



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:37 am BST

PDB ID : 3CMV
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors : Pavletich, N.P.
Deposited on : 2008-03-24
Resolution : 4.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

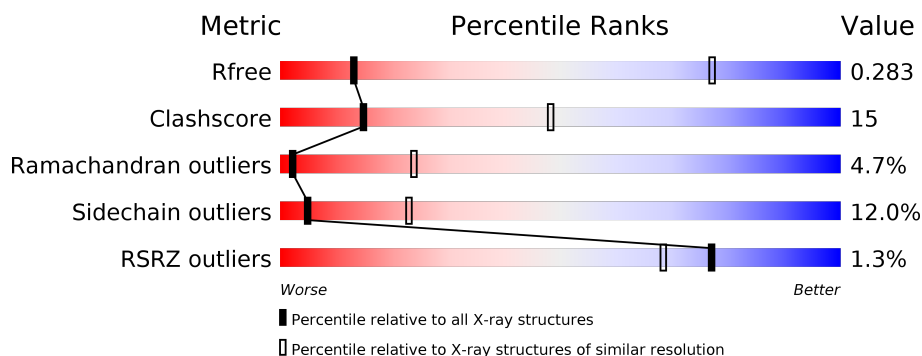
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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 on 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	1357	<div> <div>2%</div> <div>55%</div> <div>27%</div> <div>6%</div> <div>12%</div> </div>
1	B	1357	<div> <div>54%</div> <div>27%</div> <div>5%</div> <div>14%</div> </div>
1	C	1357	<div> <div>54%</div> <div>27%</div> <div>5%</div> <div>13%</div> </div>
1	D	1357	<div> <div>2%</div> <div>55%</div> <div>27%</div> <div>5%</div> <div>13%</div> </div>
1	E	1357	<div> <div>53%</div> <div>27%</div> <div>5%</div> <div>14%</div> </div>
1	F	1357	<div> <div>54%</div> <div>27%</div> <div>5%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	1357	
1	H	1357	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	B	1701	-	-	-	X
2	MG	C	701	-	-	-	X
2	MG	D	1701	-	-	-	X
2	MG	D	701	-	-	-	X
2	MG	E	701	-	-	-	X
2	MG	G	701	-	-	-	X
3	ANP	A	1400	X	-	-	-
3	ANP	A	2400	X	-	-	-
3	ANP	A	3400	X	-	-	-
3	ANP	A	400	X	-	-	-
3	ANP	B	1400	X	-	-	-
3	ANP	B	2400	X	-	-	-
3	ANP	B	3400	X	-	-	-
3	ANP	B	400	X	-	-	-
3	ANP	C	1400	X	-	-	-
3	ANP	C	2400	X	-	-	-
3	ANP	C	3400	X	-	-	-
3	ANP	C	400	X	-	-	-
3	ANP	D	1400	X	-	-	-
3	ANP	D	2400	X	-	-	-
3	ANP	D	3400	X	-	-	-
3	ANP	D	400	X	-	-	-
3	ANP	E	1400	X	-	-	-
3	ANP	E	2400	X	-	-	-
3	ANP	E	3400	X	-	-	-
3	ANP	E	400	X	-	-	-
3	ANP	F	1400	X	-	-	-
3	ANP	F	2400	X	-	-	X
3	ANP	F	3400	X	-	-	-
3	ANP	F	400	X	-	-	-
3	ANP	G	1400	X	-	-	-
3	ANP	G	2400	X	-	-	X
3	ANP	G	3400	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	G	400	X	-	-	-
3	ANP	H	1400	X	-	-	-
3	ANP	H	2400	X	-	-	-
3	ANP	H	3400	X	-	-	-
3	ANP	H	400	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 71761 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 Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1190	Total	C	N	O	S	0	0	0
			8970	5660	1553	1719	38			
1	B	1163	Total	C	N	O	S	0	0	0
			8769	5538	1519	1677	35			
1	C	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	D	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	E	1165	Total	C	N	O	S	0	0	0
			8787	5548	1521	1683	35			
1	F	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	G	1167	Total	C	N	O	S	0	0	0
			8799	5554	1523	1687	35			
1	H	1173	Total	C	N	O	S	0	0	0
			8844	5581	1531	1696	36			

There are 400 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP P0A7G6
A	27	ALA	-	linker	UNP P0A7G6
A	28	MET	-	linker	UNP P0A7G6
A	29	HIS	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6
A	988	SER	-	linker	UNP P0A7G6
A	989	THR	-	linker	UNP P0A7G6
A	990	GLY	-	linker	UNP P0A7G6
A	991	SER	-	linker	UNP P0A7G6
A	992	GLY	-	linker	UNP P0A7G6
A	993	THR	-	linker	UNP P0A7G6
A	994	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	995	GLY	-	linker	UNP P0A7G6
A	996	SER	-	linker	UNP P0A7G6
A	997	THR	-	linker	UNP P0A7G6
A	998	GLY	-	linker	UNP P0A7G6
A	999	SER	-	linker	UNP P0A7G6
A	1000	MET	-	linker	UNP P0A7G6
A	1986	THR	-	linker	UNP P0A7G6
A	1987	GLY	-	linker	UNP P0A7G6
A	1988	SER	-	linker	UNP P0A7G6
A	1989	THR	-	linker	UNP P0A7G6
A	1990	GLY	-	linker	UNP P0A7G6
A	1991	SER	-	linker	UNP P0A7G6
A	1992	MET	-	linker	UNP P0A7G6
A	1993	GLY	-	linker	UNP P0A7G6
A	1994	HIS	-	linker	UNP P0A7G6
A	1995	THR	-	linker	UNP P0A7G6
A	1996	THR	-	linker	UNP P0A7G6
A	1997	GLY	-	linker	UNP P0A7G6
A	1998	SER	-	linker	UNP P0A7G6
A	1999	MET	-	linker	UNP P0A7G6
A	2000	SER	-	linker	UNP P0A7G6
A	2985	THR	-	linker	UNP P0A7G6
A	2986	GLY	-	linker	UNP P0A7G6
A	2987	SER	-	linker	UNP P0A7G6
A	2988	THR	-	linker	UNP P0A7G6
A	2989	GLY	-	linker	UNP P0A7G6
A	2990	SER	-	linker	UNP P0A7G6
A	2991	ALA	-	linker	UNP P0A7G6
A	2992	SER	-	linker	UNP P0A7G6
A	2993	GLY	-	linker	UNP P0A7G6
A	2994	SER	-	linker	UNP P0A7G6
A	2995	SER	-	linker	UNP P0A7G6
A	2996	THR	-	linker	UNP P0A7G6
A	2997	GLY	-	linker	UNP P0A7G6
A	2998	SER	-	linker	UNP P0A7G6
A	2999	MET	-	linker	UNP P0A7G6
A	3000	SER	-	linker	UNP P0A7G6
B	26	GLY	-	linker	UNP P0A7G6
B	27	ALA	-	linker	UNP P0A7G6
B	28	MET	-	linker	UNP P0A7G6
B	29	HIS	-	linker	UNP P0A7G6
B	986	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	987	GLY	-	linker	UNP P0A7G6
B	988	SER	-	linker	UNP P0A7G6
B	989	THR	-	linker	UNP P0A7G6
B	990	GLY	-	linker	UNP P0A7G6
B	991	SER	-	linker	UNP P0A7G6
B	992	GLY	-	linker	UNP P0A7G6
B	993	THR	-	linker	UNP P0A7G6
B	994	THR	-	linker	UNP P0A7G6
B	995	GLY	-	linker	UNP P0A7G6
B	996	SER	-	linker	UNP P0A7G6
B	997	THR	-	linker	UNP P0A7G6
B	998	GLY	-	linker	UNP P0A7G6
B	999	SER	-	linker	UNP P0A7G6
B	1000	MET	-	linker	UNP P0A7G6
B	1986	THR	-	linker	UNP P0A7G6
B	1987	GLY	-	linker	UNP P0A7G6
B	1988	SER	-	linker	UNP P0A7G6
B	1989	THR	-	linker	UNP P0A7G6
B	1990	GLY	-	linker	UNP P0A7G6
B	1991	SER	-	linker	UNP P0A7G6
B	1992	MET	-	linker	UNP P0A7G6
B	1993	GLY	-	linker	UNP P0A7G6
B	1994	HIS	-	linker	UNP P0A7G6
B	1995	THR	-	linker	UNP P0A7G6
B	1996	THR	-	linker	UNP P0A7G6
B	1997	GLY	-	linker	UNP P0A7G6
B	1998	SER	-	linker	UNP P0A7G6
B	1999	MET	-	linker	UNP P0A7G6
B	2000	SER	-	linker	UNP P0A7G6
B	2985	THR	-	linker	UNP P0A7G6
B	2986	GLY	-	linker	UNP P0A7G6
B	2987	SER	-	linker	UNP P0A7G6
B	2988	THR	-	linker	UNP P0A7G6
B	2989	GLY	-	linker	UNP P0A7G6
B	2990	SER	-	linker	UNP P0A7G6
B	2991	ALA	-	linker	UNP P0A7G6
B	2992	SER	-	linker	UNP P0A7G6
B	2993	GLY	-	linker	UNP P0A7G6
B	2994	SER	-	linker	UNP P0A7G6
B	2995	SER	-	linker	UNP P0A7G6
B	2996	THR	-	linker	UNP P0A7G6
B	2997	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2998	SER	-	linker	UNP P0A7G6
B	2999	MET	-	linker	UNP P0A7G6
B	3000	SER	-	linker	UNP P0A7G6
C	26	GLY	-	linker	UNP P0A7G6
C	27	ALA	-	linker	UNP P0A7G6
C	28	MET	-	linker	UNP P0A7G6
C	29	HIS	-	linker	UNP P0A7G6
C	986	THR	-	linker	UNP P0A7G6
C	987	GLY	-	linker	UNP P0A7G6
C	988	SER	-	linker	UNP P0A7G6
C	989	THR	-	linker	UNP P0A7G6
C	990	GLY	-	linker	UNP P0A7G6
C	991	SER	-	linker	UNP P0A7G6
C	992	GLY	-	linker	UNP P0A7G6
C	993	THR	-	linker	UNP P0A7G6
C	994	THR	-	linker	UNP P0A7G6
C	995	GLY	-	linker	UNP P0A7G6
C	996	SER	-	linker	UNP P0A7G6
C	997	THR	-	linker	UNP P0A7G6
C	998	GLY	-	linker	UNP P0A7G6
C	999	SER	-	linker	UNP P0A7G6
C	1000	MET	-	linker	UNP P0A7G6
C	1986	THR	-	linker	UNP P0A7G6
C	1987	GLY	-	linker	UNP P0A7G6
C	1988	SER	-	linker	UNP P0A7G6
C	1989	THR	-	linker	UNP P0A7G6
C	1990	GLY	-	linker	UNP P0A7G6
C	1991	SER	-	linker	UNP P0A7G6
C	1992	MET	-	linker	UNP P0A7G6
C	1993	GLY	-	linker	UNP P0A7G6
C	1994	HIS	-	linker	UNP P0A7G6
C	1995	THR	-	linker	UNP P0A7G6
C	1996	THR	-	linker	UNP P0A7G6
C	1997	GLY	-	linker	UNP P0A7G6
C	1998	SER	-	linker	UNP P0A7G6
C	1999	MET	-	linker	UNP P0A7G6
C	2000	SER	-	linker	UNP P0A7G6
C	2985	THR	-	linker	UNP P0A7G6
C	2986	GLY	-	linker	UNP P0A7G6
C	2987	SER	-	linker	UNP P0A7G6
C	2988	THR	-	linker	UNP P0A7G6
C	2989	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2990	SER	-	linker	UNP P0A7G6
C	2991	ALA	-	linker	UNP P0A7G6
C	2992	SER	-	linker	UNP P0A7G6
C	2993	GLY	-	linker	UNP P0A7G6
C	2994	SER	-	linker	UNP P0A7G6
C	2995	SER	-	linker	UNP P0A7G6
C	2996	THR	-	linker	UNP P0A7G6
C	2997	GLY	-	linker	UNP P0A7G6
C	2998	SER	-	linker	UNP P0A7G6
C	2999	MET	-	linker	UNP P0A7G6
C	3000	SER	-	linker	UNP P0A7G6
D	26	GLY	-	linker	UNP P0A7G6
D	27	ALA	-	linker	UNP P0A7G6
D	28	MET	-	linker	UNP P0A7G6
D	29	HIS	-	linker	UNP P0A7G6
D	986	THR	-	linker	UNP P0A7G6
D	987	GLY	-	linker	UNP P0A7G6
D	988	SER	-	linker	UNP P0A7G6
D	989	THR	-	linker	UNP P0A7G6
D	990	GLY	-	linker	UNP P0A7G6
D	991	SER	-	linker	UNP P0A7G6
D	992	GLY	-	linker	UNP P0A7G6
D	993	THR	-	linker	UNP P0A7G6
D	994	THR	-	linker	UNP P0A7G6
D	995	GLY	-	linker	UNP P0A7G6
D	996	SER	-	linker	UNP P0A7G6
D	997	THR	-	linker	UNP P0A7G6
D	998	GLY	-	linker	UNP P0A7G6
D	999	SER	-	linker	UNP P0A7G6
D	1000	MET	-	linker	UNP P0A7G6
D	1986	THR	-	linker	UNP P0A7G6
D	1987	GLY	-	linker	UNP P0A7G6
D	1988	SER	-	linker	UNP P0A7G6
D	1989	THR	-	linker	UNP P0A7G6
D	1990	GLY	-	linker	UNP P0A7G6
D	1991	SER	-	linker	UNP P0A7G6
D	1992	MET	-	linker	UNP P0A7G6
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker	UNP P0A7G6
D	2000	SER	-	linker	UNP P0A7G6
D	2985	THR	-	linker	UNP P0A7G6
D	2986	GLY	-	linker	UNP P0A7G6
D	2987	SER	-	linker	UNP P0A7G6
D	2988	THR	-	linker	UNP P0A7G6
D	2989	GLY	-	linker	UNP P0A7G6
D	2990	SER	-	linker	UNP P0A7G6
D	2991	ALA	-	linker	UNP P0A7G6
D	2992	SER	-	linker	UNP P0A7G6
D	2993	GLY	-	linker	UNP P0A7G6
D	2994	SER	-	linker	UNP P0A7G6
D	2995	SER	-	linker	UNP P0A7G6
D	2996	THR	-	linker	UNP P0A7G6
D	2997	GLY	-	linker	UNP P0A7G6
D	2998	SER	-	linker	UNP P0A7G6
D	2999	MET	-	linker	UNP P0A7G6
D	3000	SER	-	linker	UNP P0A7G6
E	26	GLY	-	linker	UNP P0A7G6
E	27	ALA	-	linker	UNP P0A7G6
E	28	MET	-	linker	UNP P0A7G6
E	29	HIS	-	linker	UNP P0A7G6
E	986	THR	-	linker	UNP P0A7G6
E	987	GLY	-	linker	UNP P0A7G6
E	988	SER	-	linker	UNP P0A7G6
E	989	THR	-	linker	UNP P0A7G6
E	990	GLY	-	linker	UNP P0A7G6
E	991	SER	-	linker	UNP P0A7G6
E	992	GLY	-	linker	UNP P0A7G6
E	993	THR	-	linker	UNP P0A7G6
E	994	THR	-	linker	UNP P0A7G6
E	995	GLY	-	linker	UNP P0A7G6
E	996	SER	-	linker	UNP P0A7G6
E	997	THR	-	linker	UNP P0A7G6
E	998	GLY	-	linker	UNP P0A7G6
E	999	SER	-	linker	UNP P0A7G6
E	1000	MET	-	linker	UNP P0A7G6
E	1986	THR	-	linker	UNP P0A7G6
E	1987	GLY	-	linker	UNP P0A7G6
E	1988	SER	-	linker	UNP P0A7G6
E	1989	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1990	GLY	-	linker	UNP P0A7G6
E	1991	SER	-	linker	UNP P0A7G6
E	1992	MET	-	linker	UNP P0A7G6
E	1993	GLY	-	linker	UNP P0A7G6
E	1994	HIS	-	linker	UNP P0A7G6
E	1995	THR	-	linker	UNP P0A7G6
E	1996	THR	-	linker	UNP P0A7G6
E	1997	GLY	-	linker	UNP P0A7G6
E	1998	SER	-	linker	UNP P0A7G6
E	1999	MET	-	linker	UNP P0A7G6
E	2000	SER	-	linker	UNP P0A7G6
E	2985	THR	-	linker	UNP P0A7G6
E	2986	GLY	-	linker	UNP P0A7G6
E	2987	SER	-	linker	UNP P0A7G6
E	2988	THR	-	linker	UNP P0A7G6
E	2989	GLY	-	linker	UNP P0A7G6
E	2990	SER	-	linker	UNP P0A7G6
E	2991	ALA	-	linker	UNP P0A7G6
E	2992	SER	-	linker	UNP P0A7G6
E	2993	GLY	-	linker	UNP P0A7G6
E	2994	SER	-	linker	UNP P0A7G6
E	2995	SER	-	linker	UNP P0A7G6
E	2996	THR	-	linker	UNP P0A7G6
E	2997	GLY	-	linker	UNP P0A7G6
E	2998	SER	-	linker	UNP P0A7G6
E	2999	MET	-	linker	UNP P0A7G6
E	3000	SER	-	linker	UNP P0A7G6
F	26	GLY	-	linker	UNP P0A7G6
F	27	ALA	-	linker	UNP P0A7G6
F	28	MET	-	linker	UNP P0A7G6
F	29	HIS	-	linker	UNP P0A7G6
F	986	THR	-	linker	UNP P0A7G6
F	987	GLY	-	linker	UNP P0A7G6
F	988	SER	-	linker	UNP P0A7G6
F	989	THR	-	linker	UNP P0A7G6
F	990	GLY	-	linker	UNP P0A7G6
F	991	SER	-	linker	UNP P0A7G6
F	992	GLY	-	linker	UNP P0A7G6
F	993	THR	-	linker	UNP P0A7G6
F	994	THR	-	linker	UNP P0A7G6
F	995	GLY	-	linker	UNP P0A7G6
F	996	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	997	THR	-	linker	UNP P0A7G6
F	998	GLY	-	linker	UNP P0A7G6
F	999	SER	-	linker	UNP P0A7G6
F	1000	MET	-	linker	UNP P0A7G6
F	1986	THR	-	linker	UNP P0A7G6
F	1987	GLY	-	linker	UNP P0A7G6
F	1988	SER	-	linker	UNP P0A7G6
F	1989	THR	-	linker	UNP P0A7G6
F	1990	GLY	-	linker	UNP P0A7G6
F	1991	SER	-	linker	UNP P0A7G6
F	1992	MET	-	linker	UNP P0A7G6
F	1993	GLY	-	linker	UNP P0A7G6
F	1994	HIS	-	linker	UNP P0A7G6
F	1995	THR	-	linker	UNP P0A7G6
F	1996	THR	-	linker	UNP P0A7G6
F	1997	GLY	-	linker	UNP P0A7G6
F	1998	SER	-	linker	UNP P0A7G6
F	1999	MET	-	linker	UNP P0A7G6
F	2000	SER	-	linker	UNP P0A7G6
F	2985	THR	-	linker	UNP P0A7G6
F	2986	GLY	-	linker	UNP P0A7G6
F	2987	SER	-	linker	UNP P0A7G6
F	2988	THR	-	linker	UNP P0A7G6
F	2989	GLY	-	linker	UNP P0A7G6
F	2990	SER	-	linker	UNP P0A7G6
F	2991	ALA	-	linker	UNP P0A7G6
F	2992	SER	-	linker	UNP P0A7G6
F	2993	GLY	-	linker	UNP P0A7G6
F	2994	SER	-	linker	UNP P0A7G6
F	2995	SER	-	linker	UNP P0A7G6
F	2996	THR	-	linker	UNP P0A7G6
F	2997	GLY	-	linker	UNP P0A7G6
F	2998	SER	-	linker	UNP P0A7G6
F	2999	MET	-	linker	UNP P0A7G6
F	3000	SER	-	linker	UNP P0A7G6
G	26	GLY	-	linker	UNP P0A7G6
G	27	ALA	-	linker	UNP P0A7G6
G	28	MET	-	linker	UNP P0A7G6
G	29	HIS	-	linker	UNP P0A7G6
G	986	THR	-	linker	UNP P0A7G6
G	987	GLY	-	linker	UNP P0A7G6
G	988	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	989	THR	-	linker	UNP P0A7G6
G	990	GLY	-	linker	UNP P0A7G6
G	991	SER	-	linker	UNP P0A7G6
G	992	GLY	-	linker	UNP P0A7G6
G	993	THR	-	linker	UNP P0A7G6
G	994	THR	-	linker	UNP P0A7G6
G	995	GLY	-	linker	UNP P0A7G6
G	996	SER	-	linker	UNP P0A7G6
G	997	THR	-	linker	UNP P0A7G6
G	998	GLY	-	linker	UNP P0A7G6
G	999	SER	-	linker	UNP P0A7G6
G	1000	MET	-	linker	UNP P0A7G6
G	1986	THR	-	linker	UNP P0A7G6
G	1987	GLY	-	linker	UNP P0A7G6
G	1988	SER	-	linker	UNP P0A7G6
G	1989	THR	-	linker	UNP P0A7G6
G	1990	GLY	-	linker	UNP P0A7G6
G	1991	SER	-	linker	UNP P0A7G6
G	1992	MET	-	linker	UNP P0A7G6
G	1993	GLY	-	linker	UNP P0A7G6
G	1994	HIS	-	linker	UNP P0A7G6
G	1995	THR	-	linker	UNP P0A7G6
G	1996	THR	-	linker	UNP P0A7G6
G	1997	GLY	-	linker	UNP P0A7G6
G	1998	SER	-	linker	UNP P0A7G6
G	1999	MET	-	linker	UNP P0A7G6
G	2000	SER	-	linker	UNP P0A7G6
G	2985	THR	-	linker	UNP P0A7G6
G	2986	GLY	-	linker	UNP P0A7G6
G	2987	SER	-	linker	UNP P0A7G6
G	2988	THR	-	linker	UNP P0A7G6
G	2989	GLY	-	linker	UNP P0A7G6
G	2990	SER	-	linker	UNP P0A7G6
G	2991	ALA	-	linker	UNP P0A7G6
G	2992	SER	-	linker	UNP P0A7G6
G	2993	GLY	-	linker	UNP P0A7G6
G	2994	SER	-	linker	UNP P0A7G6
G	2995	SER	-	linker	UNP P0A7G6
G	2996	THR	-	linker	UNP P0A7G6
G	2997	GLY	-	linker	UNP P0A7G6
G	2998	SER	-	linker	UNP P0A7G6
G	2999	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	3000	SER	-	linker	UNP P0A7G6
H	26	GLY	-	linker	UNP P0A7G6
H	27	ALA	-	linker	UNP P0A7G6
H	28	MET	-	linker	UNP P0A7G6
H	29	HIS	-	linker	UNP P0A7G6
H	986	THR	-	linker	UNP P0A7G6
H	987	GLY	-	linker	UNP P0A7G6
H	988	SER	-	linker	UNP P0A7G6
H	989	THR	-	linker	UNP P0A7G6
H	990	GLY	-	linker	UNP P0A7G6
H	991	SER	-	linker	UNP P0A7G6
H	992	GLY	-	linker	UNP P0A7G6
H	993	THR	-	linker	UNP P0A7G6
H	994	THR	-	linker	UNP P0A7G6
H	995	GLY	-	linker	UNP P0A7G6
H	996	SER	-	linker	UNP P0A7G6
H	997	THR	-	linker	UNP P0A7G6
H	998	GLY	-	linker	UNP P0A7G6
H	999	SER	-	linker	UNP P0A7G6
H	1000	MET	-	linker	UNP P0A7G6
H	1986	THR	-	linker	UNP P0A7G6
H	1987	GLY	-	linker	UNP P0A7G6
H	1988	SER	-	linker	UNP P0A7G6
H	1989	THR	-	linker	UNP P0A7G6
H	1990	GLY	-	linker	UNP P0A7G6
H	1991	SER	-	linker	UNP P0A7G6
H	1992	MET	-	linker	UNP P0A7G6
H	1993	GLY	-	linker	UNP P0A7G6
H	1994	HIS	-	linker	UNP P0A7G6
H	1995	THR	-	linker	UNP P0A7G6
H	1996	THR	-	linker	UNP P0A7G6
H	1997	GLY	-	linker	UNP P0A7G6
H	1998	SER	-	linker	UNP P0A7G6
H	1999	MET	-	linker	UNP P0A7G6
H	2000	SER	-	linker	UNP P0A7G6
H	2985	THR	-	linker	UNP P0A7G6
H	2986	GLY	-	linker	UNP P0A7G6
H	2987	SER	-	linker	UNP P0A7G6
H	2988	THR	-	linker	UNP P0A7G6
H	2989	GLY	-	linker	UNP P0A7G6
H	2990	SER	-	linker	UNP P0A7G6
H	2991	ALA	-	linker	UNP P0A7G6

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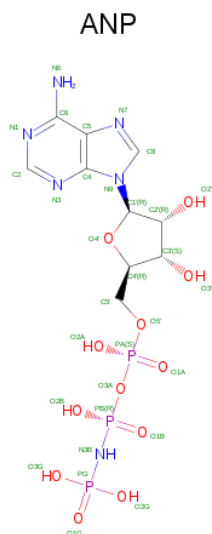
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Chain	Residue	Modelled	Actual	Comment	Reference
H	2992	SER	-	linker	UNP P0A7G6
H	2993	GLY	-	linker	UNP P0A7G6
H	2994	SER	-	linker	UNP P0A7G6
H	2995	SER	-	linker	UNP P0A7G6
H	2996	THR	-	linker	UNP P0A7G6
H	2997	GLY	-	linker	UNP P0A7G6
H	2998	SER	-	linker	UNP P0A7G6
H	2999	MET	-	linker	UNP P0A7G6
H	3000	SER	-	linker	UNP P0A7G6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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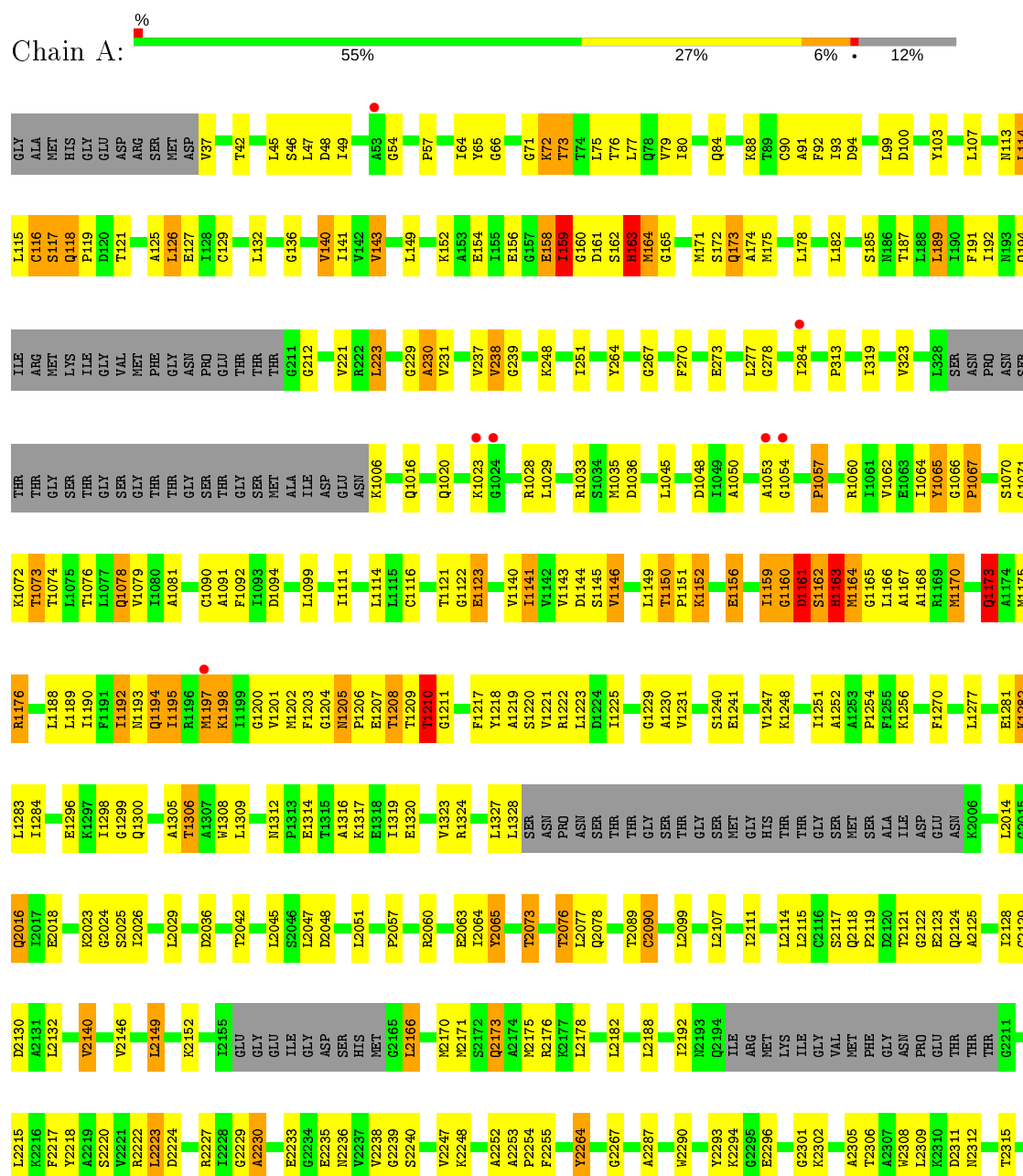
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

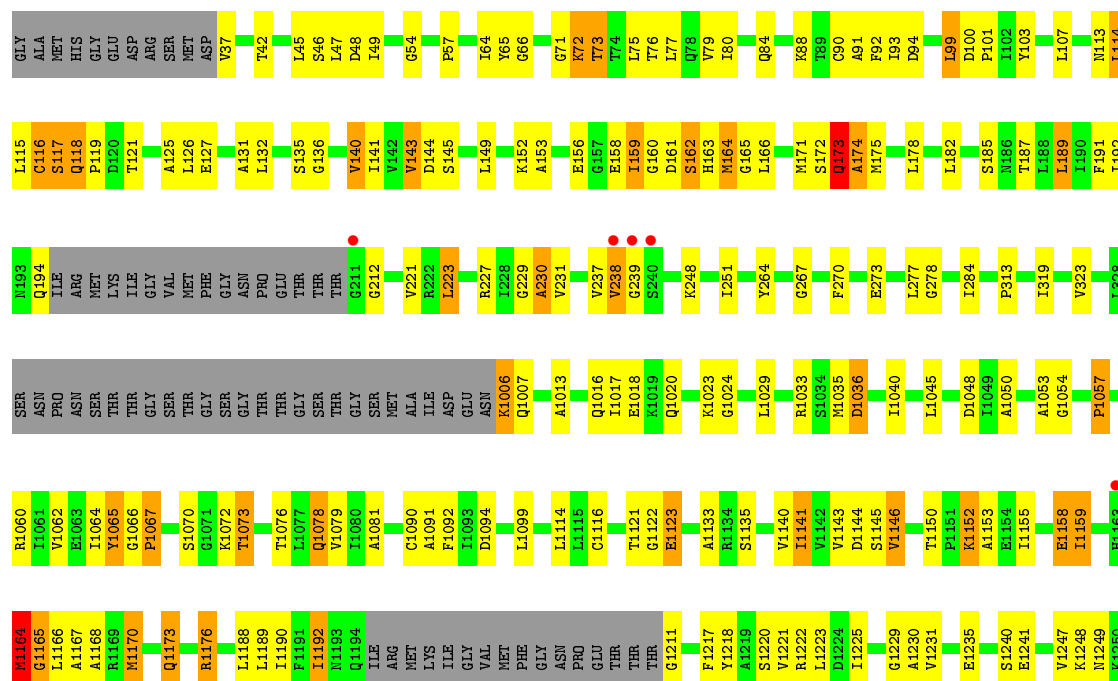
3 Residue-property plots

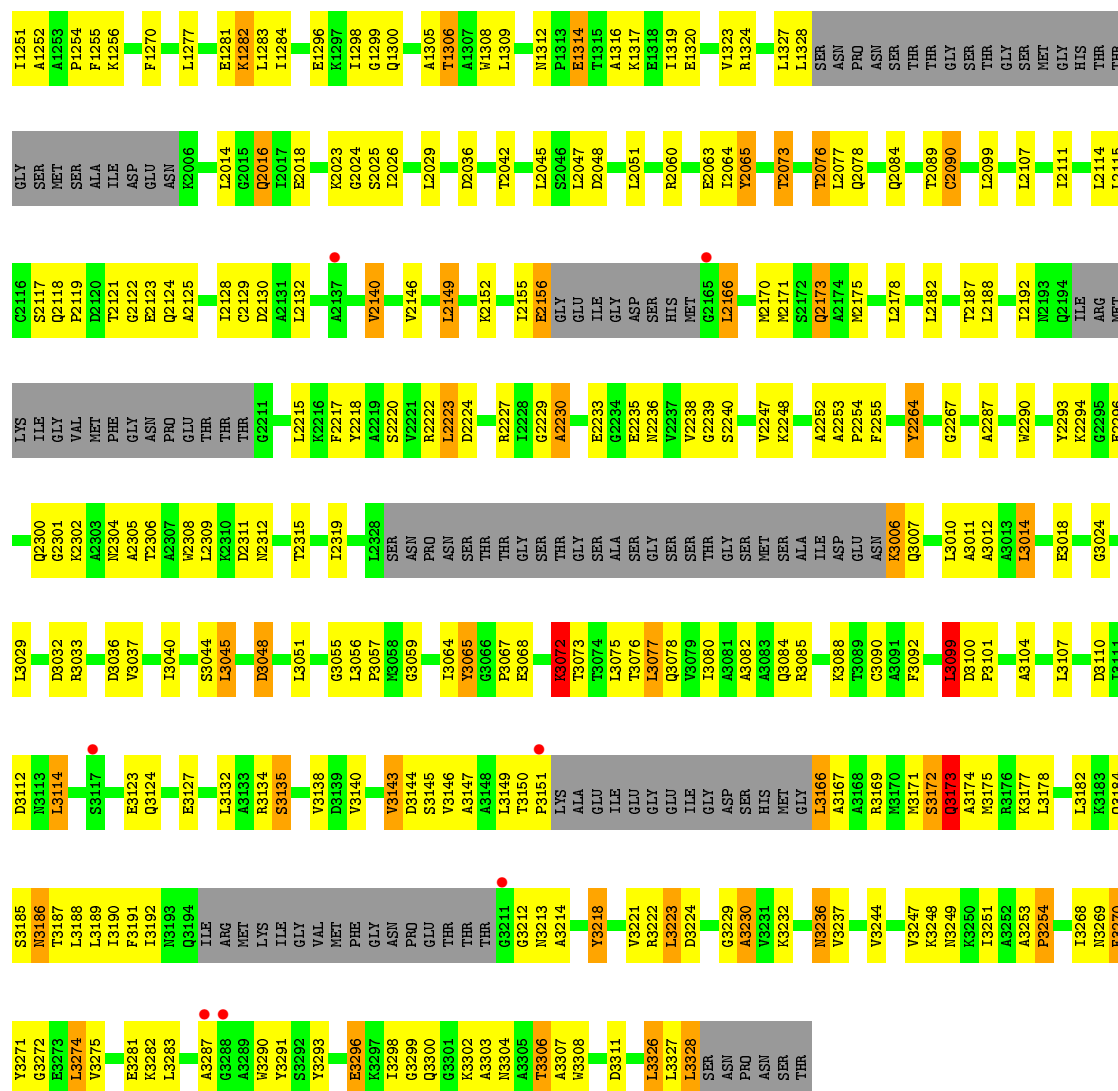
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Protein recA

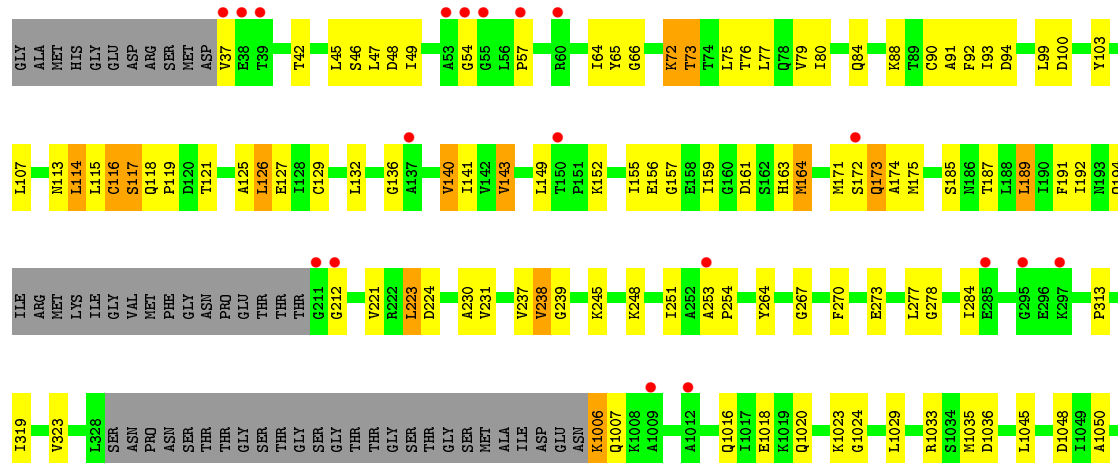


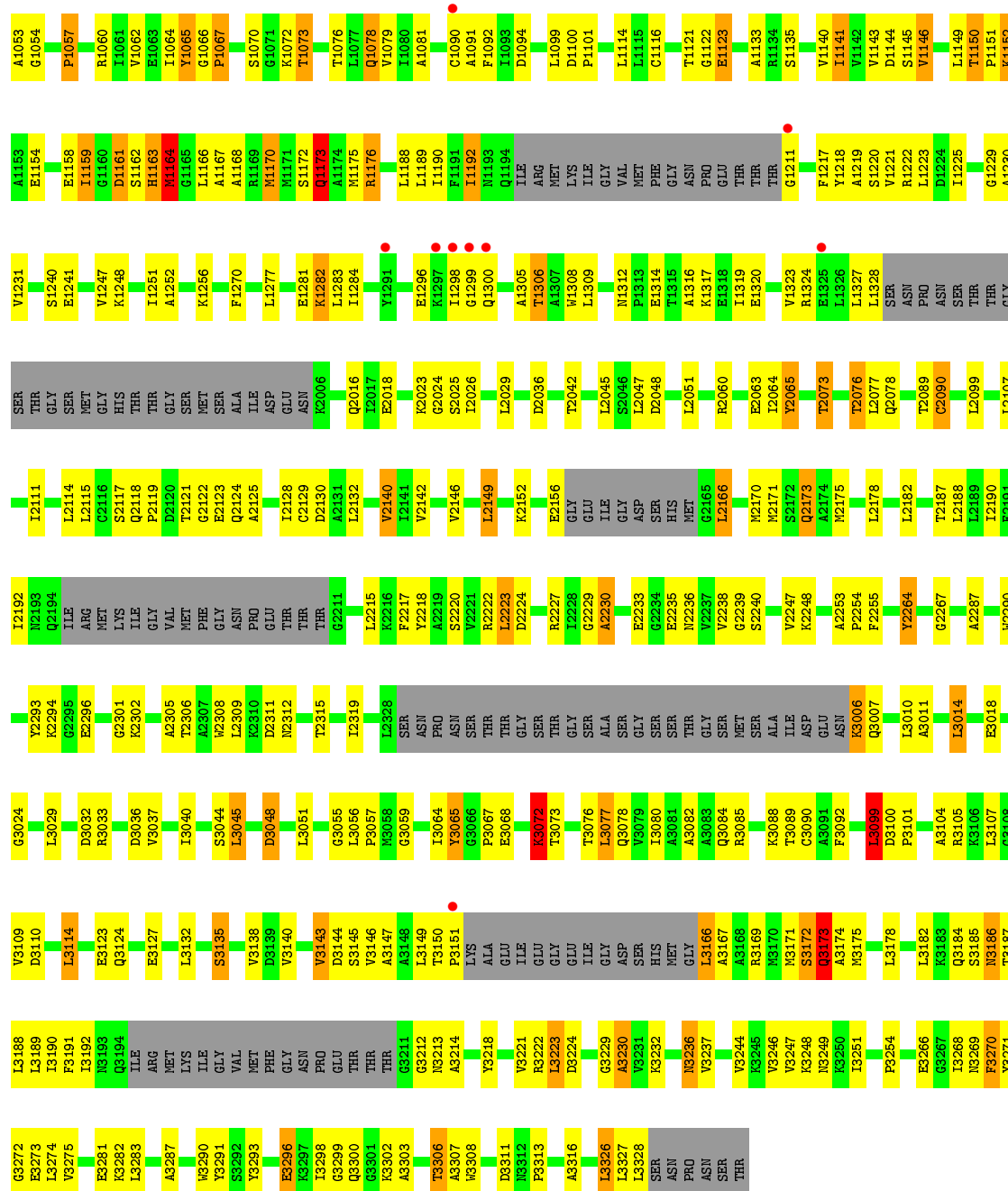




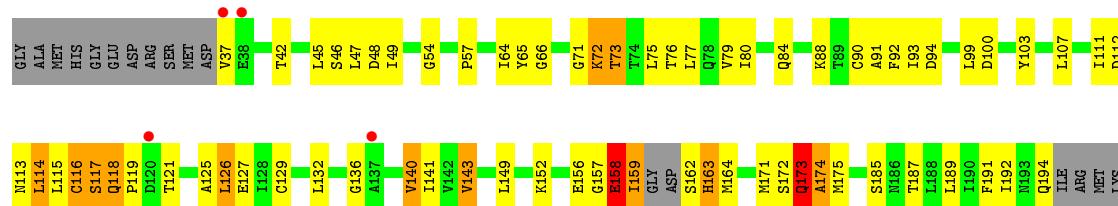


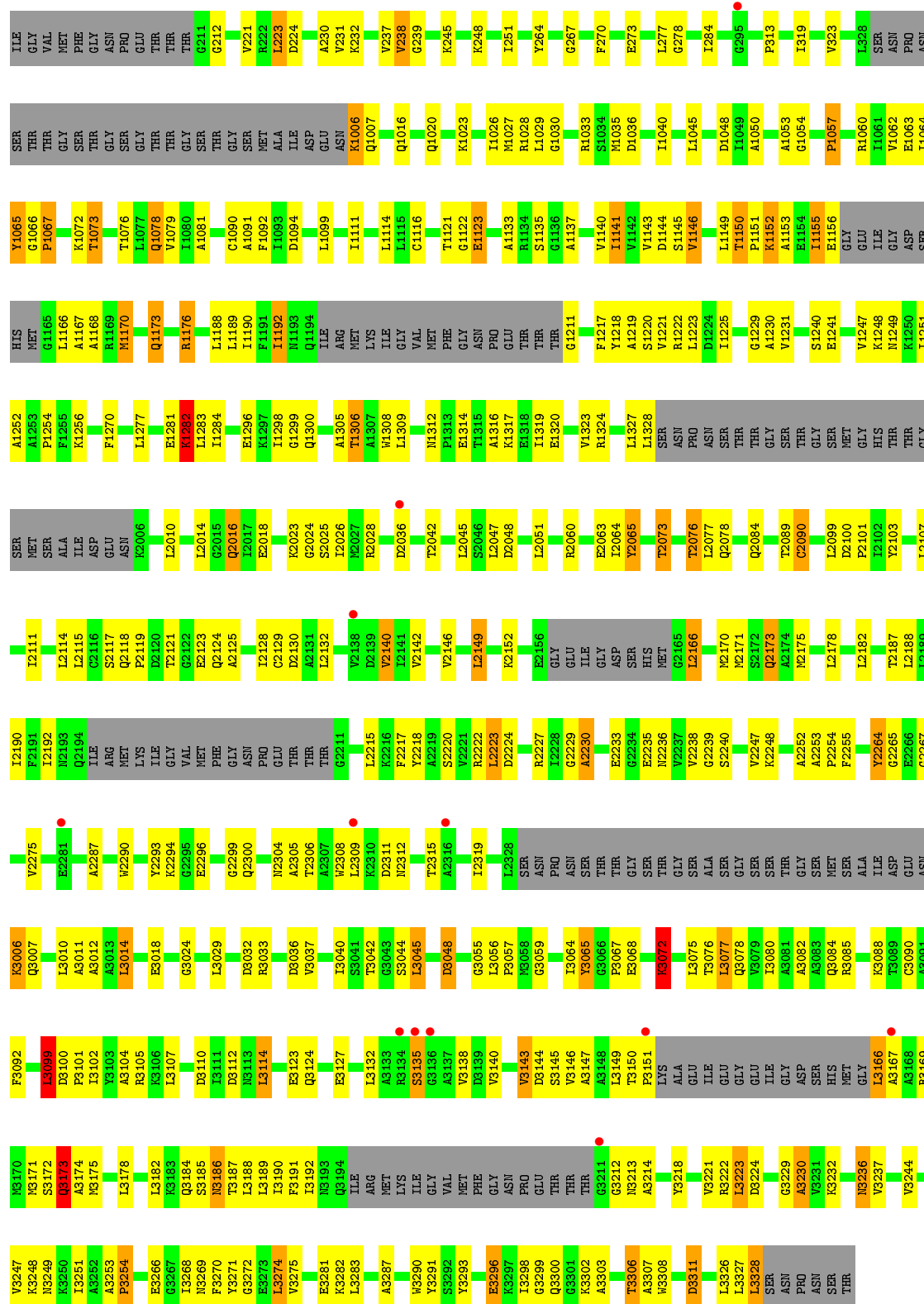
Molecule 1: Protein recA





• Molecule 1: Protein recA





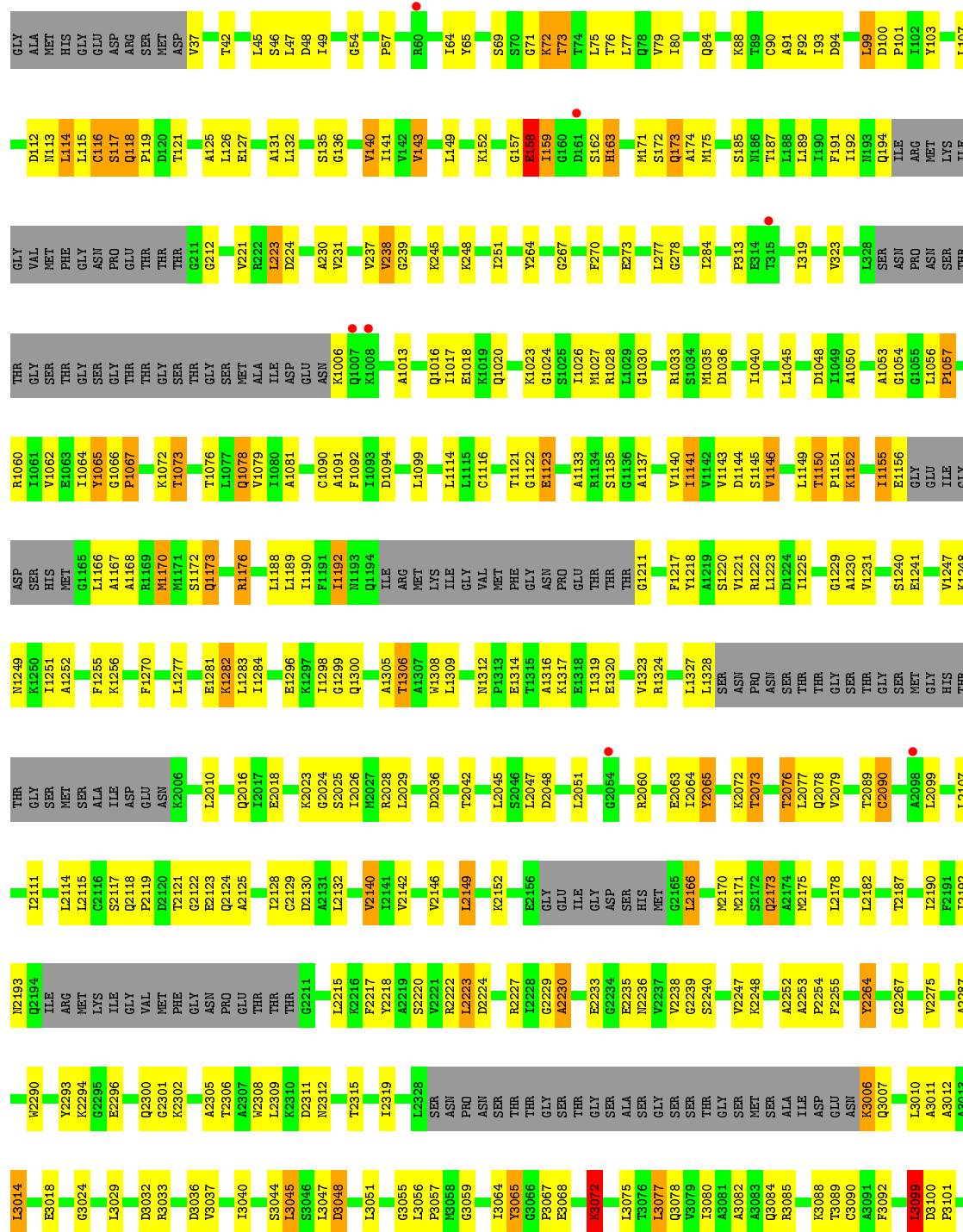
- Molecule 1: Protein recA





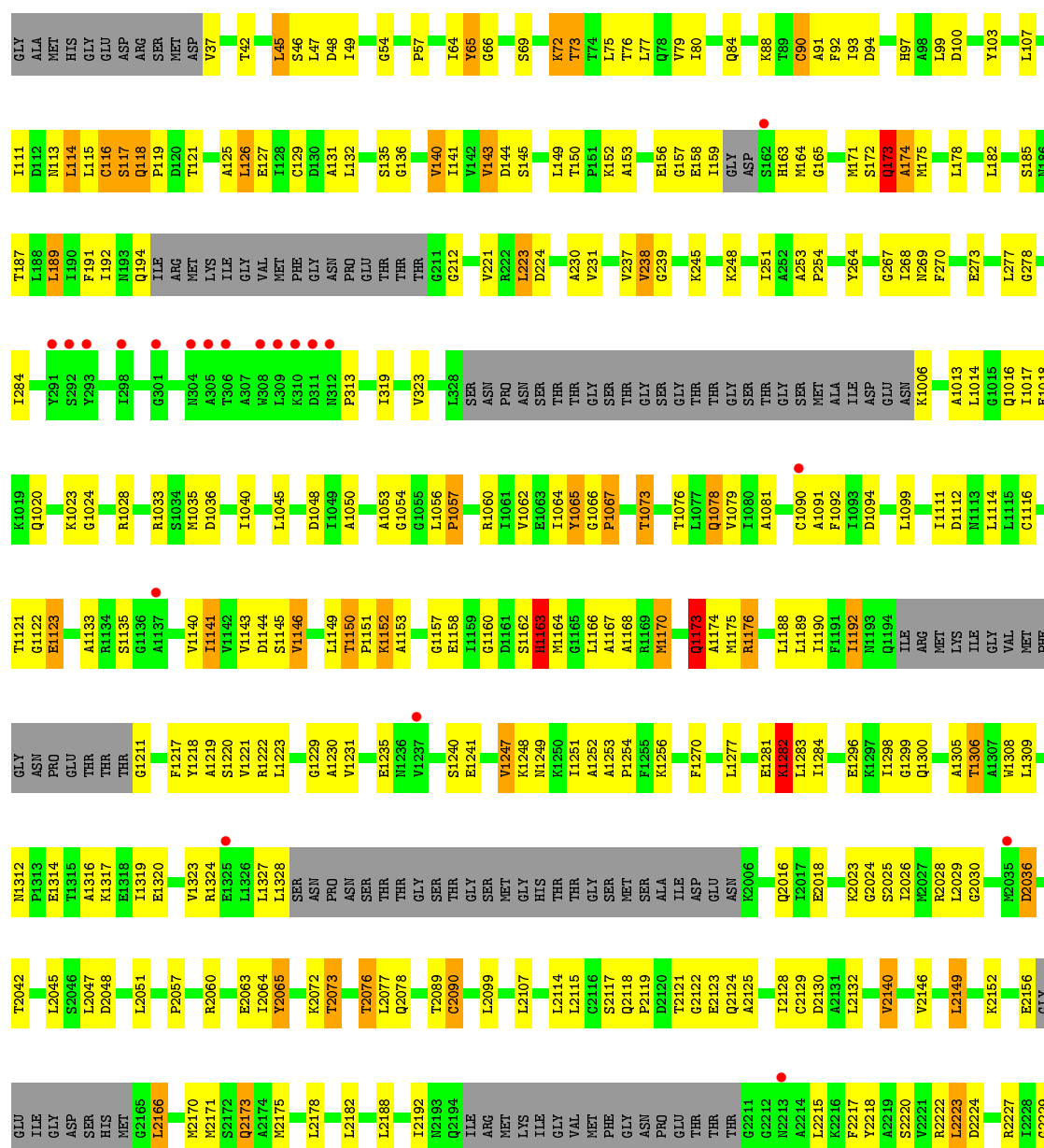


• Molecule 1: Protein recA





• Molecule 1: Protein recA



W3308	Y3218	ALA	K3072	THR	A2230
D3311	V3221	GLU	L3075	THR	E2233
N3312	R3222	ILE	T3076	GLY	G2234
P3313	L3223	GLU	L3077	THR	E2235
A3316	D3224	GLU	Q3078	GLY	N2236
		ILE	V3079	SER	V2237
	G3229	GLY	I3080	ALA	V2238
L3326	A3230	ASP	A3081	SER	G2239
L3327	V3231	SER	A3082	GLY	S2240
L3328	K3232	HIS	A3083	SER	
SER	N3236	MET	Q3084	SER	V2247
ASN	V3237	GLY	R3085	THR	K2248
PRO		L3166		GLY	
ASN	V3244	A3167	K3088	SER	A2252
SER		A3168	T3089	MET	A2253
THR	V3247	R3169	G3090	SER	P2254
	K3248	R3170	A3091	ALA	F2255
	N3249	R3171	F3092	ILE	K2256
	R3250	S3172	L3099	ASP	
	I3251	K3173	D3100	GLU	Y2264
	A3252	A3174	P3101	ASN	
A3253	P3254	R3175	I3102	K3006	G2267
		L3178	R3183	Q3007	
	Y3264	L3182	A3104	L3010	V2275
	G3265	K3183		A3011	
	E3266	Q3184	L3107	L3014	A2287
	G3267	S3185	G3108	W2290	
	I3268	N3186	V3109	Y2293	
	N3269	T3187	D3110	K2294	
	F3270	L3188	I3111	G2295	
	Y3271	L3189	D3112	E2296	
		T3190	N3113		
	L3274	F3191	L3114	G2299	
	V3275	I3192	E3123	Q2300	
		R3193	Q3124	G2301	
	E3281	I3194	E3127	K2302	
	K3282	ILE		A2303	
	L3283	ARG	L3132	N2304	
		MET	S3135	T2306	
	A3287	LYS	V3138	A2307	
		ILE	D3139	L2307	
	W3290	GLY	V3140	W2308	
	Y3291	VAL	V3143	L2309	
	S3292	MET	D3144	K2310	
	Y3293	PHE	S3145	D2311	
		GLY	V3146	N2312	
	E3296	ASN	A3147		
	K3297	PRO	L3148	G3055	
	I3298	GLU	D3149	L3056	
	G3299	THR	T3150	P3057	
	Q3300	THR	V3151	M3058	
	G3301	THR	A3151	G3059	
	K3302	THR	A3148		
	A3303	G3212	L3149	L3064	
		R3213	T3150	Y3065	
	T3306	A3214	P3151	G3066	
A3307			LYS	P3067	
				ASN	
				SER	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	176.60 Å 189.80 Å 424.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.30 39.93 – 4.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-4.30) 92.7 (39.93-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 4.28 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.261 0.274 , 0.283	Depositor DCC
R_{free} test set	1946 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	170.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 116.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	71761	wwPDB-VP
Average B, all atoms (Å ²)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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, ANP

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	0.81	6/9068 (0.1%)	0.80	10/12192 (0.1%)
1	B	0.76	4/8861 (0.0%)	0.76	1/11910 (0.0%)
1	C	0.77	0/8951	0.77	4/12033 (0.0%)
1	D	0.74	3/8951 (0.0%)	0.75	4/12033 (0.0%)
1	E	0.72	1/8879 (0.0%)	0.75	2/11934 (0.0%)
1	F	0.77	4/8951 (0.0%)	0.77	2/12033 (0.0%)
1	G	0.77	2/8892 (0.0%)	0.76	3/11953 (0.0%)
1	H	0.72	2/8938 (0.0%)	0.75	3/12014 (0.0%)
All	All	0.76	22/71491 (0.0%)	0.77	29/96102 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	3
1	C	0	4
1	D	0	7
1	E	0	6
1	F	0	6
1	G	0	5
1	H	0	4
All	All	0	46

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	HIS	N-CA	7.46	1.61	1.46
1	B	3266	GLU	CG-CD	6.68	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1164	MET	CB-CG	6.66	1.72	1.51
1	D	156	GLU	CG-CD	5.97	1.60	1.51
1	F	3270	PHE	CE1-CZ	5.74	1.48	1.37

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	MET	C-N-CA	-8.01	105.48	122.30
1	D	2166	LEU	CA-CB-CG	7.24	131.94	115.30
1	G	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	H	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	E	2166	LEU	CA-CB-CG	7.21	131.89	115.30

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1161	ASP	Peptide
1	A	1163	HIS	Peptide
1	A	158	GLU	Peptide
1	A	161	ASP	Peptide
1	A	163	HIS	Peptide

5.2 Too-close contacts

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	8970	0	9264	308	1
1	B	8769	0	9070	275	0
1	C	8856	0	9139	294	1
1	D	8856	0	9139	268	0
1	E	8787	0	9082	304	0
1	F	8856	0	9139	314	0
1	G	8799	0	9090	269	0
1	H	8844	0	9131	304	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	124	0	52	7	0
3	B	124	0	52	2	0
3	C	124	0	52	3	0
3	D	124	0	52	2	0
3	E	124	0	52	3	0
3	F	124	0	52	9	0
3	G	124	0	52	4	0
3	H	124	0	52	4	0
All	All	71761	0	73470	2200	1

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 15.

The worst 5 of 2200 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:A:1204:GLY:HA2	1:B:3115:LEU:CD2	1.50	1.42
1:A:1194:GLN:O	1:A:1195:ILE:CG2	1.73	1.37
1:A:162:SER:O	1:A:165:GLY:CA	1.71	1.35
1:A:1194:GLN:O	1:A:1195:ILE:CB	1.81	1.27
1:A:1194:GLN:O	1:A:1195:ILE:HG22	1.25	1.22

All (1) 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:A:1161:ASP:OD1	1:C:1314:GLU:OE2[4_456]	2.05	0.15

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	1172/1357 (86%)	923 (79%)	191 (16%)	58 (5%)	2	23
1	B	1139/1357 (84%)	915 (80%)	172 (15%)	52 (5%)	2	24
1	C	1155/1357 (85%)	919 (80%)	178 (15%)	58 (5%)	2	23
1	D	1155/1357 (85%)	923 (80%)	179 (16%)	53 (5%)	2	24
1	E	1141/1357 (84%)	910 (80%)	178 (16%)	53 (5%)	2	24
1	F	1155/1357 (85%)	913 (79%)	188 (16%)	54 (5%)	2	24
1	G	1145/1357 (84%)	914 (80%)	179 (16%)	52 (4%)	2	24
1	H	1151/1357 (85%)	914 (79%)	180 (16%)	57 (5%)	2	23
All	All	9213/10856 (85%)	7331 (80%)	1445 (16%)	437 (5%)	2	24

5 of 437 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	A	99	LEU
1	A	238	VAL
1	A	1099	LEU
1	A	1146	VAL

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	930/1065 (87%)	813 (87%)	117 (13%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	908/1065 (85%)	801 (88%)	107 (12%)	5	23
1	C	917/1065 (86%)	805 (88%)	112 (12%)	5	23
1	D	917/1065 (86%)	810 (88%)	107 (12%)	5	23
1	E	910/1065 (85%)	801 (88%)	109 (12%)	5	23
1	F	917/1065 (86%)	812 (88%)	105 (12%)	5	24
1	G	911/1065 (86%)	800 (88%)	111 (12%)	5	23
1	H	916/1065 (86%)	806 (88%)	110 (12%)	5	23
All	All	7326/8520 (86%)	6448 (88%)	878 (12%)	5	23

5 of 878 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2089	THR
1	E	1282	LYS
1	H	1221	VAL
1	D	2264	TYR
1	E	65	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2300	GLN
1	E	2236	ASN
1	H	2020	GLN
1	D	3181	ASN
1	E	173	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 32 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ANP	G	3400	-	29,33,33	2.11	8 (27%)	31,52,52	2.32	8 (25%)
3	ANP	D	3400	-	29,33,33	1.99	8 (27%)	31,52,52	2.37	8 (25%)
3	ANP	E	400	-	29,33,33	2.00	9 (31%)	31,52,52	1.86	8 (25%)
3	ANP	B	400	-	29,33,33	2.01	8 (27%)	31,52,52	1.83	9 (29%)
3	ANP	E	2400	-	29,33,33	2.07	9 (31%)	31,52,52	1.99	7 (22%)
3	ANP	H	2400	-	29,33,33	2.01	11 (37%)	31,52,52	1.99	7 (22%)
3	ANP	E	3400	2	29,33,33	1.81	8 (27%)	31,52,52	2.40	10 (32%)
3	ANP	B	3400	-	29,33,33	1.95	7 (24%)	31,52,52	2.43	9 (29%)
3	ANP	C	3400	-	29,33,33	2.14	8 (27%)	31,52,52	2.30	9 (29%)
3	ANP	C	1400	-	29,33,33	2.11	8 (27%)	31,52,52	2.02	8 (25%)
3	ANP	B	2400	-	29,33,33	2.01	8 (27%)	31,52,52	2.00	7 (22%)
3	ANP	B	1400	-	29,33,33	2.00	7 (24%)	31,52,52	2.02	7 (22%)
3	ANP	H	400	-	29,33,33	1.96	8 (27%)	31,52,52	1.84	7 (22%)
3	ANP	H	1400	-	29,33,33	2.09	8 (27%)	31,52,52	1.91	8 (25%)
3	ANP	A	400	-	29,33,33	2.07	9 (31%)	31,52,52	1.84	7 (22%)
3	ANP	G	1400	-	29,33,33	2.01	7 (24%)	31,52,52	1.95	8 (25%)
3	ANP	G	2400	-	29,33,33	2.06	8 (27%)	31,52,52	1.99	7 (22%)
3	ANP	G	400	-	29,33,33	1.99	7 (24%)	31,52,52	1.89	7 (22%)
3	ANP	F	3400	-	29,33,33	1.98	10 (34%)	31,52,52	2.34	9 (29%)
3	ANP	D	2400	-	29,33,33	2.02	8 (27%)	31,52,52	1.98	7 (22%)
3	ANP	D	1400	-	29,33,33	1.99	7 (24%)	31,52,52	1.97	8 (25%)
3	ANP	F	1400	-	29,33,33	2.10	9 (31%)	31,52,52	2.01	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	D	400	-	29,33,33	2.07	11 (37%)	31,52,52	1.85	8 (25%)
3	ANP	F	400	-	29,33,33	1.95	8 (27%)	31,52,52	1.85	7 (22%)
3	ANP	F	2400	-	29,33,33	1.91	9 (31%)	31,52,52	1.99	7 (22%)
3	ANP	H	3400	-	29,33,33	2.07	8 (27%)	31,52,52	2.44	9 (29%)
3	ANP	A	1400	-	29,33,33	1.95	10 (34%)	31,52,52	1.96	7 (22%)
3	ANP	A	2400	-	29,33,33	2.04	8 (27%)	31,52,52	2.01	7 (22%)
3	ANP	C	2400	-	29,33,33	1.96	7 (24%)	31,52,52	1.99	7 (22%)
3	ANP	A	3400	-	29,33,33	1.96	7 (24%)	31,52,52	2.35	9 (29%)
3	ANP	C	400	-	29,33,33	1.85	7 (24%)	31,52,52	1.91	7 (22%)
3	ANP	E	1400	-	29,33,33	2.05	9 (31%)	31,52,52	1.99	7 (22%)

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	ANP	G	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	D	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	E	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	B	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	E	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	H	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	E	3400	2	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	B	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	C	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	C	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	B	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	B	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	H	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	H	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	A	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	G	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	G	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	G	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	F	3400	-	1/1/7/8	7/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	D	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	D	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	F	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	D	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	F	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	F	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	H	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	A	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	A	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	C	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	A	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	C	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	E	1400	-	1/1/7/8	10/14/38/38	0/3/3/3

The worst 5 of 264 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3400	ANP	PG-N3B	5.90	1.78	1.63
3	H	3400	ANP	PG-N3B	5.54	1.77	1.63
3	G	3400	ANP	PG-N3B	5.49	1.77	1.63
3	C	3400	ANP	PB-N3B	5.45	1.77	1.63
3	G	3400	ANP	PB-N3B	5.33	1.77	1.63

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3400	ANP	O1G-PG-N3B	-7.84	100.23	111.77
3	F	3400	ANP	O1G-PG-N3B	-7.45	100.81	111.77
3	H	3400	ANP	O1G-PG-N3B	-7.29	101.03	111.77
3	A	3400	ANP	O1G-PG-N3B	-7.10	101.32	111.77
3	G	3400	ANP	O1G-PG-N3B	-7.08	101.34	111.77

5 of 32 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	3400	ANP	C4'
3	D	3400	ANP	C4'
3	E	400	ANP	C4'
3	F	3400	ANP	C4'

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Mol	Chain	Res	Type	Atom
3	E	2400	ANP	C4'

5 of 280 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	3400	ANP	PB-N3B-PG-O1G
3	G	3400	ANP	PG-N3B-PB-O1B
3	G	3400	ANP	PG-N3B-PB-O3A
3	G	3400	ANP	C5'-O5'-PA-O3A
3	D	3400	ANP	PB-N3B-PG-O1G

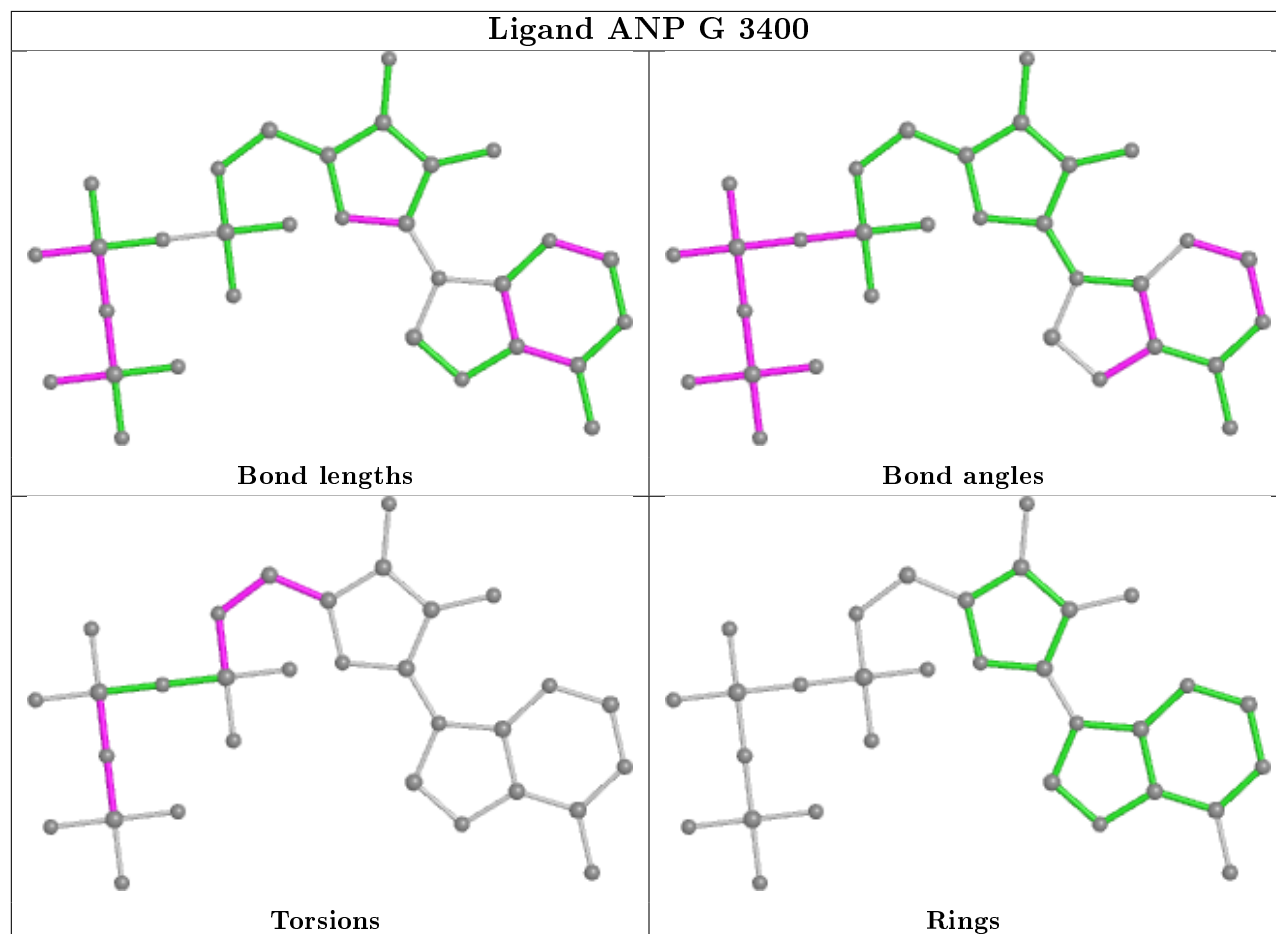
There are no ring outliers.

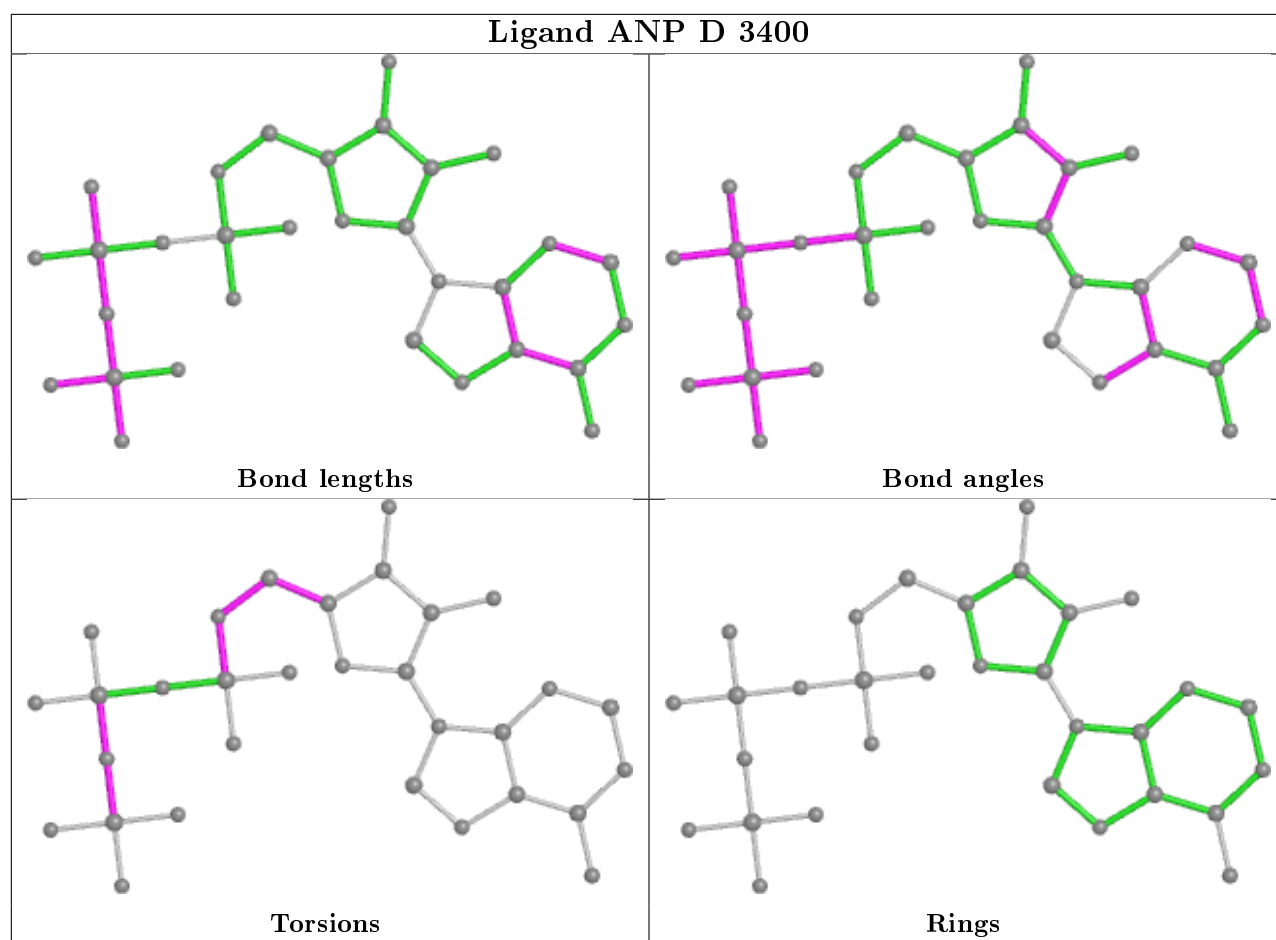
17 monomers are involved in 34 short contacts:

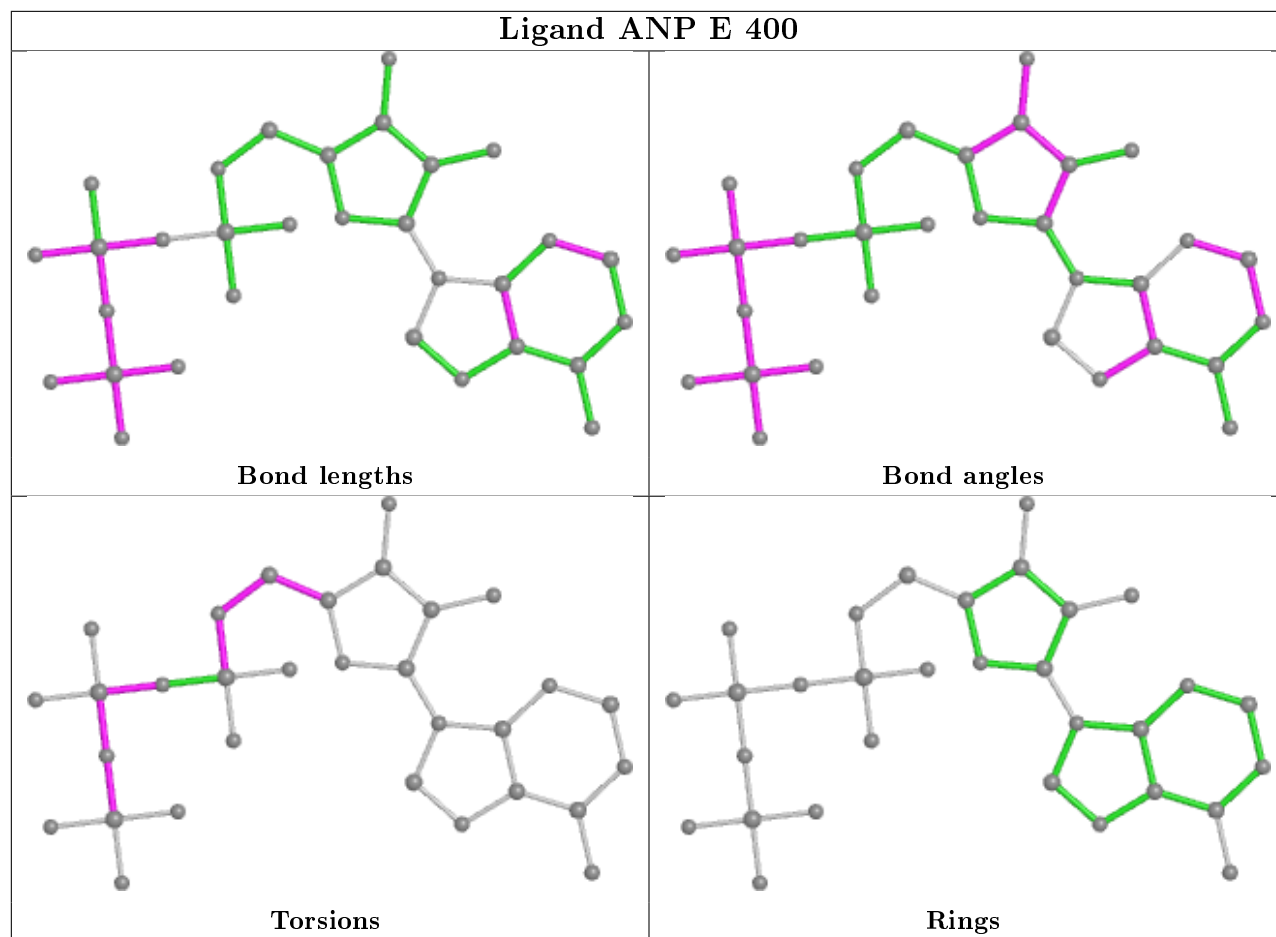
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3400	ANP	2	0
3	D	3400	ANP	2	0
3	E	400	ANP	1	0
3	B	400	ANP	1	0
3	E	3400	ANP	1	0
3	B	3400	ANP	1	0
3	C	3400	ANP	2	0
3	H	400	ANP	1	0
3	A	400	ANP	1	0
3	G	400	ANP	2	0
3	F	3400	ANP	3	0
3	F	400	ANP	6	0
3	H	3400	ANP	3	0
3	A	1400	ANP	3	0
3	A	3400	ANP	3	0
3	C	400	ANP	1	0
3	E	1400	ANP	1	0

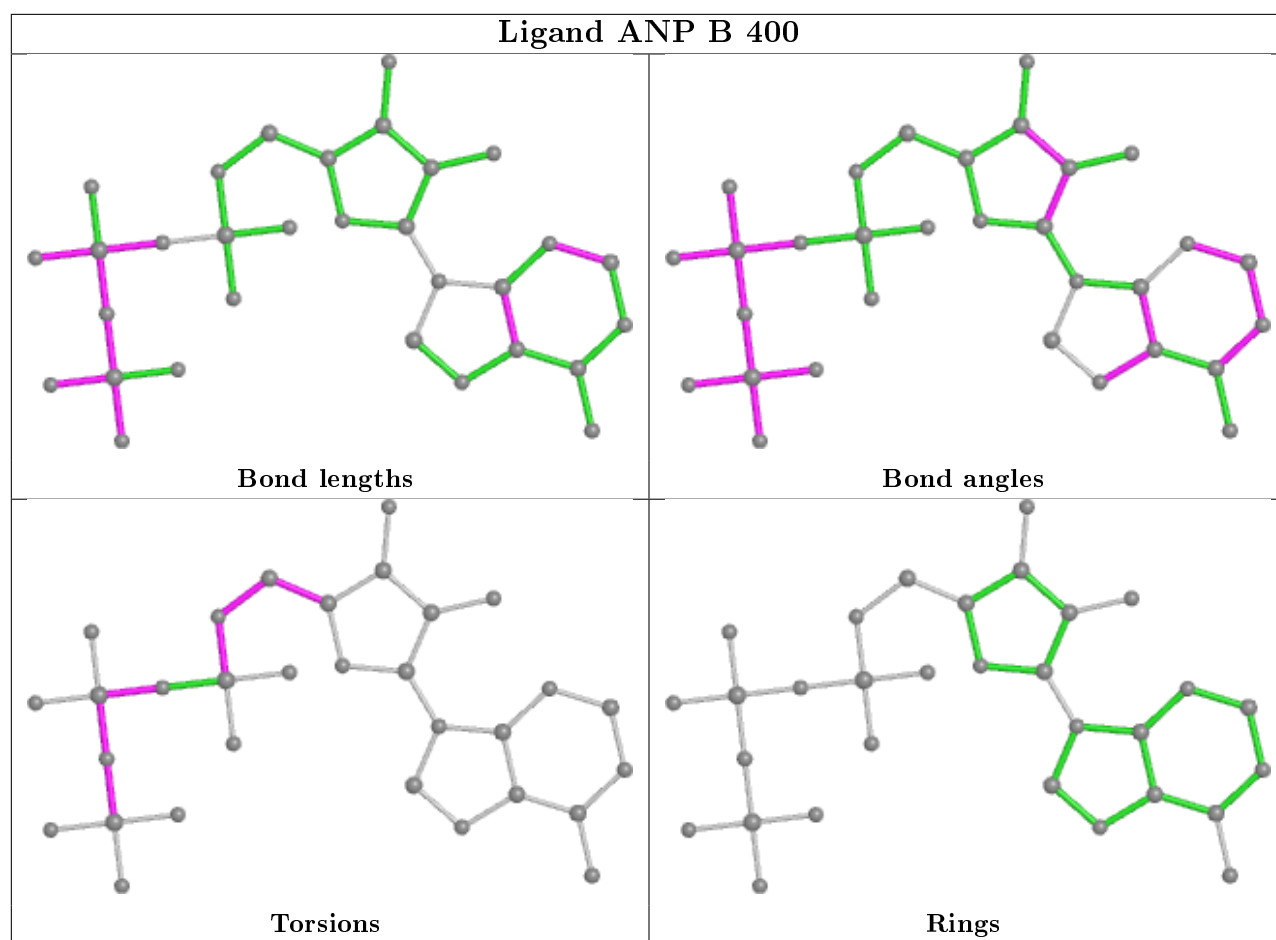
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

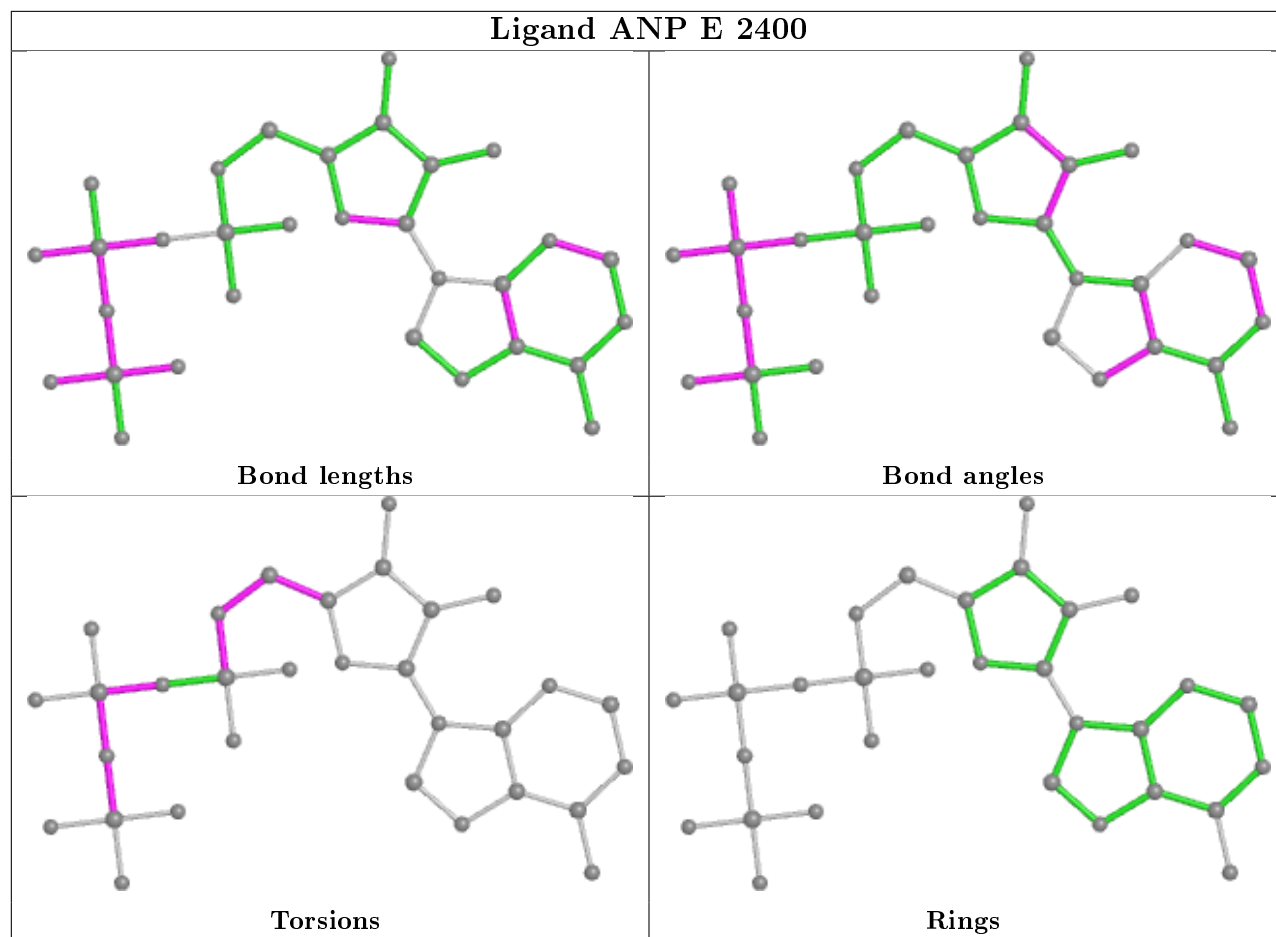
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

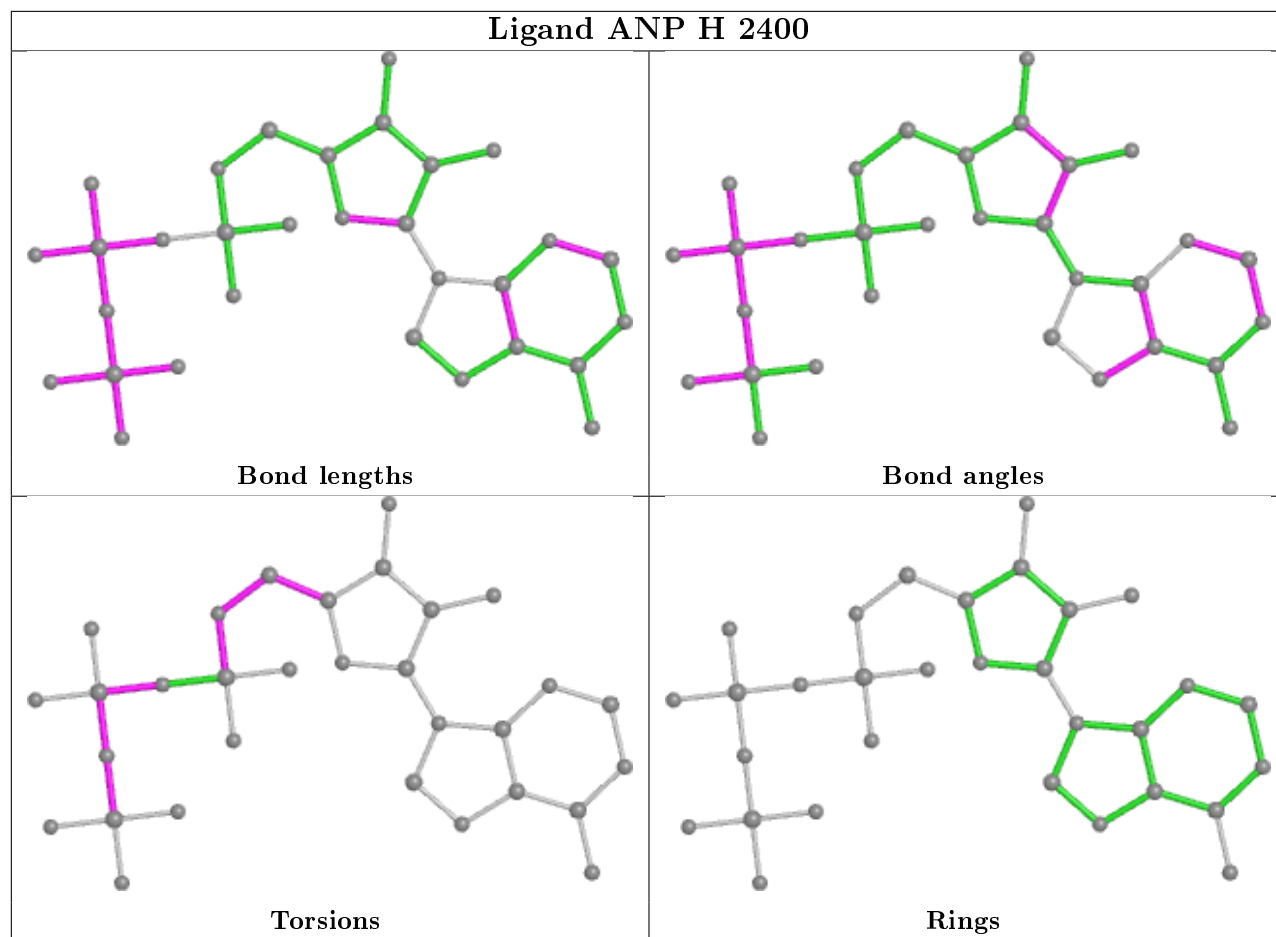


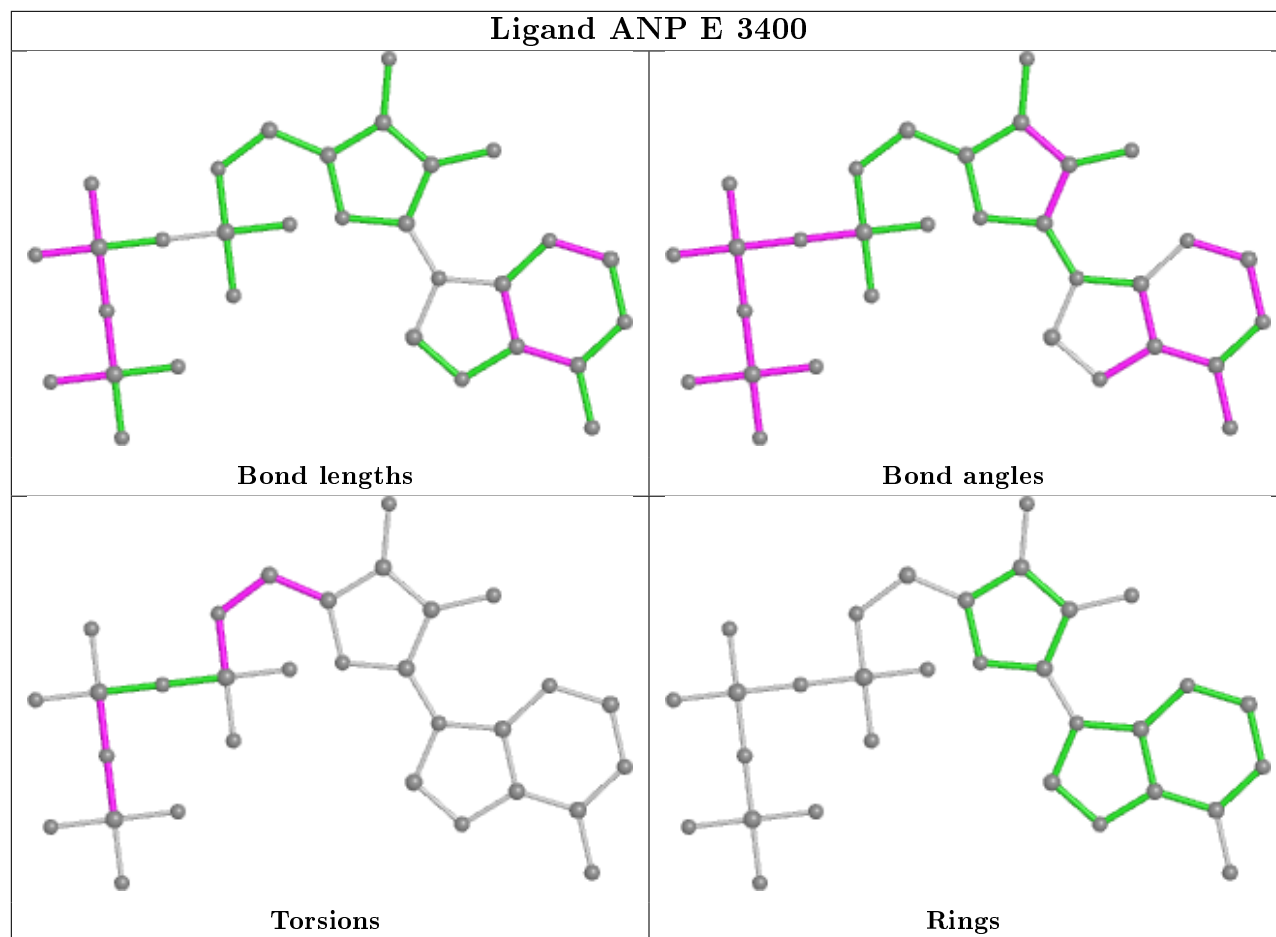


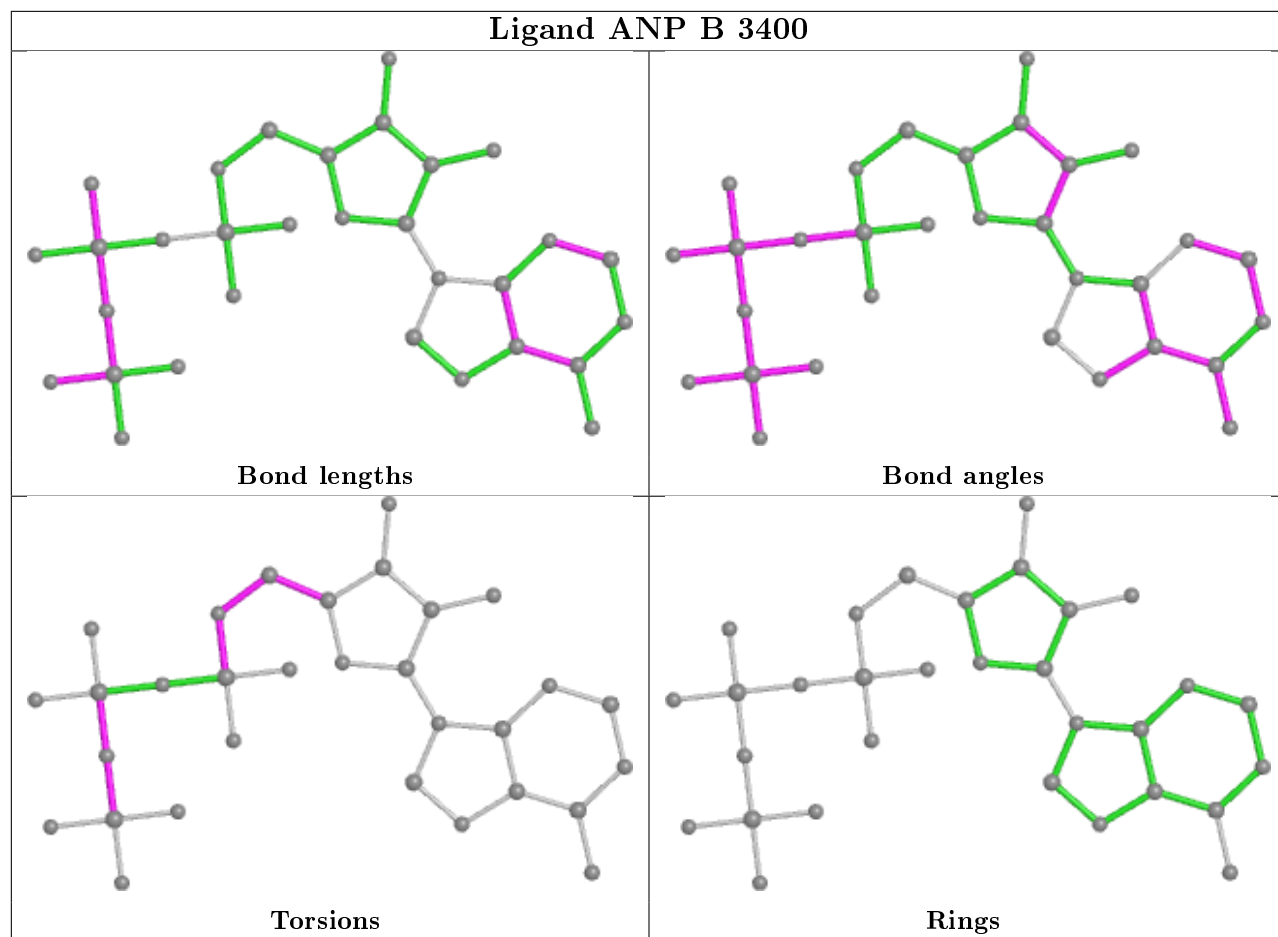


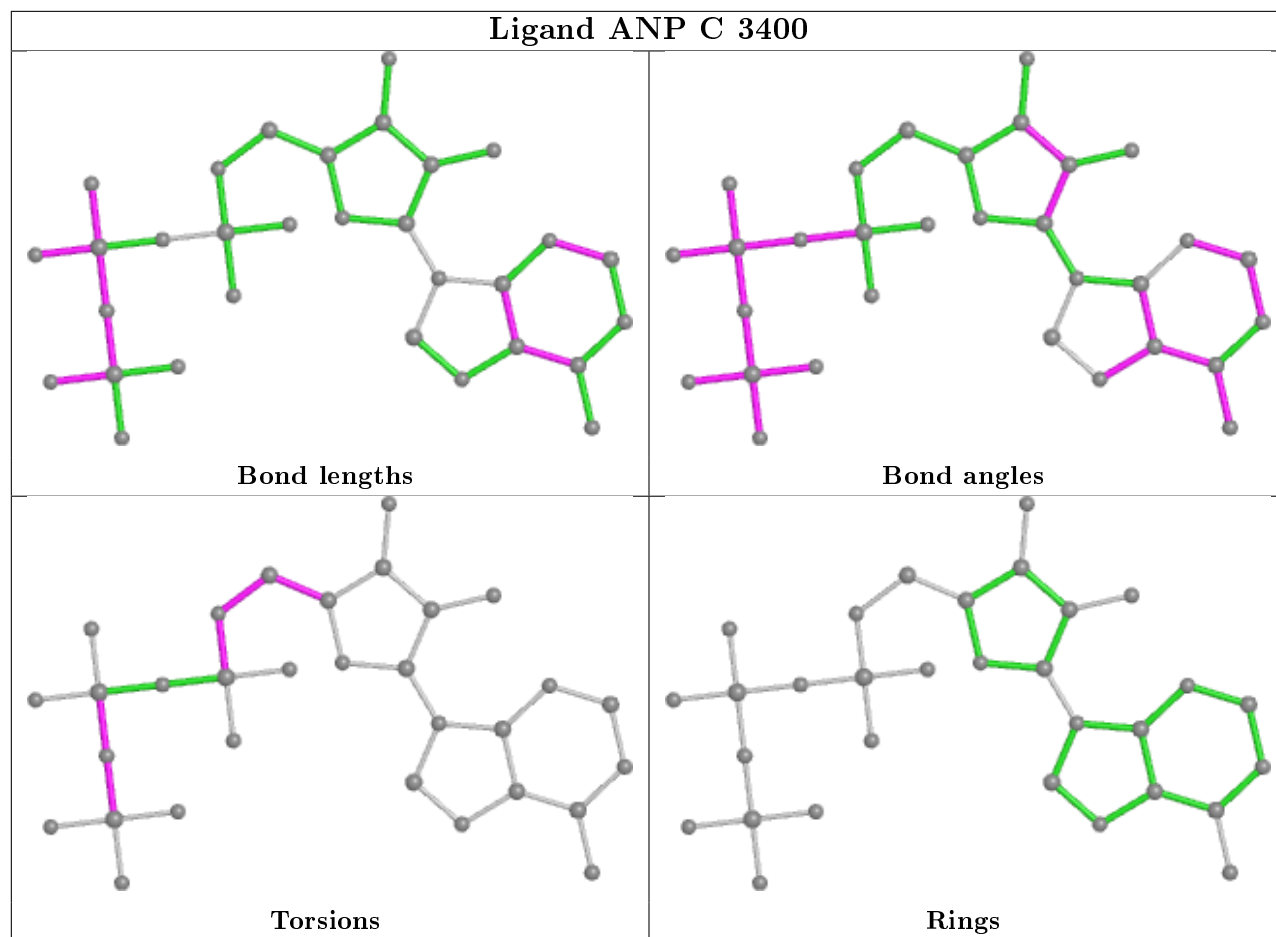


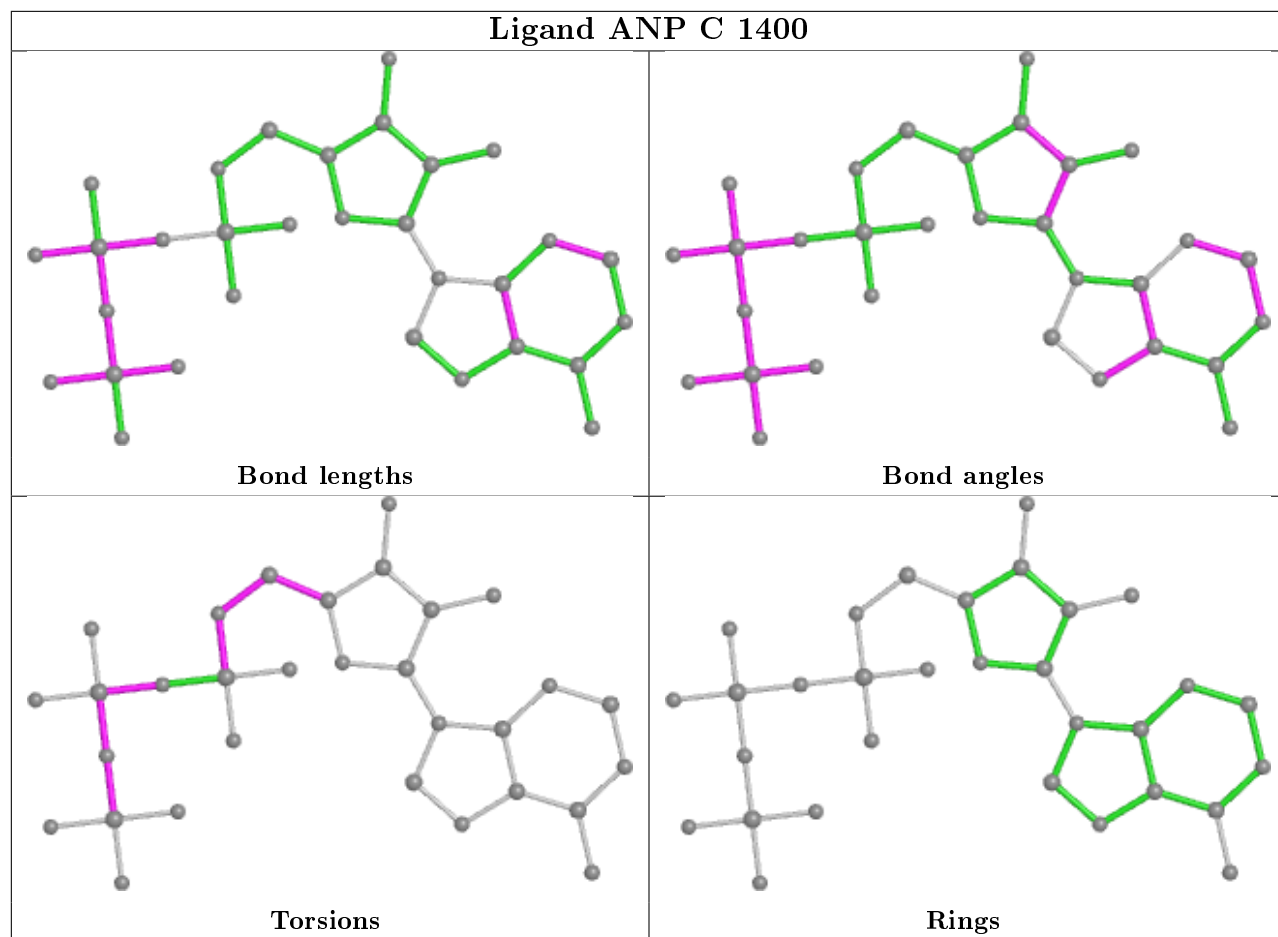


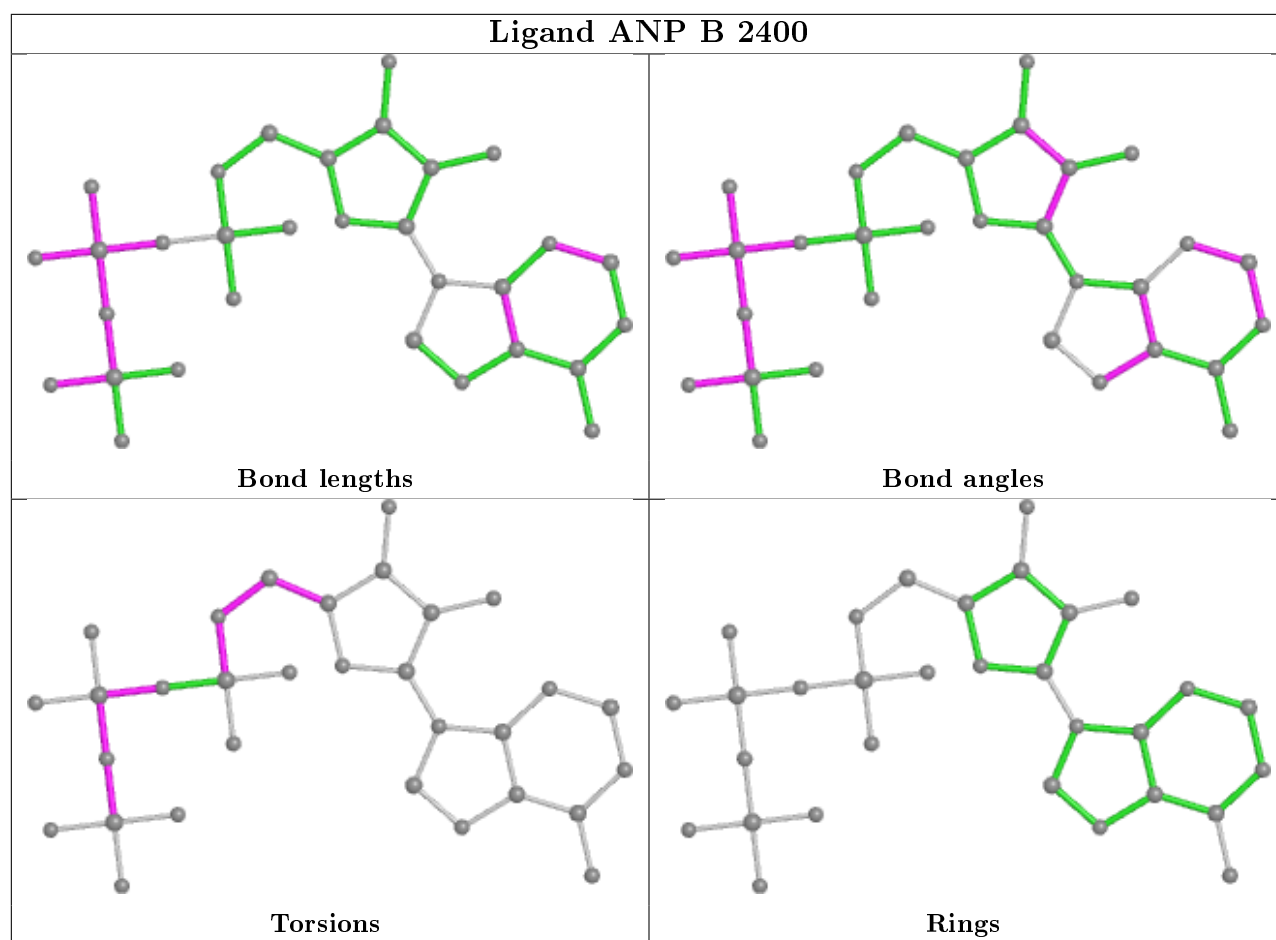


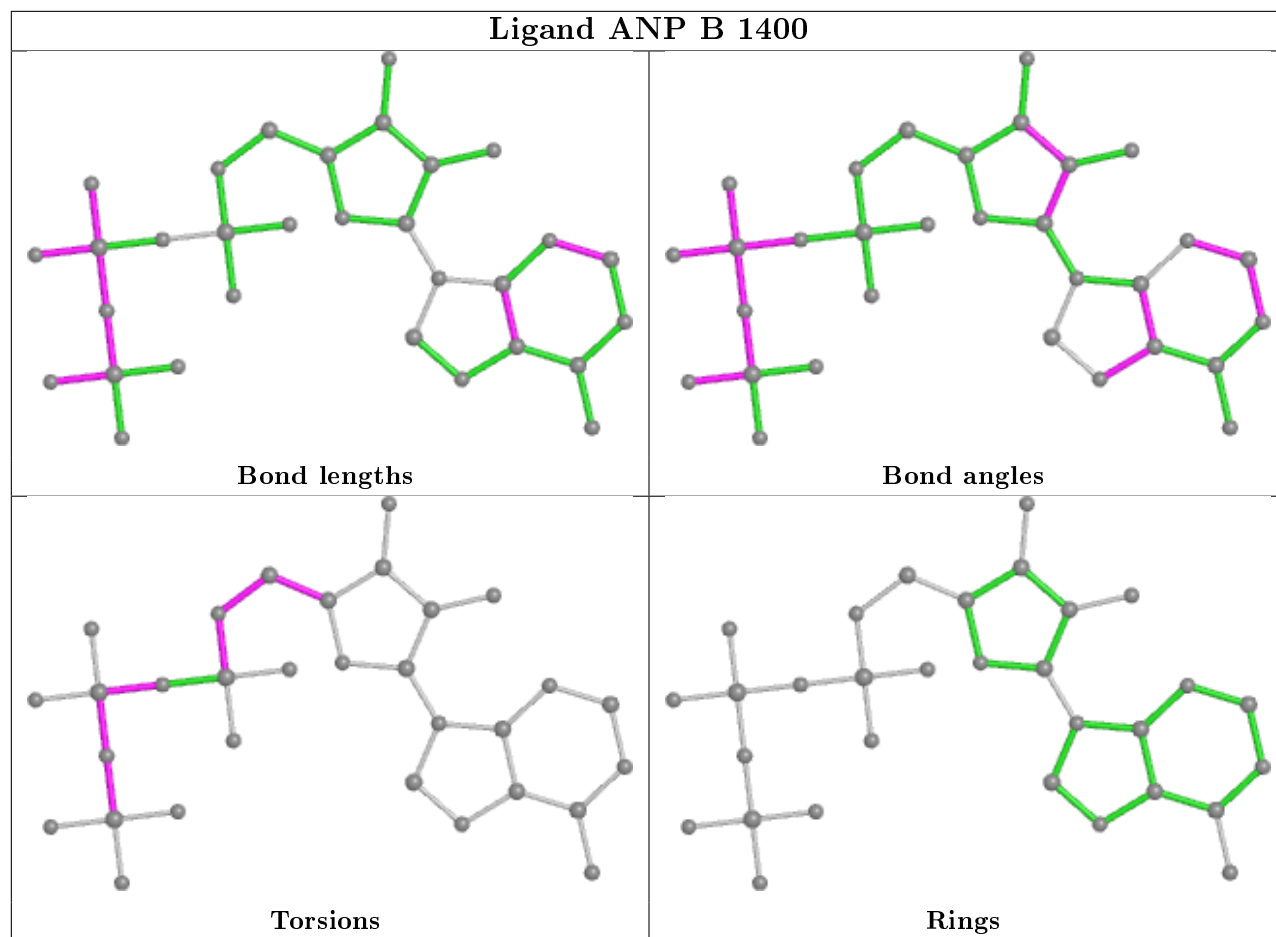


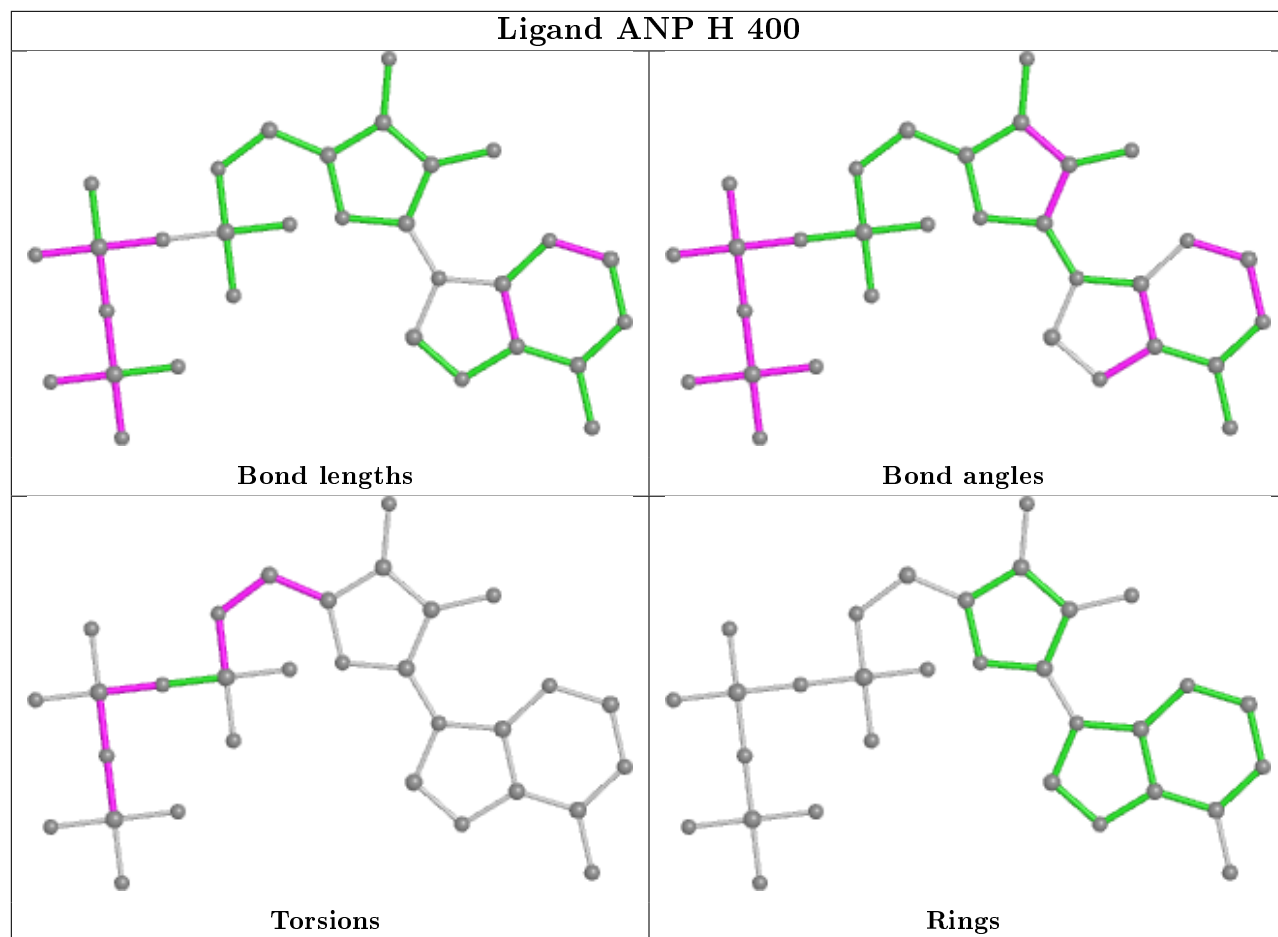


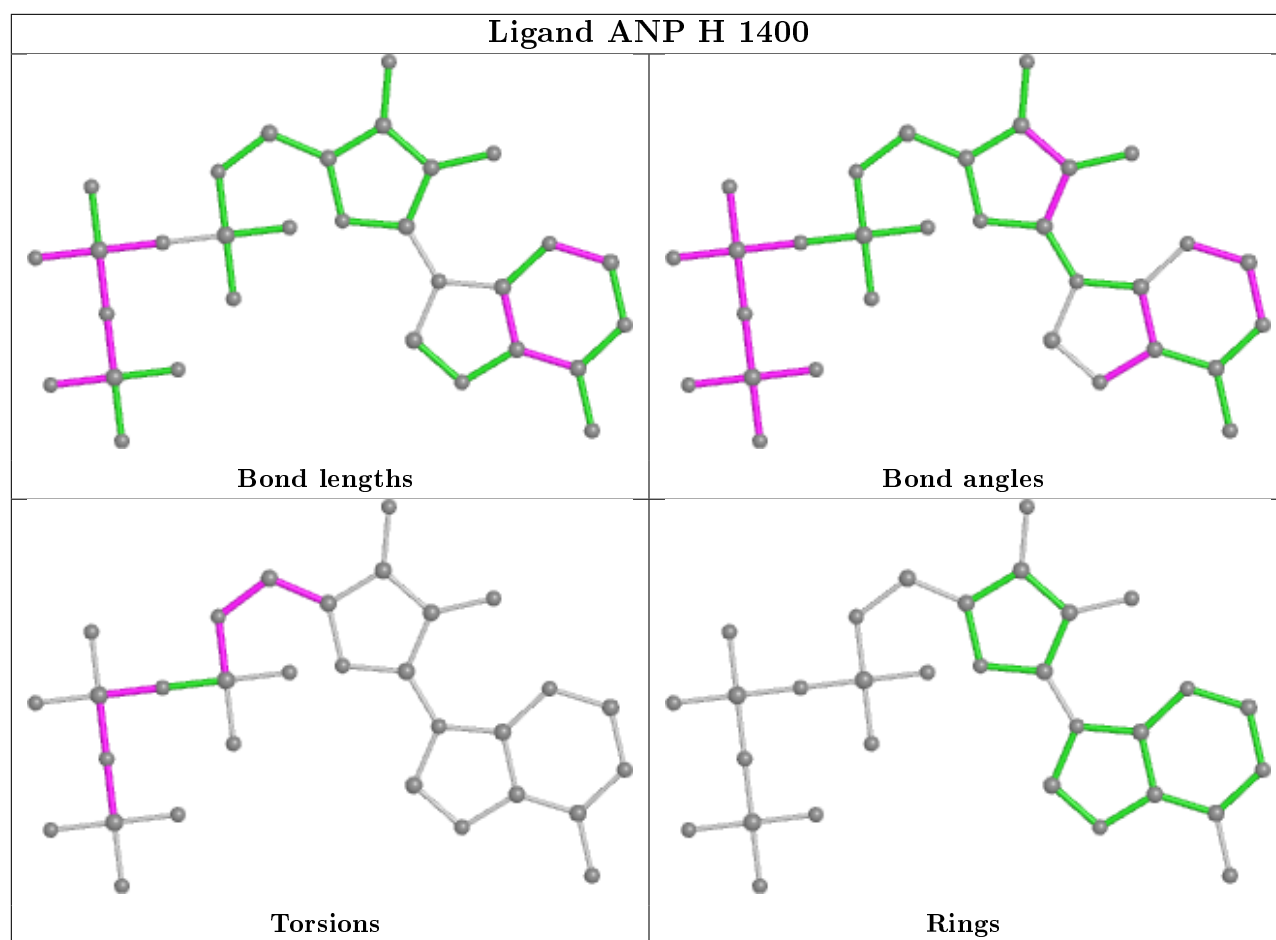


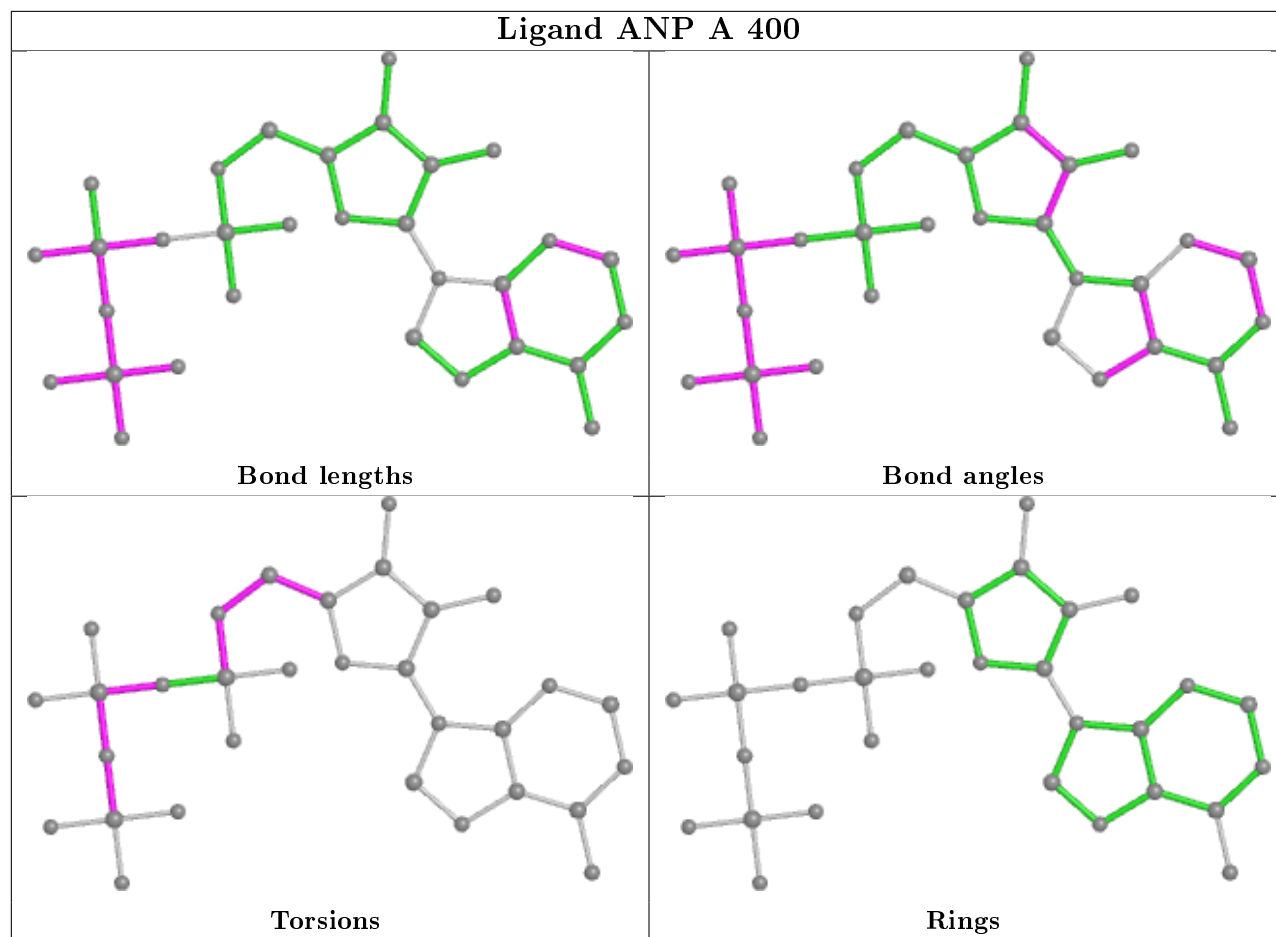


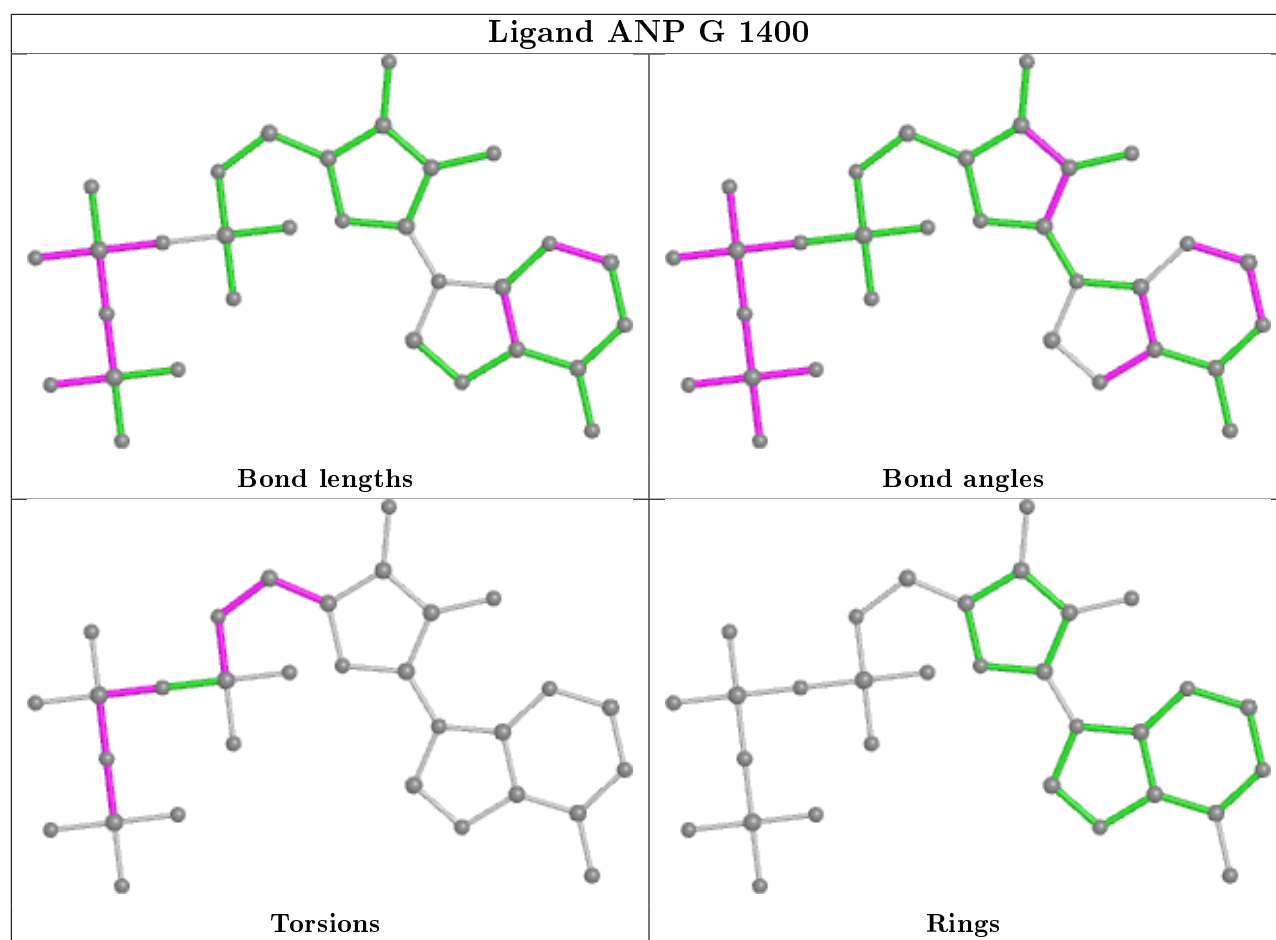


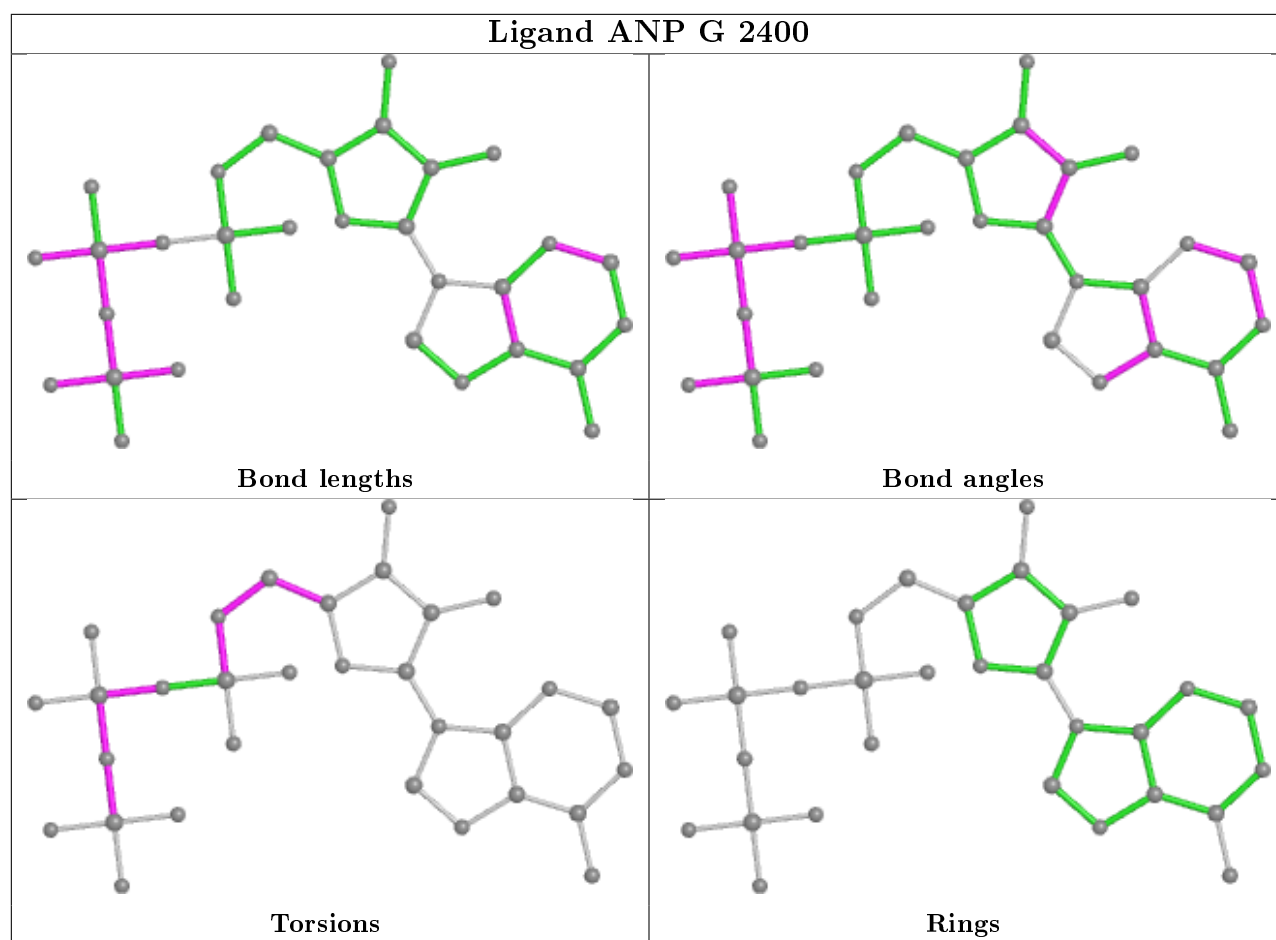


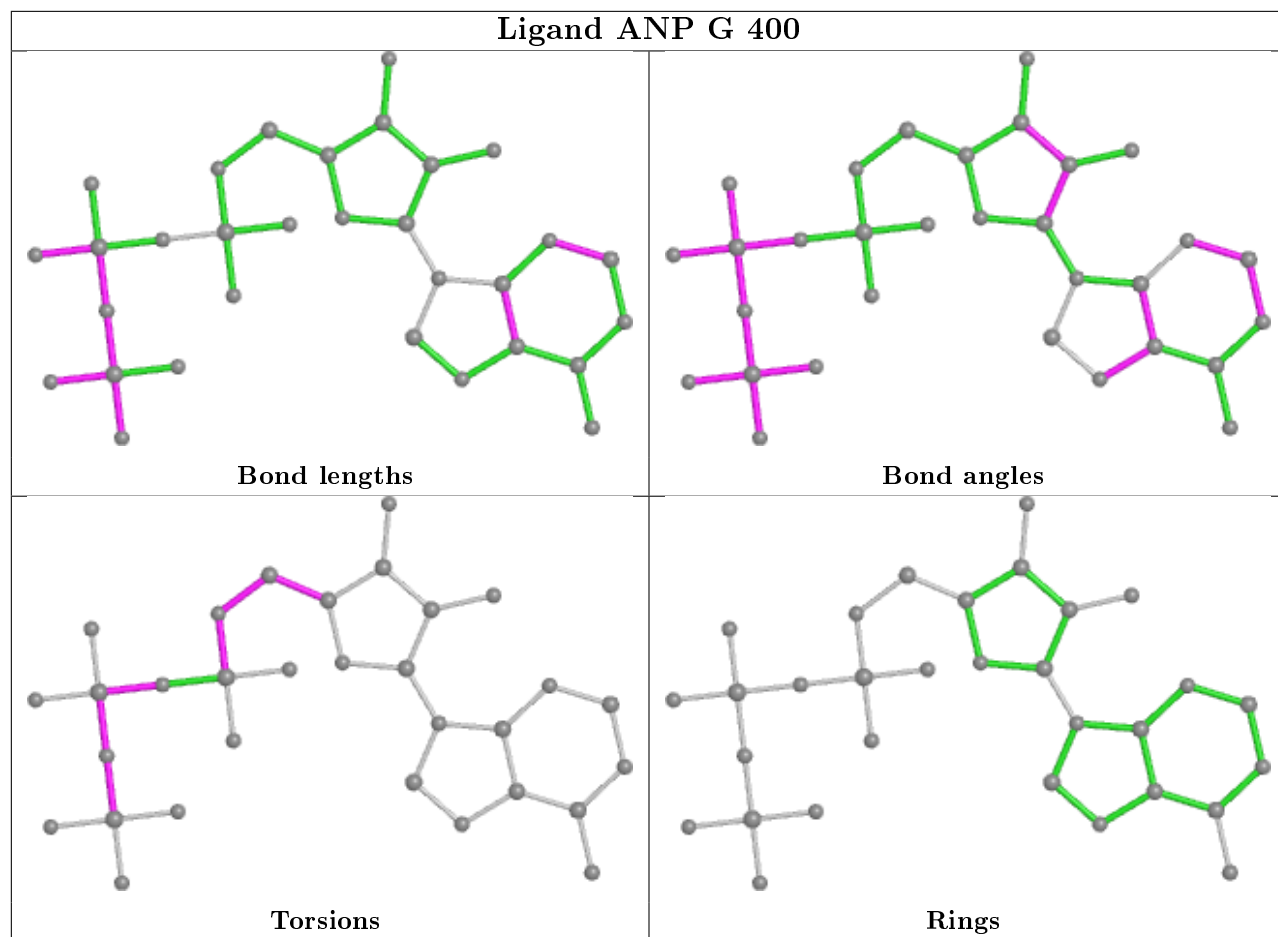


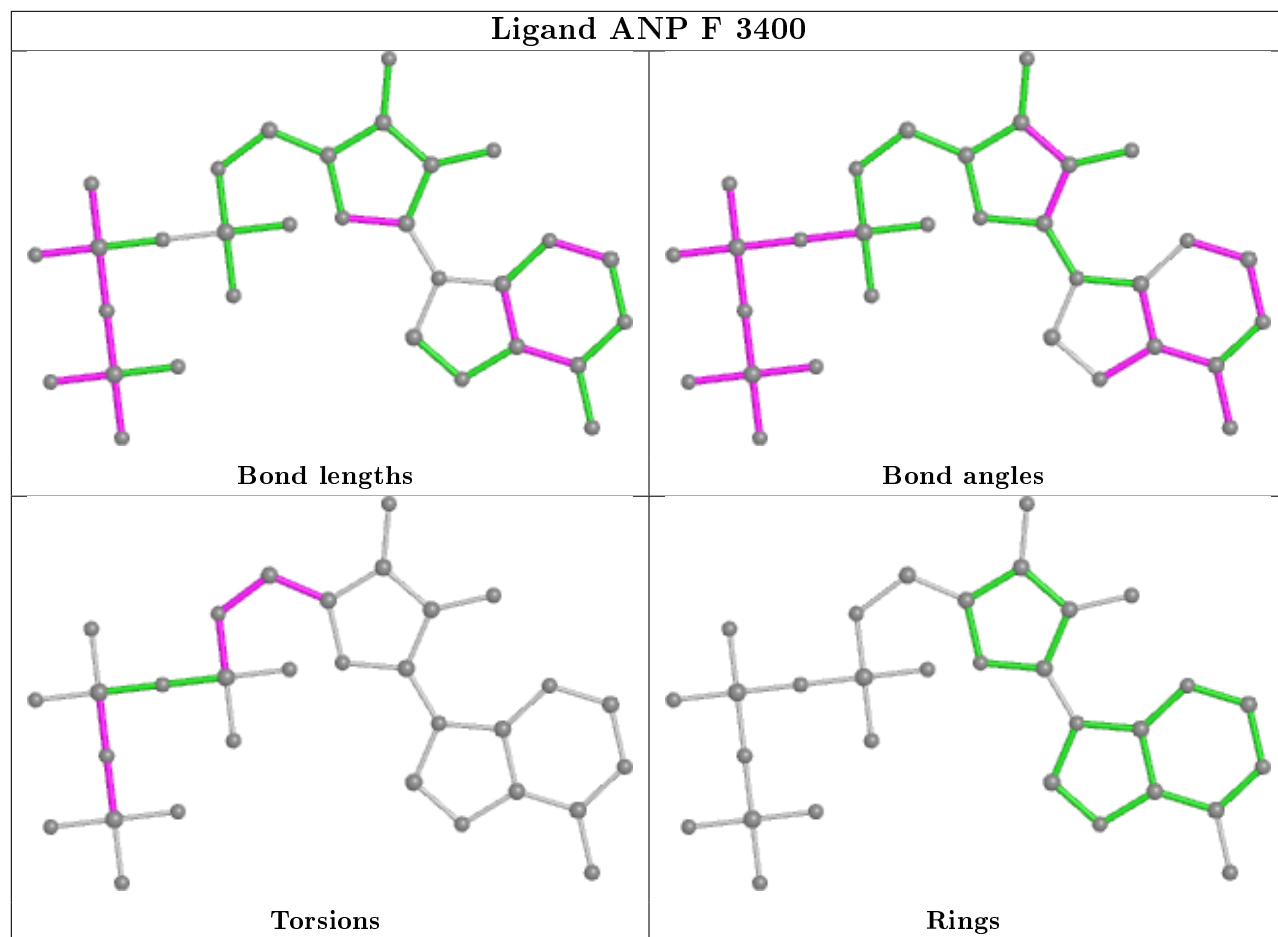


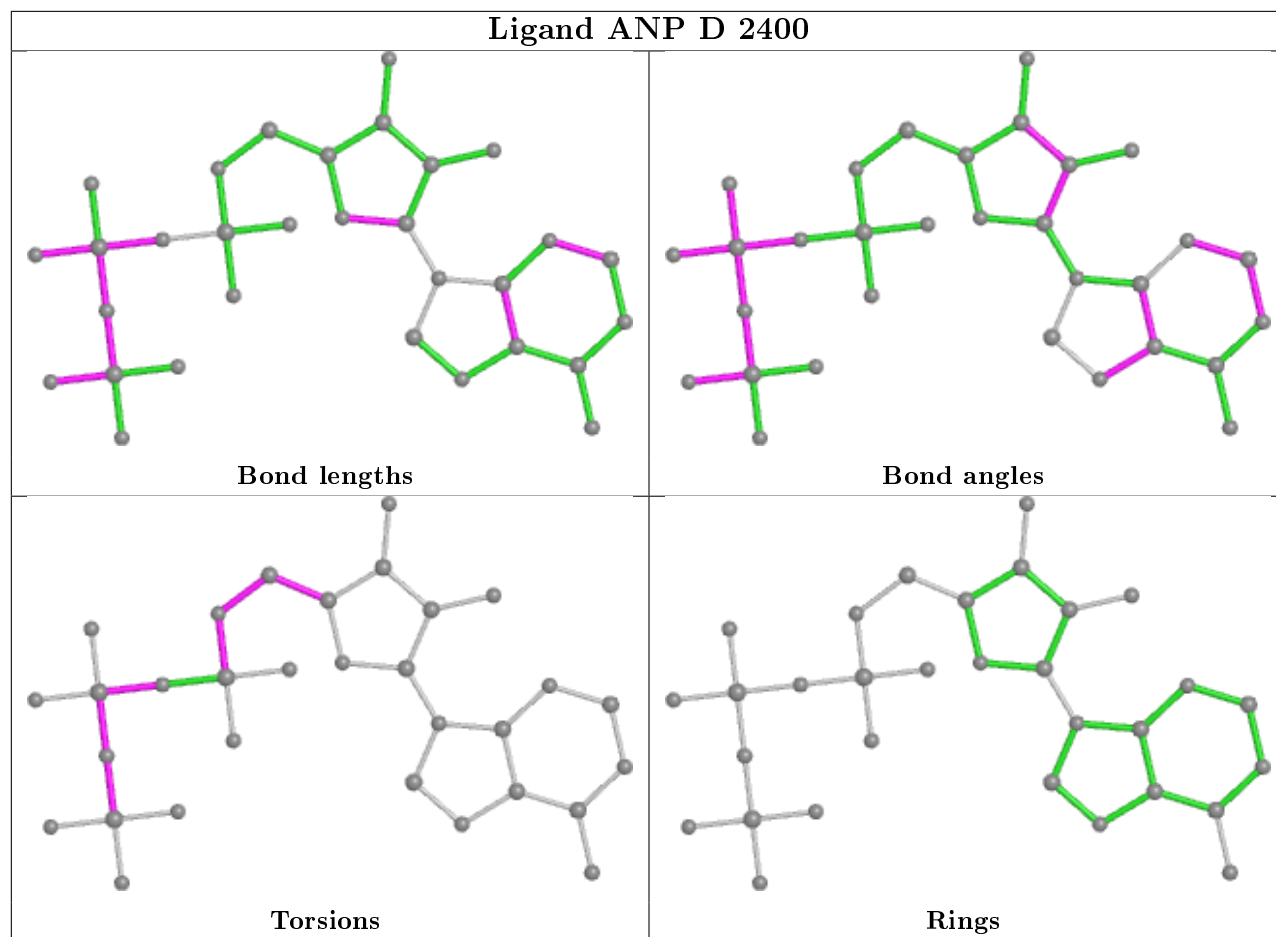


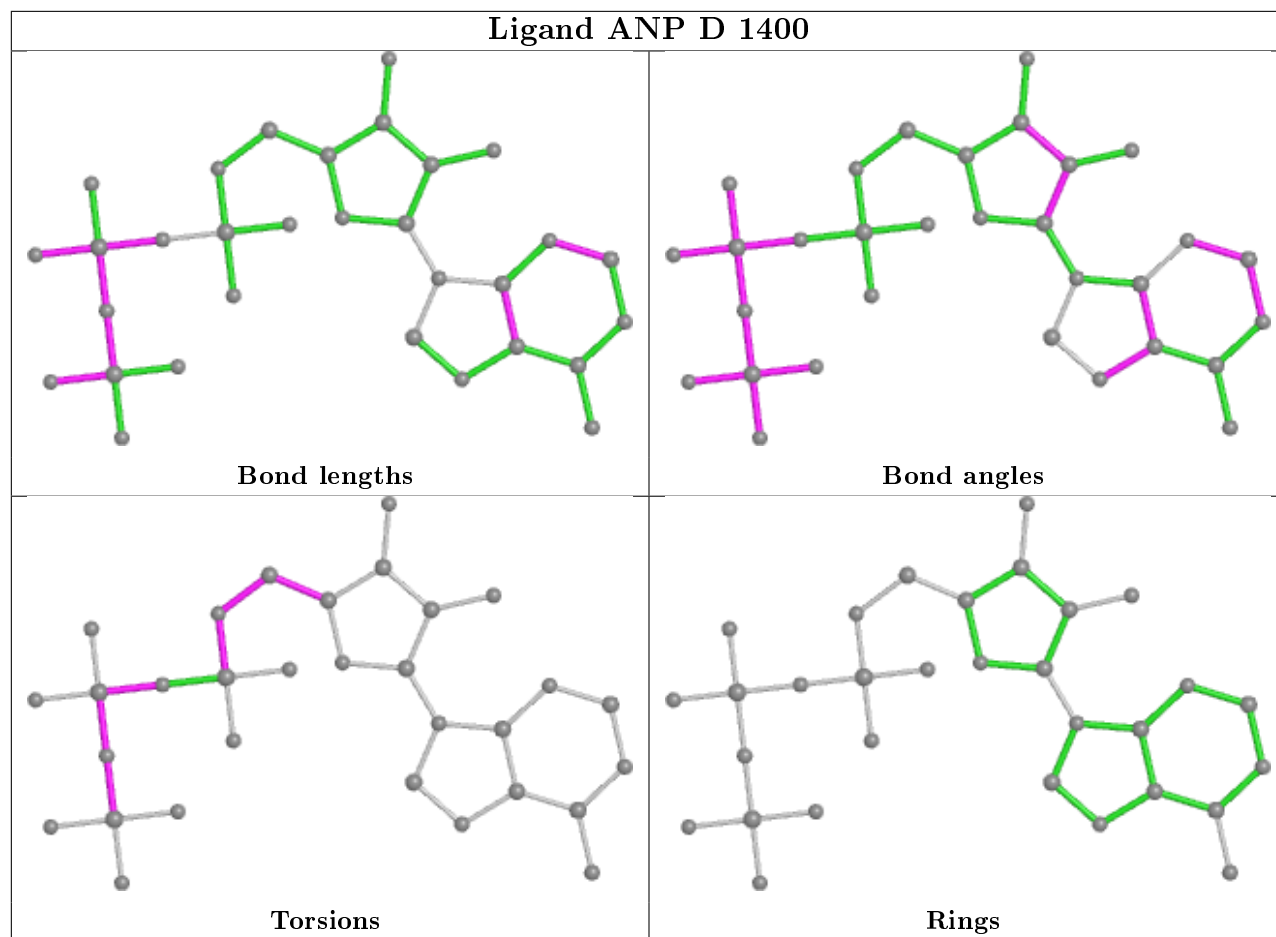


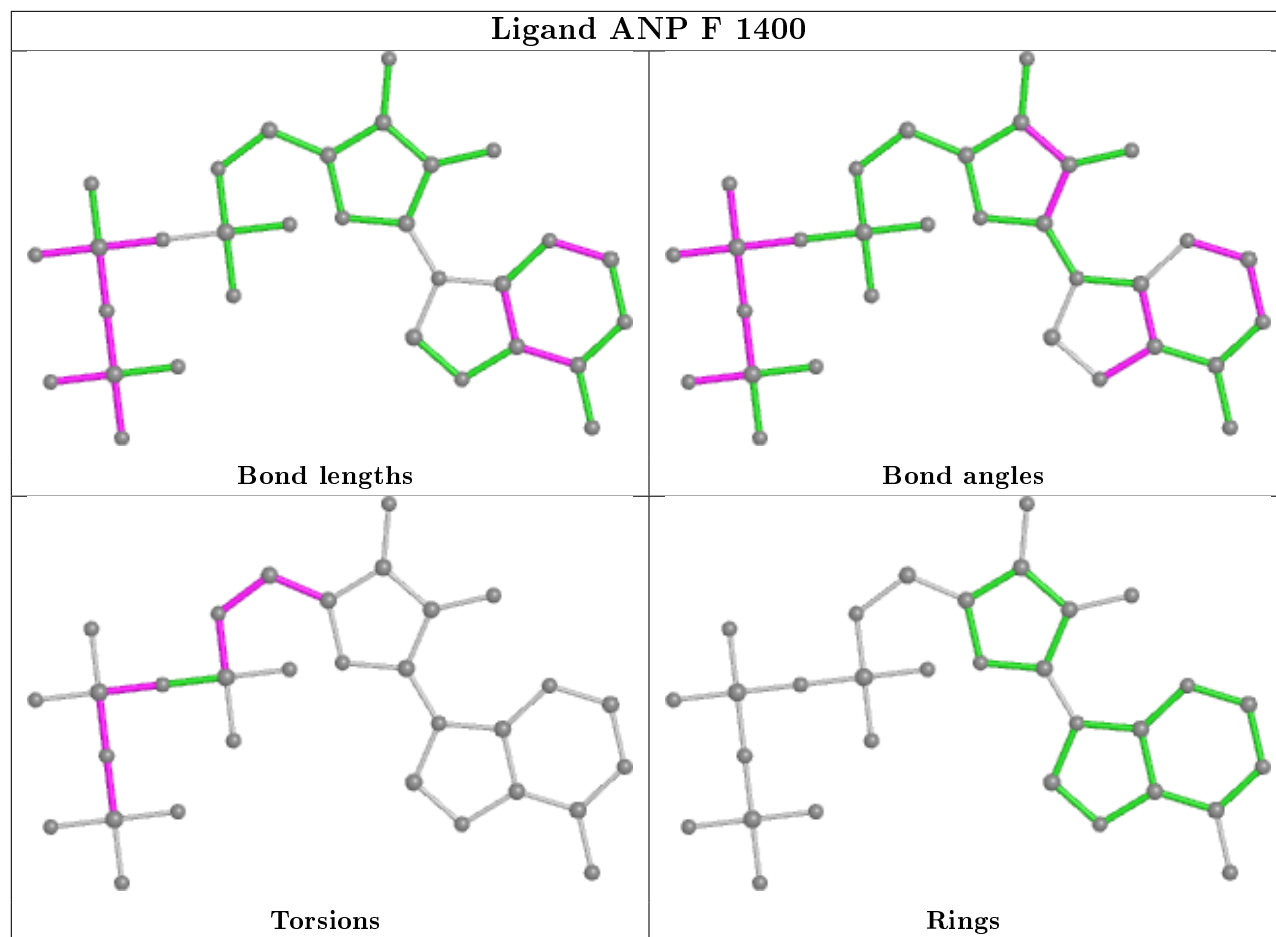


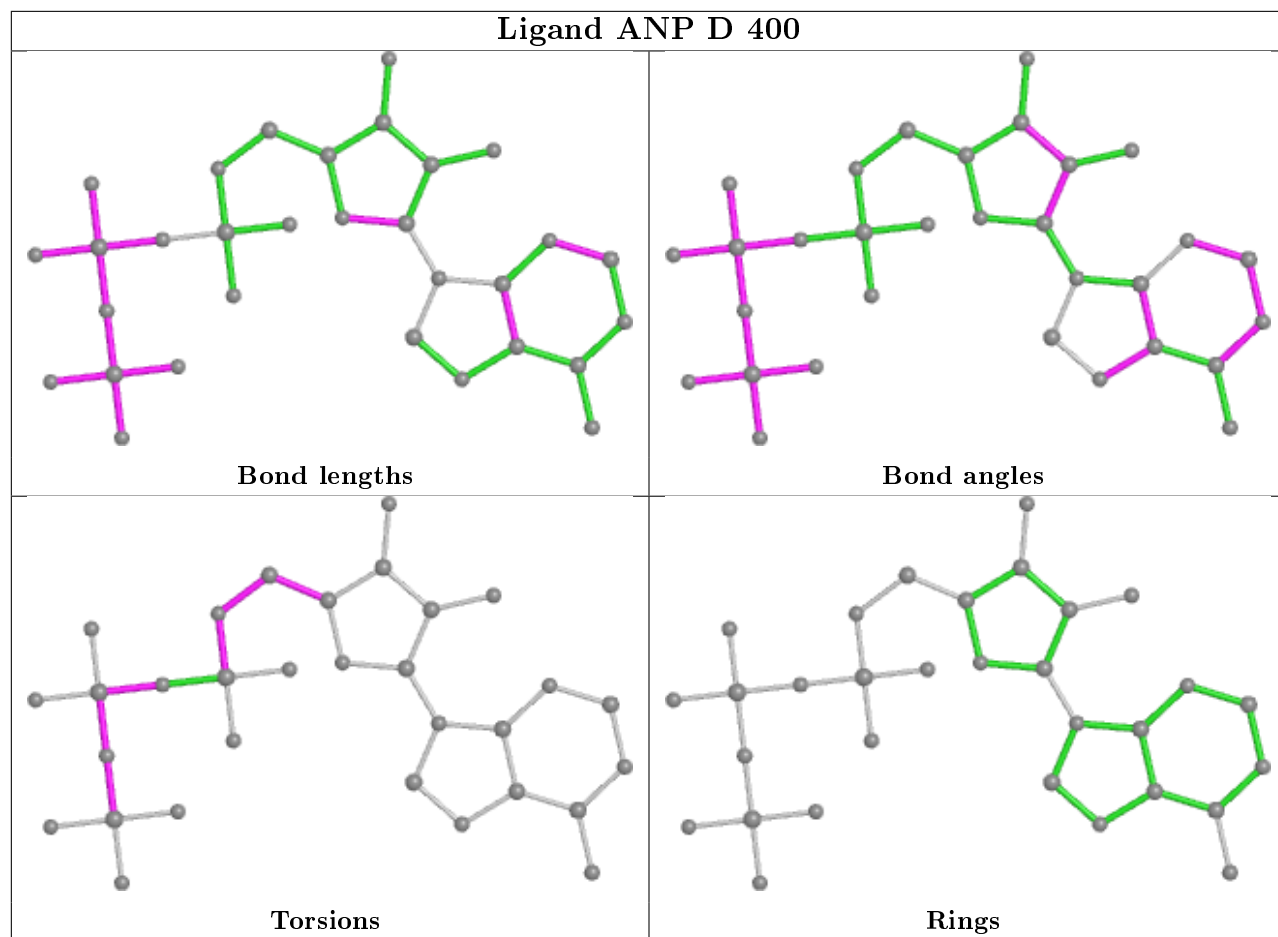


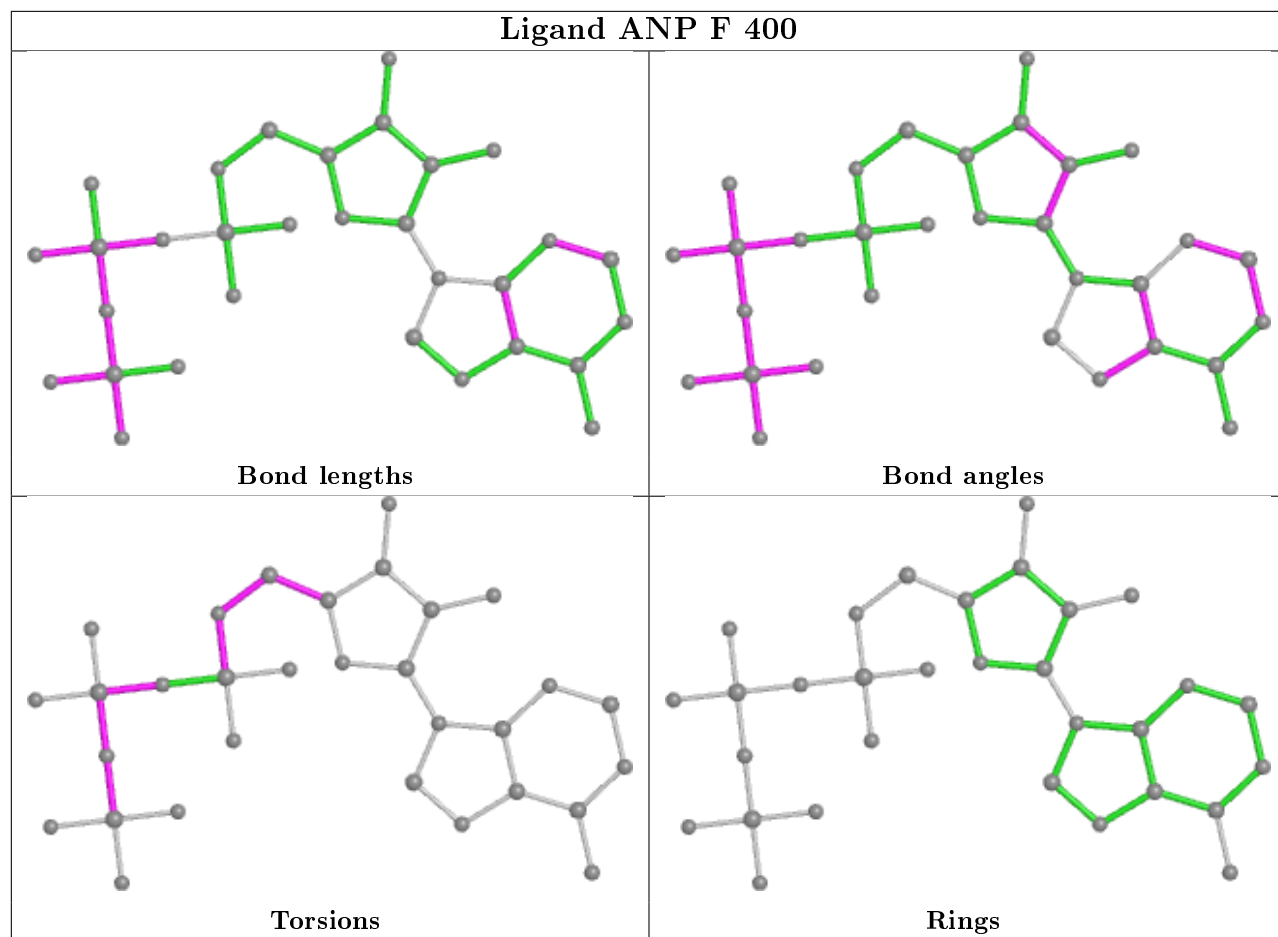


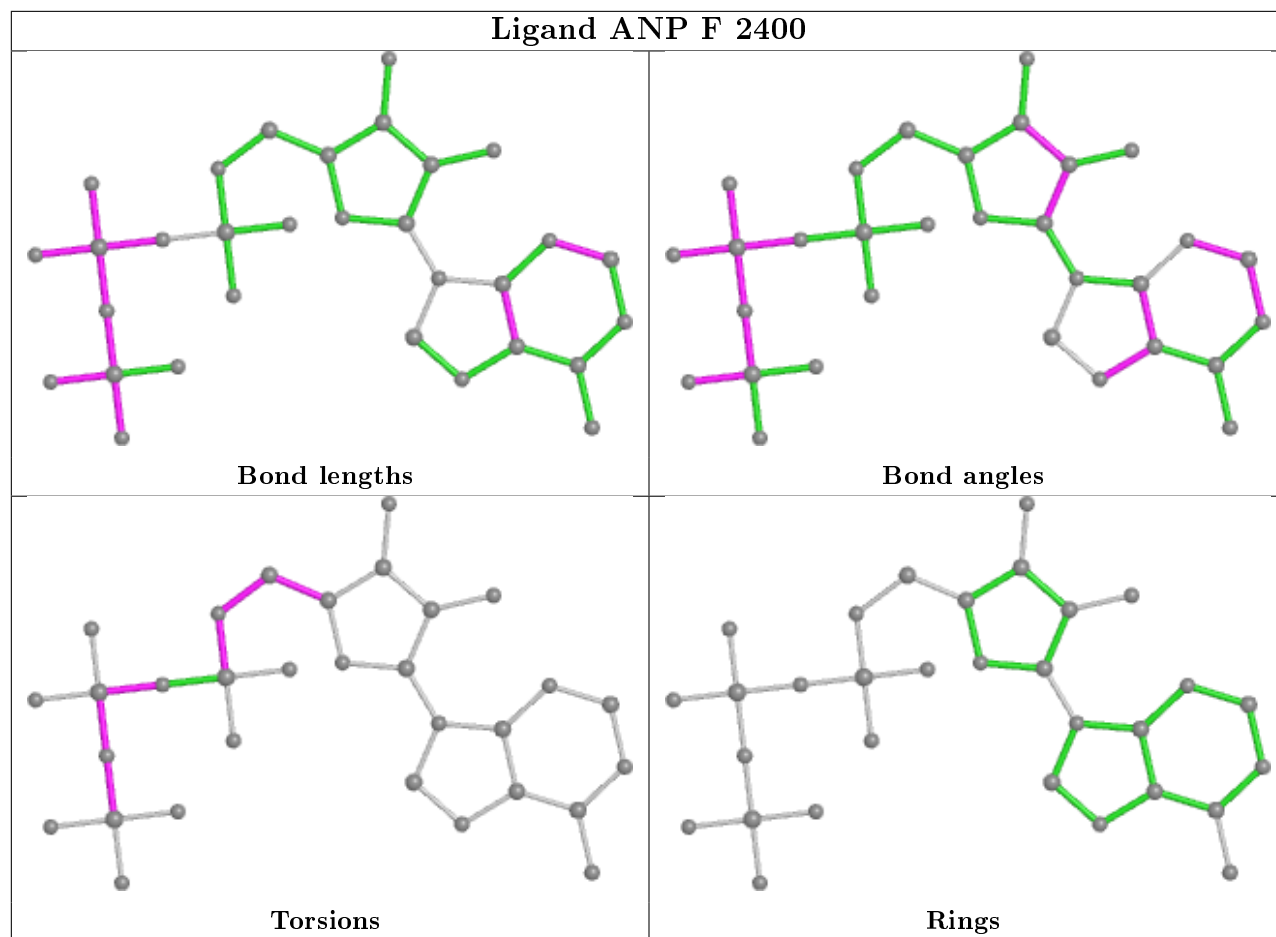


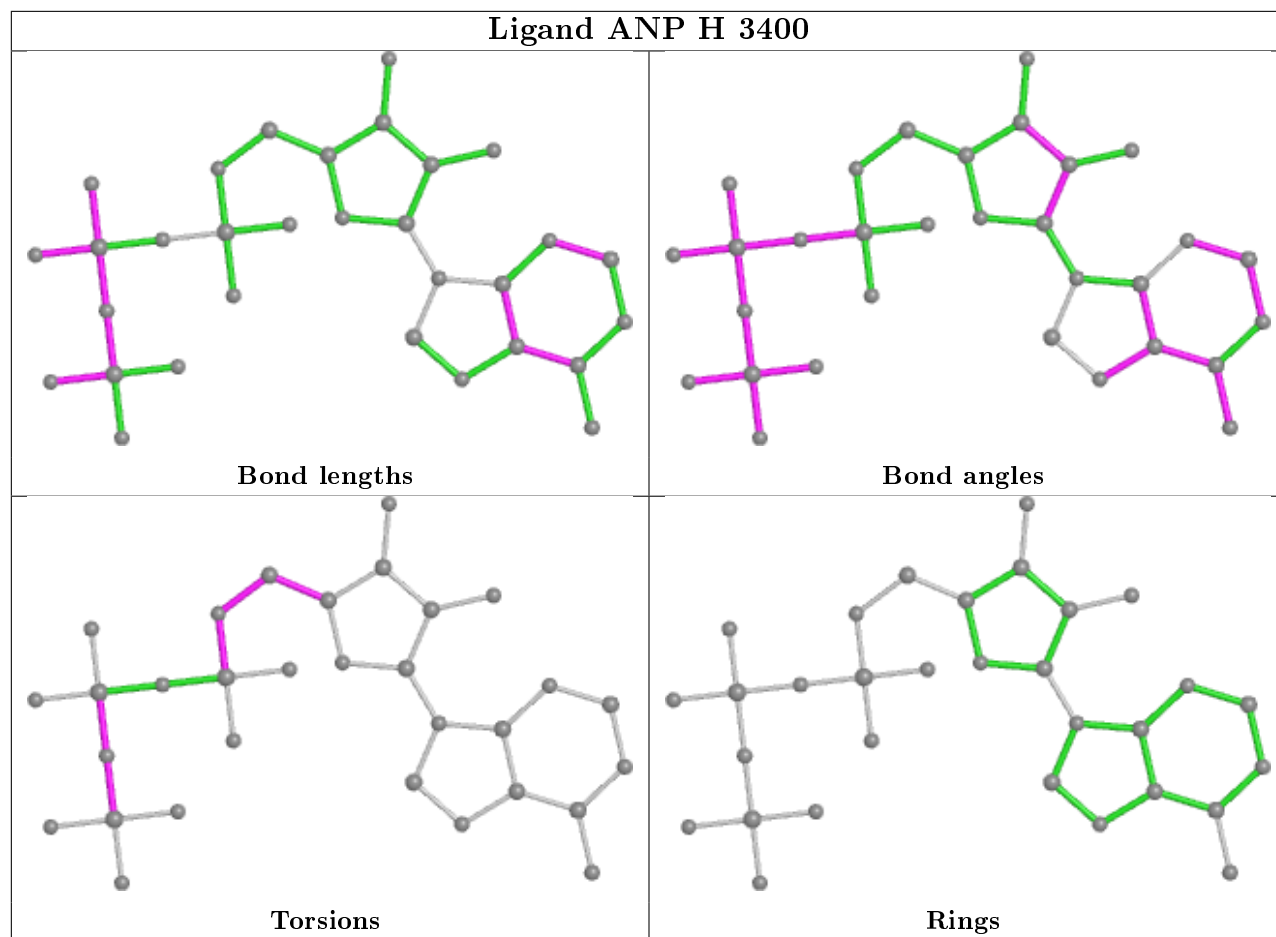


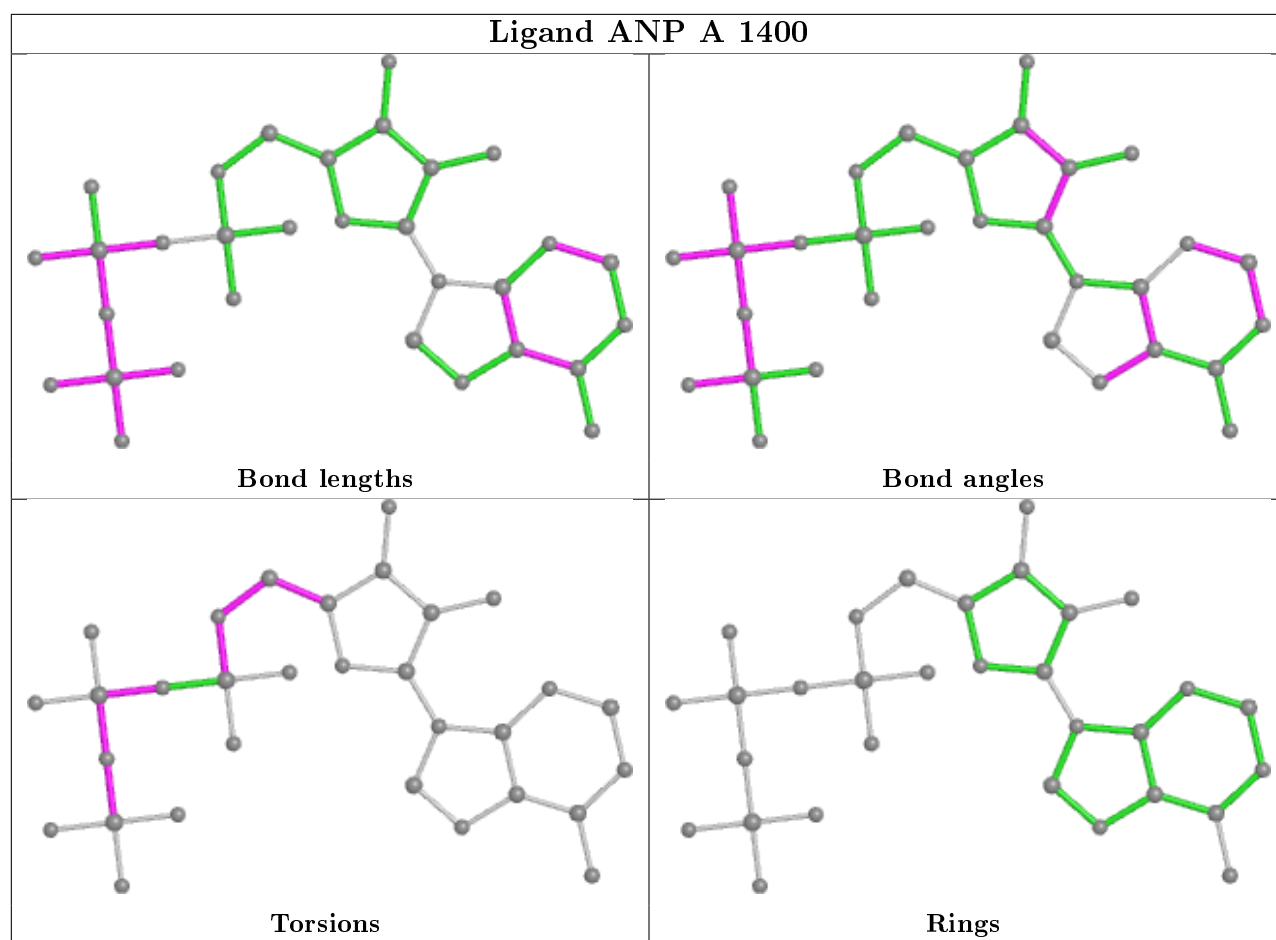


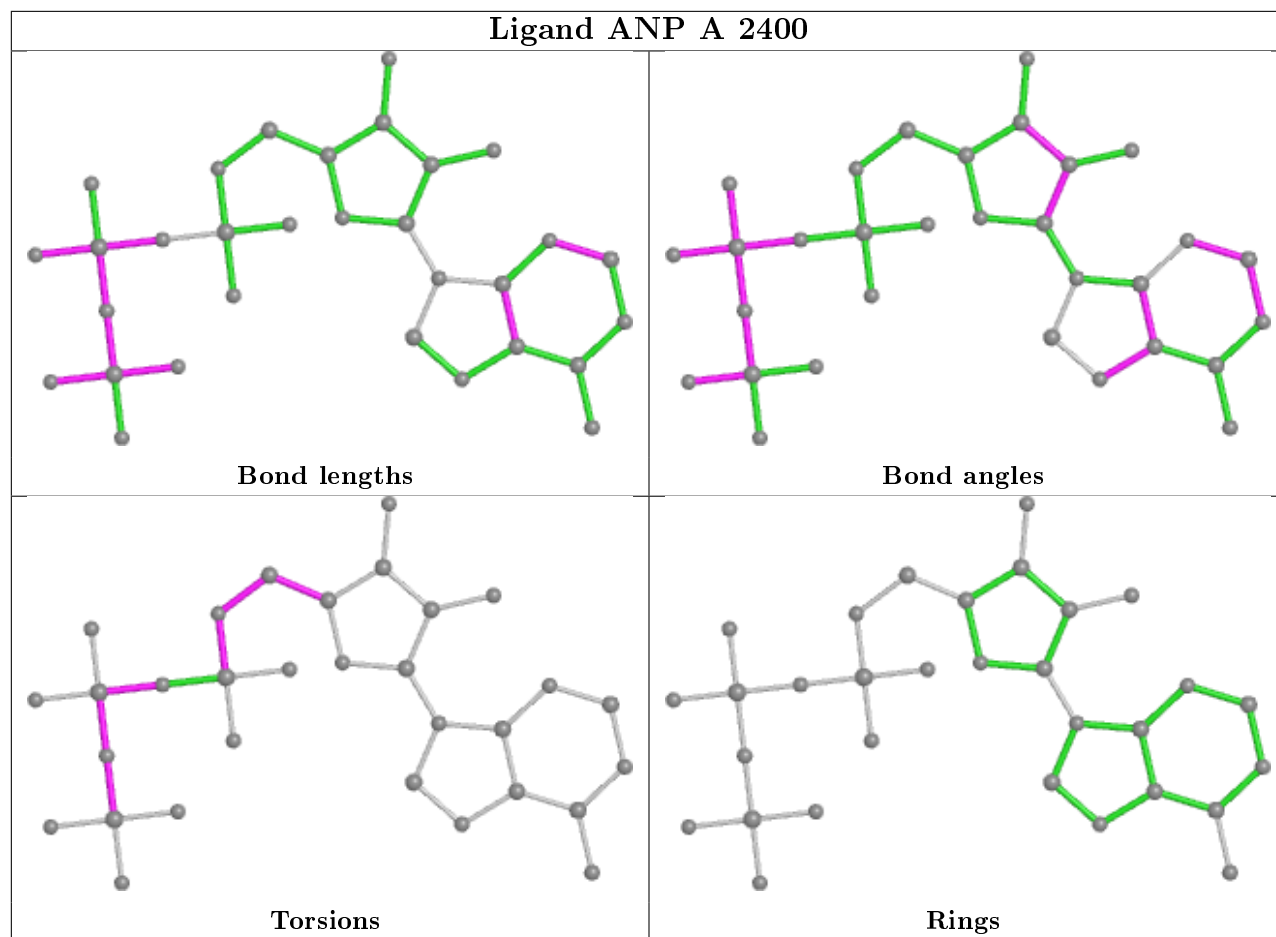


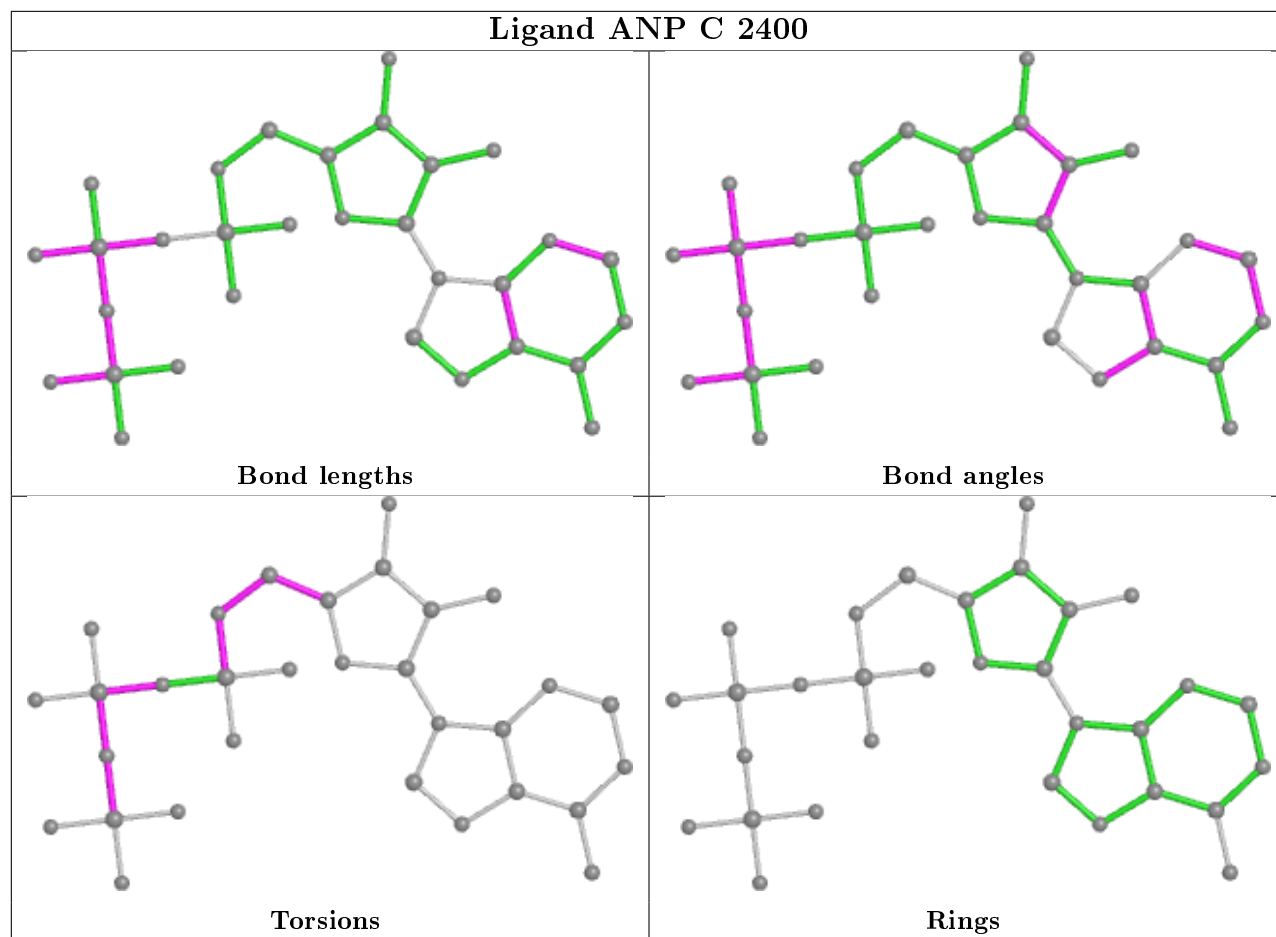


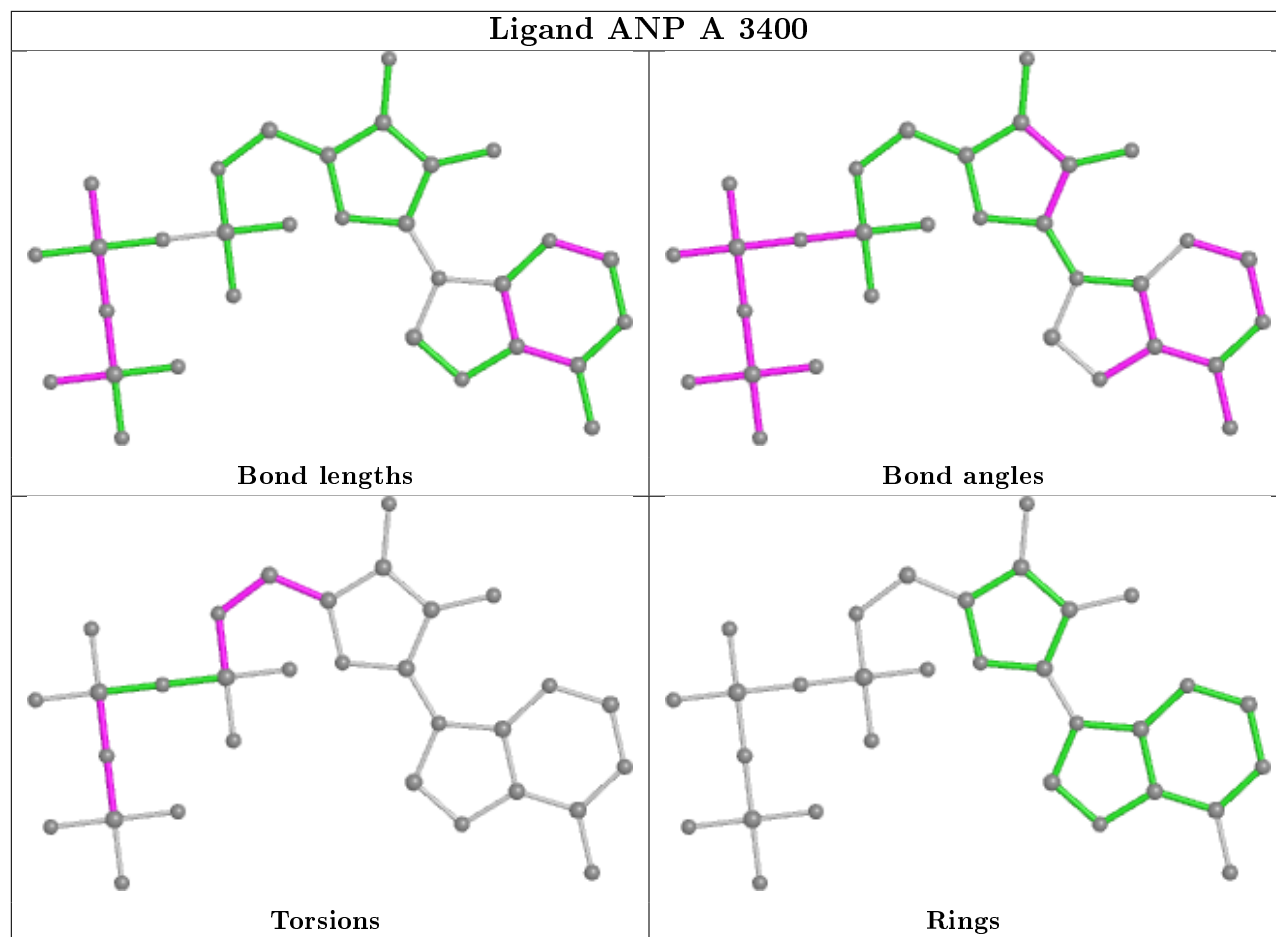


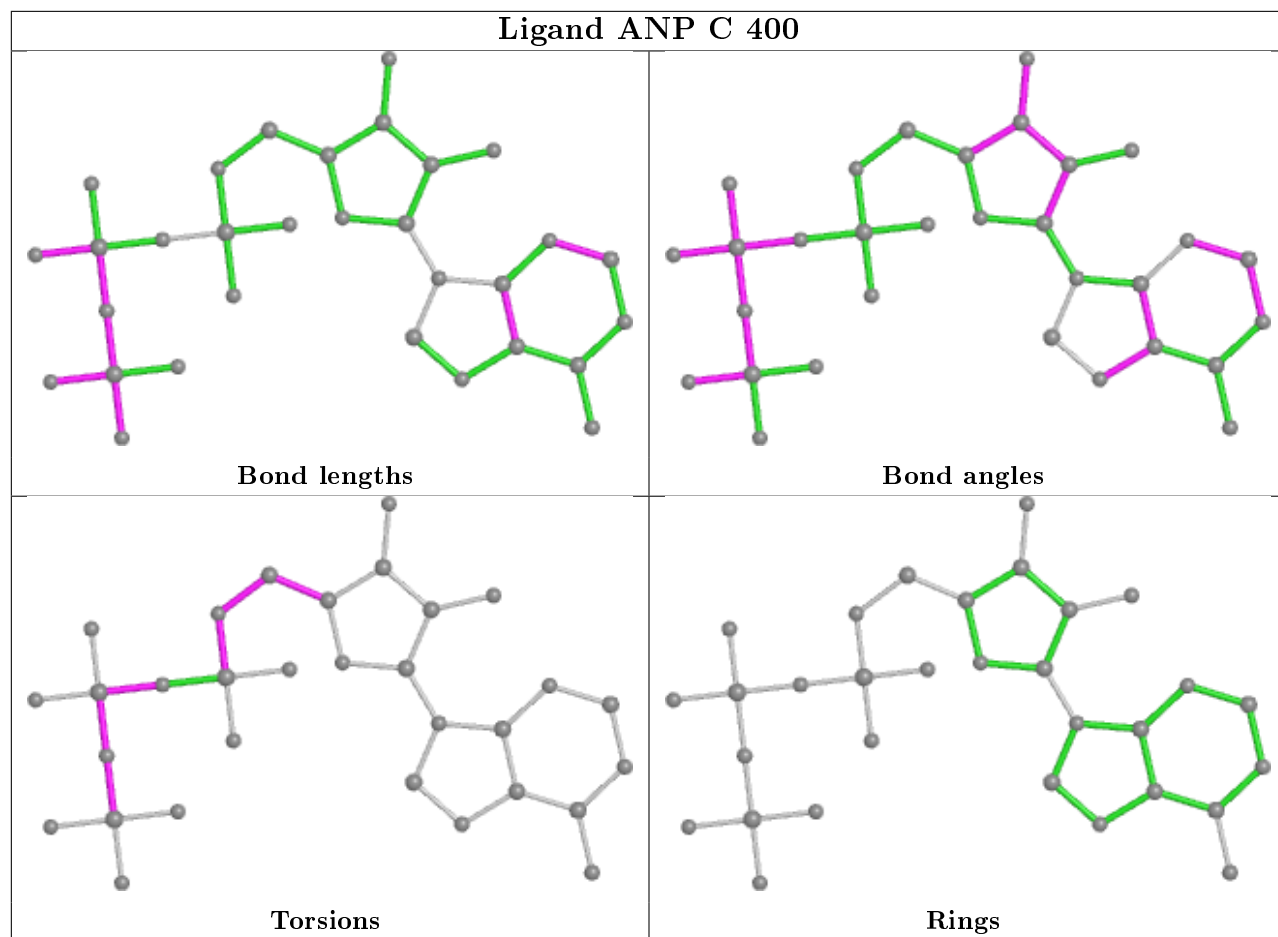


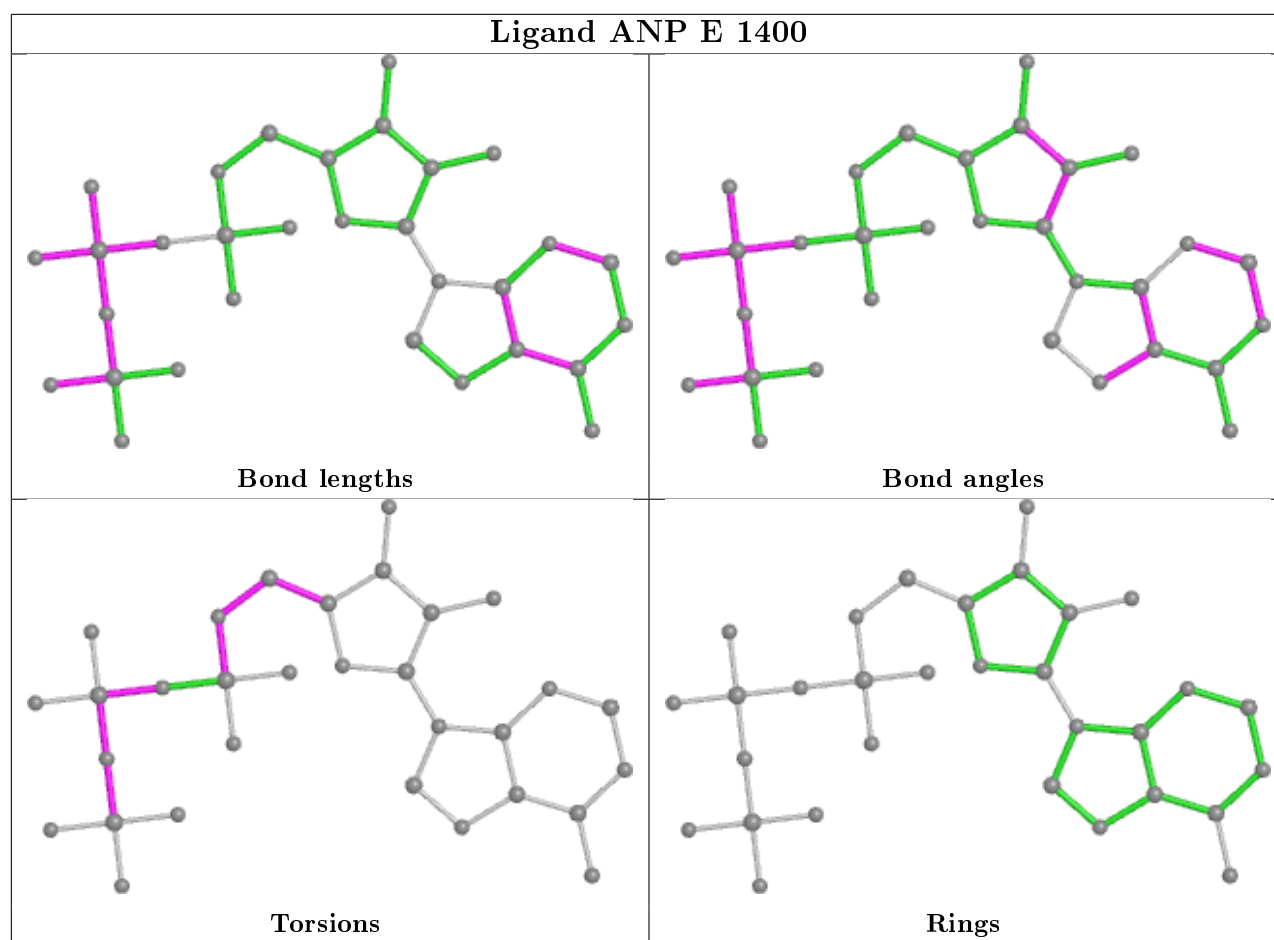












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1190/1357 (87%)	-0.16	14 (1%) 79 70	181, 217, 253, 285	0
1	B	1163/1357 (85%)	-0.31	10 (0%) 84 77	175, 217, 254, 286	0
1	C	1175/1357 (86%)	-0.23	12 (1%) 82 74	187, 216, 253, 284	0
1	D	1175/1357 (86%)	-0.15	28 (2%) 59 49	181, 218, 256, 286	0
1	E	1165/1357 (85%)	-0.18	16 (1%) 75 66	186, 218, 255, 288	0
1	F	1175/1357 (86%)	-0.19	10 (0%) 84 77	185, 217, 255, 285	0
1	G	1167/1357 (85%)	-0.22	10 (0%) 84 77	185, 216, 254, 291	0
1	H	1173/1357 (86%)	-0.21	23 (1%) 65 56	186, 218, 255, 288	0
All	All	9383/10856 (86%)	-0.21	123 (1%) 77 68	175, 217, 255, 291	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3151	PRO	6.3
1	A	3151	PRO	5.8
1	C	3151	PRO	4.9
1	E	3151	PRO	4.7
1	G	161	ASP	4.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	G	701	1/1	0.54	0.94	215,215,215,215	0
2	MG	E	701	1/1	0.57	1.16	204,204,204,204	0
2	MG	C	701	1/1	0.59	0.60	177,177,177,177	0
2	MG	D	2701	1/1	0.69	0.40	237,237,237,237	0
2	MG	B	2701	1/1	0.70	0.25	238,238,238,238	0
3	ANP	G	2400	31/31	0.72	0.41	303,308,315,315	0
3	ANP	F	2400	31/31	0.72	0.43	286,303,310,310	0
3	ANP	H	2400	31/31	0.72	0.38	298,312,316,316	0
2	MG	B	1701	1/1	0.74	0.41	214,214,214,214	0
2	MG	D	1701	1/1	0.75	1.14	212,212,212,212	0
3	ANP	D	1400	31/31	0.75	0.38	287,290,294,294	0
3	ANP	A	1400	31/31	0.76	0.36	267,280,283,283	0
2	MG	D	701	1/1	0.77	0.62	261,261,261,261	0
3	ANP	E	1400	31/31	0.79	0.31	287,293,296,296	0
3	ANP	B	2400	31/31	0.79	0.34	306,312,314,314	0
2	MG	F	2701	1/1	0.80	0.37	232,232,232,232	0
3	ANP	B	400	31/31	0.80	0.33	242,255,259,260	0
3	ANP	G	1400	31/31	0.81	0.25	279,285,289,290	0
2	MG	H	2701	1/1	0.82	0.35	271,271,271,271	0
2	MG	C	3701	1/1	0.83	0.14	140,140,140,140	0
3	ANP	F	1400	31/31	0.83	0.34	271,280,286,286	0
2	MG	E	1701	1/1	0.83	0.48	190,190,190,190	0
3	ANP	H	1400	31/31	0.83	0.31	296,299,304,304	0
3	ANP	C	1400	31/31	0.84	0.25	288,291,293,294	0
2	MG	H	1701	1/1	0.84	0.67	188,188,188,188	0
3	ANP	H	400	31/31	0.84	0.42	254,263,265,265	0
3	ANP	C	400	31/31	0.84	0.29	226,245,250,250	0
3	ANP	G	400	31/31	0.84	0.28	253,262,264,265	0
2	MG	B	701	1/1	0.84	1.12	184,184,184,184	0
3	ANP	D	400	31/31	0.84	0.29	263,273,274,274	0
3	ANP	D	2400	31/31	0.86	0.30	305,310,315,315	0
3	ANP	B	1400	31/31	0.86	0.30	275,286,290,290	0
2	MG	A	1701	1/1	0.86	0.84	181,181,181,181	0
3	ANP	F	400	31/31	0.86	0.33	243,257,263,263	0
2	MG	A	701	1/1	0.86	0.65	143,143,143,143	0
3	ANP	A	2400	31/31	0.86	0.34	308,311,315,315	0

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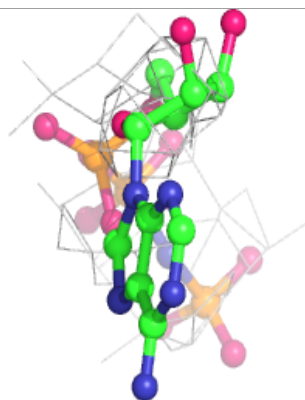
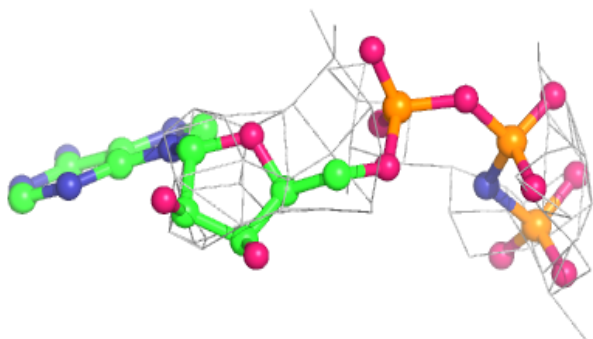
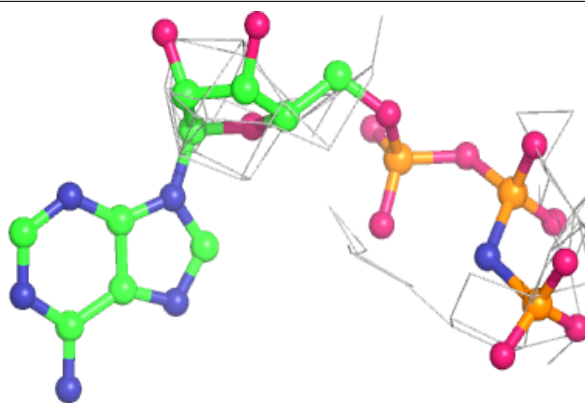
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	E	3701	1/1	0.87	0.20	131,131,131,131	0
2	MG	F	1701	1/1	0.87	0.57	175,175,175,175	0
2	MG	A	2701	1/1	0.88	0.16	247,247,247,247	0
3	ANP	A	400	31/31	0.88	0.27	246,250,255,256	0
2	MG	E	2701	1/1	0.88	0.34	228,228,228,228	0
3	ANP	C	2400	31/31	0.89	0.28	296,309,314,315	0
3	ANP	E	400	31/31	0.89	0.26	256,261,264,265	0
2	MG	G	1701	1/1	0.89	0.56	191,191,191,191	0
3	ANP	H	3400	31/31	0.90	0.18	180,187,196,197	0
3	ANP	E	2400	31/31	0.90	0.25	307,317,320,320	0
3	ANP	G	3400	31/31	0.91	0.19	153,176,191,192	0
3	ANP	D	3400	31/31	0.92	0.16	149,170,188,189	0
3	ANP	F	3400	31/31	0.92	0.20	148,171,183,183	0
2	MG	G	2701	1/1	0.92	0.45	192,192,192,192	0
2	MG	H	701	1/1	0.92	0.18	200,200,200,200	0
3	ANP	C	3400	31/31	0.93	0.14	176,190,200,200	0
2	MG	C	2701	1/1	0.93	0.26	211,211,211,211	0
3	ANP	B	3400	31/31	0.93	0.17	143,159,176,178	0
2	MG	F	701	1/1	0.94	0.56	189,189,189,189	0
3	ANP	E	3400	31/31	0.94	0.19	163,180,187,187	0
3	ANP	A	3400	31/31	0.94	0.17	152,165,180,181	0
2	MG	H	3701	1/1	0.95	0.15	121,121,121,121	0
2	MG	D	3701	1/1	0.95	0.14	108,108,108,108	0
2	MG	B	3701	1/1	0.96	0.17	69,69,69,69	0
2	MG	C	1701	1/1	0.96	0.18	132,132,132,132	0
2	MG	A	3701	1/1	0.97	0.09	116,116,116,116	0
2	MG	G	3701	1/1	0.97	0.10	100,100,100,100	0
2	MG	F	3701	1/1	0.98	0.09	77,77,77,77	0

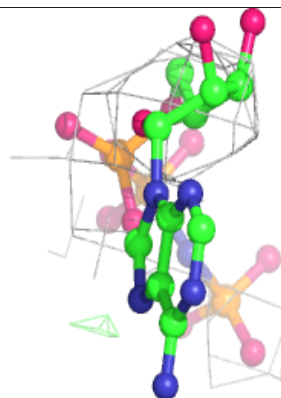
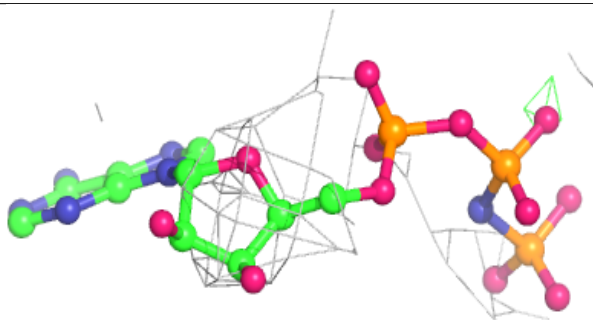
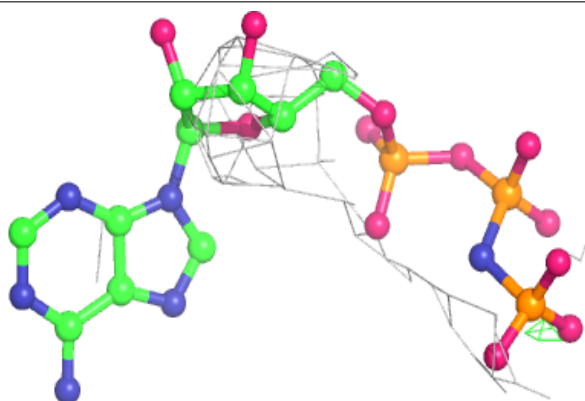
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ANP G 2400:

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

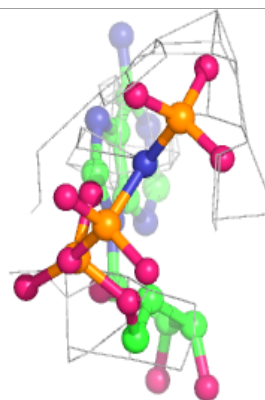
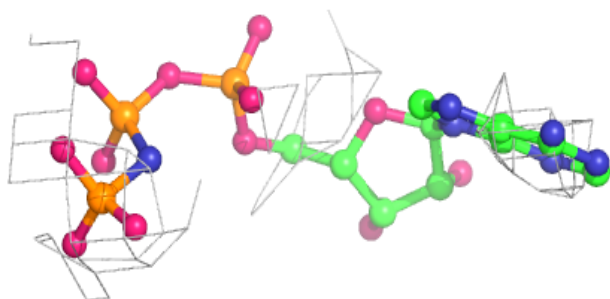
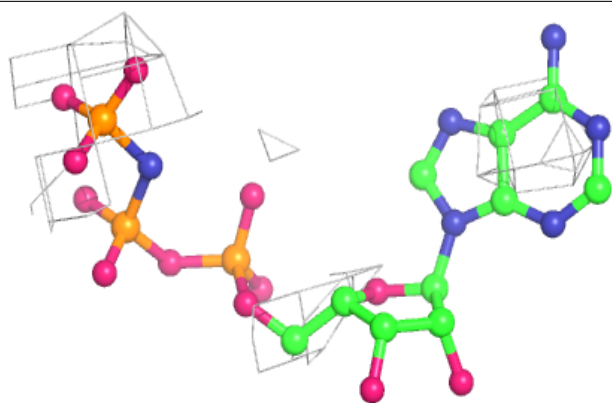
**Electron density around ANP F 2400:**

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

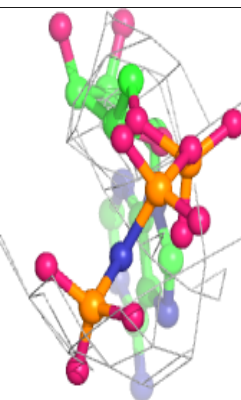
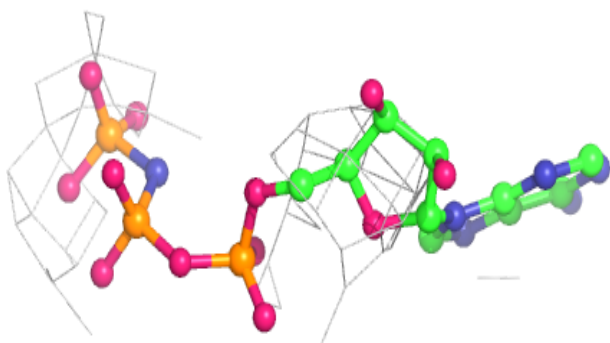
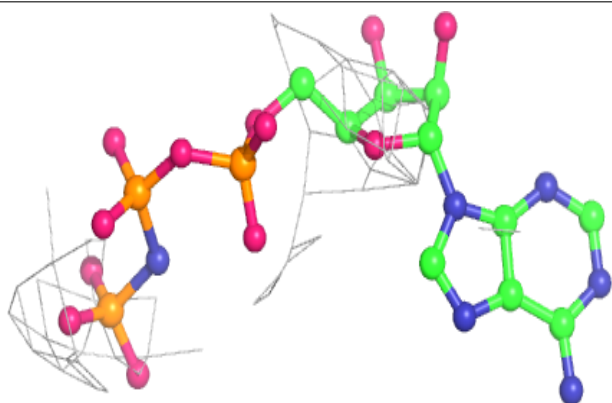


Electron density around ANP H 2400:

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

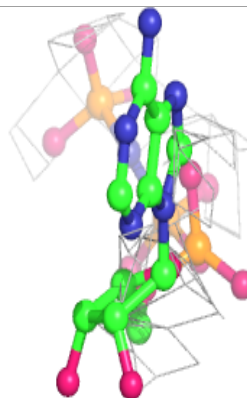
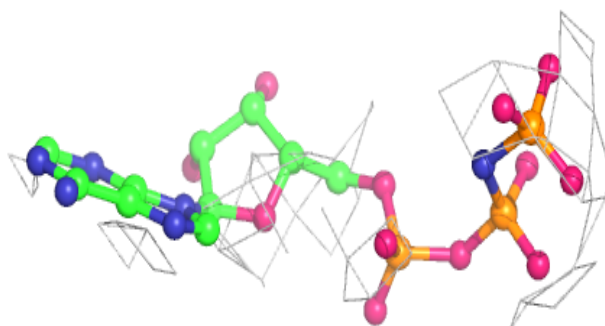
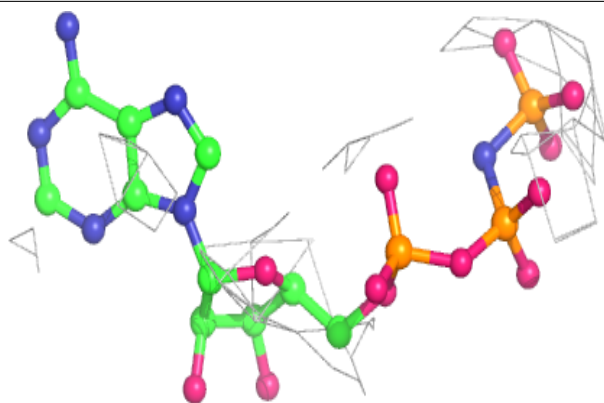
**Electron density around ANP D 1400:**

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

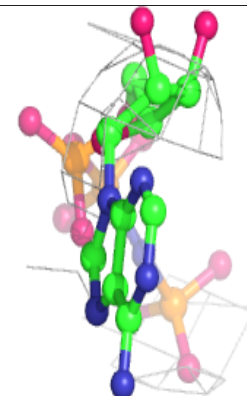
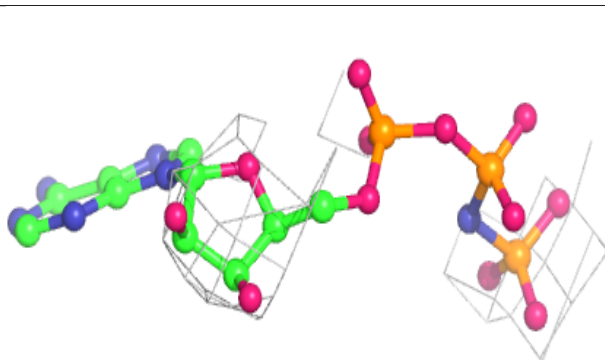
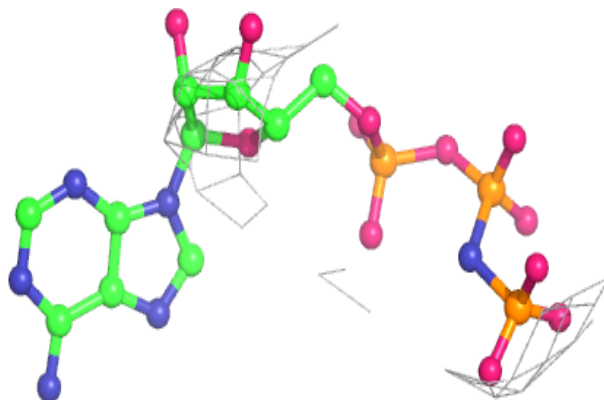


Electron density around ANP A 1400:

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

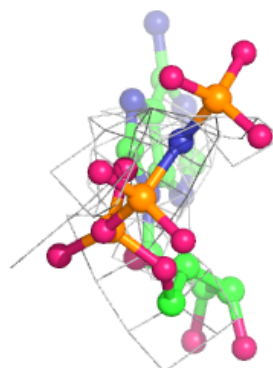
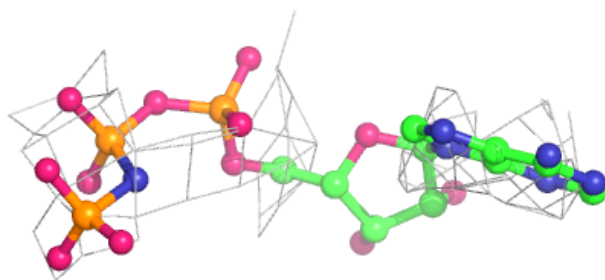
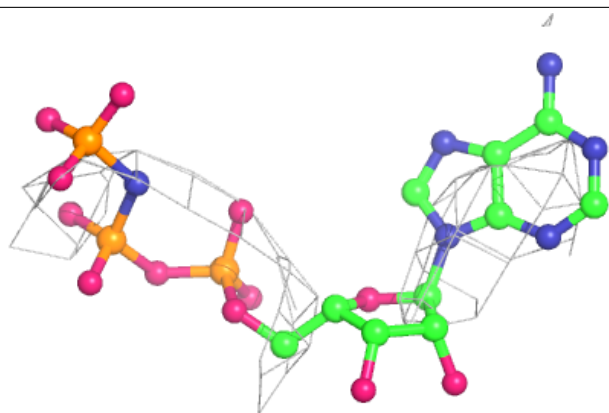
**Electron density around ANP E 1400:**

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

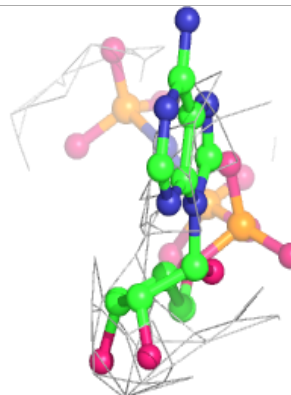
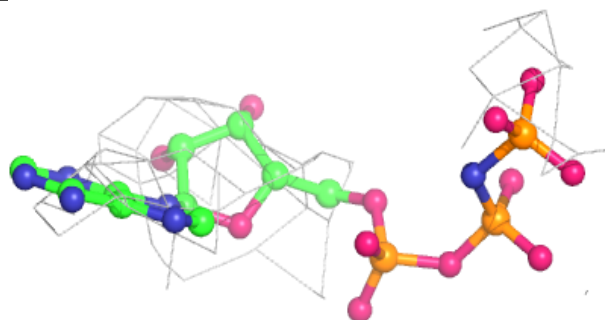
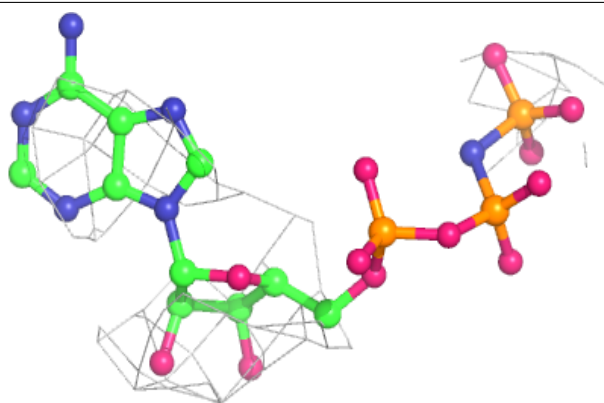


Electron density around ANP B 2400:

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

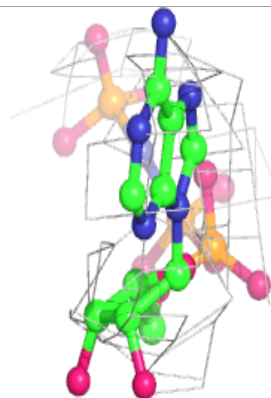
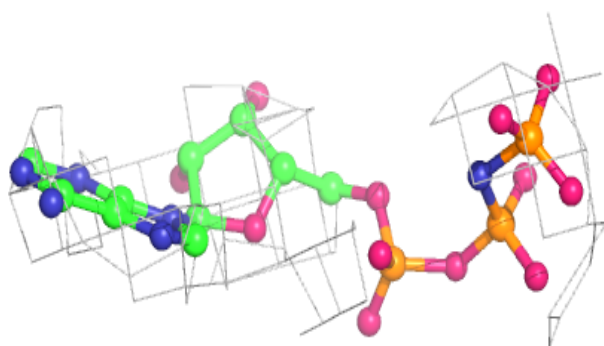
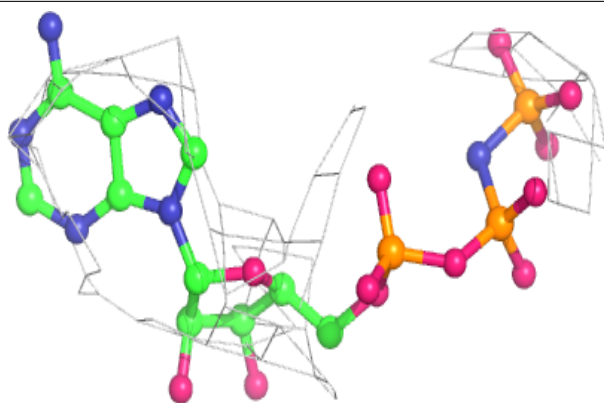
**Electron density around ANP B 400:**

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

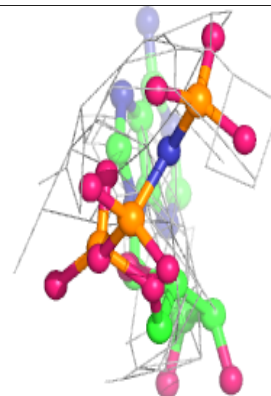
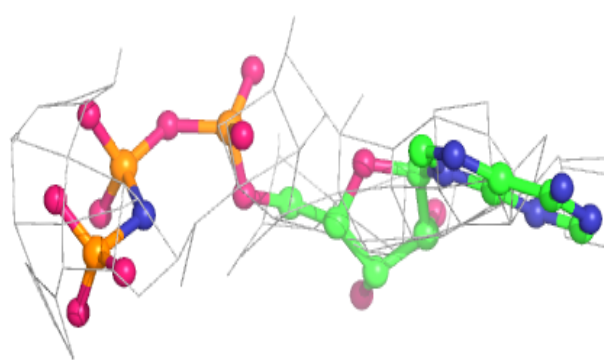
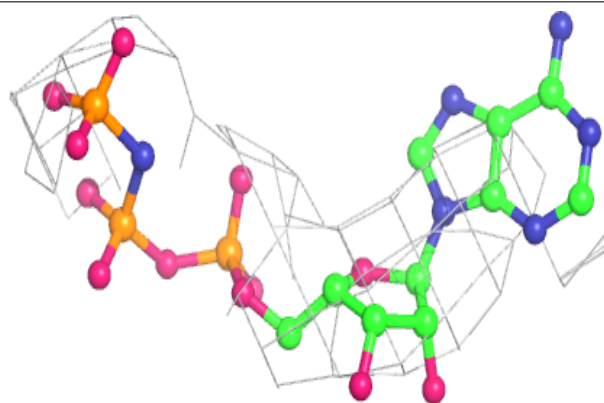


Electron density around ANP G 1400:

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

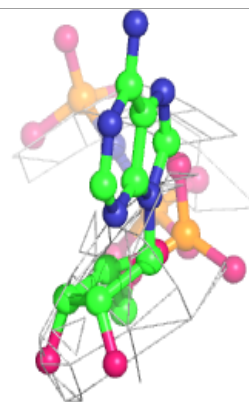
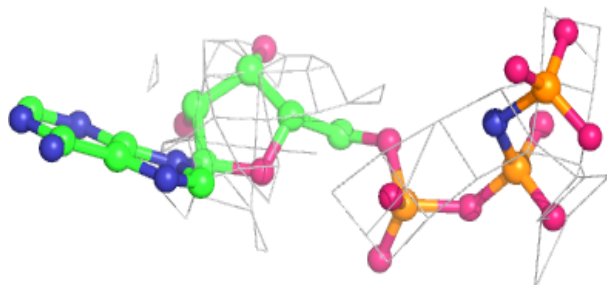
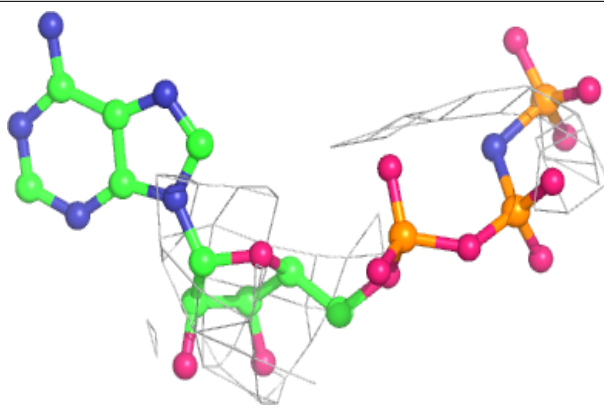
**Electron density around ANP F 1400:**

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

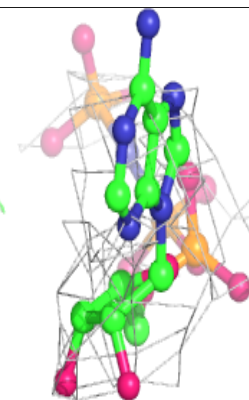
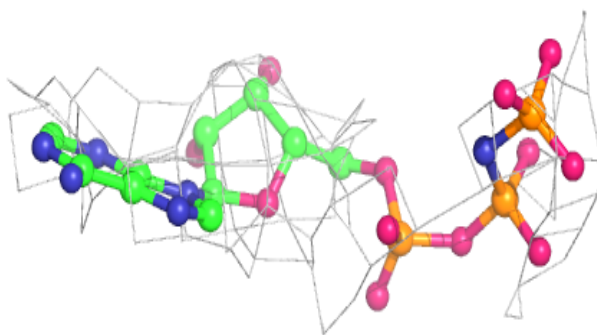
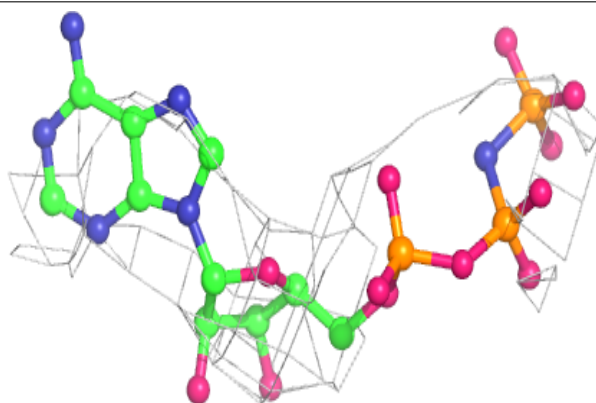


Electron density around ANP H 1400:

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

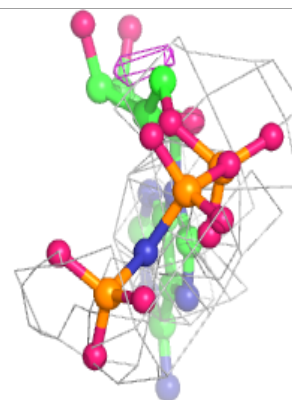
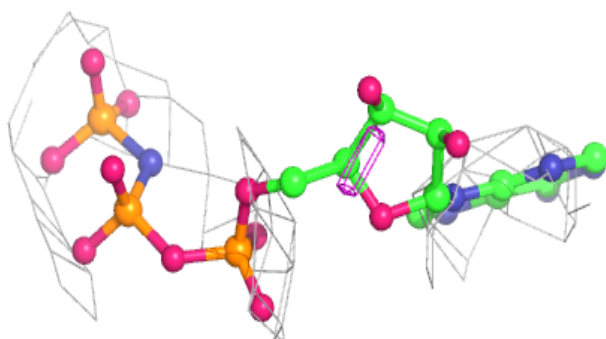
**Electron density around ANP C 1400:**

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

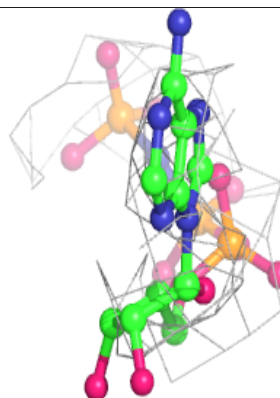
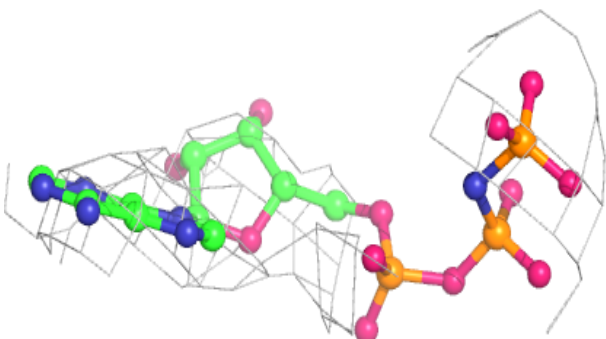
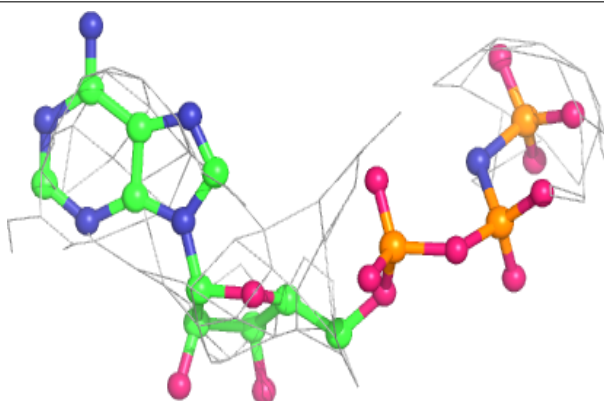


Electron density around ANP H 400:

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

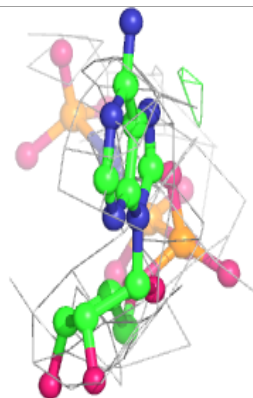
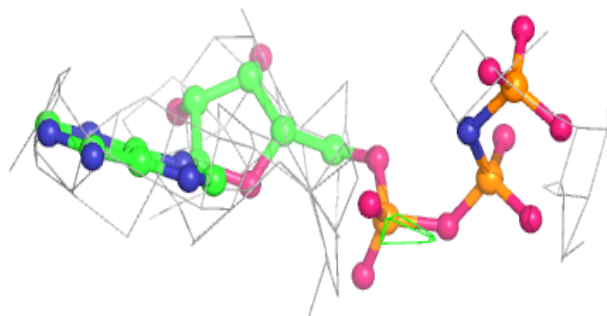
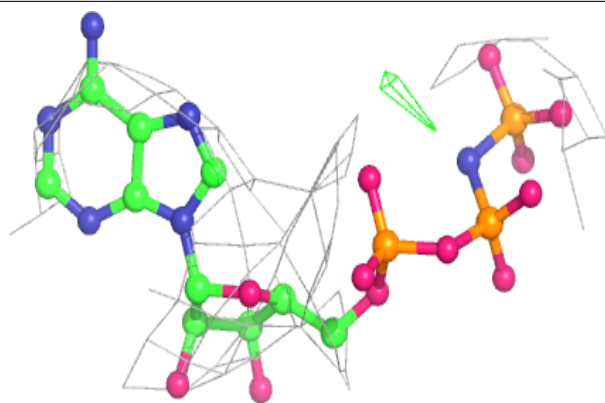
**Electron density around ANP C 400:**

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

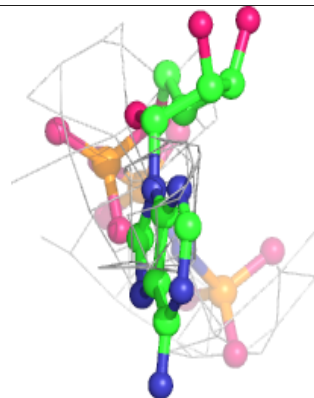
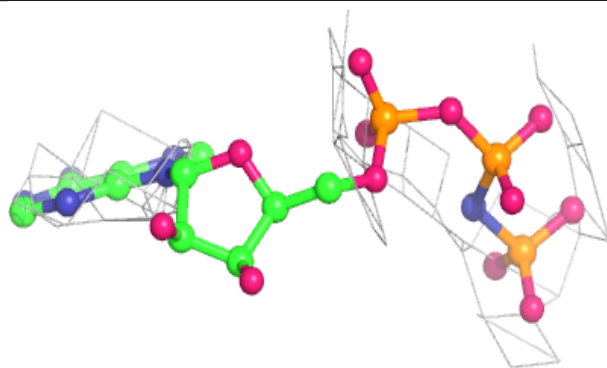
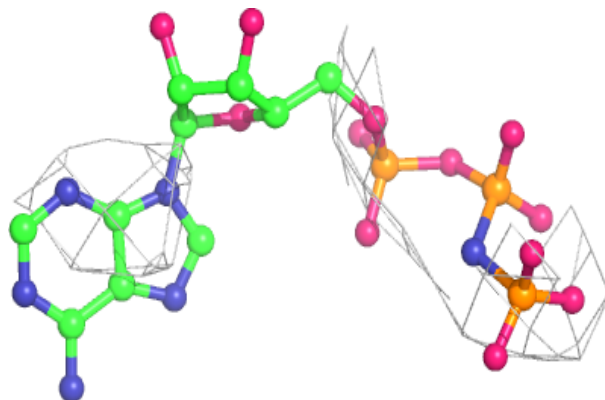


Electron density around ANP G 400:

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

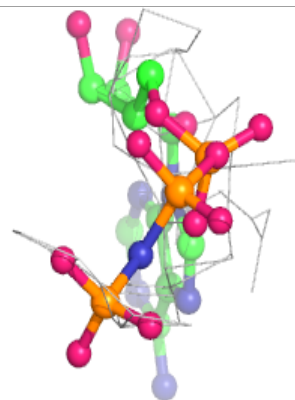
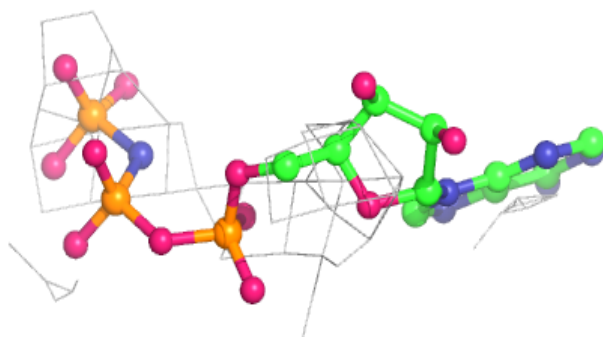
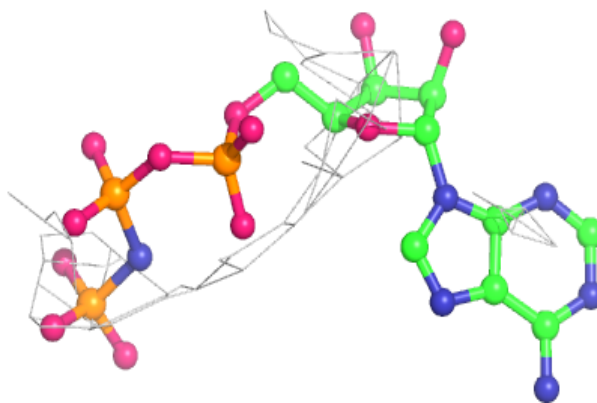
**Electron density around ANP D 400:**

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

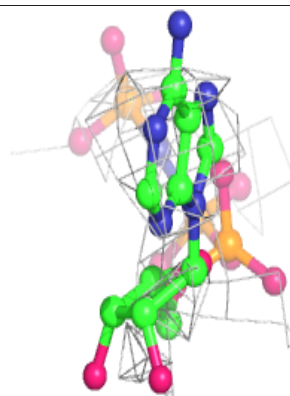
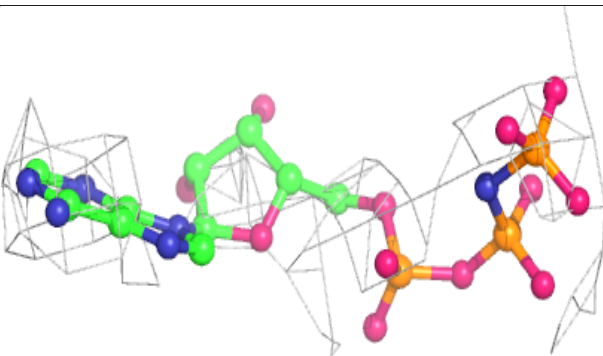
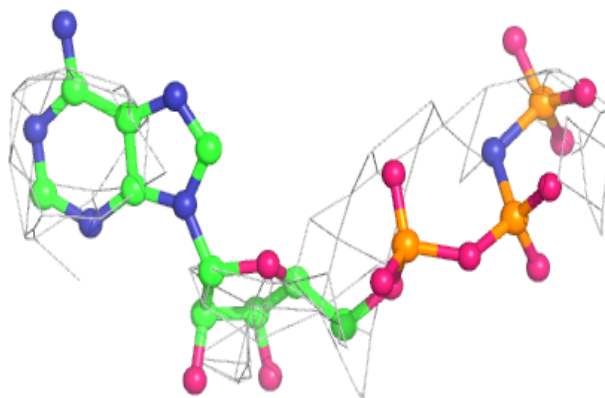


Electron density around ANP D 2400:

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

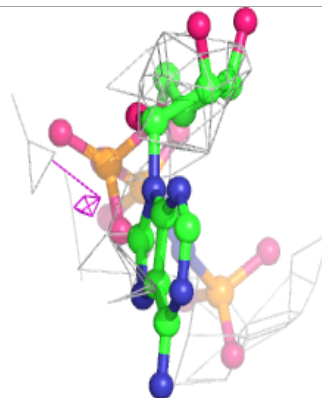
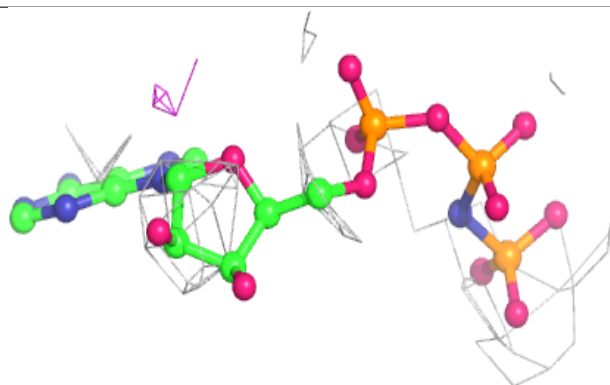
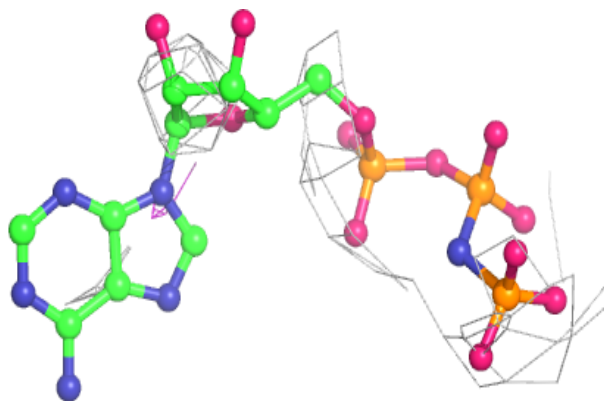
**Electron density around ANP B 1400:**

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

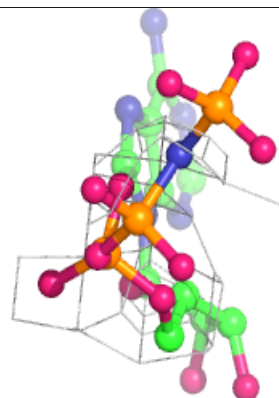
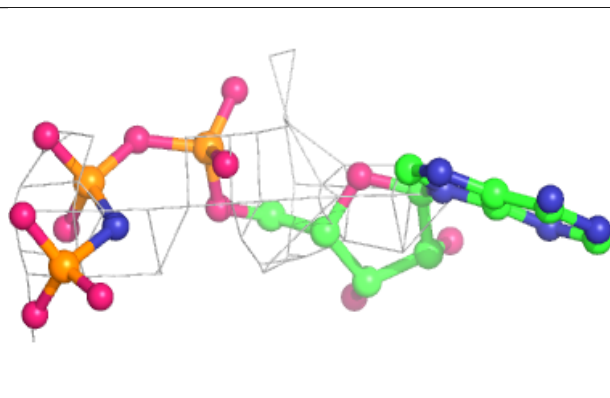
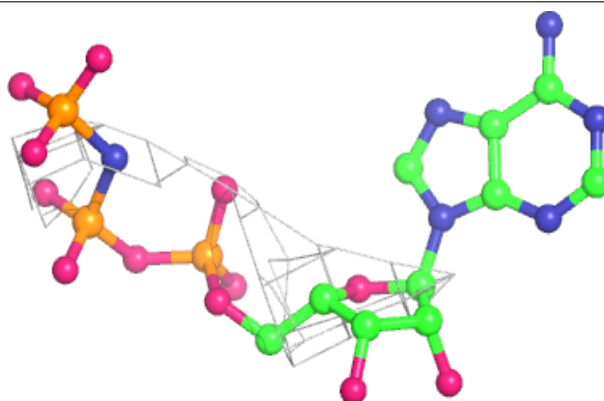


Electron density around ANP F 400:

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

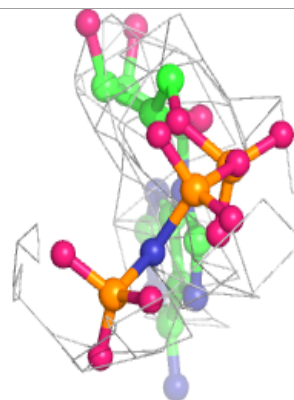
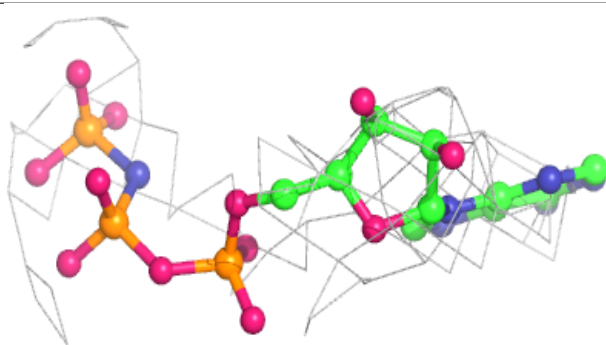
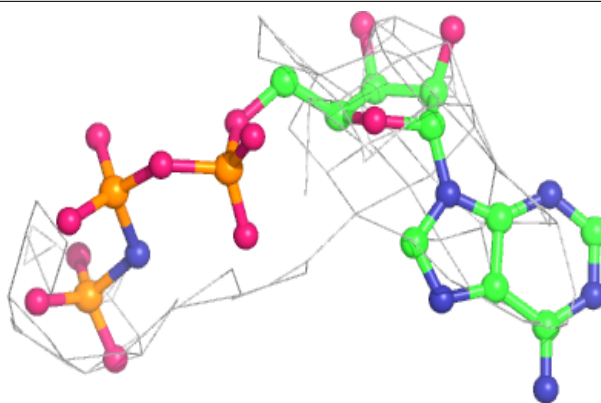
**Electron density around ANP A 2400:**

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

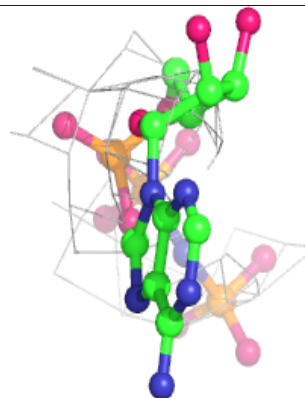
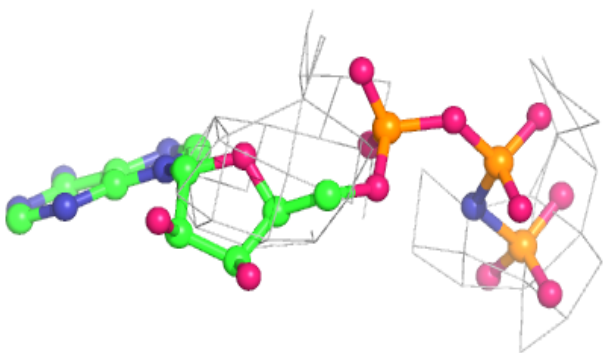
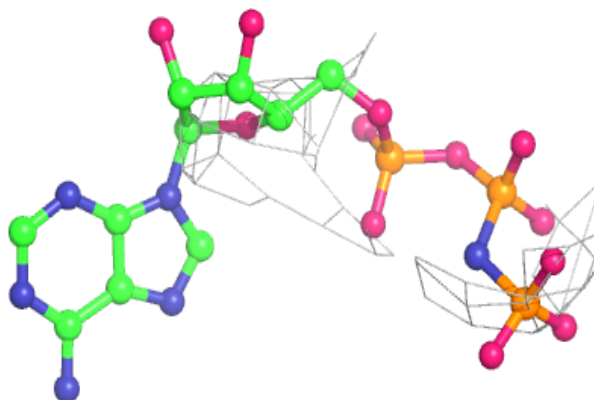


Electron density around ANP A 400:

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

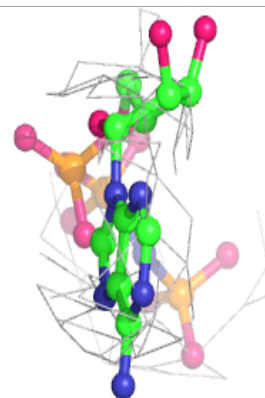
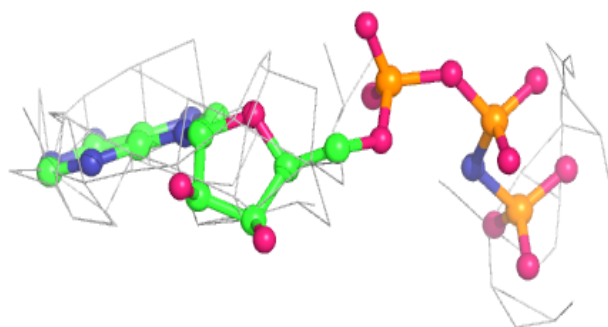
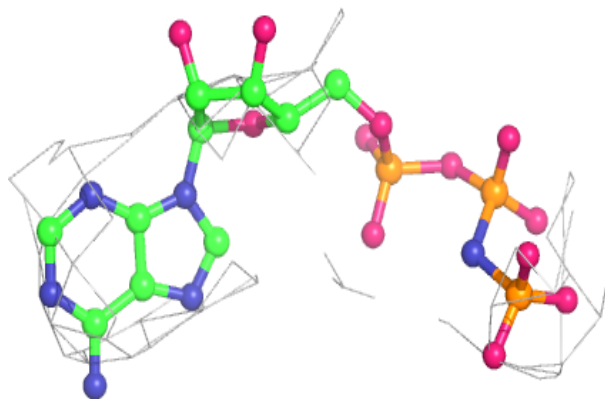
**Electron density around ANP C 2400:**

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

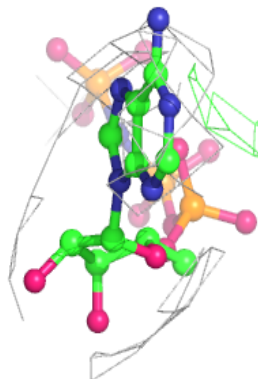
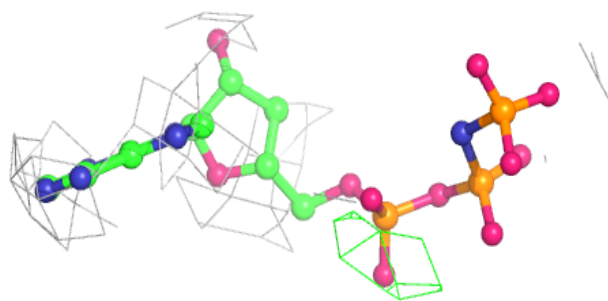
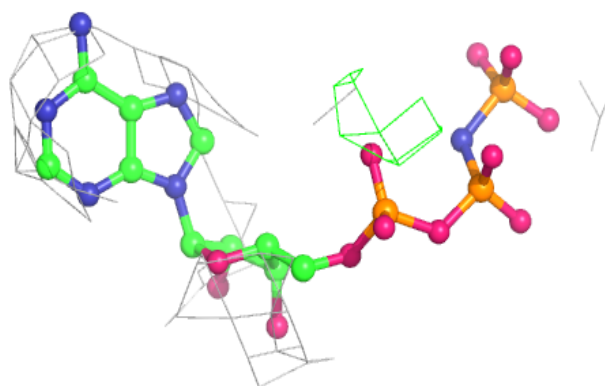


Electron density around ANP E 400:

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

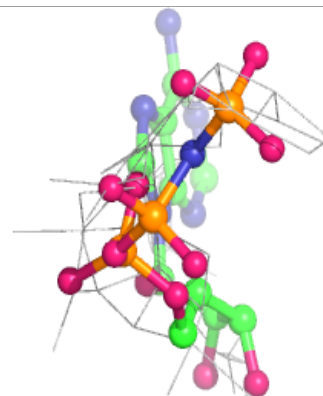
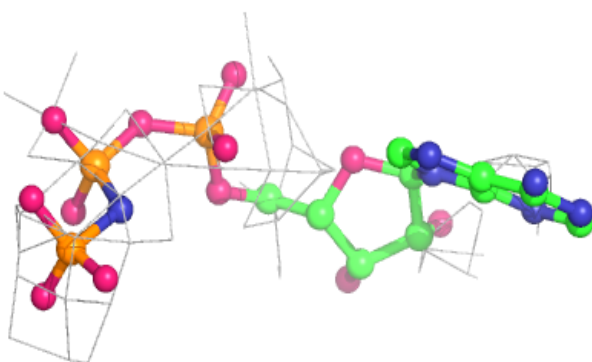
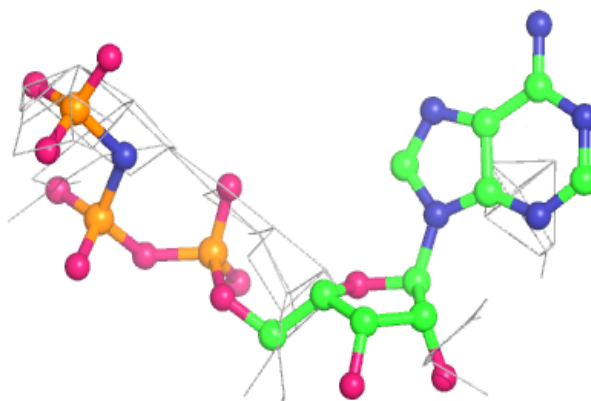
**Electron density around ANP H 3400:**

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

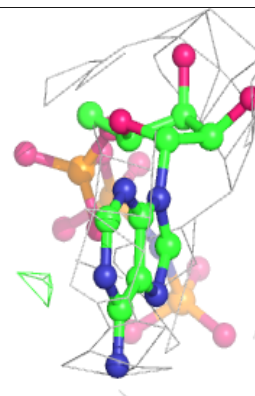
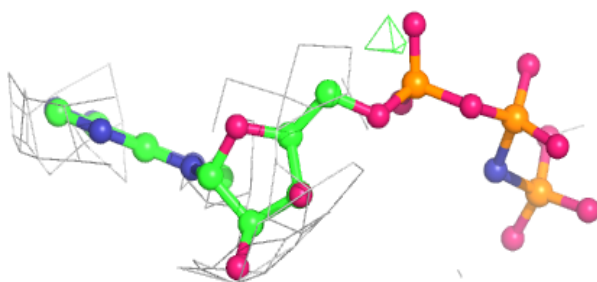


Electron density around ANP E 2400:

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

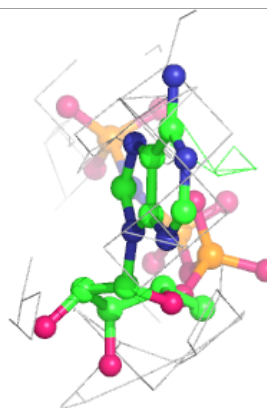
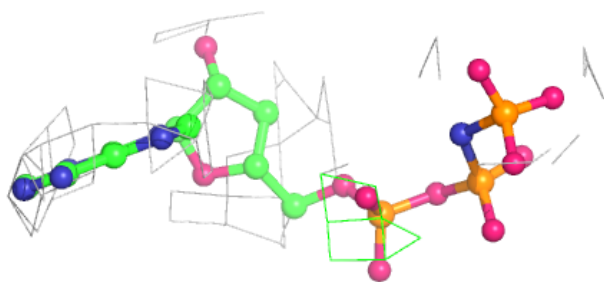
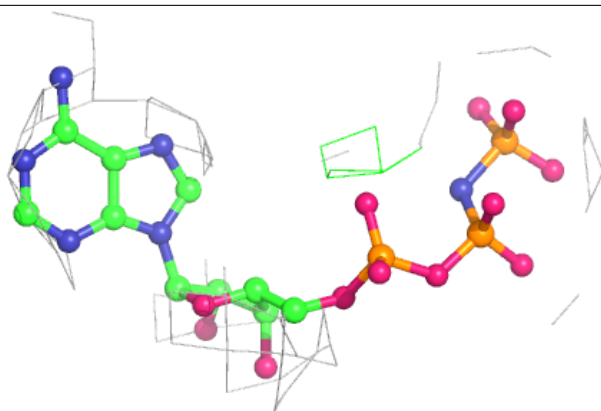
**Electron density around ANP G 3400:**

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

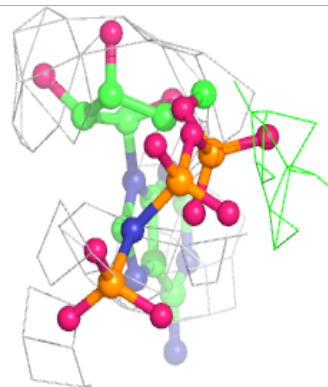
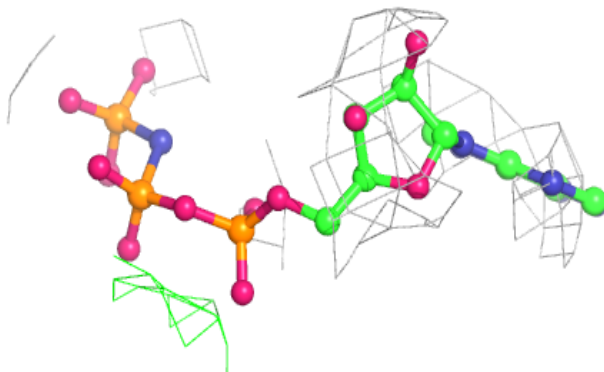
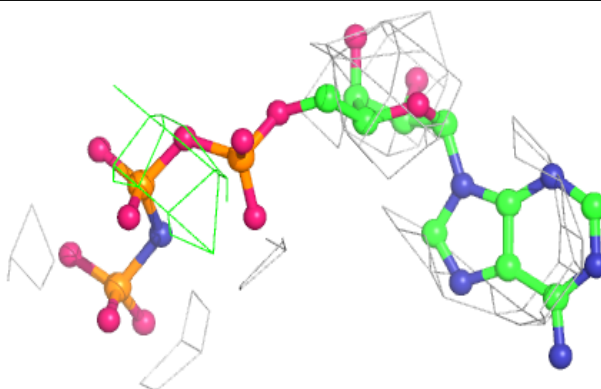


Electron density around ANP D 3400:

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

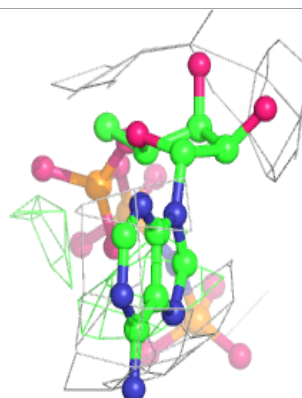
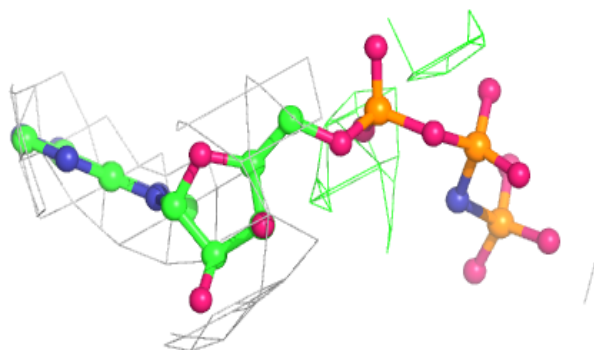
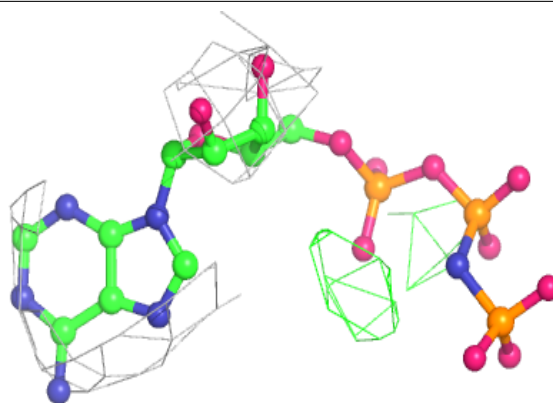
**Electron density around ANP F 3400:**

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

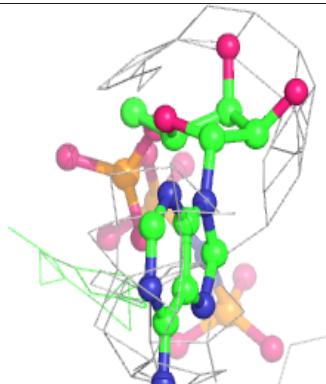
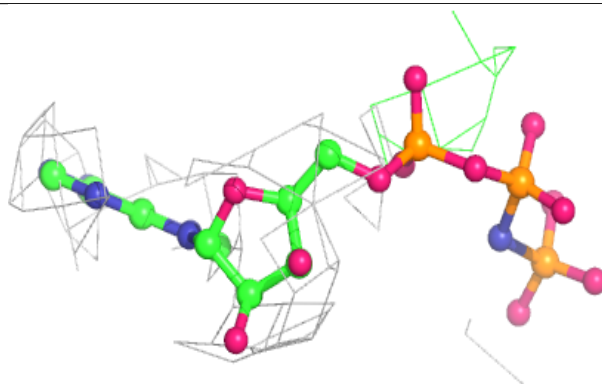
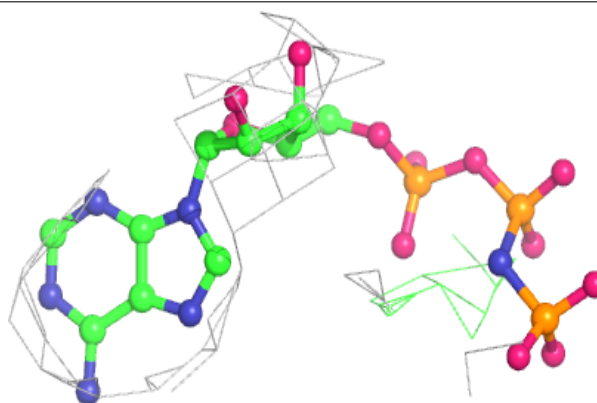


Electron density around ANP C 3400:

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

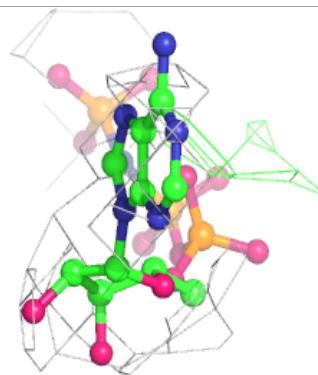
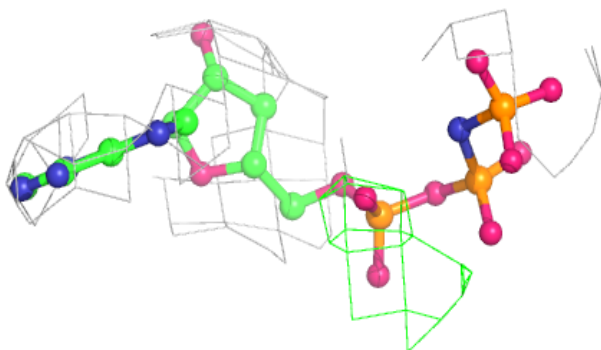
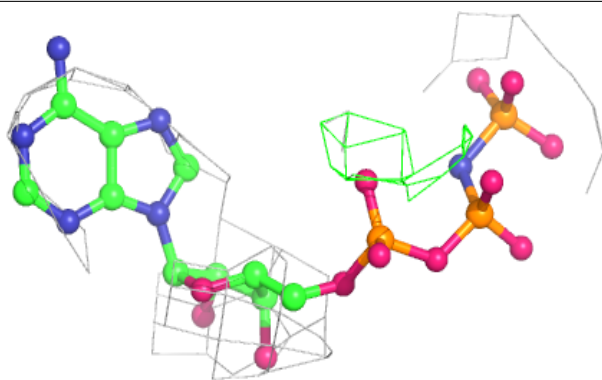
**Electron density around ANP B 3400:**

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

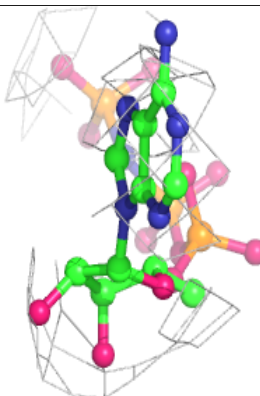
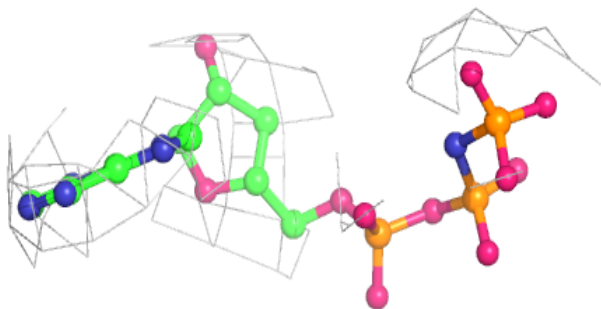
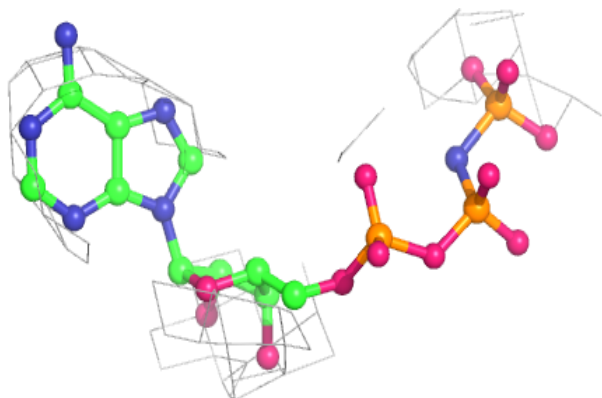


Electron density around ANP E 3400:

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

**Electron density around ANP A 3400:**

$2mF_o-DF_c$ (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.