ring outliers.

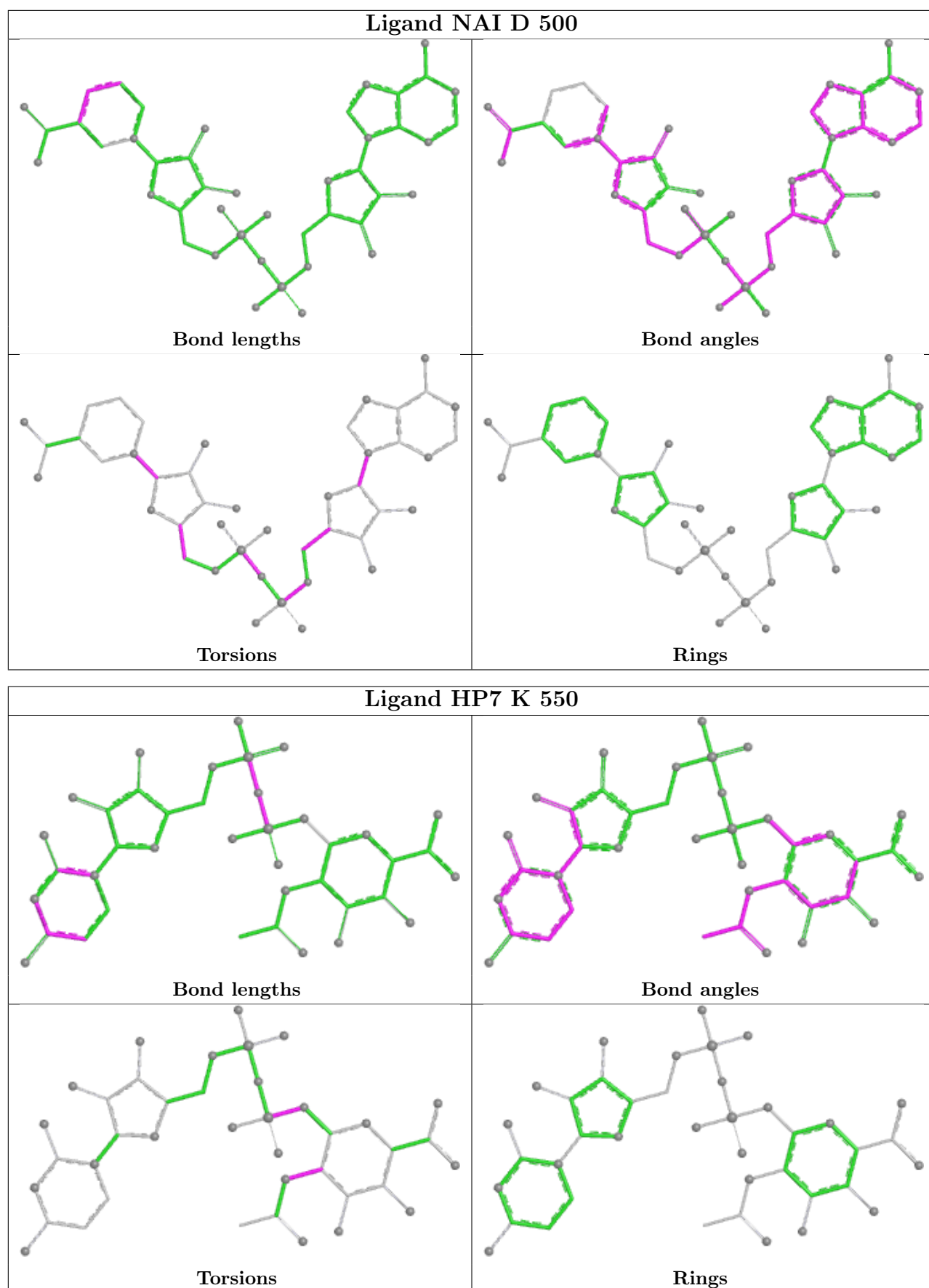
31 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	550	HP7	1	0
2	D	500	NAI	7	0
3	K	550	HP7	6	0
3	P	550	HP7	1	0
2	H	500	NAI	8	0
2	I	500	NAI	12	0
3	O	550	HP7	2	0
2	L	500	NAI	6	0
2	E	500	NAI	7	0
3	N	550	HP7	1	0
3	J	550	HP7	3	0
2	M	500	NAI	4	0
3	E	550	HP7	5	0
2	K	500	NAI	4	0
2	P	500	NAI	5	0
3	I	550	HP7	3	0
2	O	500	NAI	3	0
2	J	500	NAI	7	0
2	F	500	NAI	4	0
3	A	550	HP7	2	0
3	F	550	HP7	2	0
2	B	500	NAI	6	0
3	M	550	HP7	4	0
3	G	550	HP7	2	0
3	D	550	HP7	1	0
2	C	500	NAI	6	0
3	H	550	HP7	3	0
2	A	500	NAI	1	0
2	G	500	NAI	4	0
2	N	500	NAI	4	0
3	C	550	HP7	1	0

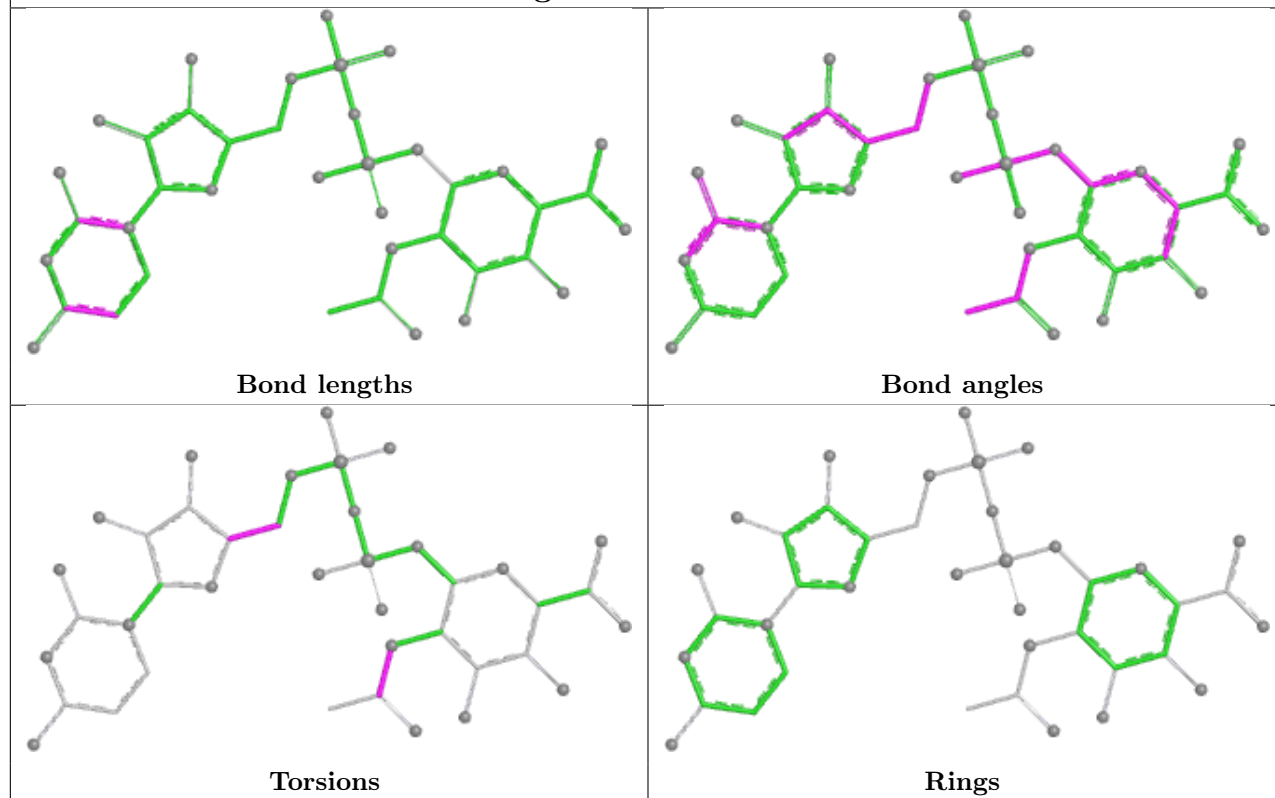
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

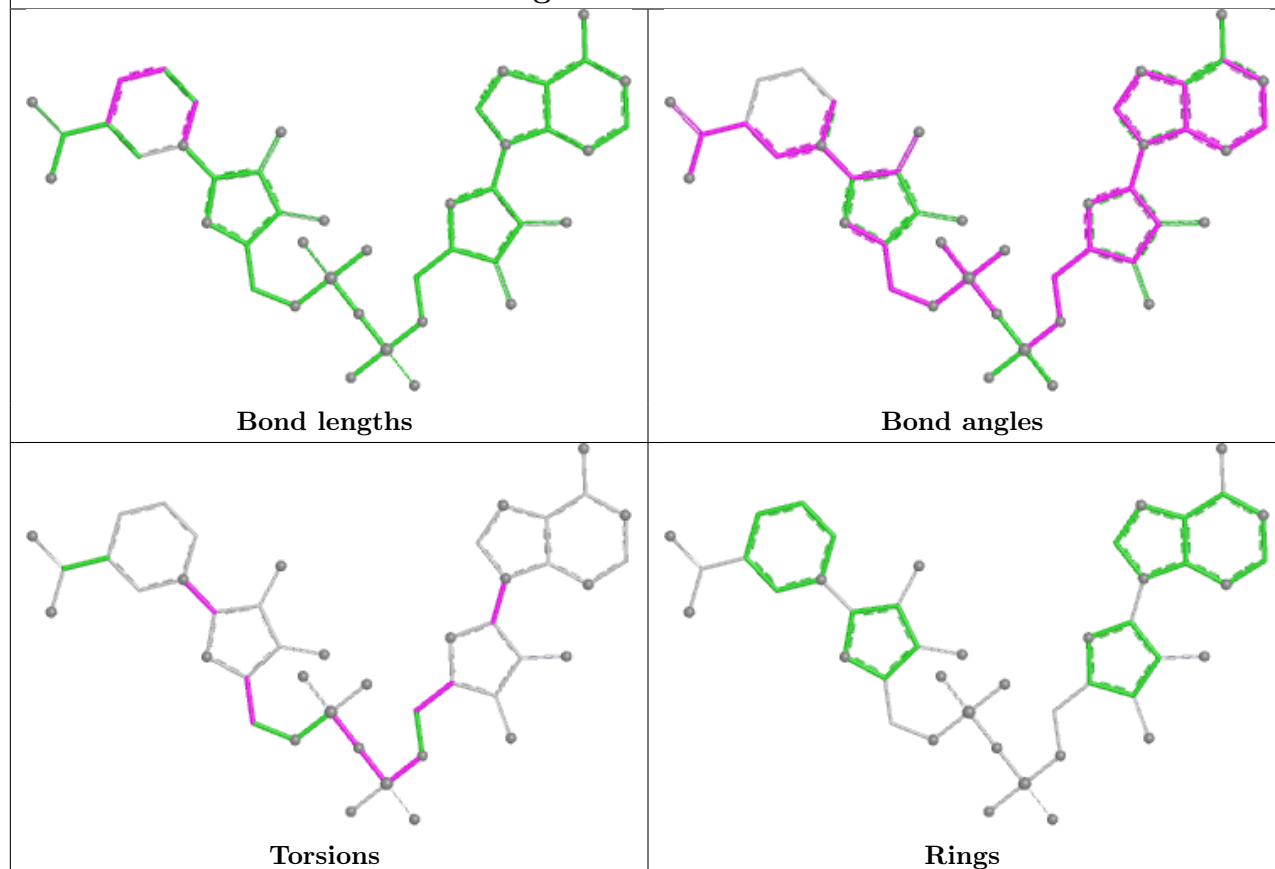


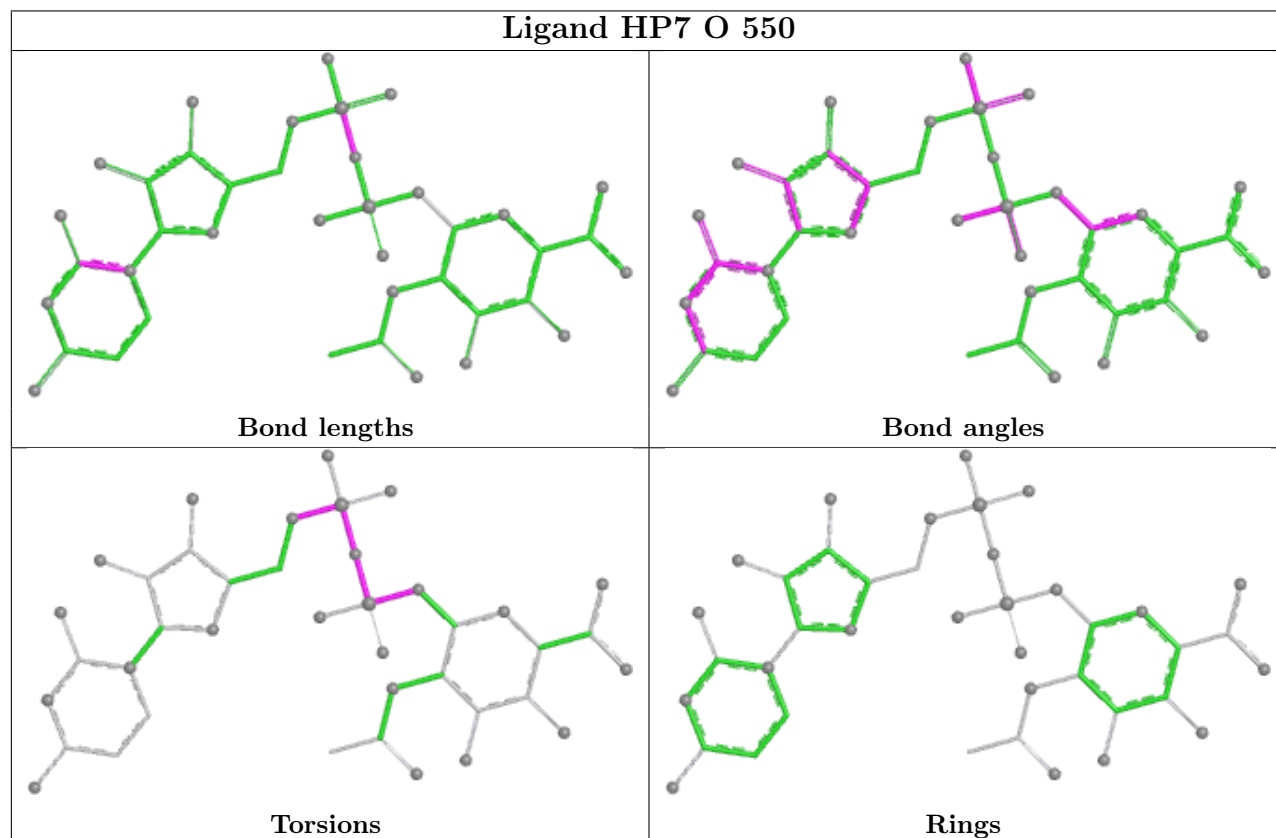
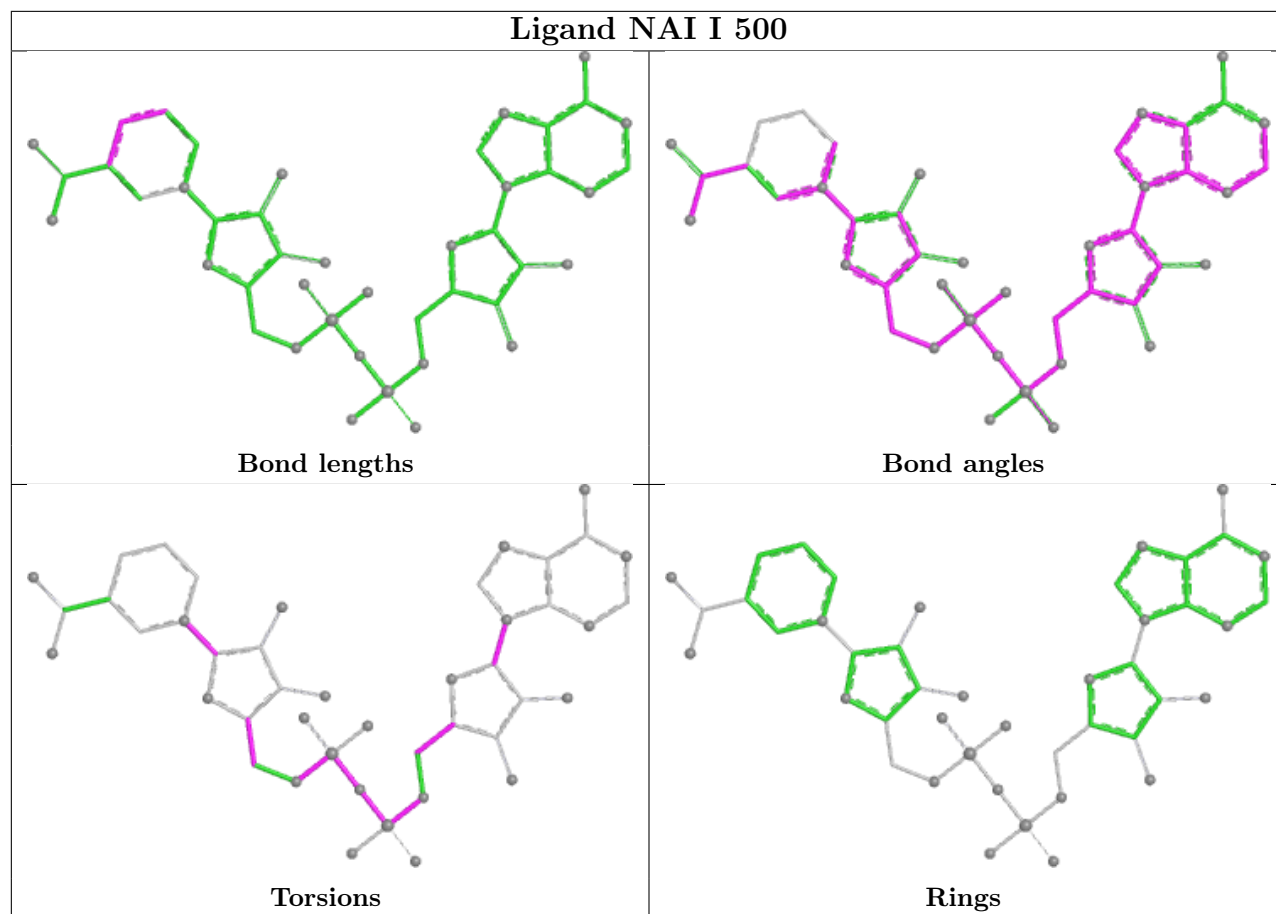


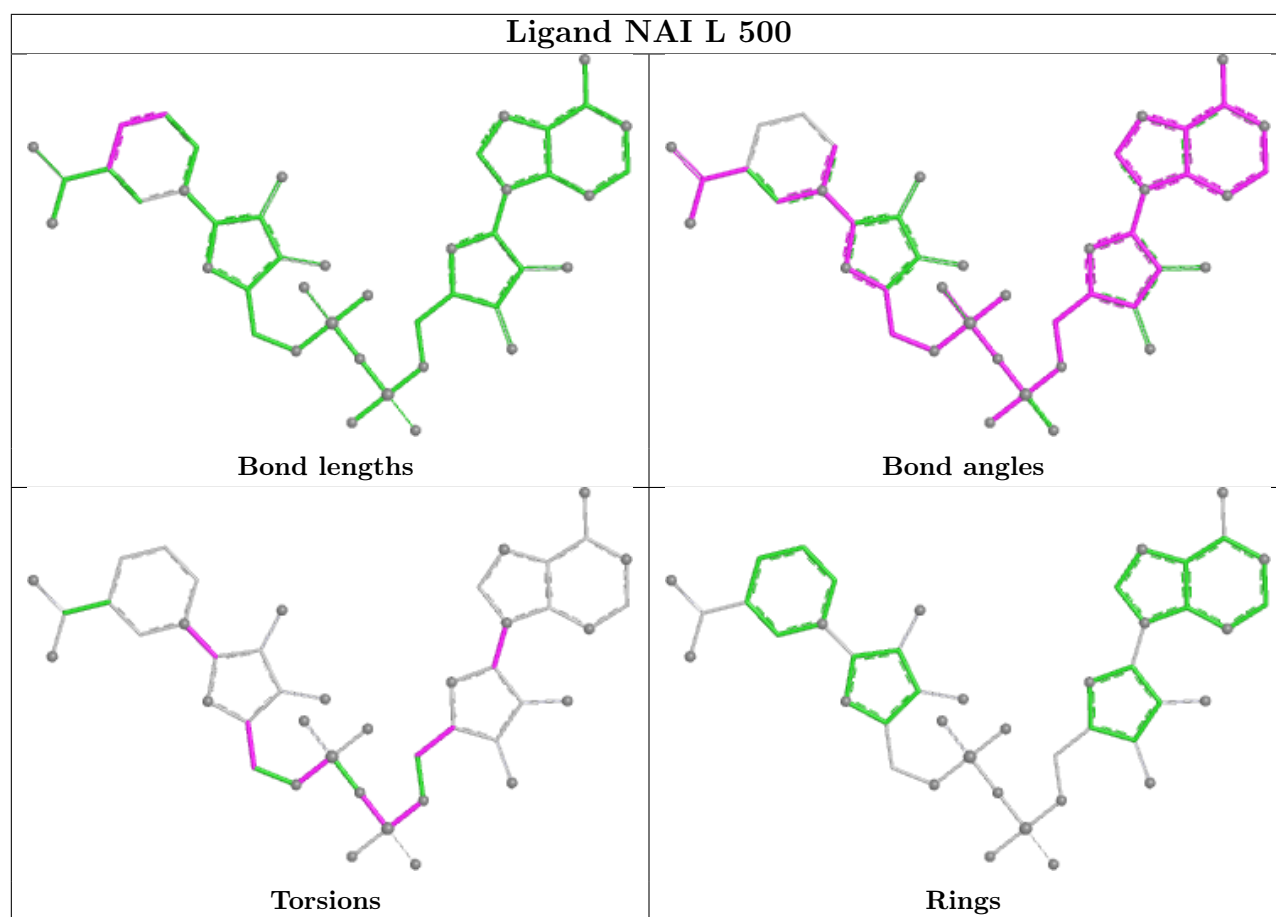
Ligand HP7 P 550

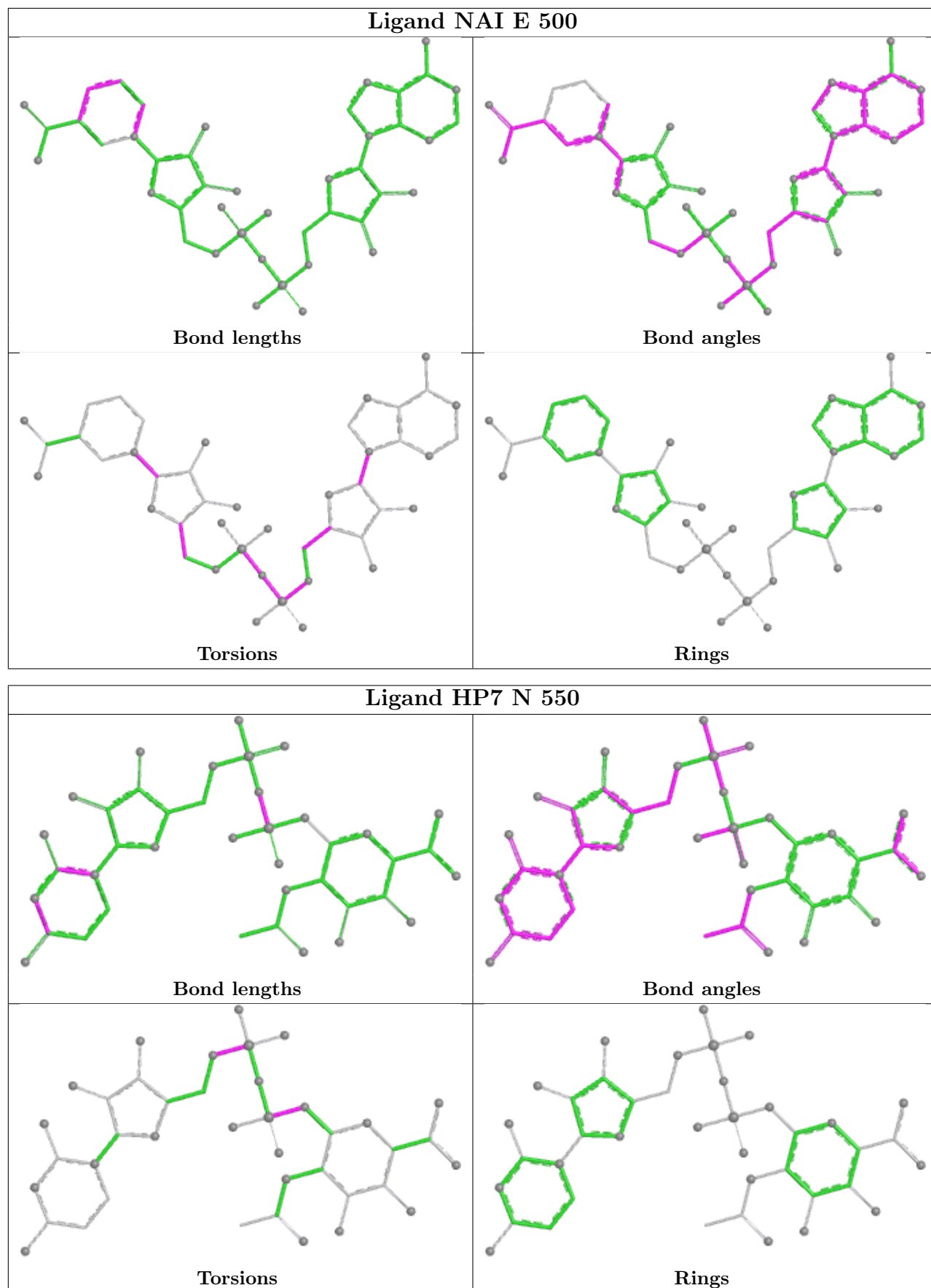


Ligand NAI H 500

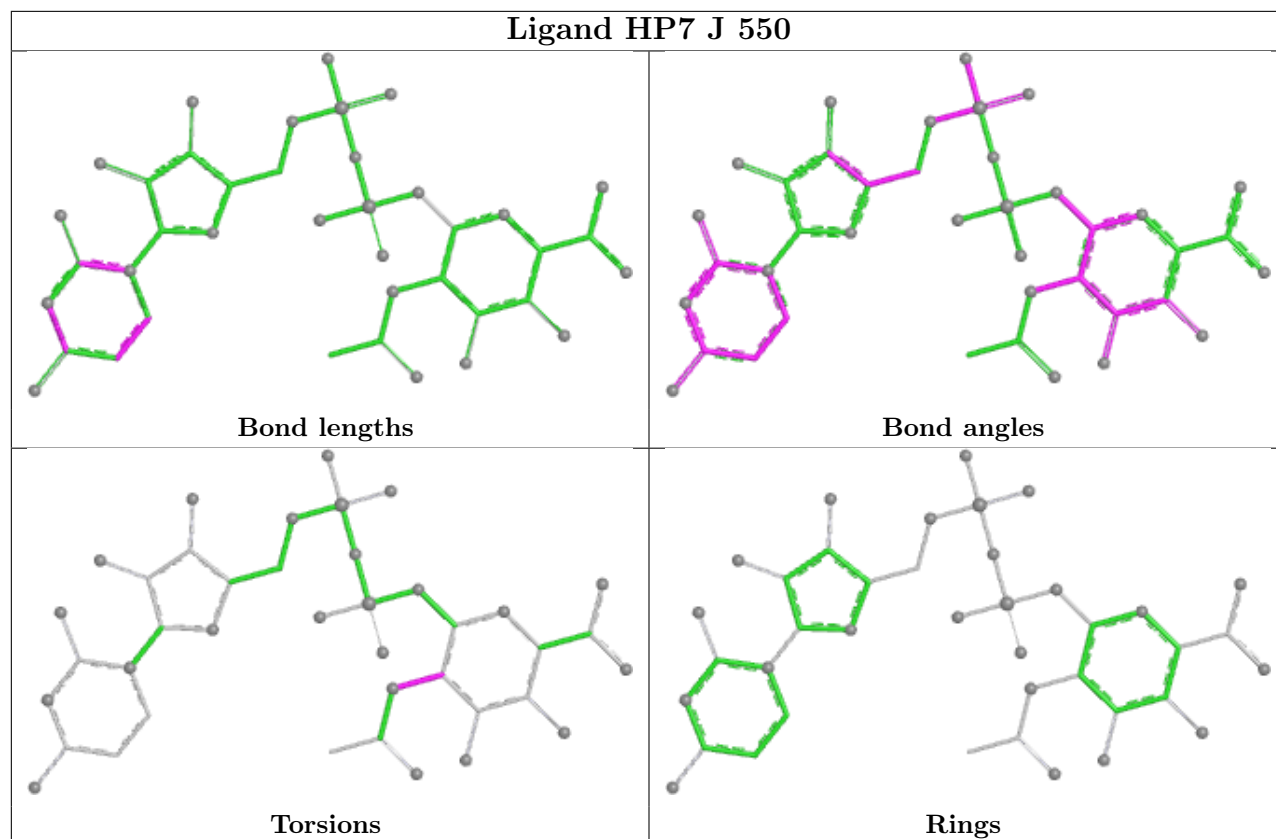




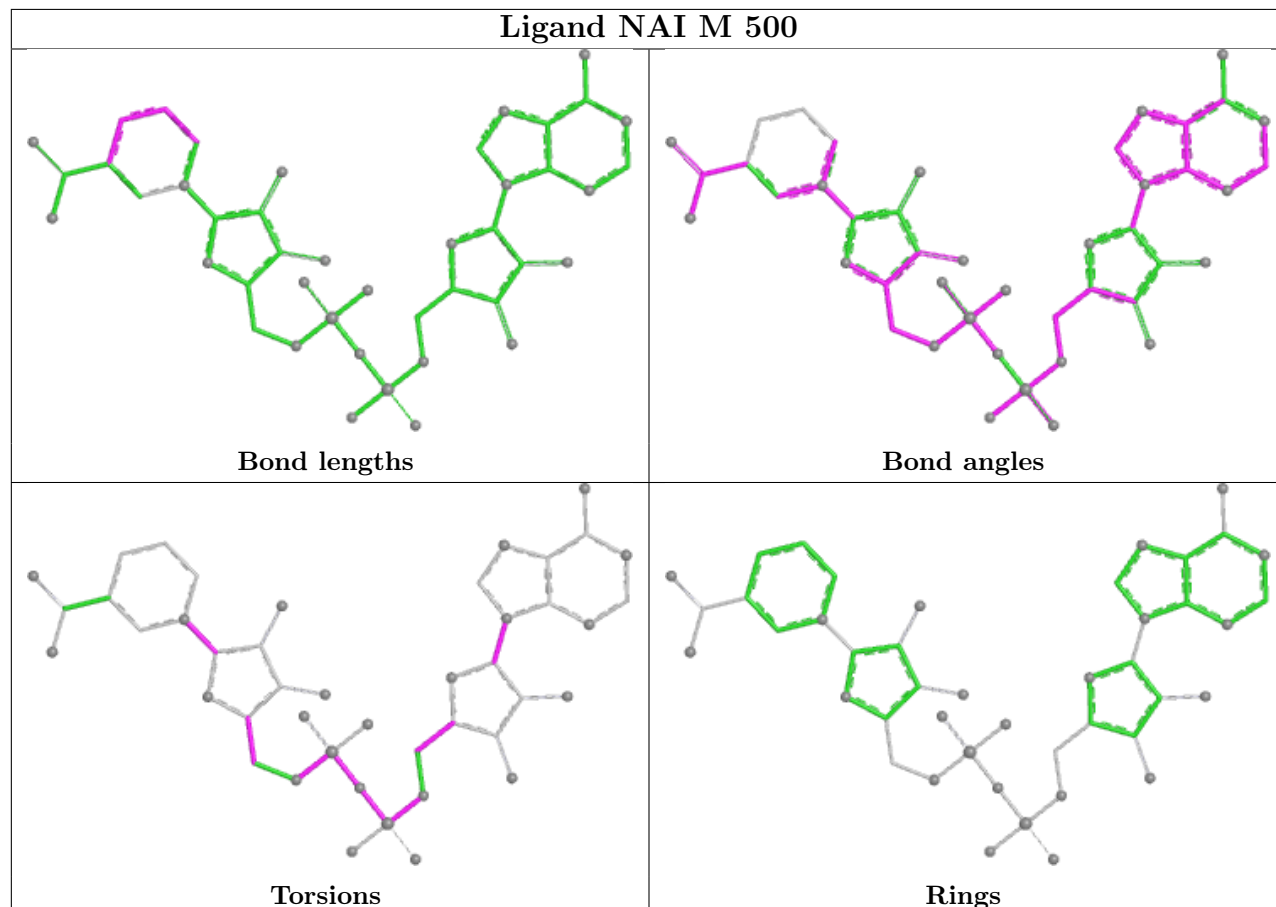


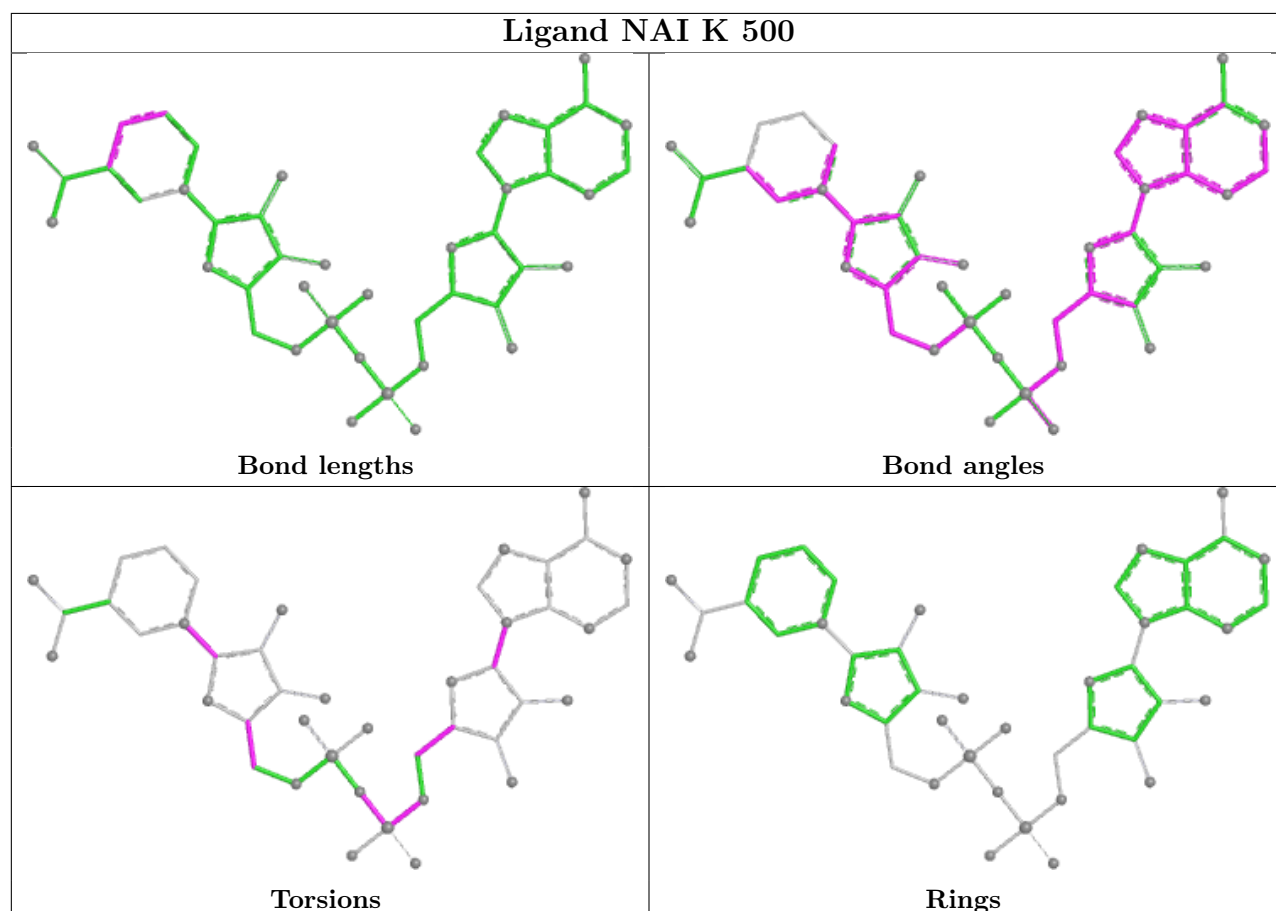
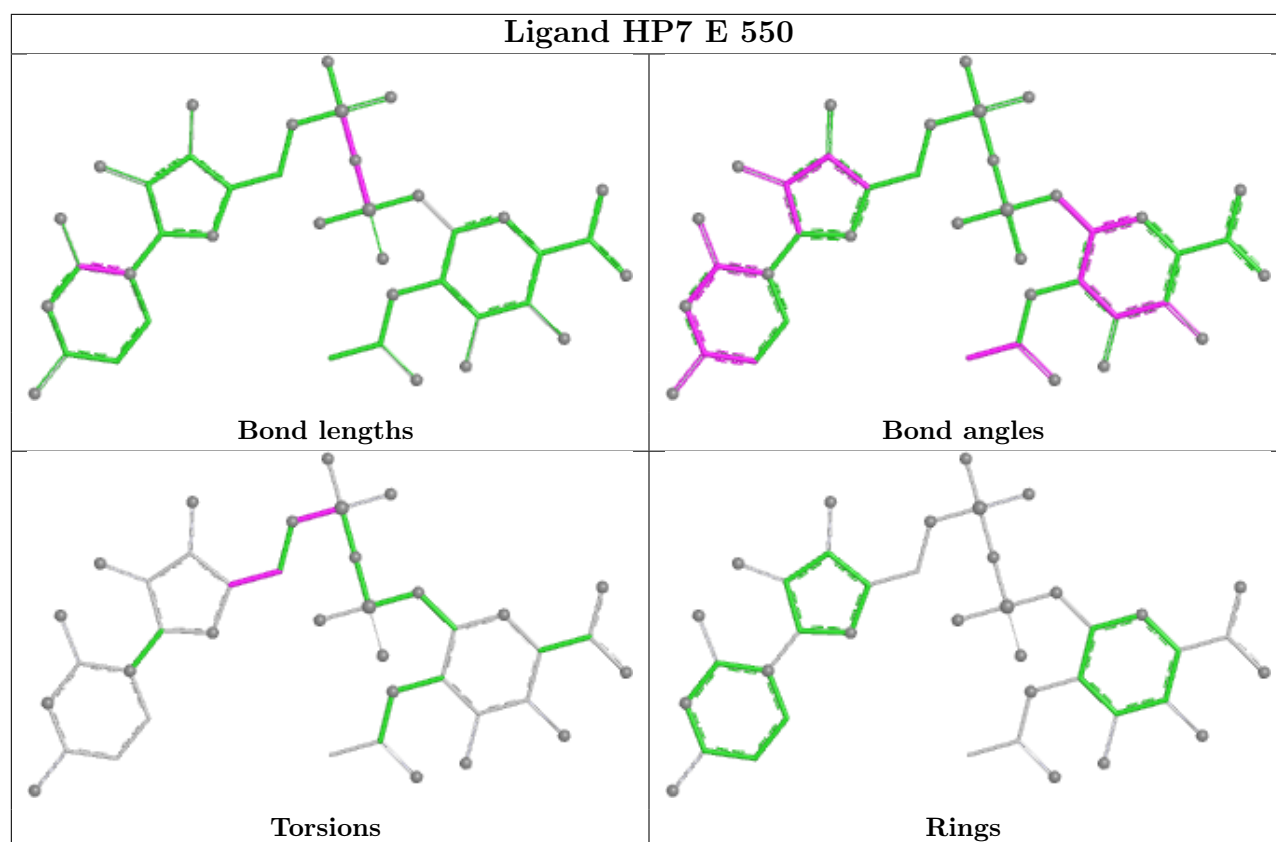


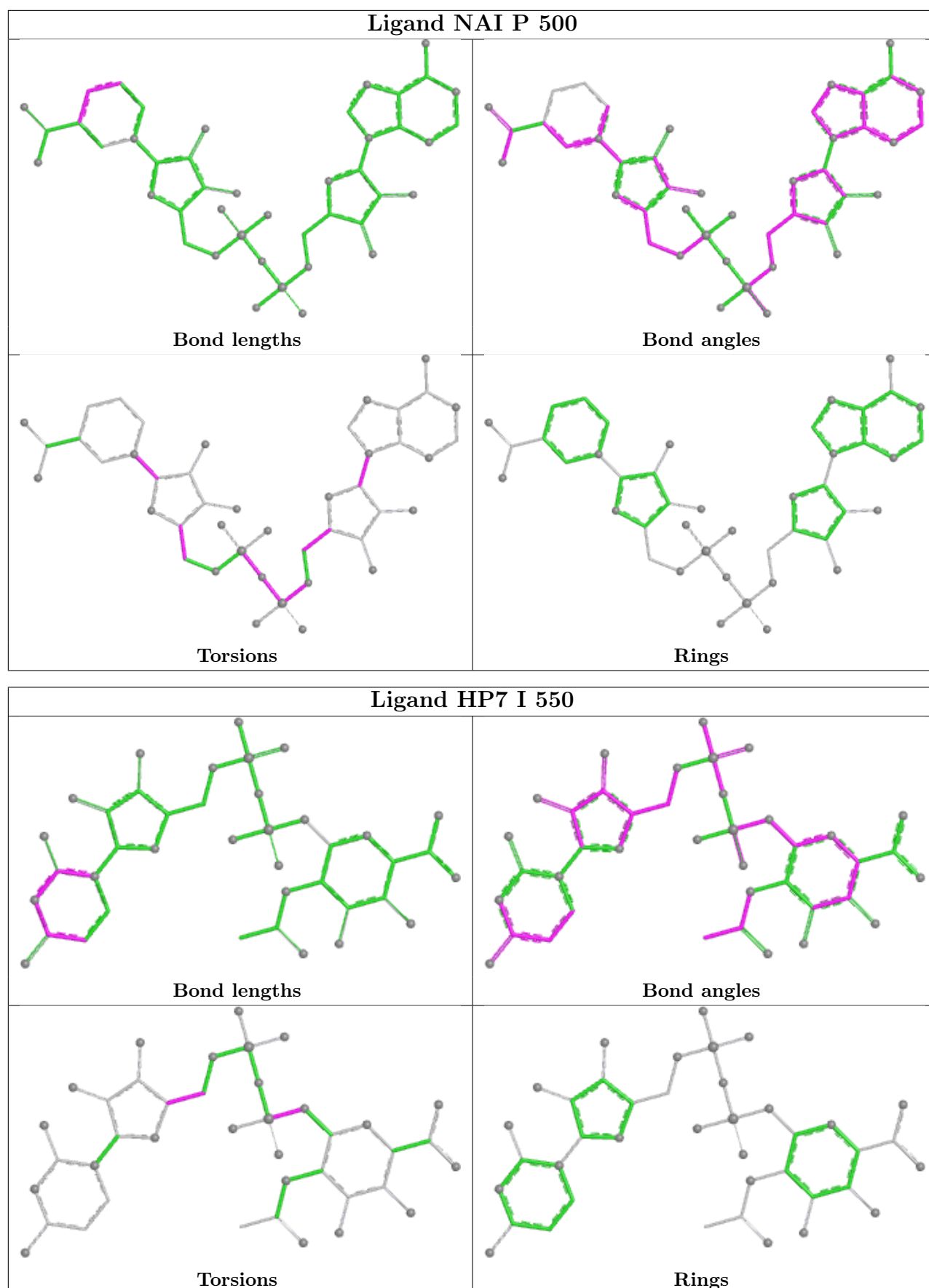
Ligand HP7 J 550

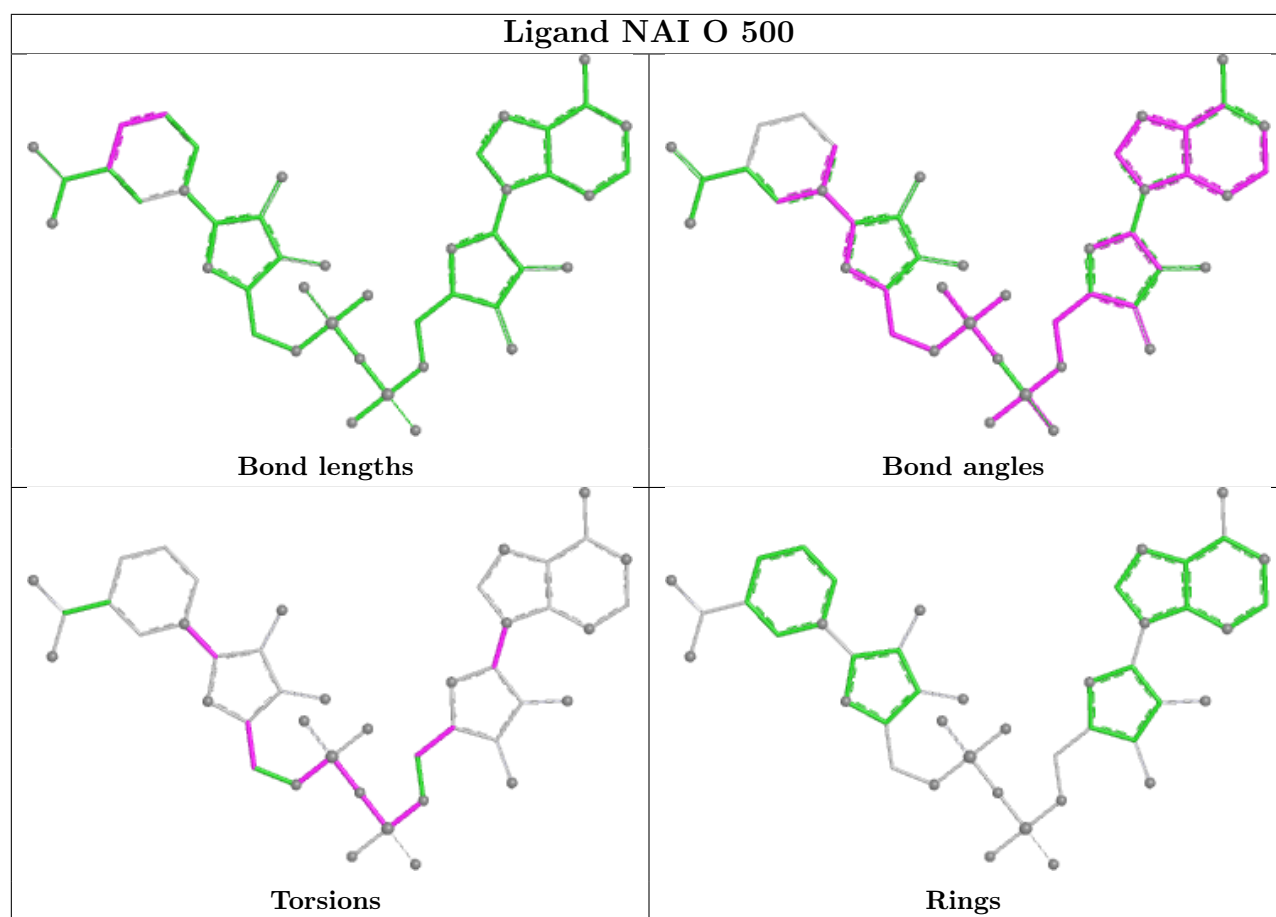


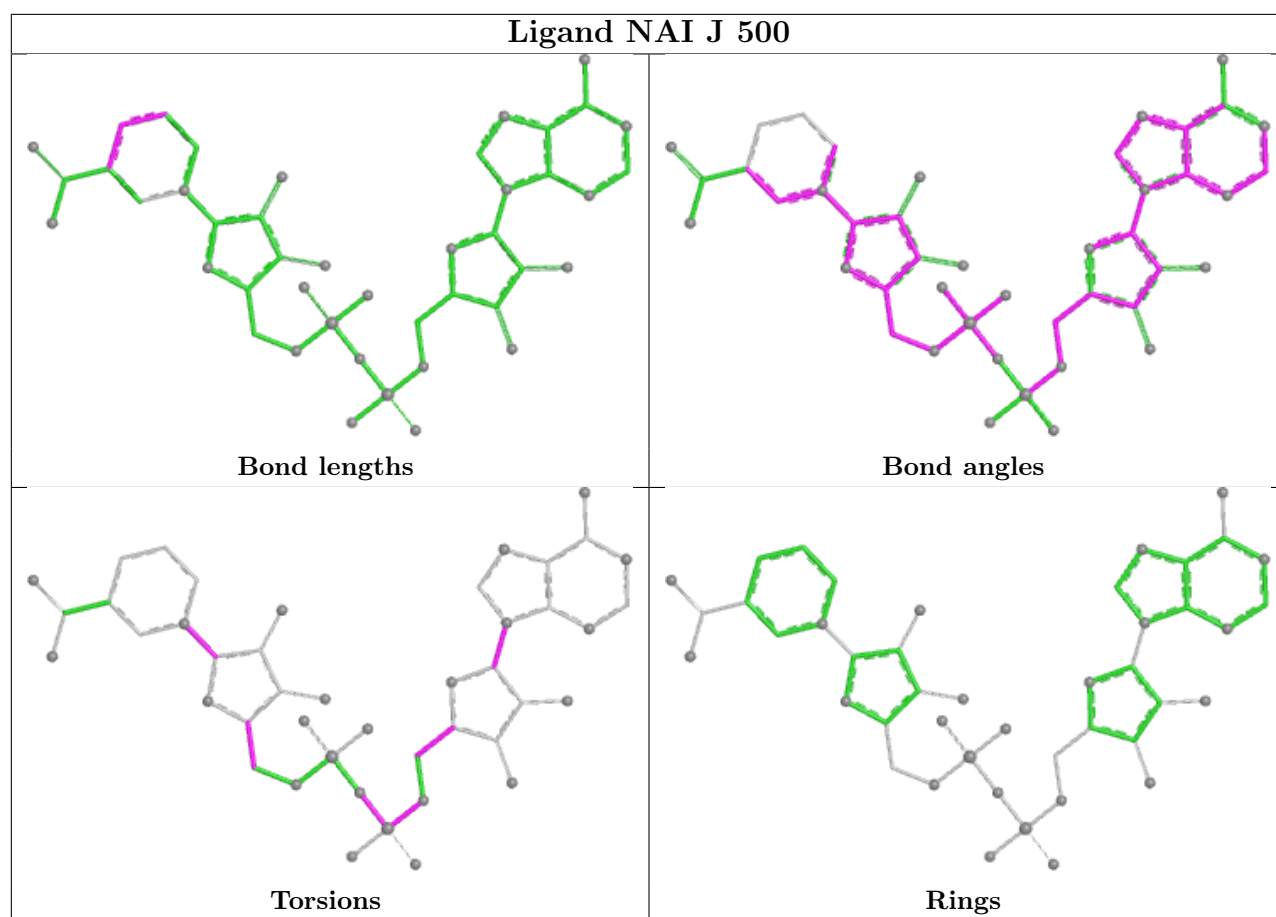
Ligand NAI M 500

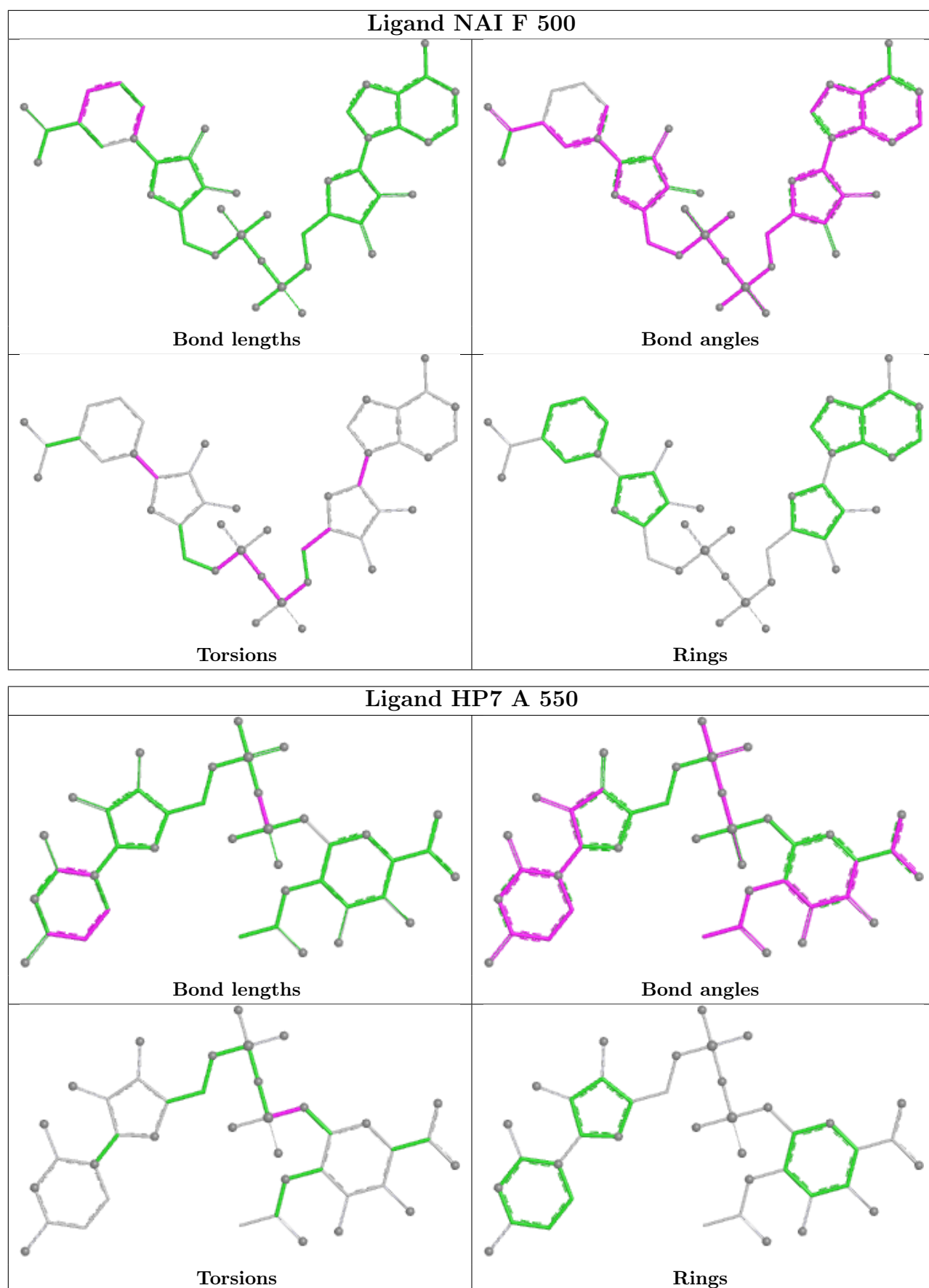




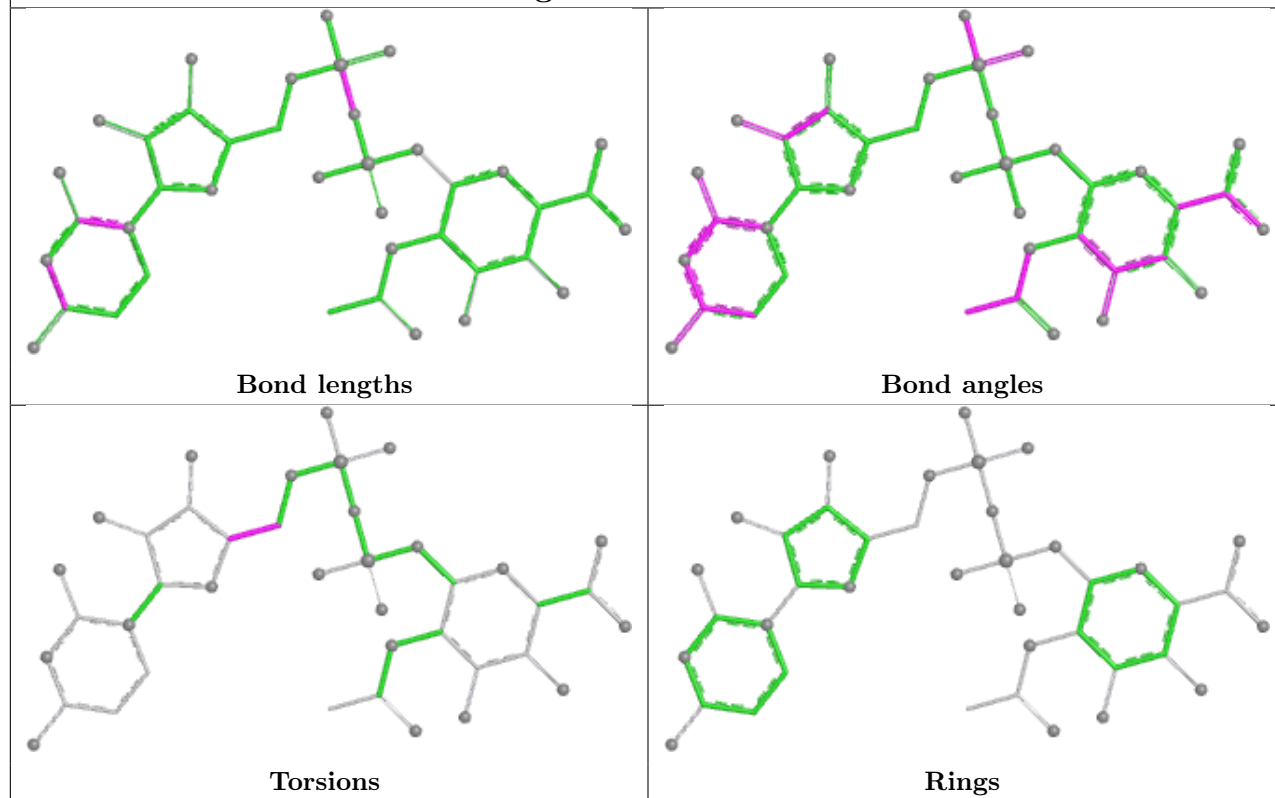




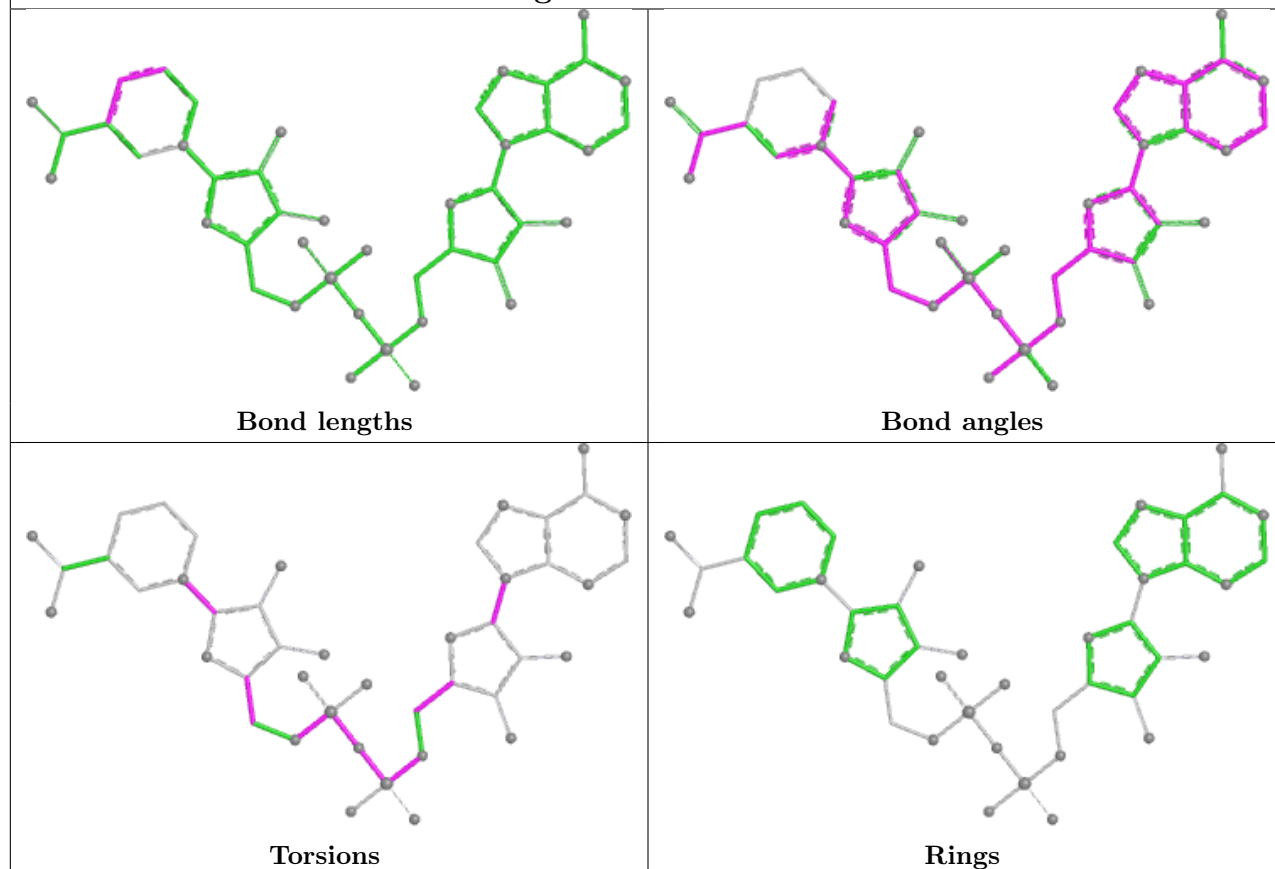


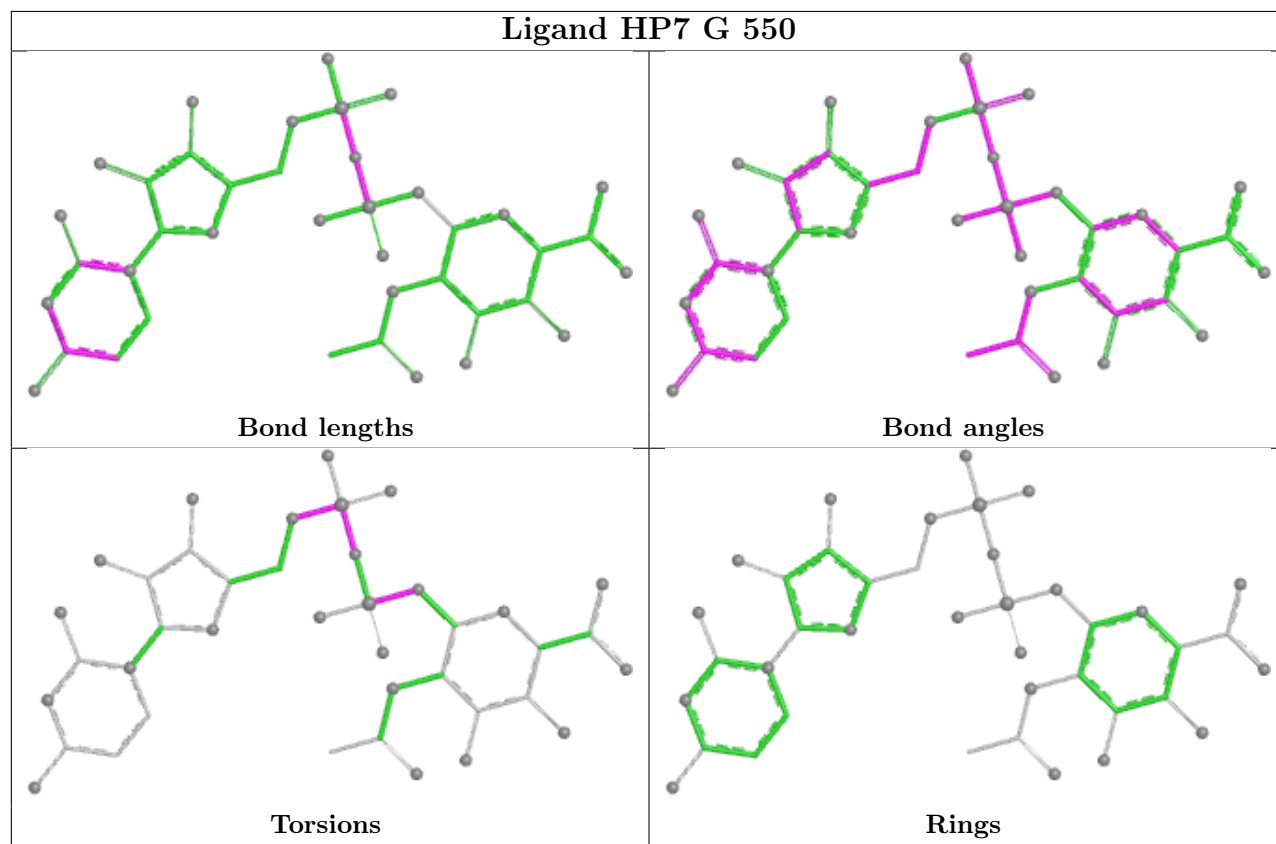
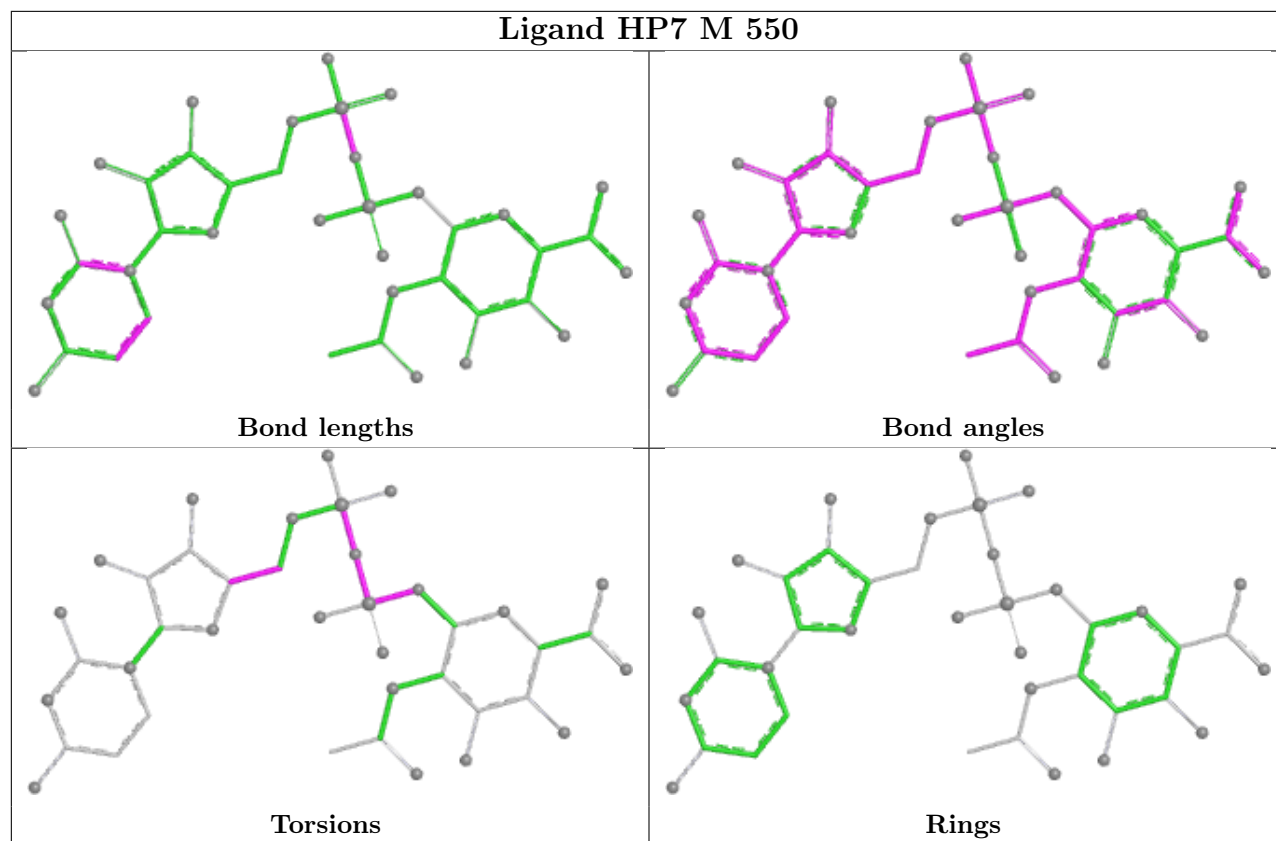


Ligand HP7 F 550

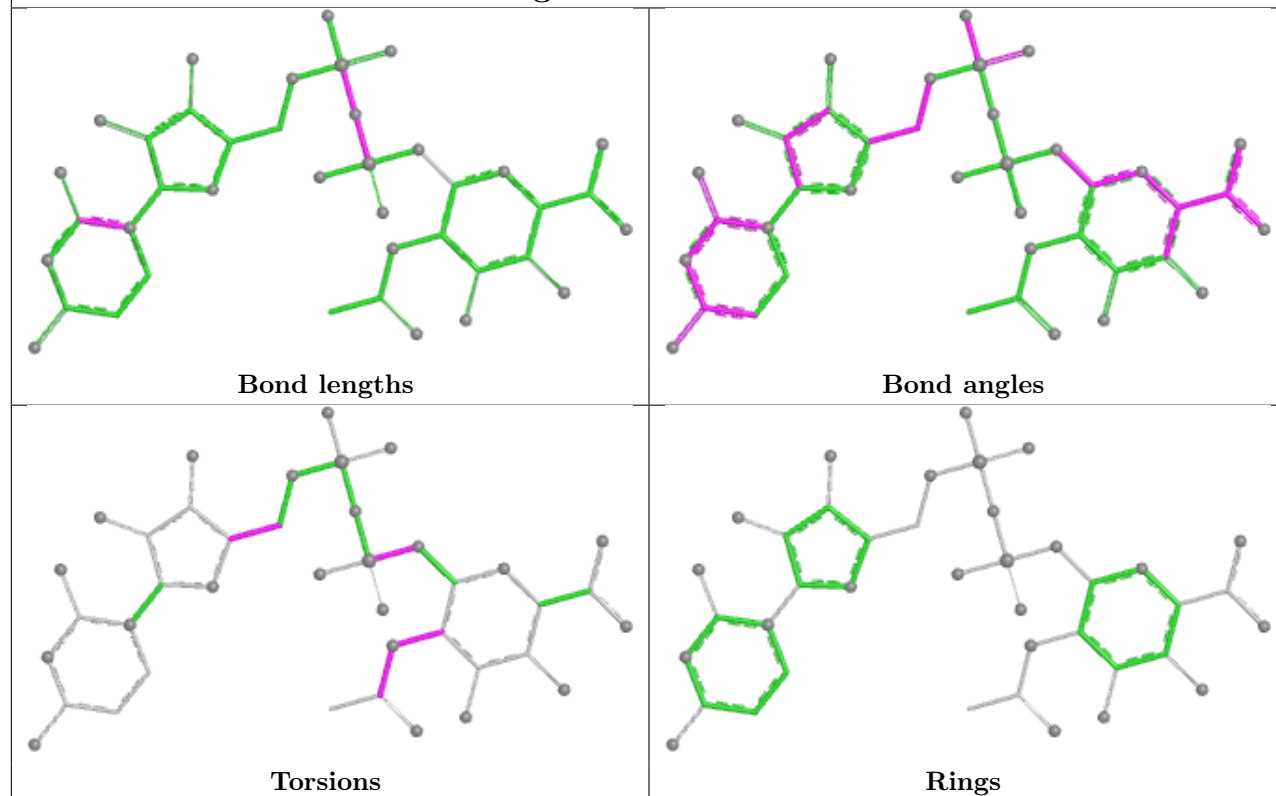


Ligand NAI B 500

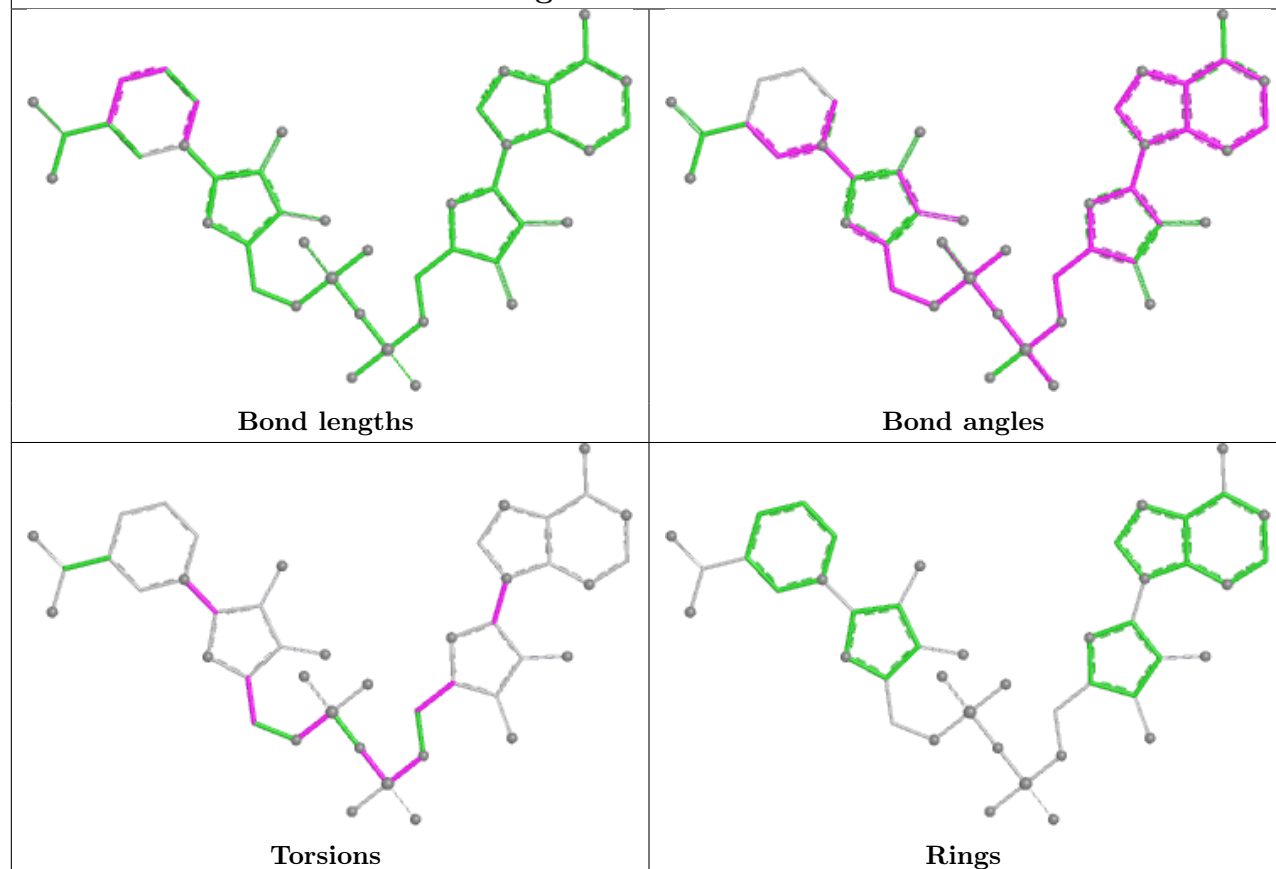




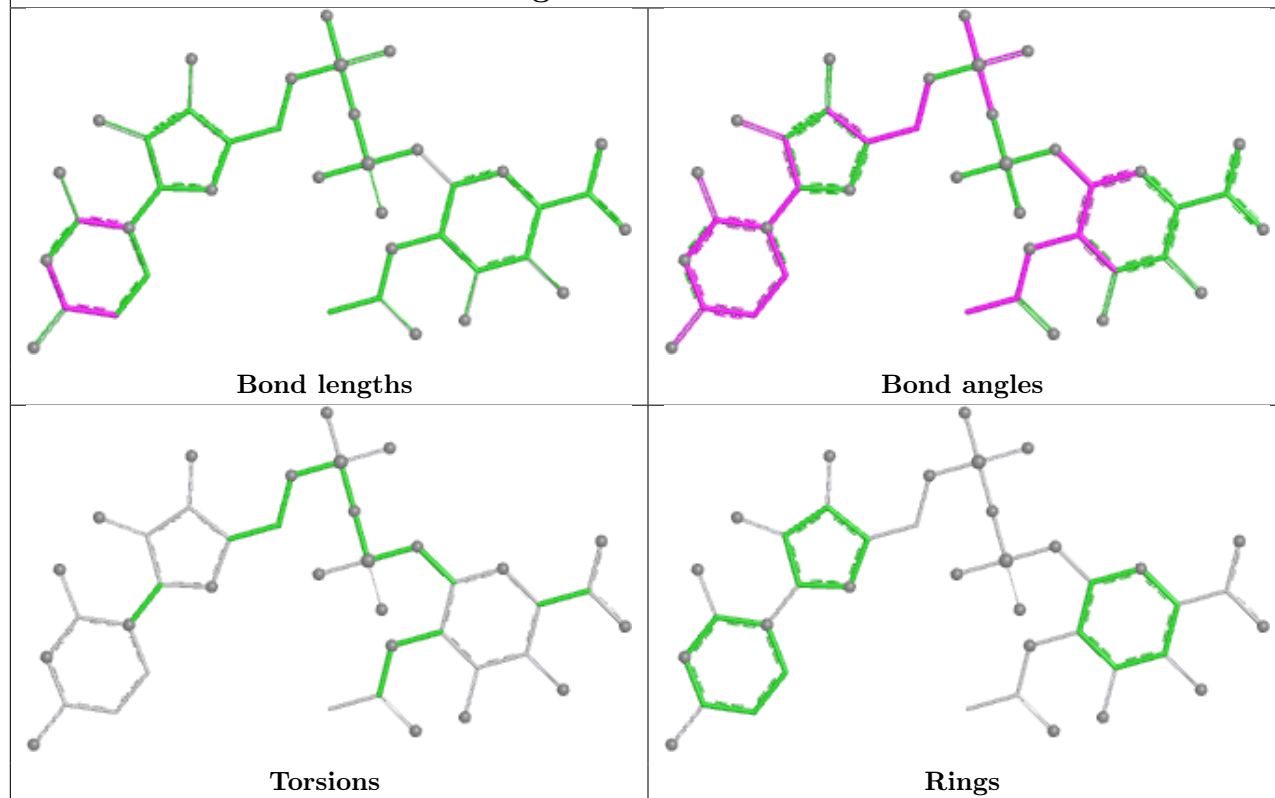
Ligand HP7 D 550



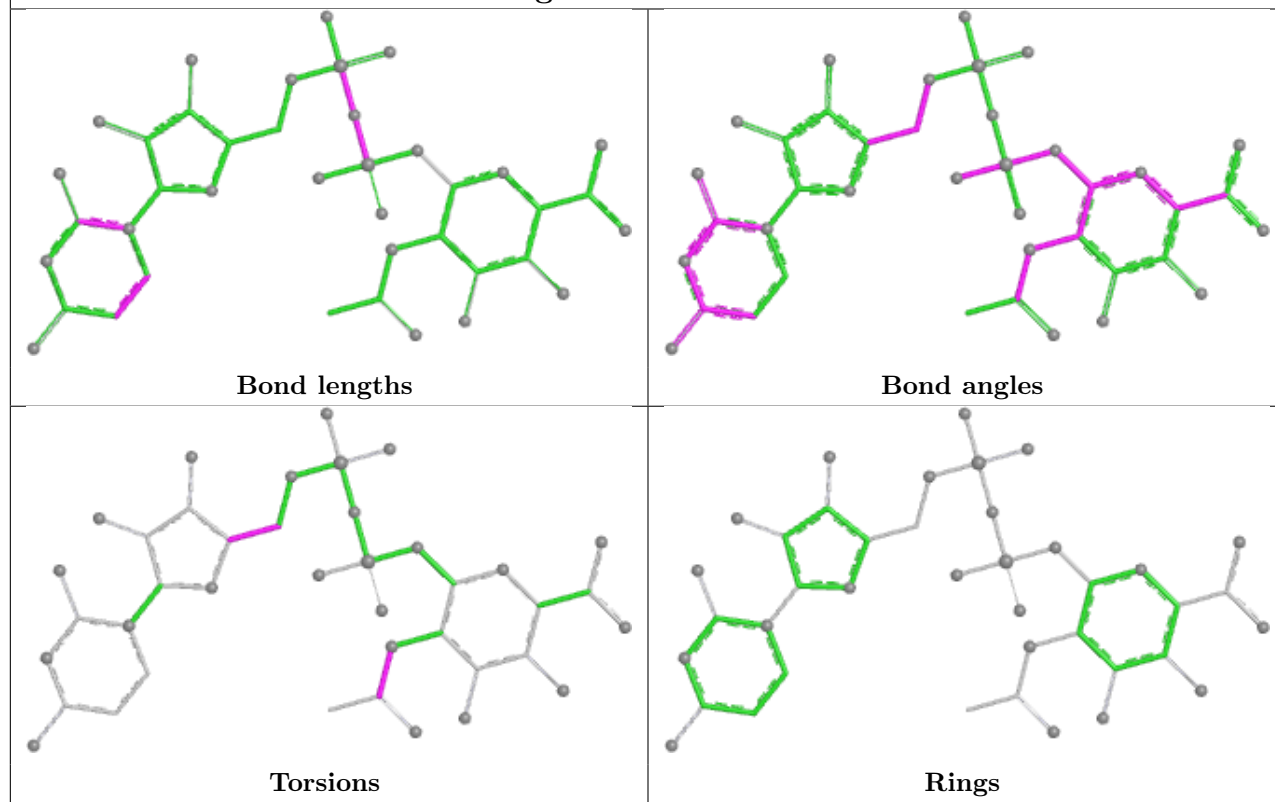
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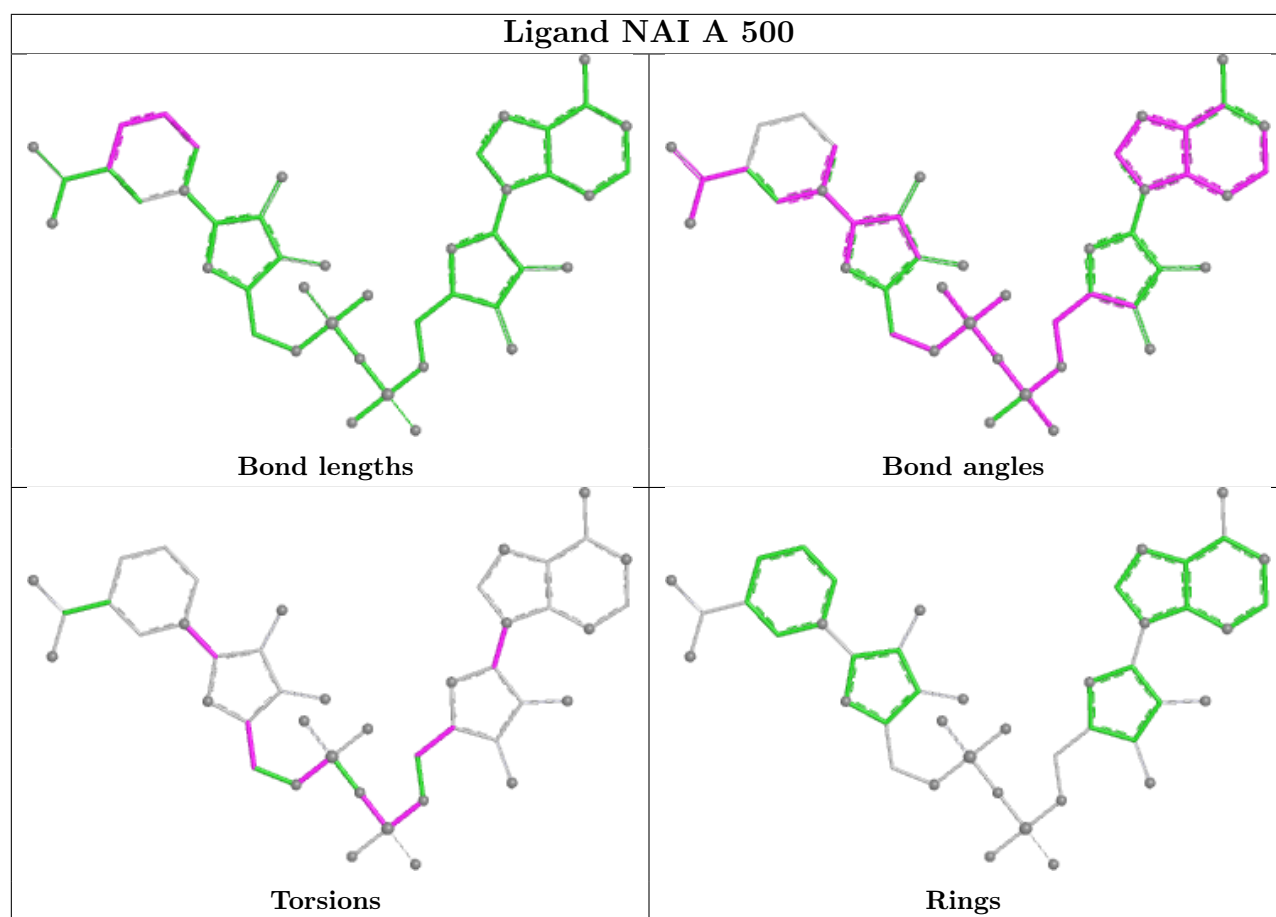


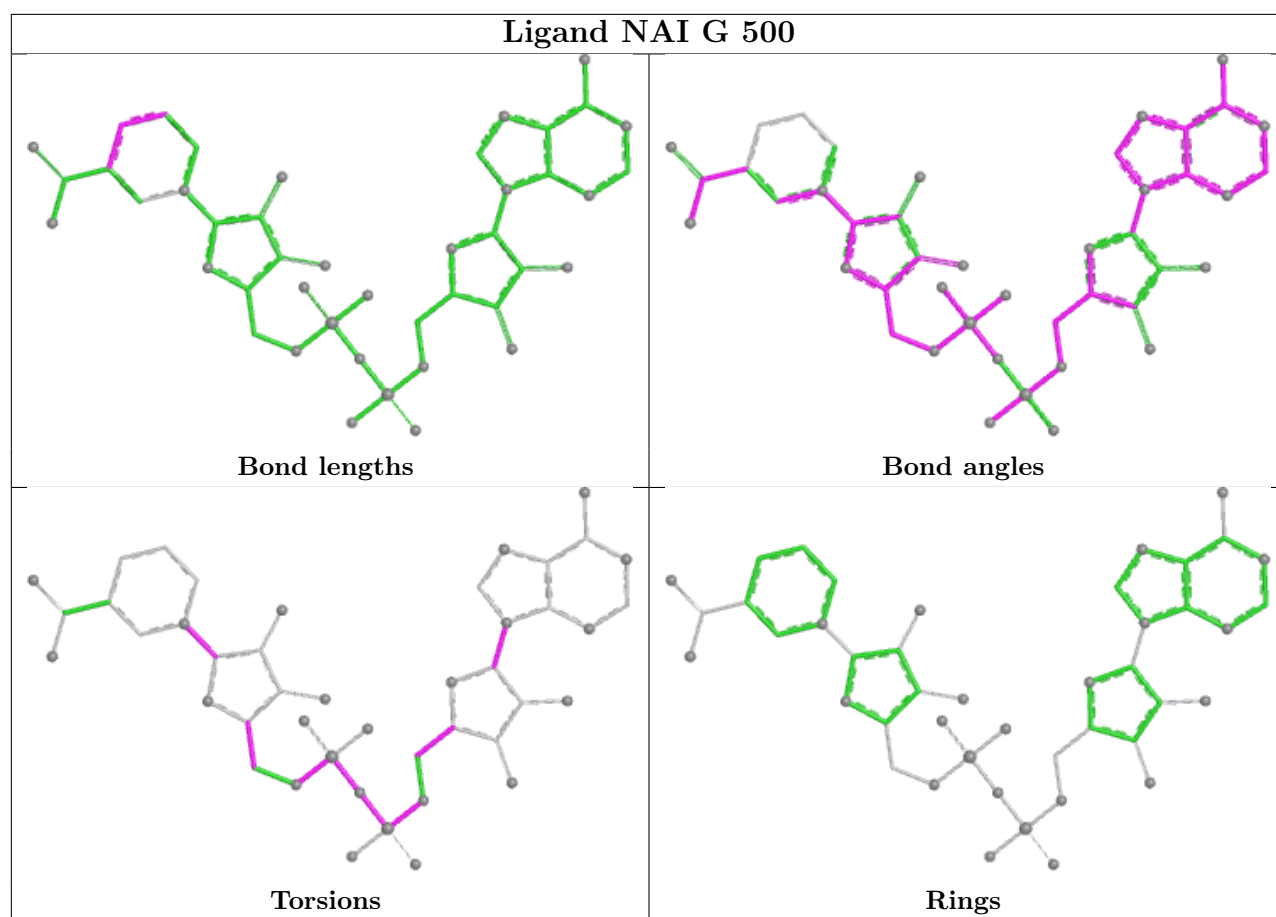
Ligand HP7 H 550

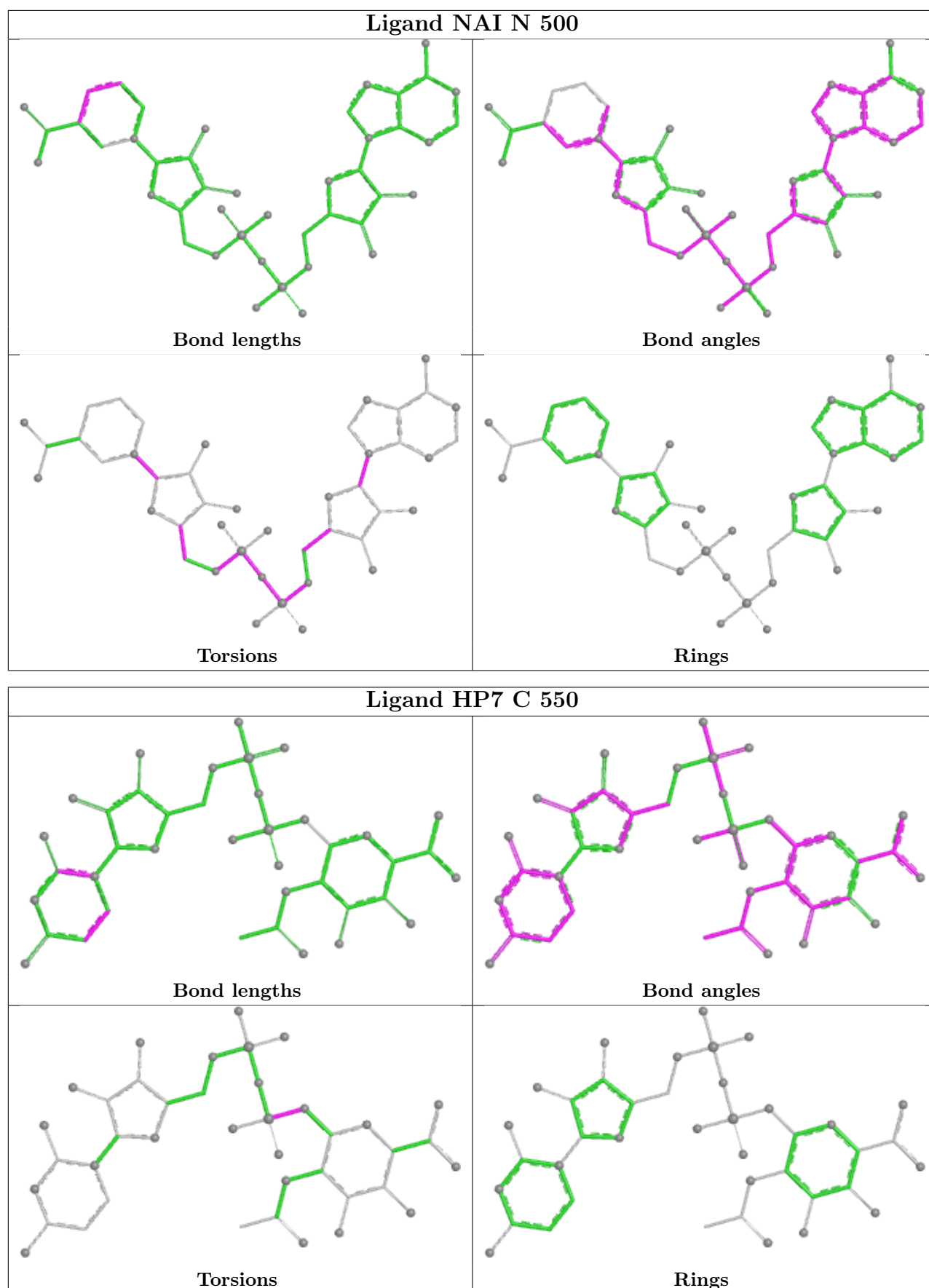


Ligand HP7 L 550









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	346/370 (93%)	-0.48	0 100 100	16, 29, 45, 62	0
1	B	329/370 (88%)	-0.24	1 (0%) 90 92	12, 37, 68, 94	2 (0%)
1	C	347/370 (93%)	-0.34	2 (0%) 85 88	13, 34, 62, 82	0
1	D	343/370 (92%)	-0.12	11 (3%) 50 54	14, 39, 75, 90	1 (0%)
1	E	321/370 (86%)	0.06	4 (1%) 76 80	16, 46, 74, 89	0
1	F	327/370 (88%)	-0.18	3 (0%) 81 84	16, 38, 69, 87	0
1	G	342/370 (92%)	-0.43	2 (0%) 85 88	13, 31, 59, 75	0
1	H	342/370 (92%)	-0.19	5 (1%) 72 76	10, 36, 72, 88	1 (0%)
1	I	342/370 (92%)	-0.09	3 (0%) 81 84	17, 39, 72, 91	0
1	J	346/370 (93%)	-0.13	5 (1%) 73 77	20, 40, 73, 86	0
1	K	322/370 (87%)	-0.02	6 (1%) 66 70	15, 42, 75, 97	0
1	L	321/370 (86%)	0.12	12 (3%) 45 50	16, 47, 82, 93	1 (0%)
1	M	346/370 (93%)	-0.41	4 (1%) 76 80	12, 31, 61, 84	0
1	N	342/370 (92%)	-0.29	1 (0%) 90 92	13, 34, 69, 80	0
1	O	334/370 (90%)	-0.21	1 (0%) 90 92	16, 39, 64, 86	0
1	P	322/370 (87%)	-0.10	6 (1%) 66 70	16, 40, 74, 93	0
All	All	5372/5920 (90%)	-0.19	66 (1%) 76 80	10, 37, 72, 97	5 (0%)

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	279	PRO	5.8
1	E	303	LEU	5.4
1	L	30	ALA	5.2
1	D	299	PHE	4.4
1	K	33	GLY	4.2

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($\text{\AA}^2$)	Q<0.9
3	HP7	E	550	40/40	0.91	0.10	32,64,100,100	0
3	HP7	P	550	40/40	0.92	0.10	28,48,100,100	0
3	HP7	L	550	40/40	0.93	0.10	20,56,100,100	0
3	HP7	O	550	40/40	0.93	0.10	22,56,100,100	0
3	HP7	F	550	40/40	0.93	0.10	24,43,100,100	0
3	HP7	K	550	40/40	0.94	0.09	17,53,100,100	0
3	HP7	B	550	40/40	0.94	0.08	25,45,100,100	0
3	HP7	D	550	40/40	0.95	0.09	23,47,99,100	0
2	NAI	L	500	44/44	0.95	0.09	23,40,63,100	0
2	NAI	B	500	44/44	0.95	0.08	21,36,58,79	0
3	HP7	H	550	40/40	0.95	0.07	21,34,59,90	0
2	NAI	N	500	44/44	0.96	0.07	17,32,48,63	0
2	NAI	O	500	44/44	0.96	0.07	19,35,52,63	0
3	HP7	I	550	40/40	0.96	0.07	19,40,82,100	0
3	HP7	J	550	40/40	0.96	0.07	14,36,75,100	0
2	NAI	E	500	44/44	0.96	0.07	23,43,87,98	0
3	HP7	C	550	40/40	0.96	0.07	17,30,76,100	0
2	NAI	K	500	44/44	0.96	0.07	18,33,53,100	0
2	NAI	D	500	44/44	0.96	0.07	20,36,52,70	0
2	NAI	J	500	44/44	0.97	0.07	18,37,60,78	0
2	NAI	A	500	44/44	0.97	0.06	19,25,31,45	0
2	NAI	C	500	44/44	0.97	0.06	14,28,44,71	0
3	HP7	G	550	40/40	0.97	0.06	14,32,77,100	0
2	NAI	M	500	44/44	0.97	0.07	15,32,49,84	0
2	NAI	F	500	44/44	0.97	0.06	15,28,43,64	0
2	NAI	G	500	44/44	0.97	0.06	17,28,38,57	0
2	NAI	P	500	44/44	0.97	0.06	24,37,54,73	0

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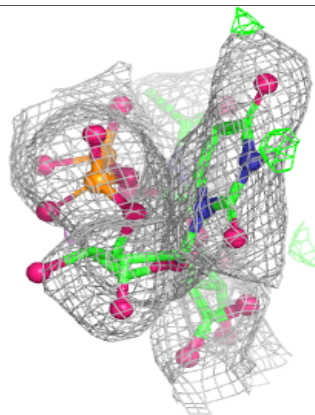
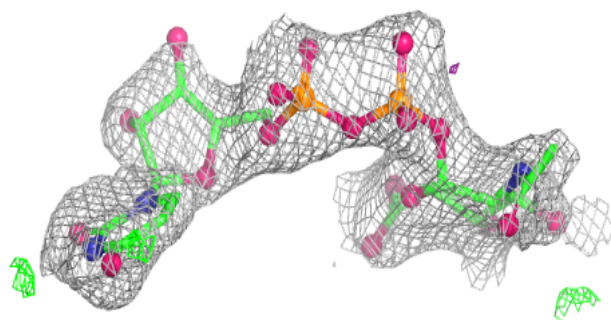
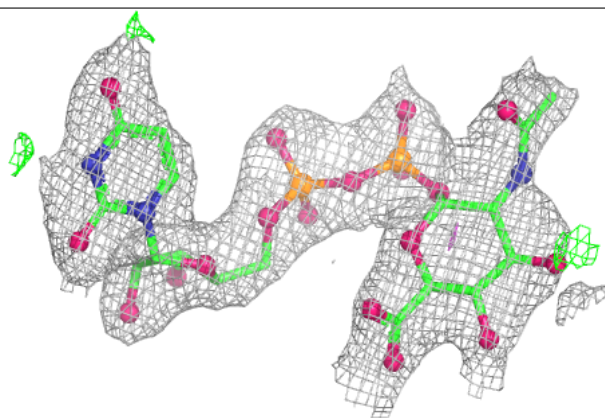
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HP7	A	550	40/40	0.97	0.06	11,25,50,100	0
3	HP7	M	550	40/40	0.97	0.06	17,31,42,59	0
3	HP7	N	550	40/40	0.97	0.05	15,27,50,56	0
2	NAI	H	500	44/44	0.97	0.07	21,34,60,100	0
2	NAI	I	500	44/44	0.97	0.06	20,35,46,59	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.

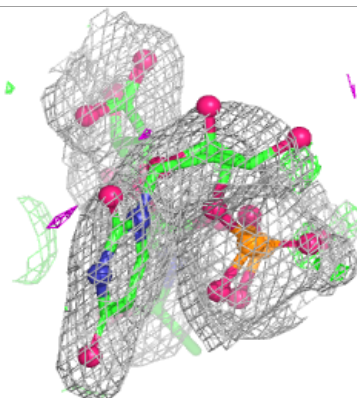
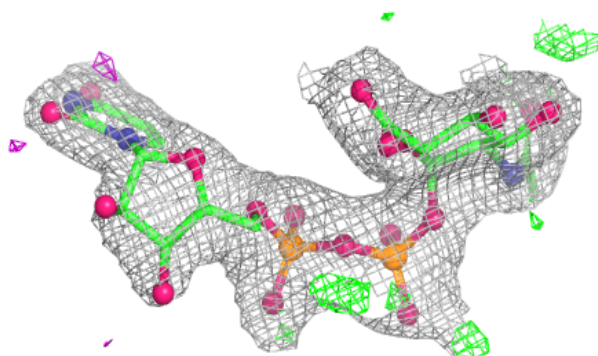
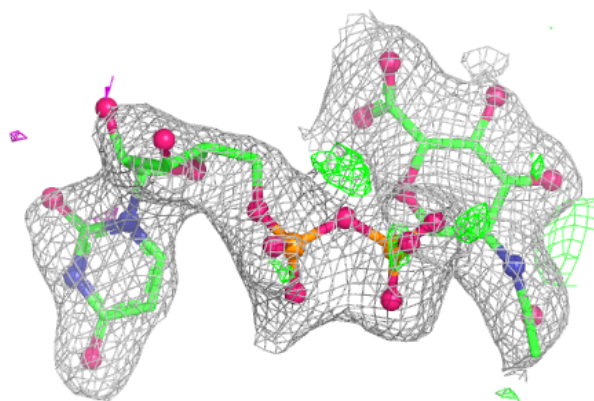
Electron density around HP7 E 550:

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

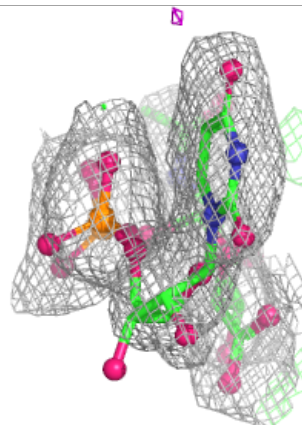
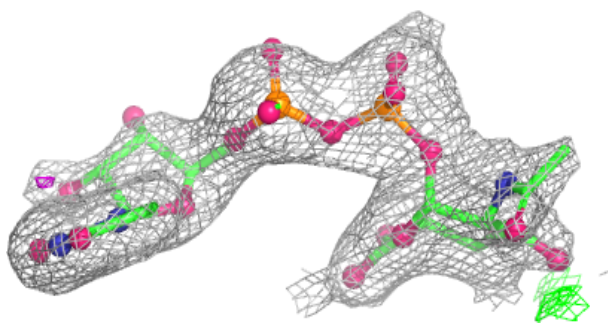
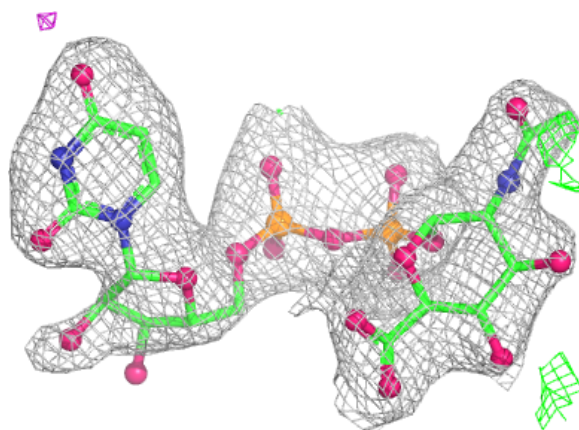


Electron density around HP7 P 550:

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and green (positive)

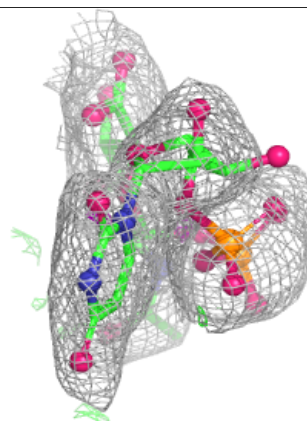
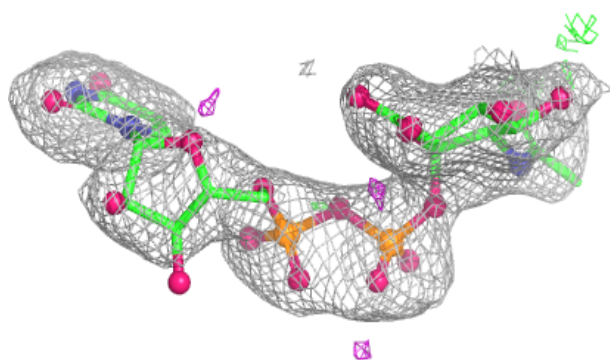
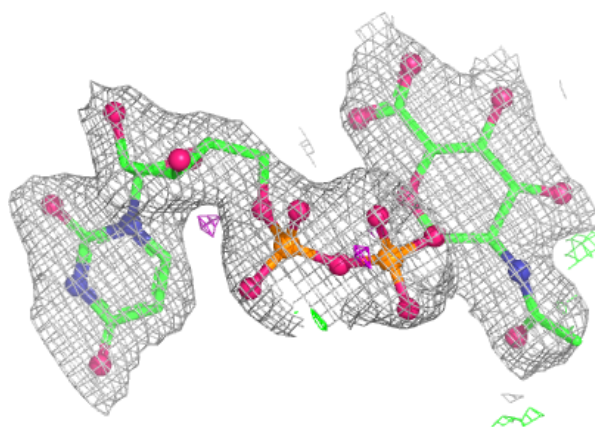
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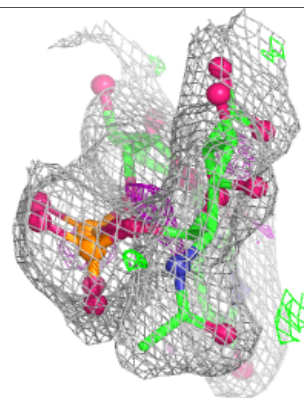
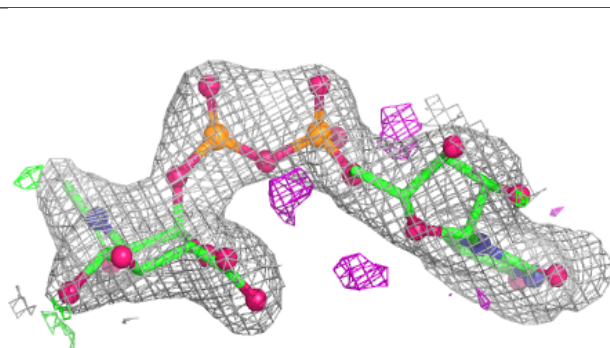
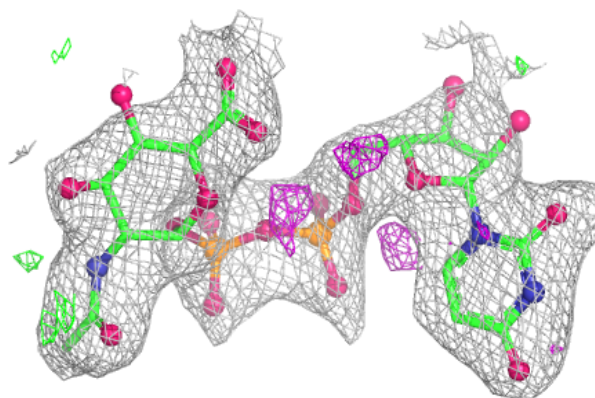


Electron density around HP7 O 550:

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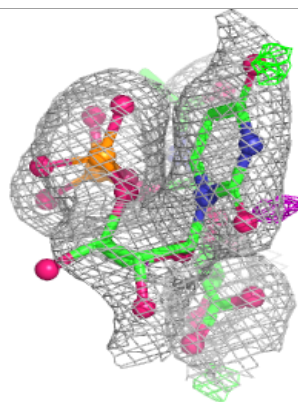
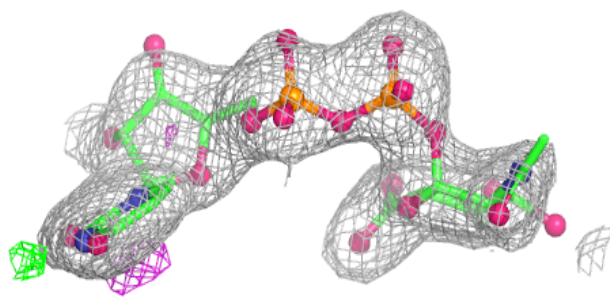
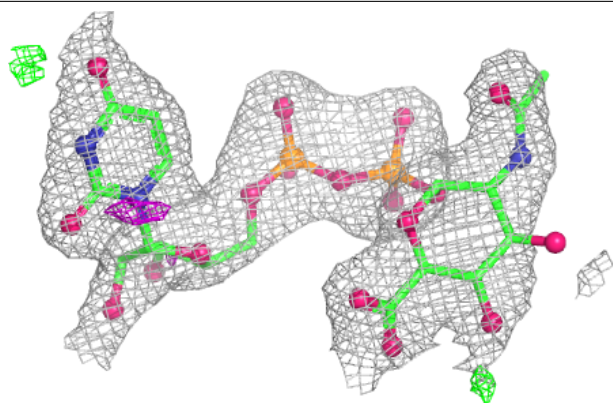
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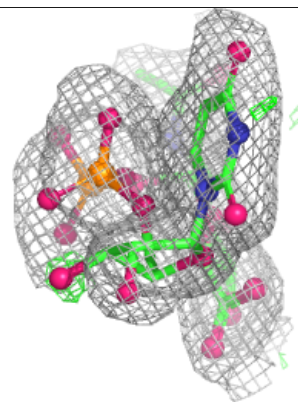
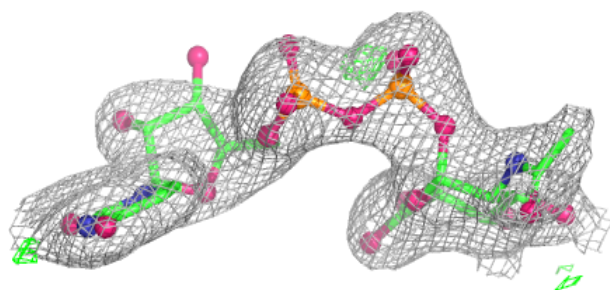
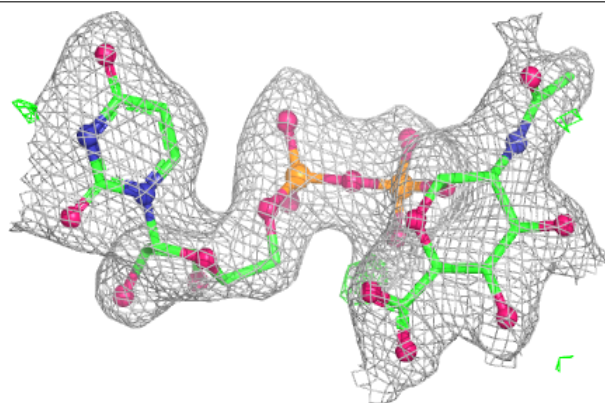


Electron density around HP7 K 550:

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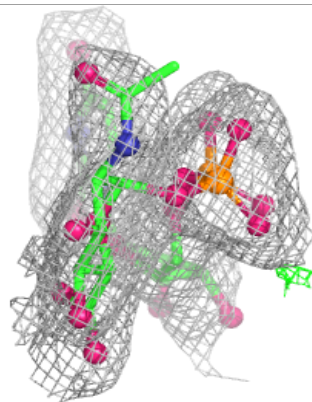
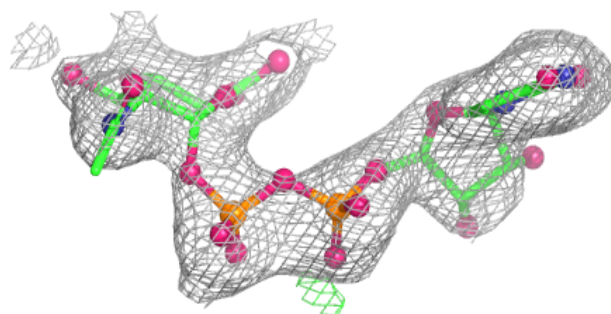
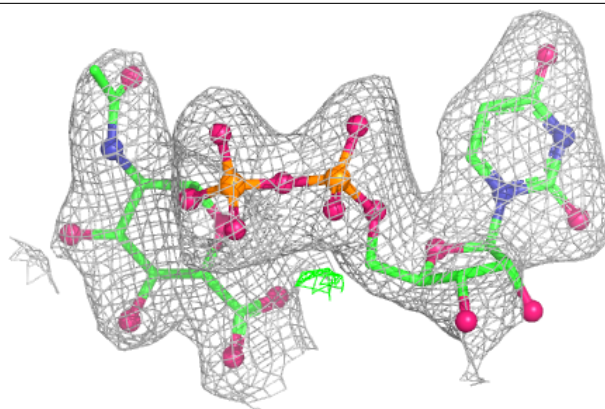
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and green (positive)

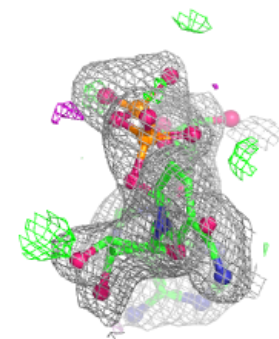
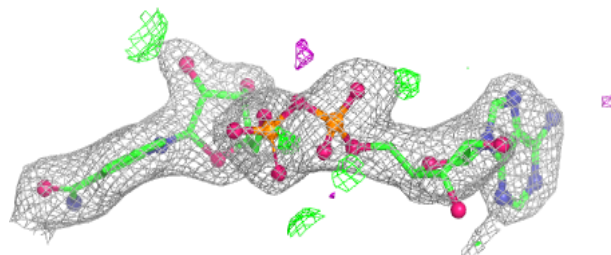
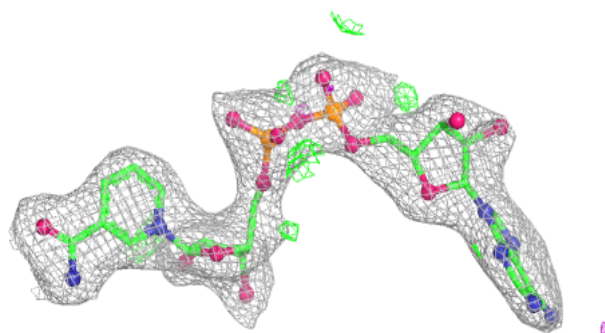


Electron density around HP7 D 550:

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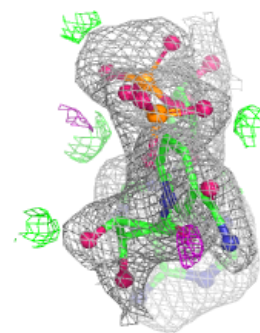
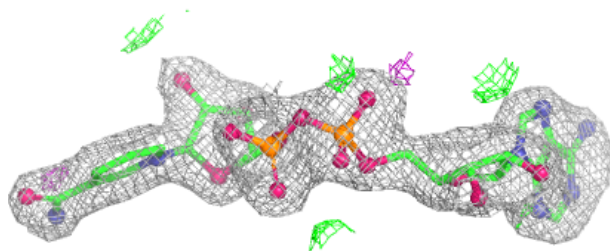
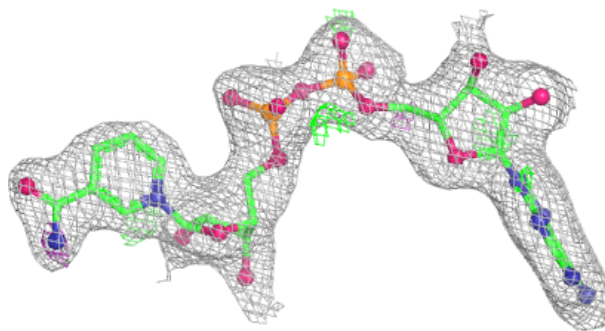
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and green (positive)

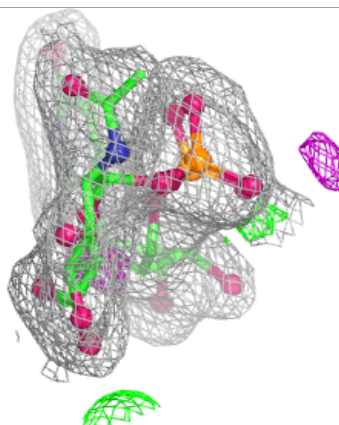
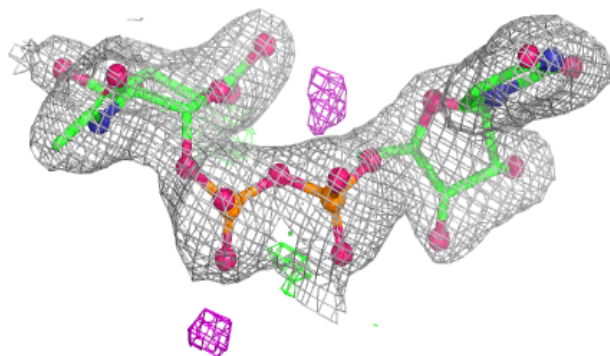
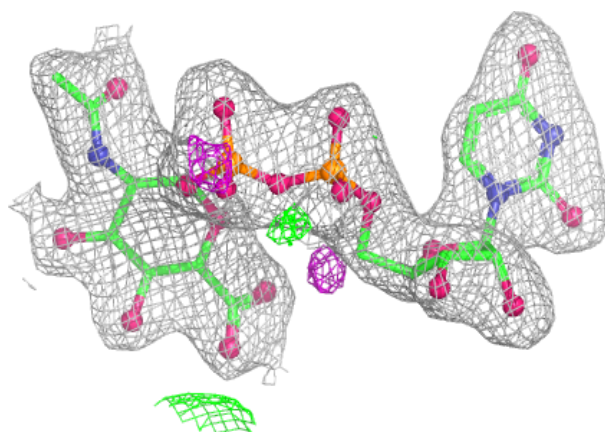


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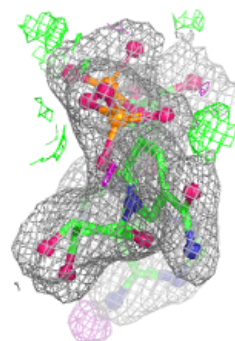
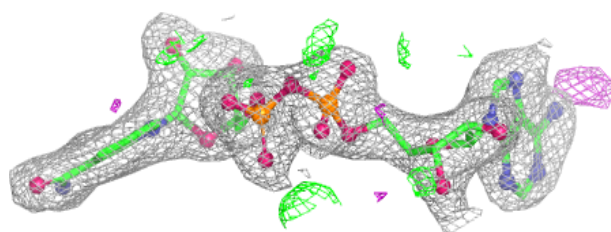
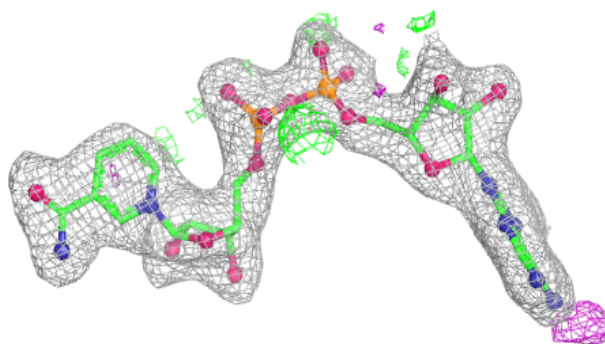
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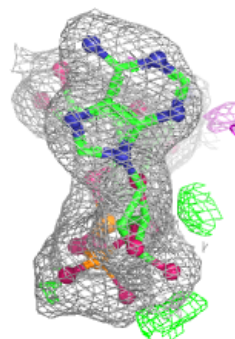
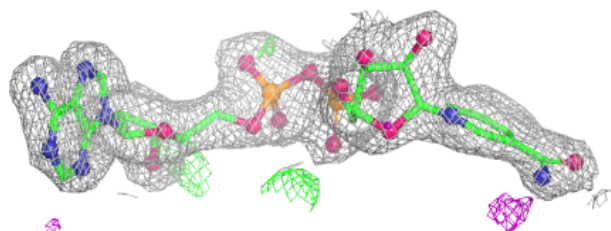
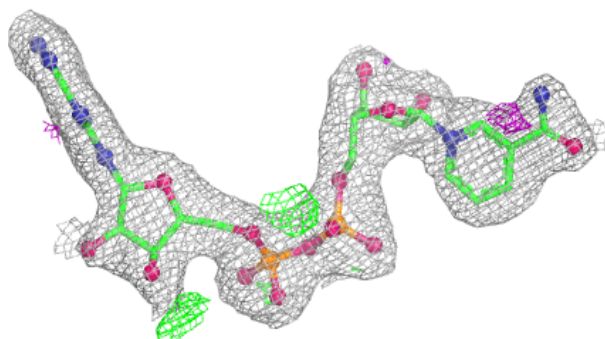


Electron density around NAI N 500:

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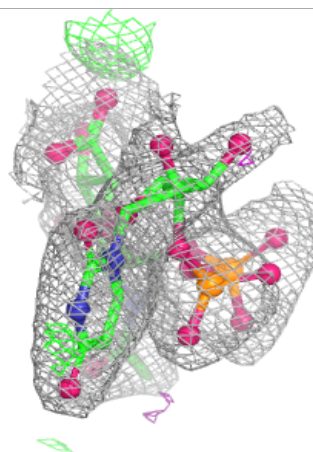
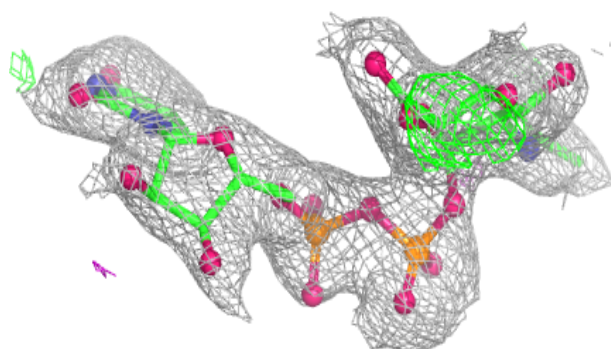
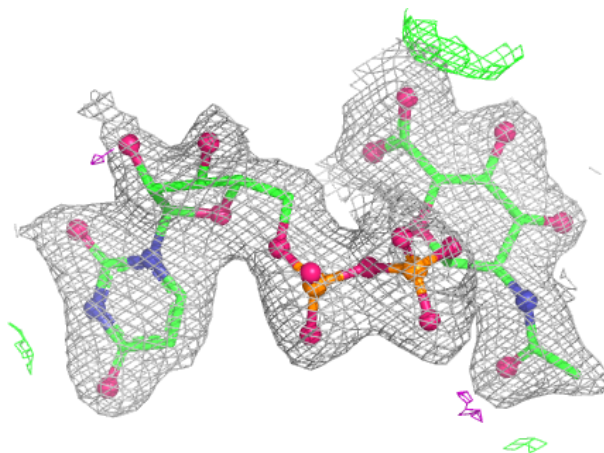
**Electron density around NAI O 500:**

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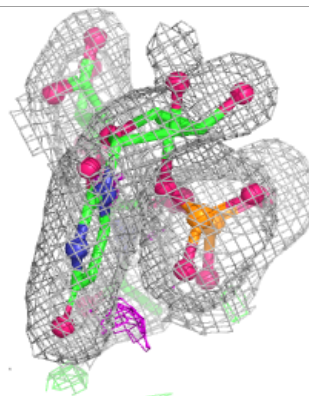
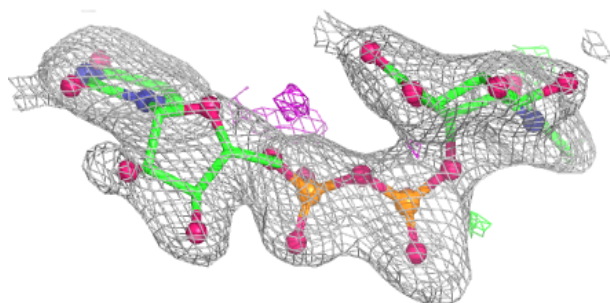
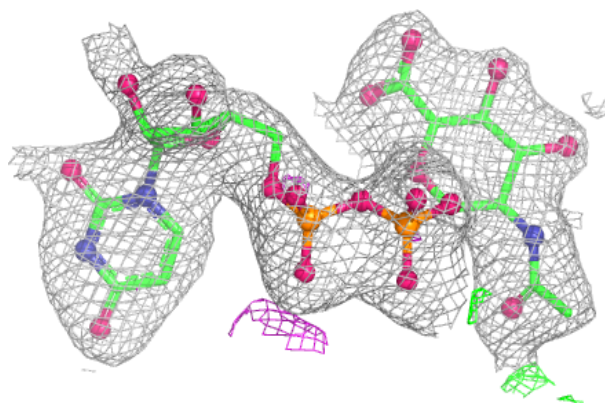
Electron density around HP7 I 550:

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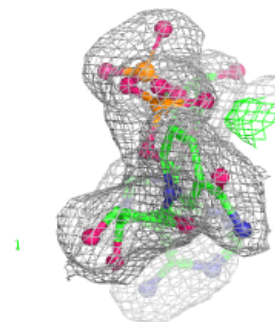
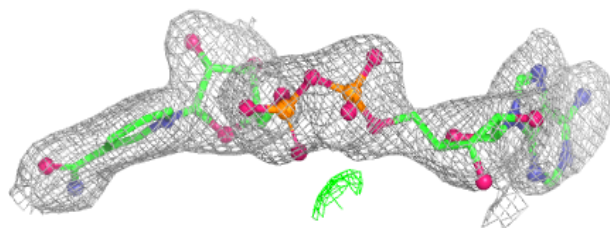
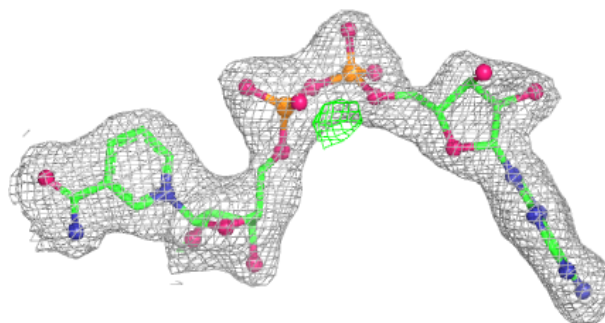


Electron density around HP7 J 550:

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

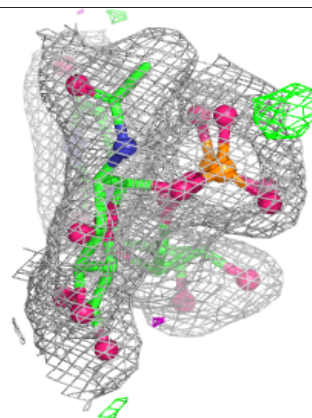
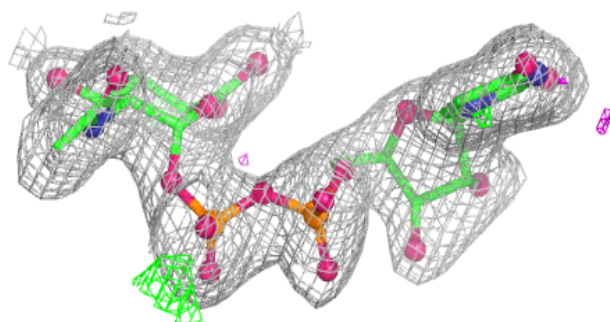
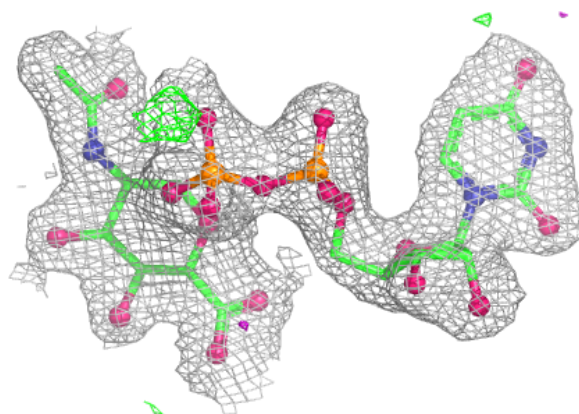
**Electron density around NAI E 500:**

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

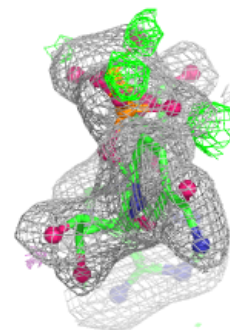
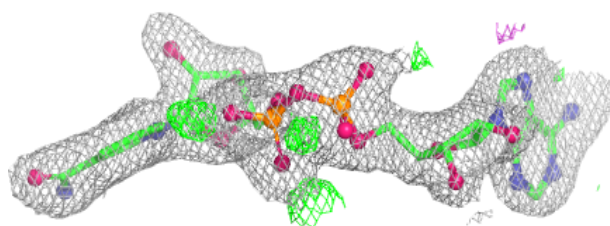
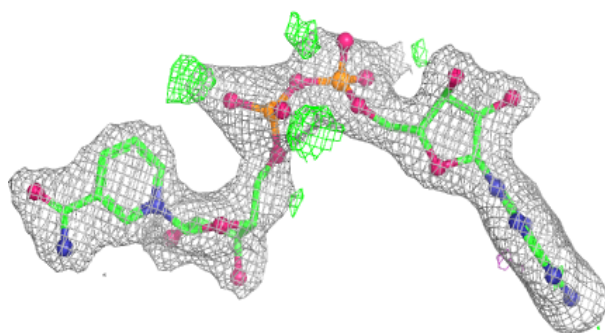


Electron density around HP7 C 550:

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

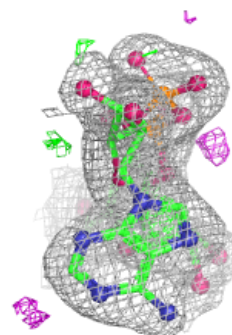
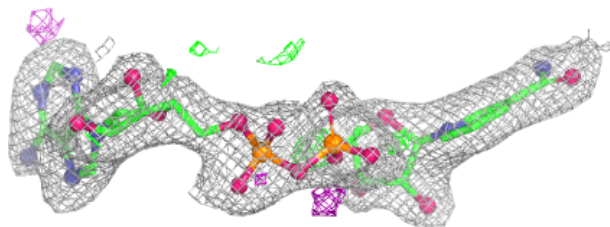
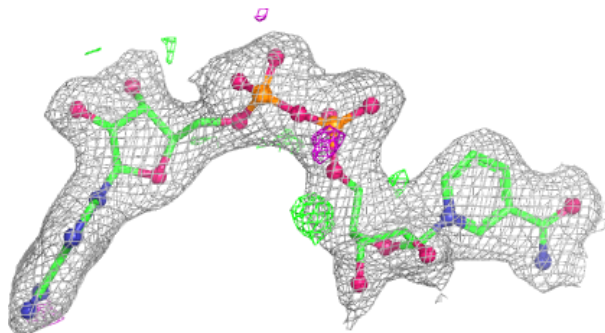
**Electron density around NAI K 500:**

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

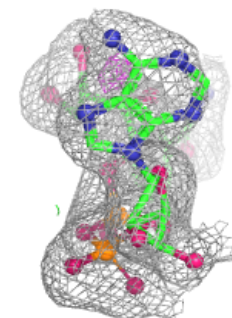
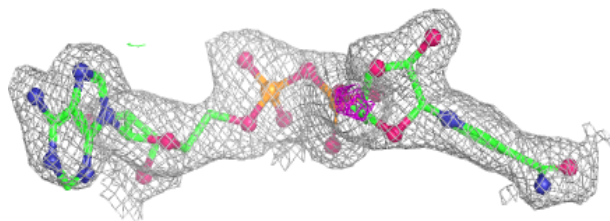
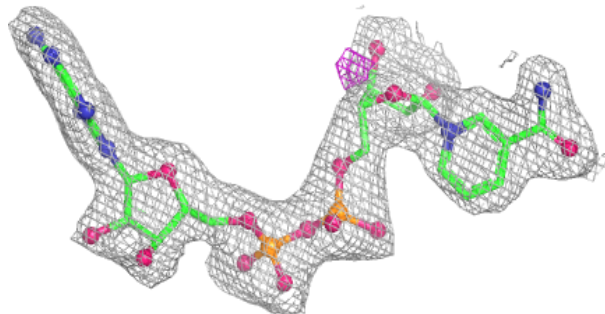


Electron density around NAI D 500:

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

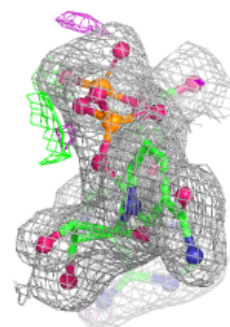
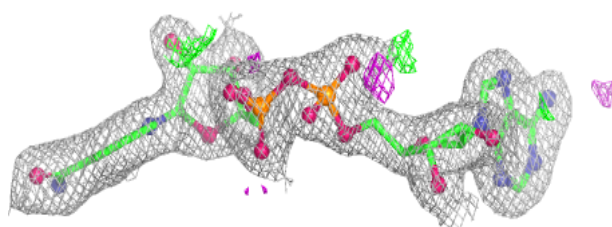
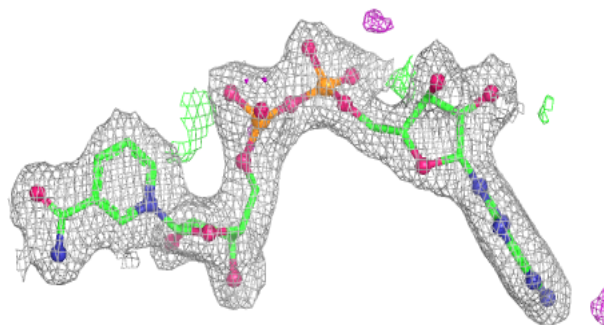
**Electron density around NAI J 500:**

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

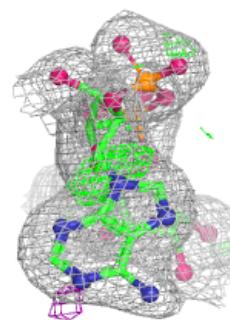
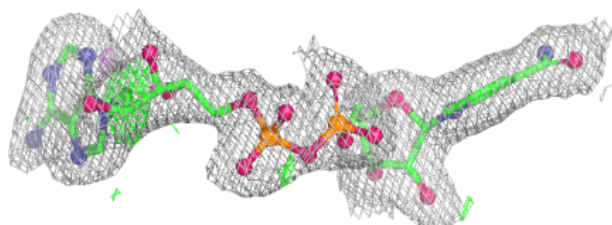
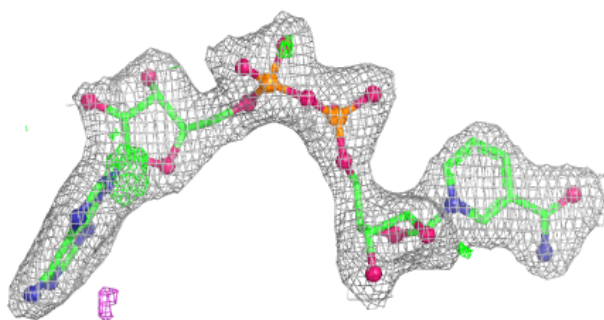


Electron density around NAI A 500:

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

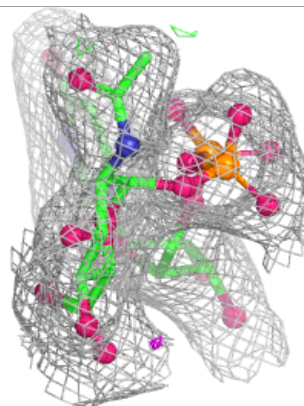
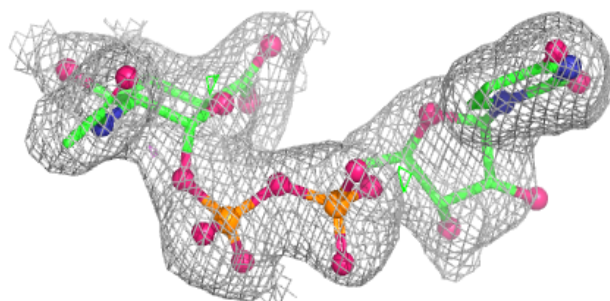
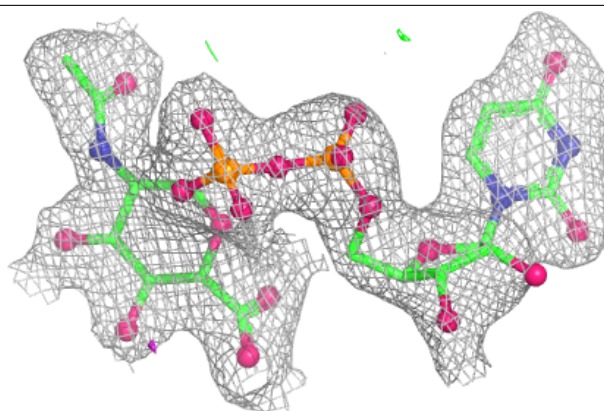
**Electron density around NAI C 500:**

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

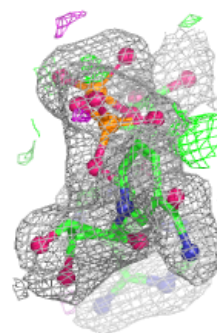
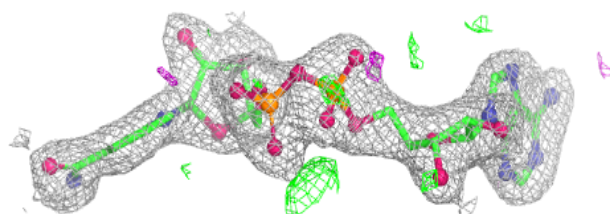
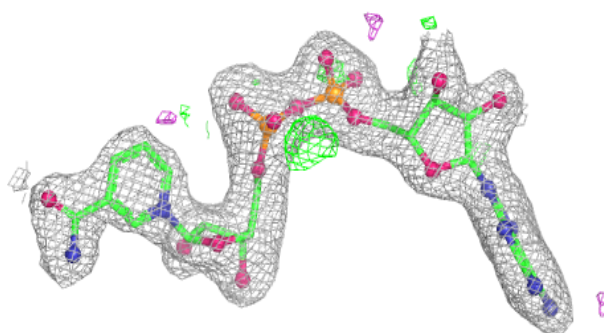


Electron density around HP7 G 550:

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

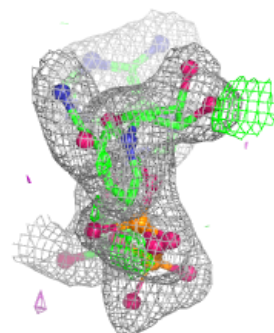
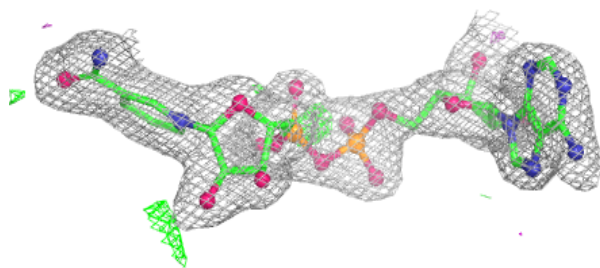
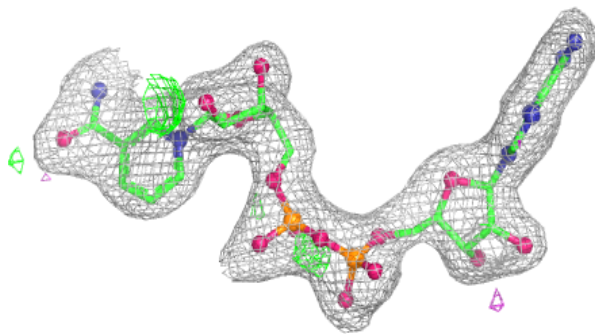
**Electron density around NAI M 500:**

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

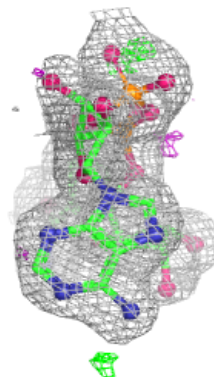
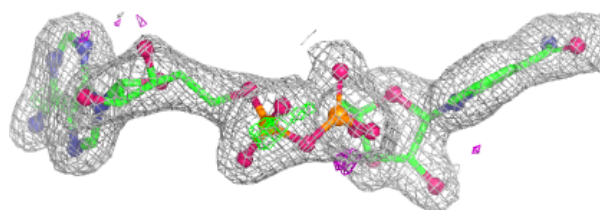
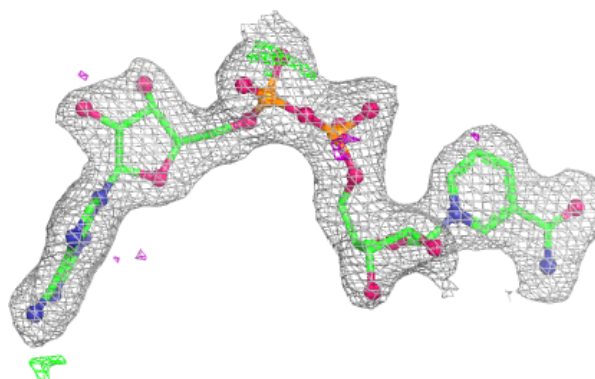


Electron density around NAI F 500:

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

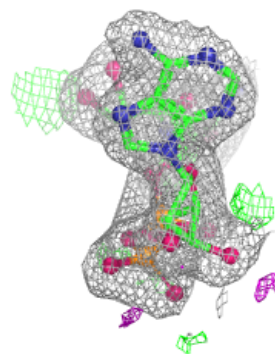
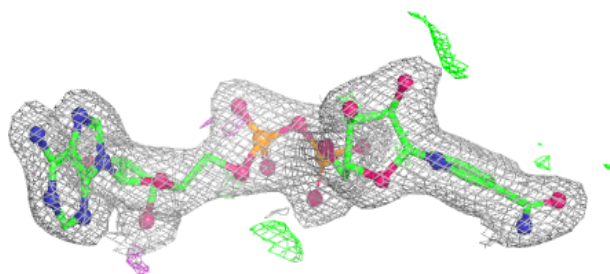
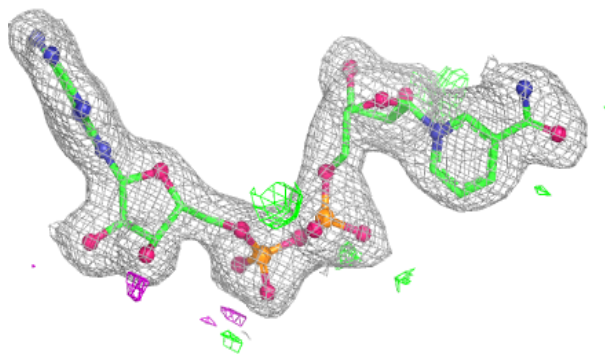
**Electron density around NAI G 500:**

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

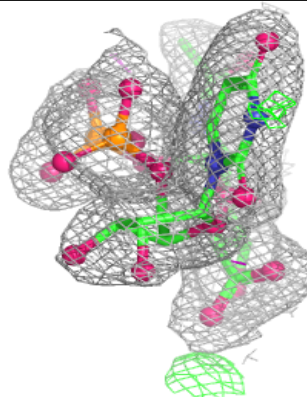
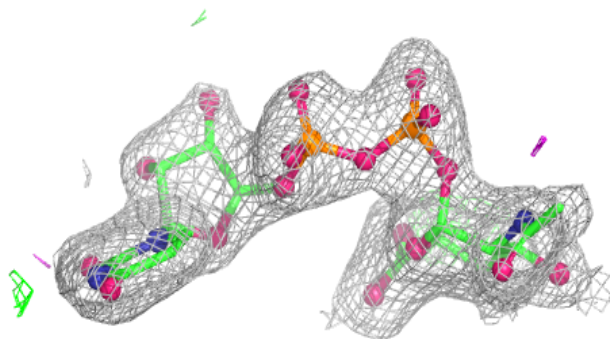
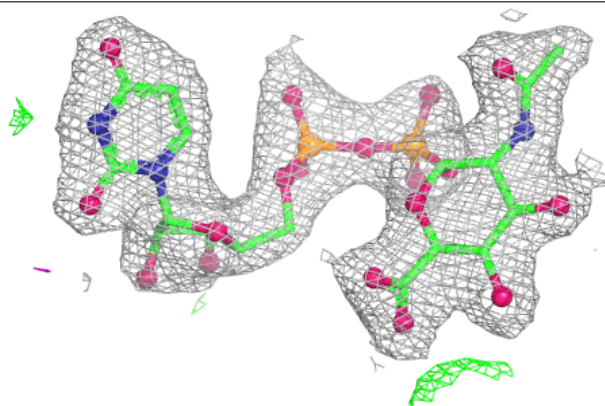


Electron density around NAI P 500:

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

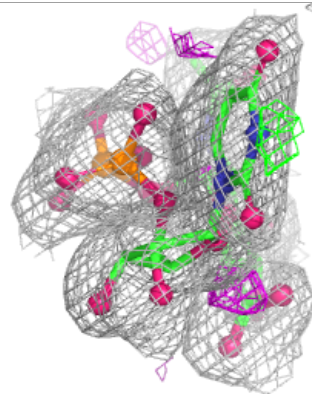
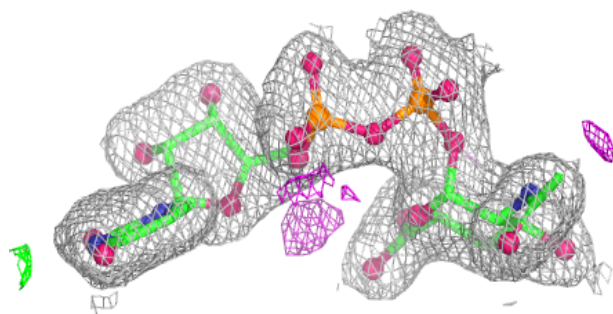
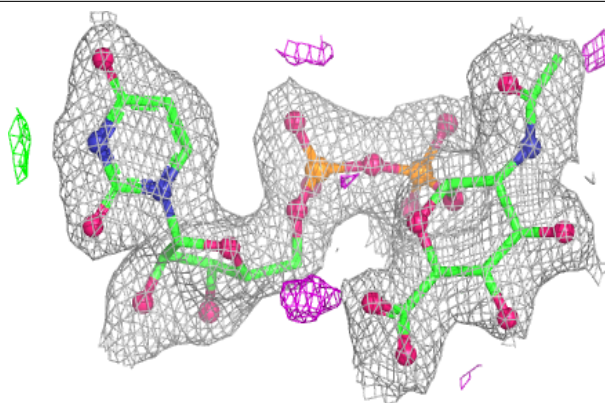
**Electron density around HP7 A 550:**

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

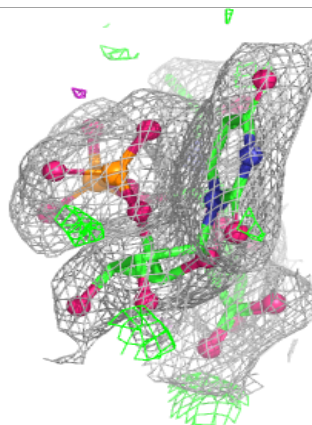
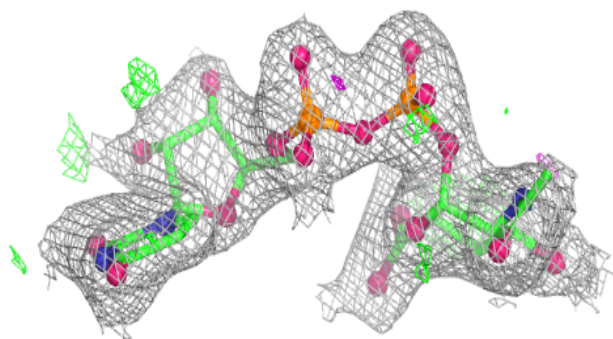
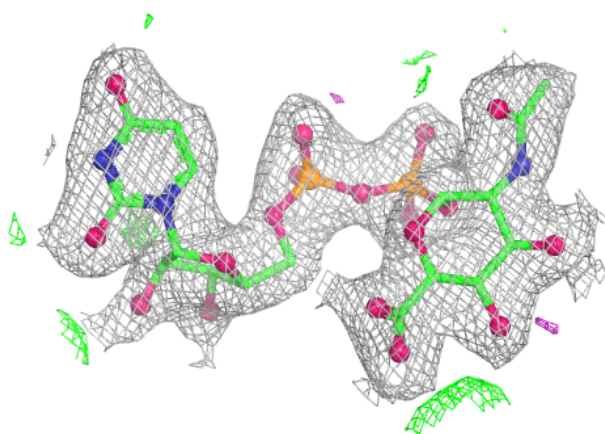


Electron density around HP7 M 550:

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

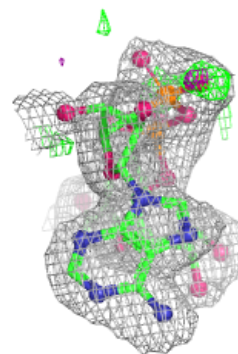
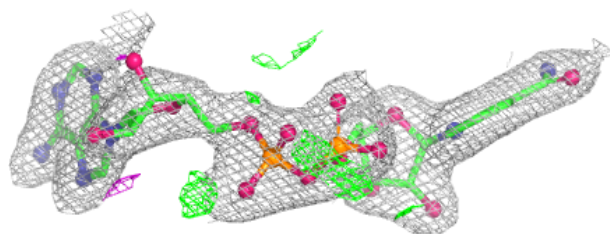
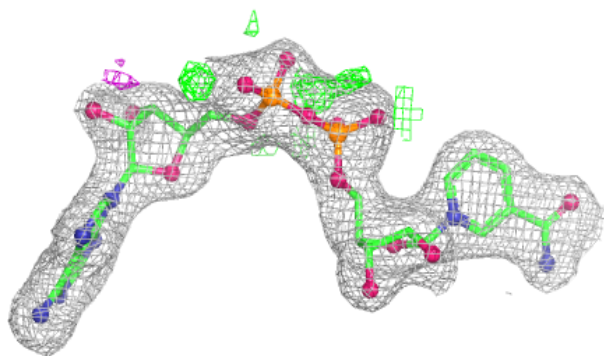
**Electron density around HP7 N 550:**

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

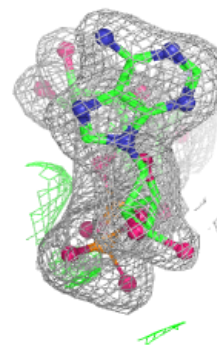
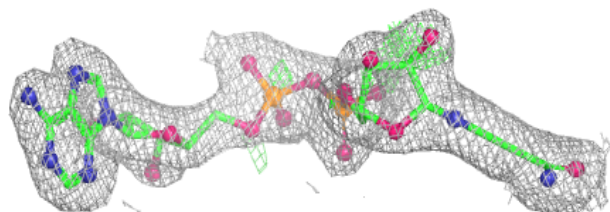
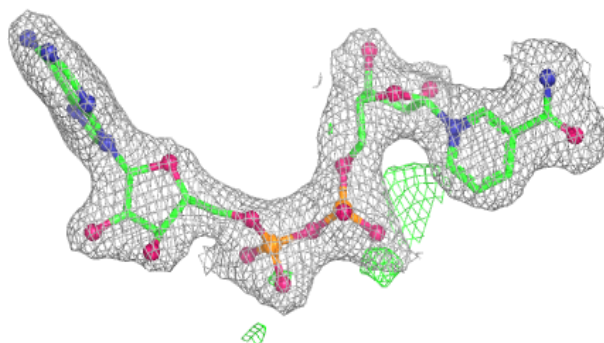


Electron density around NAI H 500:

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

**Electron density around NAI I 500:**

$2mF_o-DF_c$ (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.