



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 03:57 AM UTC

PDB ID : 3CMV / pdb_00003cmv
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 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

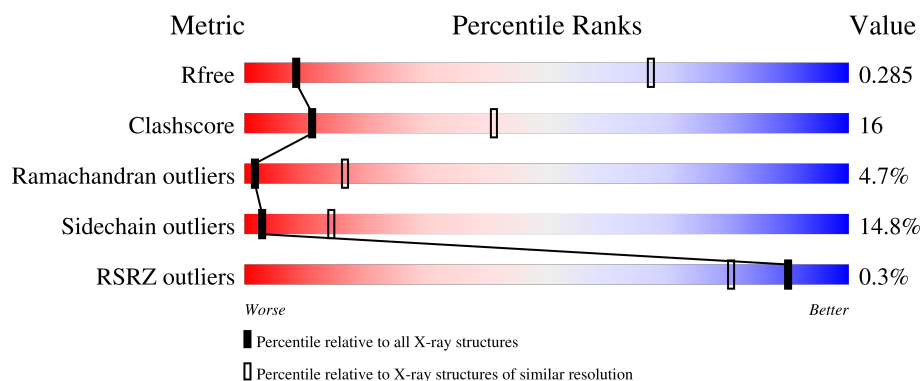
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	1357	 52% 28% 7% • 12%
1	B	1357	 51% 28% 6% • 14%
1	C	1357	 50% 29% 6% • 13%
1	D	1357	 52% 28% 6% • 13%
1	E	1357	 50% 28% 6% • 14%

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Mol	Chain	Length	Quality of chain
1	F	1357	
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
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	-	-	-
3	ANP	F	3400	X	-	-	-
3	ANP	F	400	X	-	-	-
3	ANP	G	1400	X	-	-	-
3	ANP	G	2400	X	-	-	-
3	ANP	G	3400	X	-	-	-
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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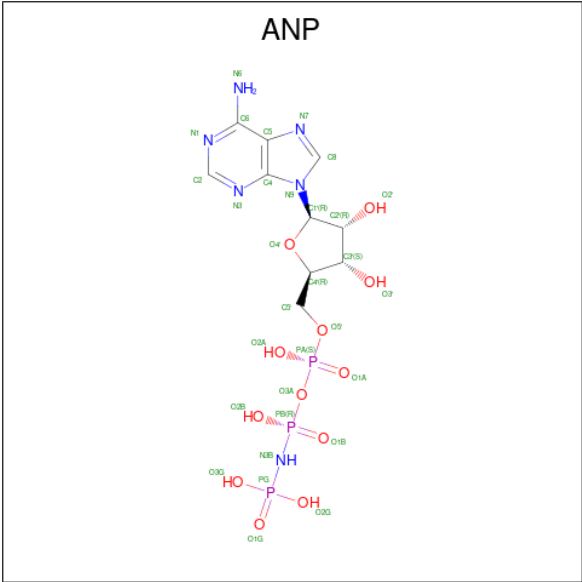
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Chain	Residue	Modelled	Actual	Comment	Reference
H	2992	SER	-	linker	UNP P0A7G6
H	2993	GLY	-	linker	UNP P0A7G6
H	2994	SER	-	linker	UNP P0A7G6
H	2995	SER	-	linker	UNP P0A7G6
H	2996	THR	-	linker	UNP P0A7G6
H	2997	GLY	-	linker	UNP P0A7G6
H	2998	SER	-	linker	UNP P0A7G6
H	2999	MET	-	linker	UNP P0A7G6
H	3000	SER	-	linker	UNP P0A7G6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	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	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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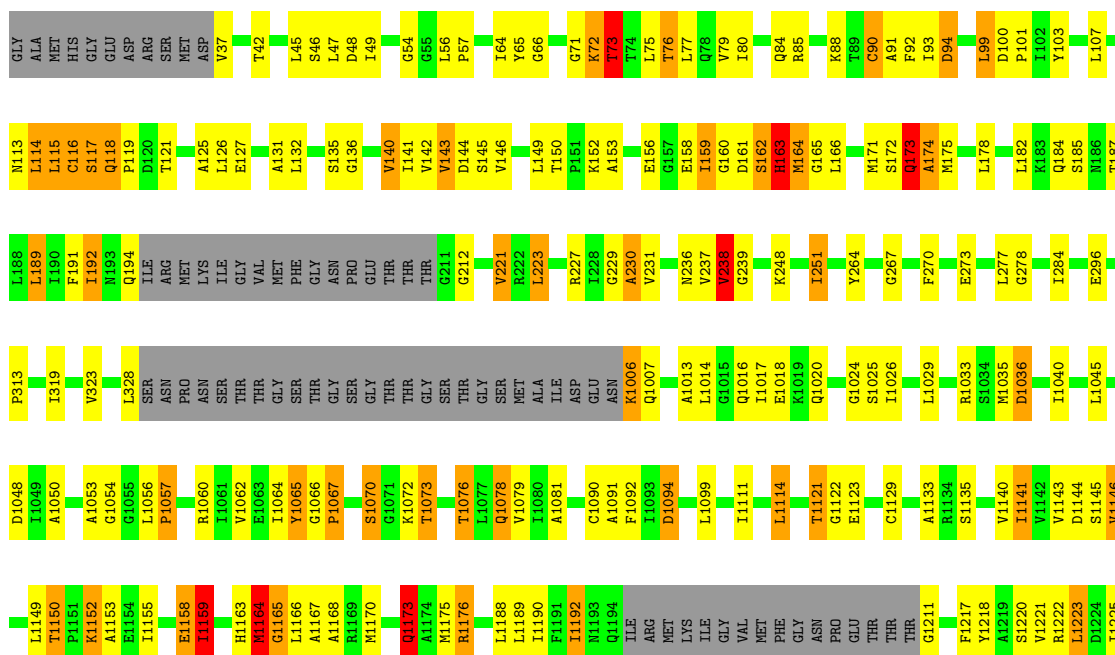
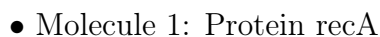
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F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

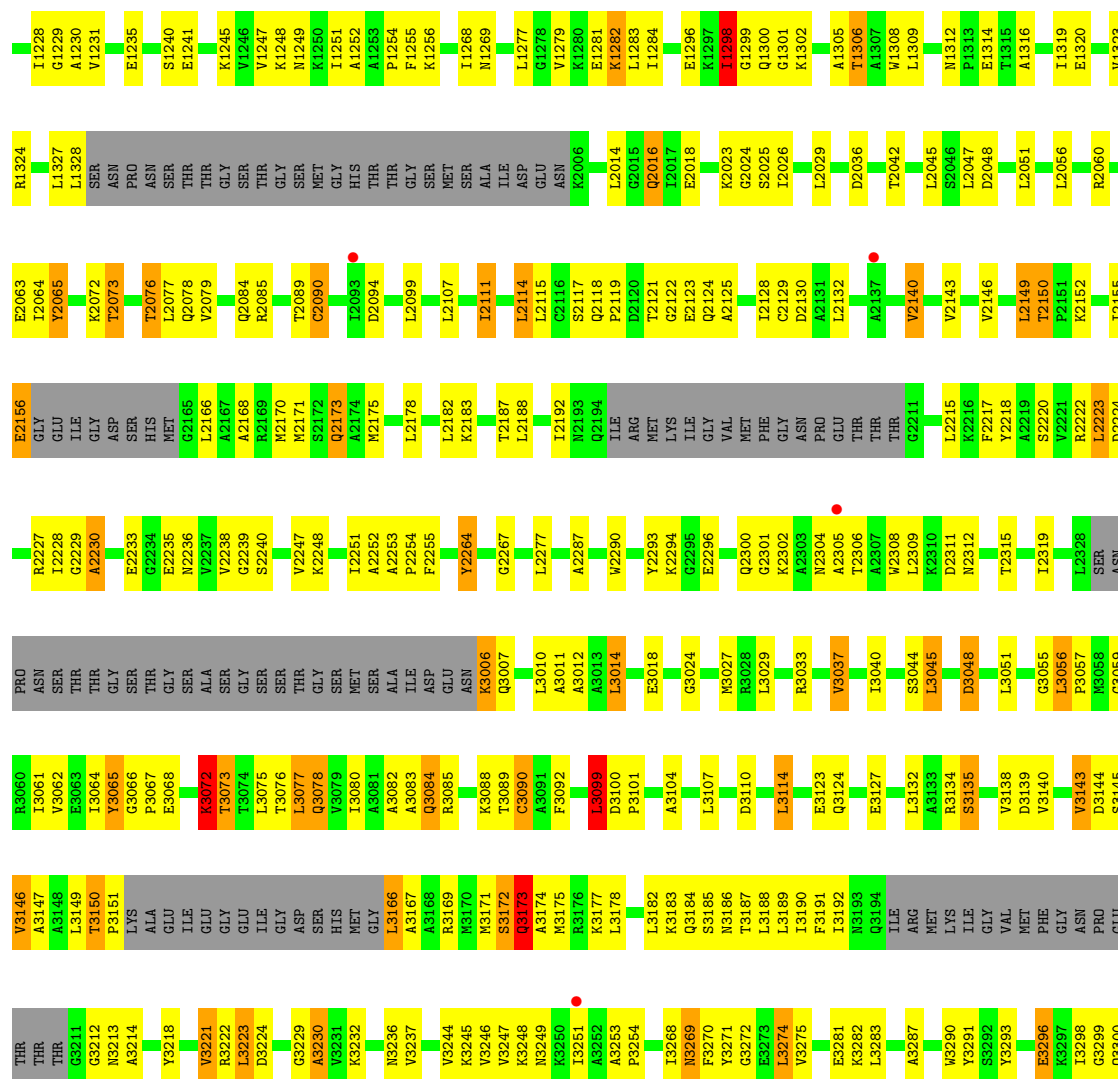
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A: 52% 28% 7% 12%



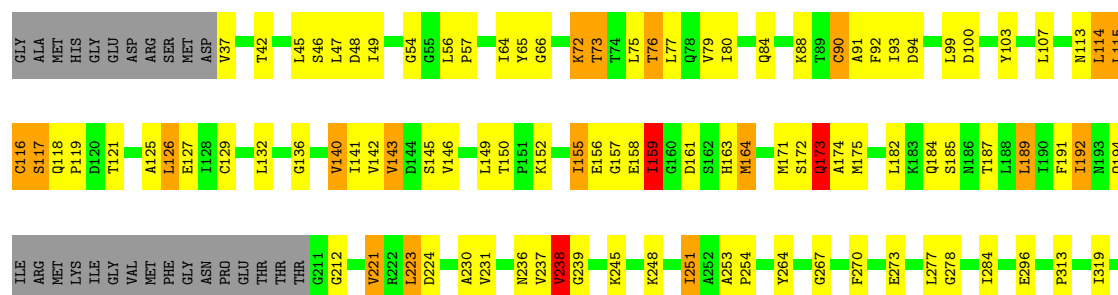






● Molecule 1: Protein recA

Chain D: 52% 28% 6% 13%

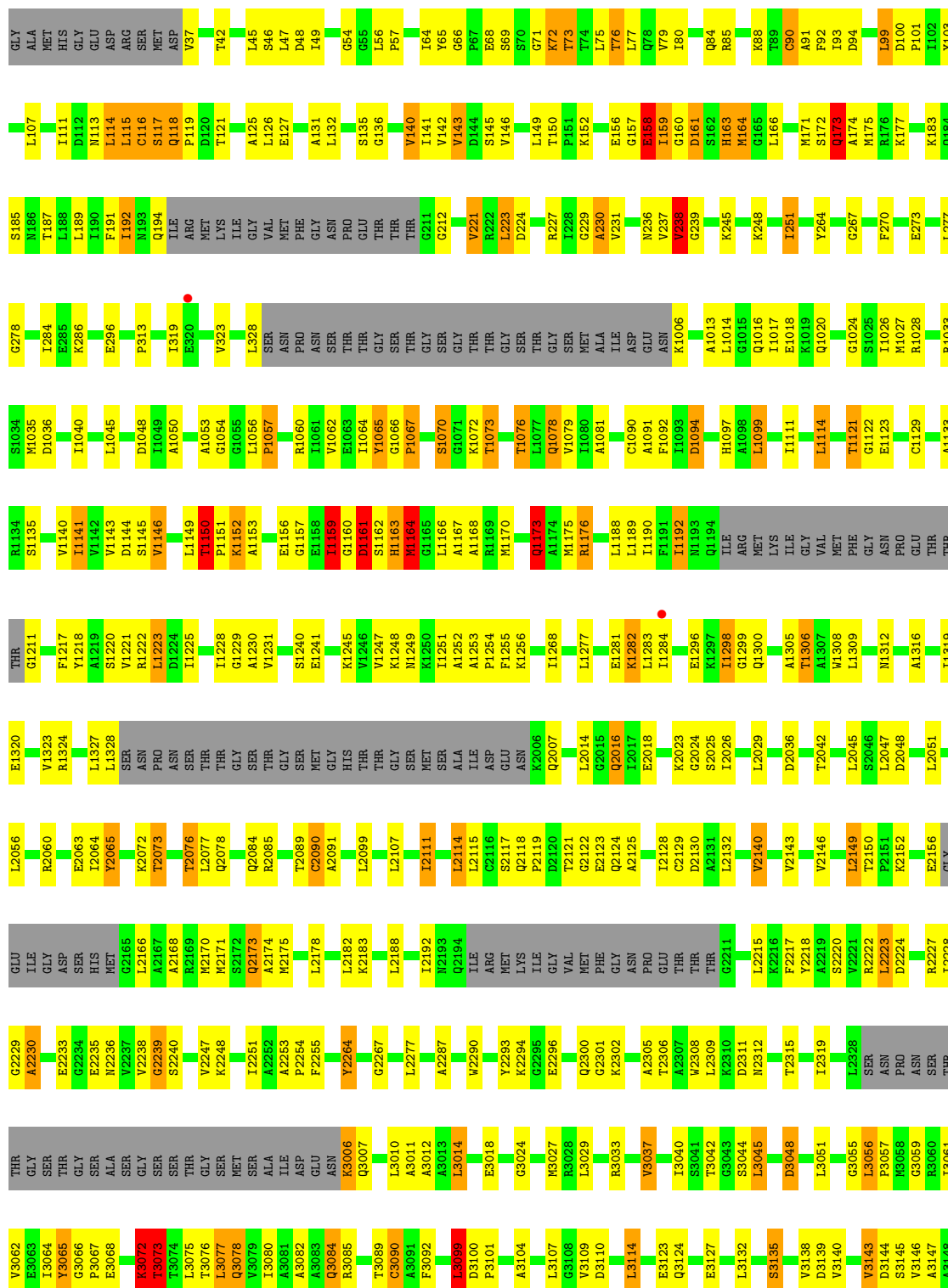


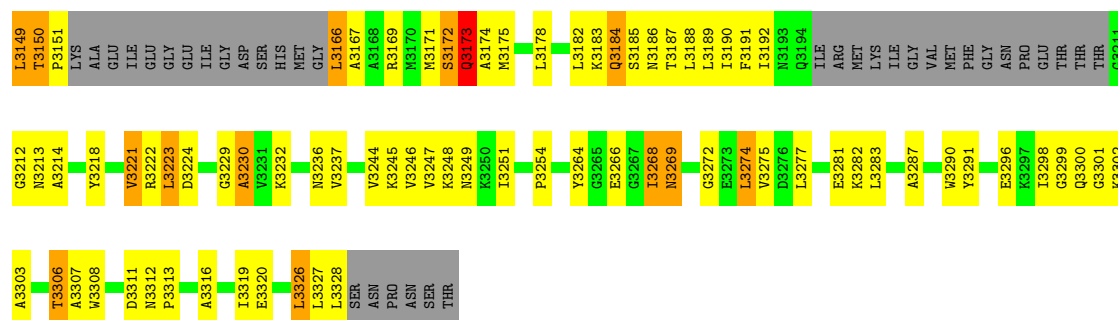




• Molecule 1: Protein recA

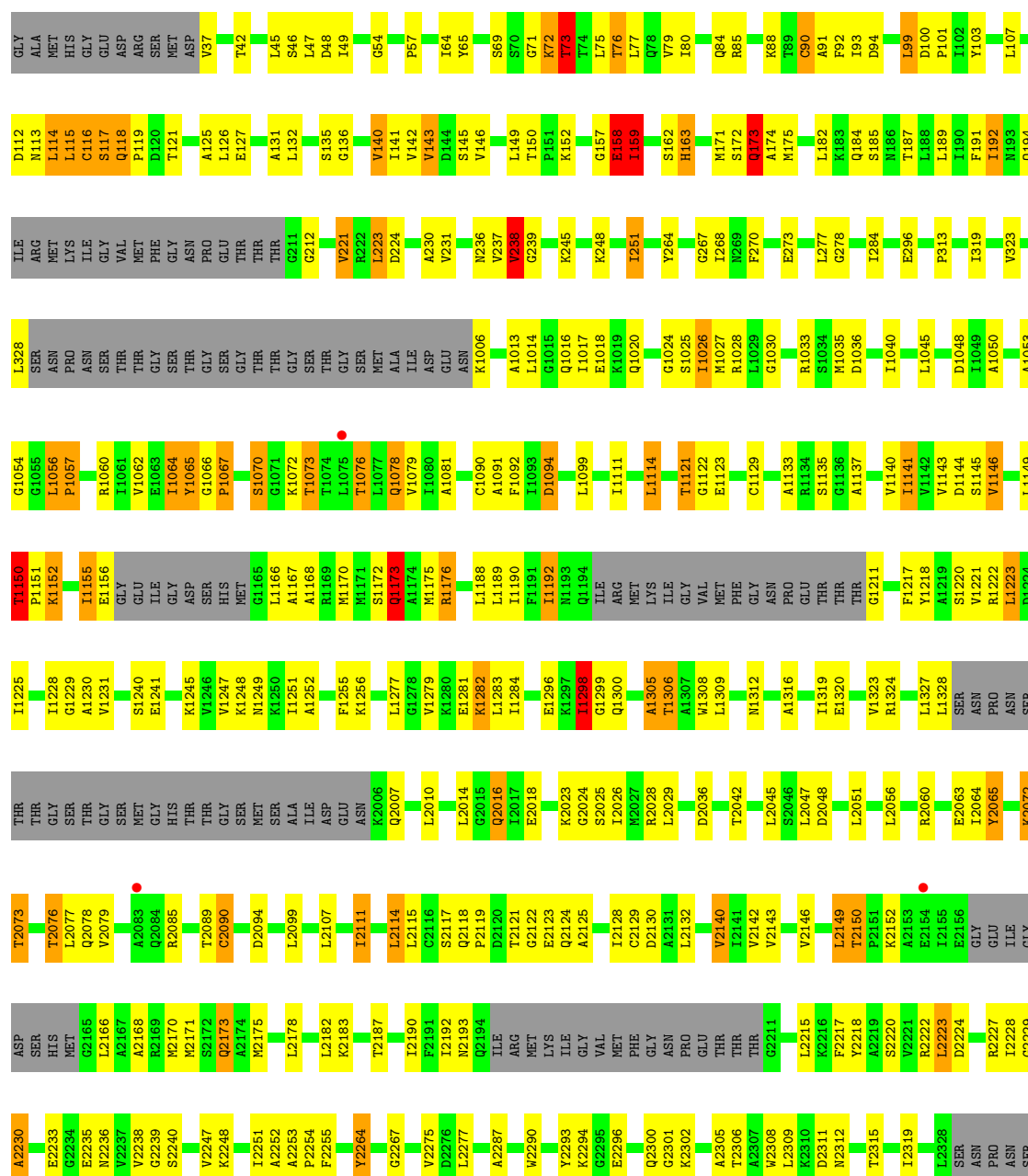
Chain F: 51% 29% 6% 13%

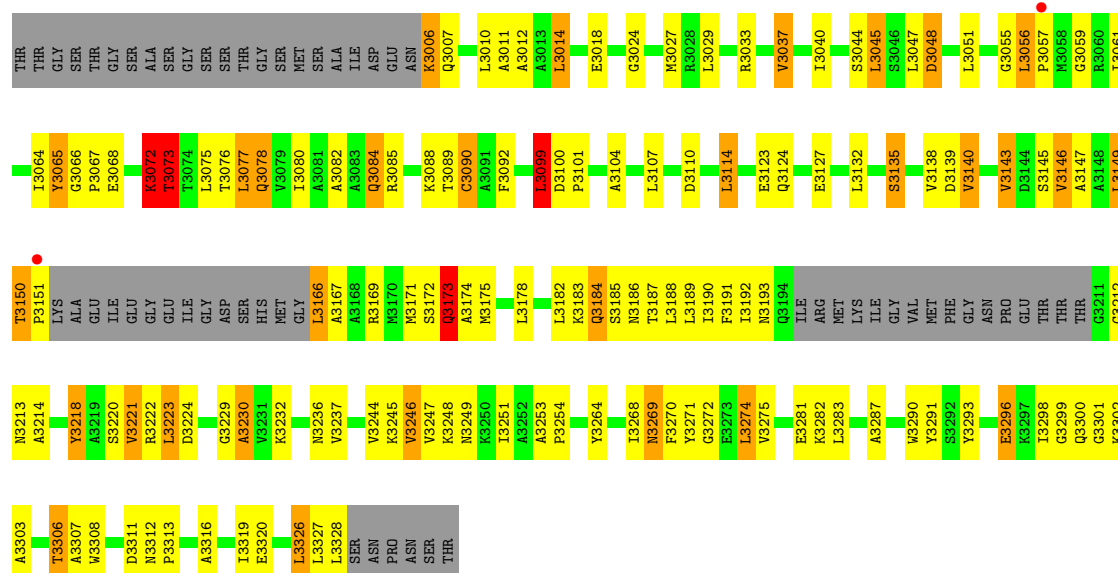




Molecule 1: Protein recA

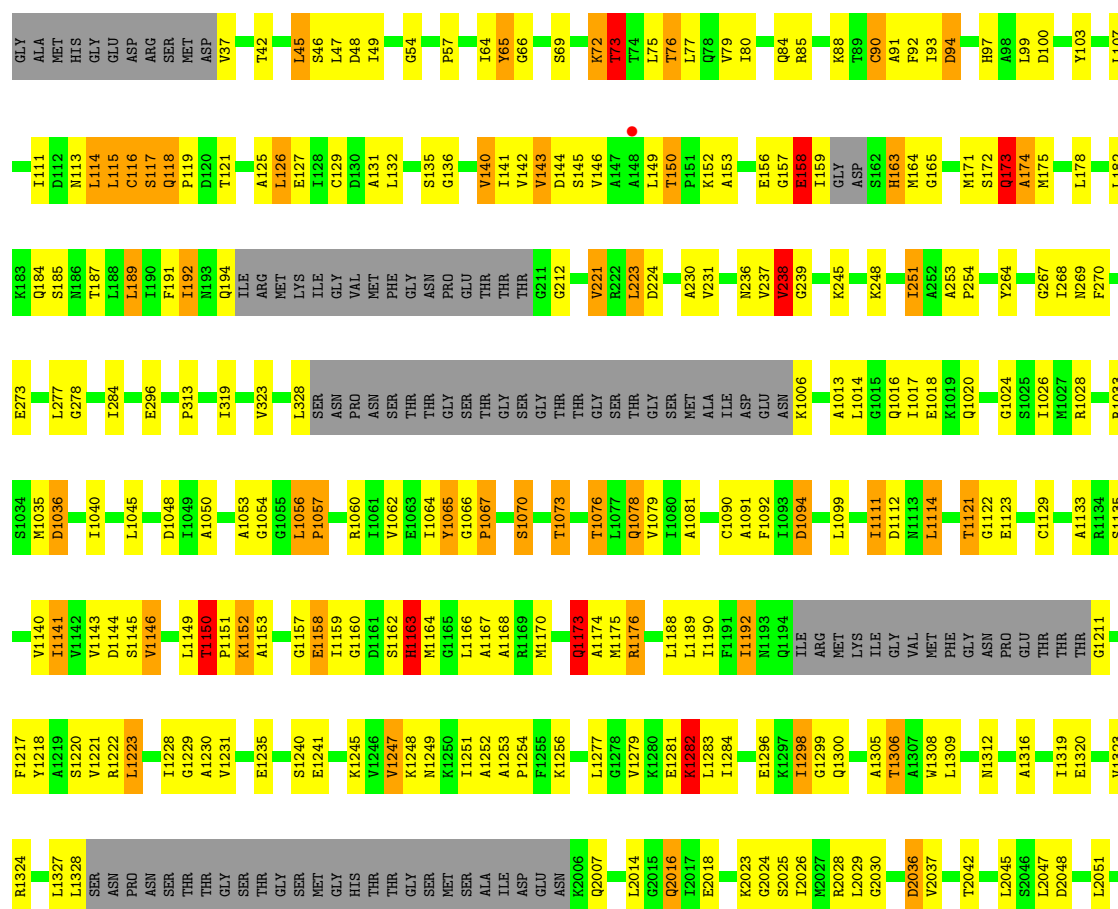
Chain G: 51% 28% 6% 14%





• Molecule 1: Protein recA

Chain H: 51% 28% 7% 14%



L2056 P2057	GLU ILE	G2229 A2230	SER ASN	H3058 G3059	V3143 D3144	PRO GLU	I3298 G3299
R2060	GLY ASP	E2233	PRO ASN	R3060 I3061	D3145 V3146	THR THR	G3300 G3301
E2063 I2064 Y2065	SER HIS MET	E2234 N2236 Y2237	THR THR GLY	V3062 E3063 I3064 Y3065	A3147 A3148 L3149 T3150 P3151	THR G3212 N3213 A3214	K3302 A3303
T2072 K2073	A2167 L2166 A2168	S2239 S2240 Y2244	THR THR GLY ALA	P3067 E3068 SER	LYS ALA GLU ILE	Y3218 V3221	T3306 A3307 W3308
T2076 L2077 Q2078 V2079	R2169 M2170 M2171 S2172 Q2173	V2247 K2248 I2251 A2252 A2253	SER ALA SER GLY SER	K3072 T3073 T3074 T3075 T3076 T3077 Q3078 V3079	GLU ILE GLU GLY ILE GLY ASP	V3222 R3222 L3223 D3224	N3311 N3312 P3313
R2085	A2174 M2175	T2251 A2252 A2253 F2255	THR THR GLY MET	A3081 A3082 A3083 Q3084 R3085	ASP HIS MET GLY	G3229 A3230 K3231 K3232	I3319 E3320
T2089 C2090	L2178 K2182 K2183	A2254 Y2264	SER GLY MET SER ALA	V3079 I3080 A3081 A3082 A3083	THR GLY MET GLY ILE	N3236 V3237	L3326 L3327
L2099	L2188	G2267	ASP GLU ASN	F3092 L3099 D3100 P3101 I3102 Y3103 A3104	L3166 A3167 A3168 R3169 M3170 M3171 S3172 D3173 A3174 M3175	N3244 K3245 V3246 V3247 K3248 N3249 K3250 I3251 A3252 P3254	SER ASN PRO ASN SER THR
L2107	T2192	V2275 D2276 L2277	GLU ASN Q3007	R3088 T3089 C3090 A3091 F3092	L3178 L3182 K3183 Q3184 S3185 N3186 T3187 L3188 L3189 I3190 F3191 I3192	Y3264 I3268 N3269 F3270 Y3271	
T2111	N2193 Q2194	A2287 W2290	L3010 A3011 A3012 A3013 L3014	L3099 D3100 P3101 I3102 Y3103 A3104	L3182 K3183 Q3184 S3185 N3186 T3187 L3188 L3189 I3190 F3191 I3192	L3274 V3275	
L2114 L2115 C2116 S2117 Q2118 P2119 D2120 T2121 G2122 F2123 Q2124 A2125	ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN	A2287 W2290 Y2293 K2294 G2295 E2296	A3011 A3012 A3013 L3014 E3018 G3024	L3107 G3108 V3109 D3110 L3114	L3182 K3183 Q3184 S3185 N3186 T3187 L3188 L3189 I3190 F3191 I3192	L3274 V3275	
T2128 C2129 D2130 A2131 L2132	PRO GLU THR THR	G2299 Q2300 Q2301 K2302 A2303 N2304 T2306	M3027 R3028 L3029 R3033 V3037	L3107 G3108 V3109 D3110 L3114	L3182 K3183 Q3184 S3185 N3186 T3187 L3188 L3189 I3190 F3191 I3192	L3274 V3275	
V2140 V2143 V2146 L2149 T2150 P2151 K2152	L2215 F2216 F2217 Y2218 A2219 S2220 V2221 R2222 T2223 D2224	A2307 H2308 L2309 K2310 D2311 N2312 T2315	I3040 S3041 T3042 G3043 S3044 L3045 D3048	E3127 Q3124 Q3124 E3127 L3132 S3135	L3182 K3183 Q3184 S3185 N3186 T3187 L3188 L3189 I3190 F3191 I3192	L3274 V3275	
E2156 GLY	R2227 I2228	T2319 L2328	G3055 L3056 P3057	V3138 D3139 V3140	L3182 K3183 Q3184 S3185 N3186 T3187 L3188 L3189 I3190 F3191 I3192	L3274 V3275	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	176.60Å 189.80Å 424.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.30 20.00 – 4.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-4.30) 91.6 (20.00-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.261 0.275 , 0.285	Depositor DCC
R_{free} test set	1946 reflections (1.99%)	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)	0.19 , 94.8	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	0.92	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: ANP, MG

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	0.99	19/9068 (0.2%)	1.14	55/12192 (0.5%)
1	B	0.90	3/8861 (0.0%)	1.08	31/11910 (0.3%)
1	C	0.92	7/8951 (0.1%)	1.09	40/12033 (0.3%)
1	D	0.86	3/8951 (0.0%)	1.08	36/12033 (0.3%)
1	E	0.85	5/8879 (0.1%)	1.08	34/11934 (0.3%)
1	F	0.92	8/8951 (0.1%)	1.09	34/12033 (0.3%)
1	G	0.91	6/8892 (0.1%)	1.09	37/11953 (0.3%)
1	H	0.87	9/8938 (0.1%)	1.09	35/12014 (0.3%)
All	All	0.90	60/71491 (0.1%)	1.09	302/96102 (0.3%)

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 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	HIS	N-CA	11.76	1.61	1.46
1	A	159	ILE	CA-C	11.04	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	159	ILE	CA-CB	8.75	1.65	1.54
1	F	1159	ILE	CA-CB	8.70	1.66	1.54
1	H	2036	ASP	CA-C	8.61	1.63	1.53

The worst 5 of 302 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	HIS	N-CA-C	11.44	128.28	110.20
1	D	1163	HIS	N-CA-C	10.76	126.00	109.96
1	A	1150	THR	CA-C-N	9.40	130.64	120.11
1	A	1150	THR	C-N-CA	9.40	130.64	120.11
1	H	158	GLU	N-CA-C	9.23	124.49	112.12

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	330	1
1	B	8769	0	9070	295	0
1	C	8856	0	9139	310	1
1	D	8856	0	9139	294	0
1	E	8787	0	9082	326	0
1	F	8856	0	9139	332	0
1	G	8799	0	9090	293	0
1	H	8844	0	9131	324	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	2368	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 16.

The worst 5 of 2368 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%)	1	16
1	B	1139/1357 (84%)	915 (80%)	172 (15%)	52 (5%)	2	17
1	C	1155/1357 (85%)	919 (80%)	178 (15%)	58 (5%)	1	16
1	D	1155/1357 (85%)	923 (80%)	179 (16%)	53 (5%)	2	17
1	E	1141/1357 (84%)	910 (80%)	178 (16%)	53 (5%)	2	17
1	F	1155/1357 (85%)	913 (79%)	188 (16%)	54 (5%)	2	16
1	G	1145/1357 (84%)	914 (80%)	179 (16%)	52 (4%)	2	17
1	H	1151/1357 (85%)	914 (79%)	180 (16%)	57 (5%)	1	16
All	All	9213/10856 (85%)	7331 (80%)	1445 (16%)	437 (5%)	2	16

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%)	791 (85%)	139 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	908/1065 (85%)	775 (85%)	133 (15%)	3	14
1	C	917/1065 (86%)	777 (85%)	140 (15%)	3	13
1	D	917/1065 (86%)	783 (85%)	134 (15%)	3	14
1	E	910/1065 (85%)	778 (86%)	132 (14%)	3	15
1	F	917/1065 (86%)	784 (86%)	133 (14%)	3	15
1	G	911/1065 (86%)	777 (85%)	134 (15%)	3	14
1	H	916/1065 (86%)	780 (85%)	136 (15%)	3	14
All	All	7326/8520 (86%)	6245 (85%)	1081 (15%)	3	14

5 of 1081 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3127	GLU
1	H	115	LEU
1	G	3114	LEU
1	H	2264	TYR
1	C	3078	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	173	GLN
1	H	2236	ASN
1	G	1124	GLN
1	G	3257	GLN
1	H	3257	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 oligosaccharides 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	2400	-	33,33,33	2.22	10 (30%)	45,52,52	2.26	12 (26%)
3	ANP	C	3400	-	33,33,33	2.32	8 (24%)	45,52,52	2.48	13 (28%)
3	ANP	D	1400	-	33,33,33	2.18	9 (27%)	45,52,52	2.30	13 (28%)
3	ANP	H	2400	-	33,33,33	2.17	12 (36%)	45,52,52	2.25	12 (26%)
3	ANP	H	1400	-	33,33,33	2.27	9 (27%)	45,52,52	2.25	13 (28%)
3	ANP	B	400	-	33,33,33	2.21	9 (27%)	45,52,52	2.10	14 (31%)
3	ANP	A	400	-	33,33,33	2.26	12 (36%)	45,52,52	2.13	12 (26%)
3	ANP	C	400	-	33,33,33	2.06	10 (30%)	45,52,52	2.14	12 (26%)
3	ANP	F	3400	-	33,33,33	2.14	9 (27%)	45,52,52	2.48	12 (26%)
3	ANP	A	3400	-	33,33,33	2.16	7 (21%)	45,52,52	2.55	13 (28%)
3	ANP	C	2400	-	33,33,33	2.12	11 (33%)	45,52,52	2.26	12 (26%)
3	ANP	D	2400	-	33,33,33	2.19	9 (27%)	45,52,52	2.26	12 (26%)
3	ANP	G	3400	-	33,33,33	2.27	8 (24%)	45,52,52	2.51	14 (31%)
3	ANP	C	1400	-	33,33,33	2.27	10 (30%)	45,52,52	2.31	13 (28%)
3	ANP	H	400	-	33,33,33	2.14	10 (30%)	45,52,52	2.11	12 (26%)
3	ANP	H	3400	-	33,33,33	2.25	9 (27%)	45,52,52	2.68	14 (31%)
3	ANP	G	1400	-	33,33,33	2.17	11 (33%)	45,52,52	2.26	13 (28%)
3	ANP	B	3400	-	33,33,33	2.15	9 (27%)	45,52,52	2.59	16 (35%)
3	ANP	E	400	-	33,33,33	2.18	12 (36%)	45,52,52	2.16	13 (28%)
3	ANP	F	2400	-	33,33,33	2.09	12 (36%)	45,52,52	2.26	12 (26%)
3	ANP	F	1400	-	33,33,33	2.27	11 (33%)	45,52,52	2.31	12 (26%)
3	ANP	D	3400	-	33,33,33	2.18	8 (24%)	45,52,52	2.56	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	E	2400	-	33,33,33	2.23	10 (30%)	45,52,52	2.25	12 (26%)
3	ANP	E	1400	-	33,33,33	2.26	11 (33%)	45,52,52	2.32	12 (26%)
3	ANP	B	2400	-	33,33,33	2.17	12 (36%)	45,52,52	2.28	12 (26%)
3	ANP	E	3400	2	33,33,33	2.00	9 (27%)	45,52,52	2.59	16 (35%)
3	ANP	G	400	-	33,33,33	2.16	9 (27%)	45,52,52	2.13	12 (26%)
3	ANP	D	400	-	33,33,33	2.26	12 (36%)	45,52,52	2.07	12 (26%)
3	ANP	A	2400	-	33,33,33	2.20	9 (27%)	45,52,52	2.28	12 (26%)
3	ANP	A	1400	-	33,33,33	2.12	10 (30%)	45,52,52	2.30	12 (26%)
3	ANP	F	400	-	33,33,33	2.15	10 (30%)	45,52,52	2.08	12 (26%)
3	ANP	B	1400	-	33,33,33	2.17	9 (27%)	45,52,52	2.31	12 (26%)

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	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	C	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	D	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	H	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	H	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	B	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	A	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	C	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	F	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	A	3400	-	1/1/7/8	7/18/38/38	0/3/3/3
3	ANP	C	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	D	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	G	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	C	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	H	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	H	3400	-	1/1/7/8	7/18/38/38	0/3/3/3
3	ANP	G	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	B	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	E	400	-	1/1/7/8	9/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	F	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	F	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	D	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	E	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	E	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	B	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	E	3400	2	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	G	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	D	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	A	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	A	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	F	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	B	1400	-	1/1/7/8	9/18/38/38	0/3/3/3

The worst 5 of 316 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3400	ANP	C5-C4	6.30	1.50	1.39
3	D	3400	ANP	C5-C4	6.10	1.50	1.39
3	G	3400	ANP	C5-C4	6.04	1.49	1.39
3	C	3400	ANP	C5-C4	6.03	1.49	1.39
3	C	3400	ANP	PG-N3B	5.90	1.78	1.63

The worst 5 of 406 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	H	3400	ANP	C5-C4-N3	-7.72	116.08	126.72
3	B	3400	ANP	C5-C4-N3	-7.61	116.24	126.72
3	E	3400	ANP	C5-C4-N3	-7.57	116.29	126.72
3	F	3400	ANP	O1G-PG-N3B	-7.45	100.81	111.77

5 of 32 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	400	ANP	C4'
3	A	1400	ANP	C4'
3	A	2400	ANP	C4'
3	A	3400	ANP	C4'

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Mol	Chain	Res	Type	Atom
3	B	400	ANP	C4'

5 of 278 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	ANP	PB-N3B-PG-O1G
3	A	400	ANP	PG-N3B-PB-O1B
3	A	400	ANP	PG-N3B-PB-O3A
3	A	400	ANP	PA-O3A-PB-O2B
3	A	400	ANP	C5'-O5'-PA-O2A

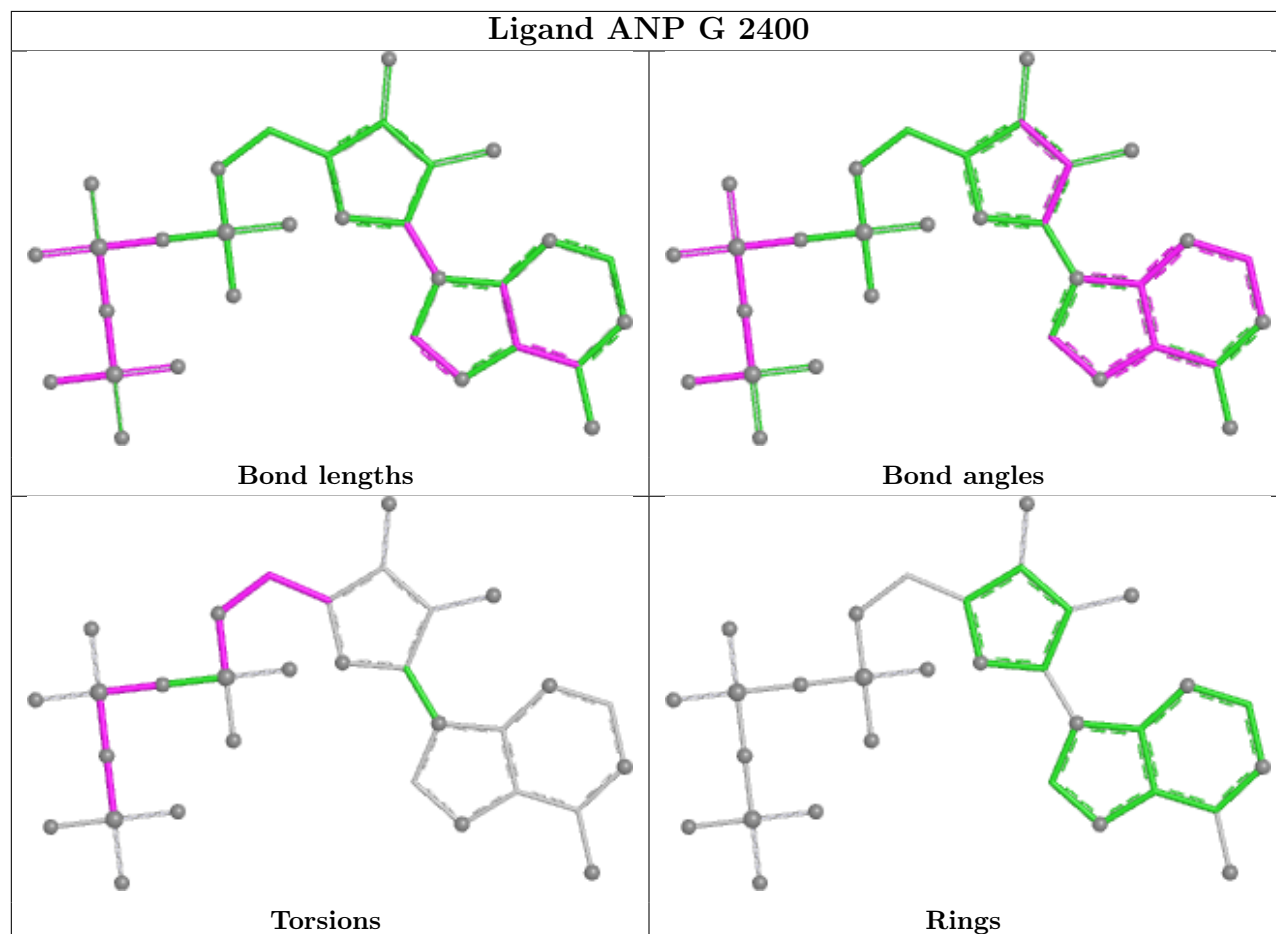
There are no ring outliers.

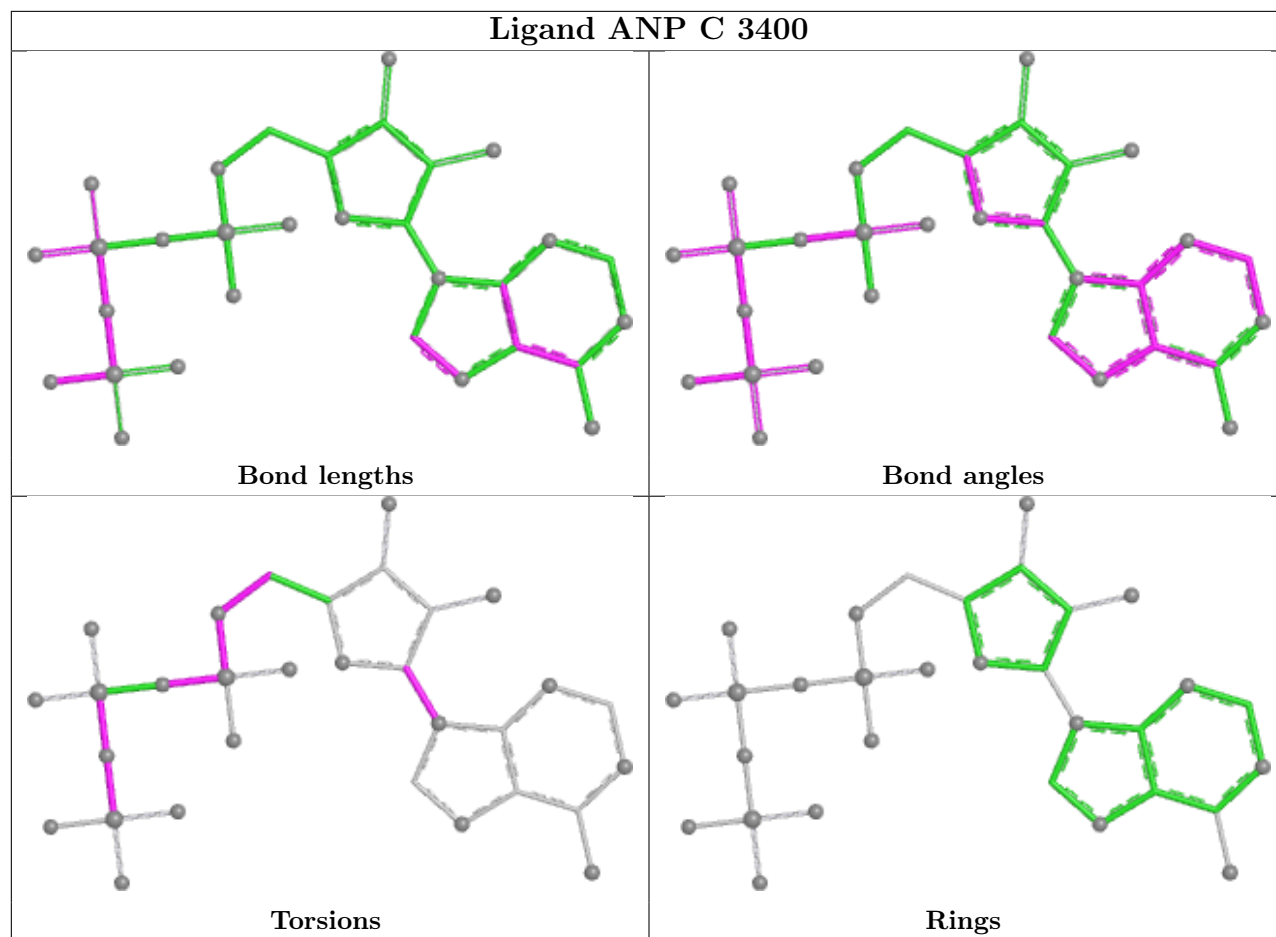
17 monomers are involved in 34 short contacts:

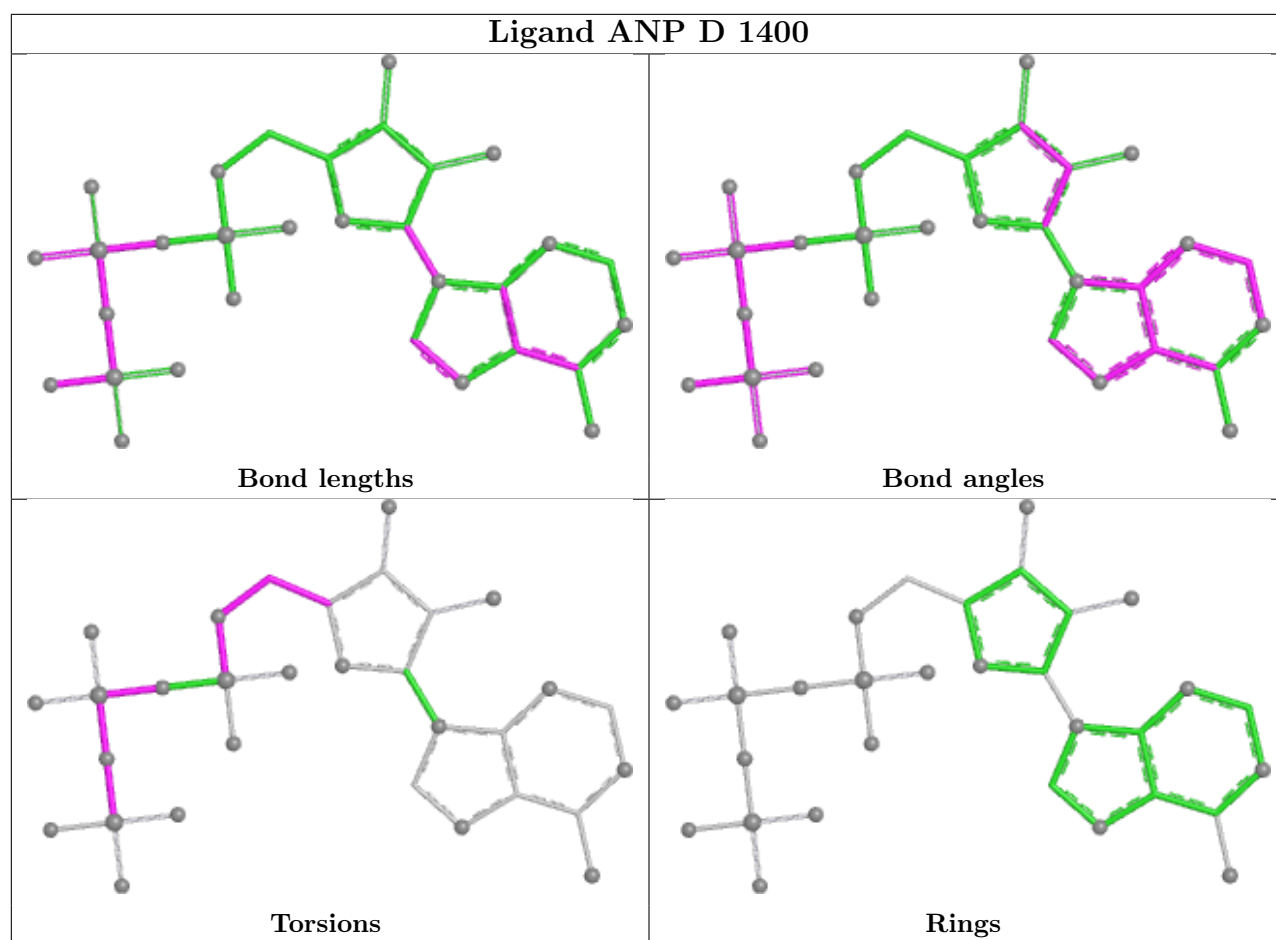
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3400	ANP	2	0
3	B	400	ANP	1	0
3	A	400	ANP	1	0
3	C	400	ANP	1	0
3	F	3400	ANP	3	0
3	A	3400	ANP	3	0
3	G	3400	ANP	2	0
3	H	400	ANP	1	0
3	H	3400	ANP	3	0
3	B	3400	ANP	1	0
3	E	400	ANP	1	0
3	D	3400	ANP	2	0
3	E	1400	ANP	1	0
3	E	3400	ANP	1	0
3	G	400	ANP	2	0
3	A	1400	ANP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

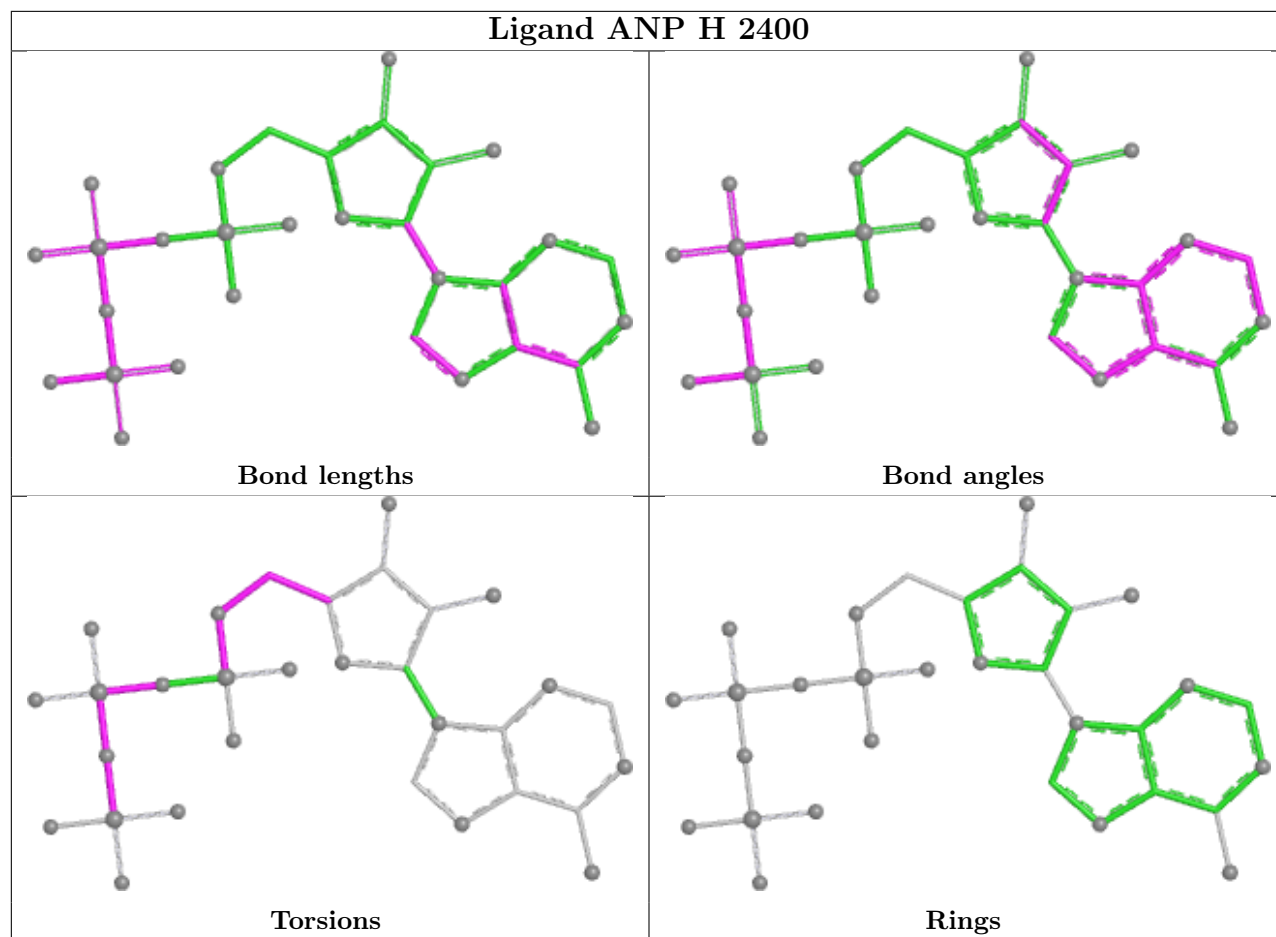
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

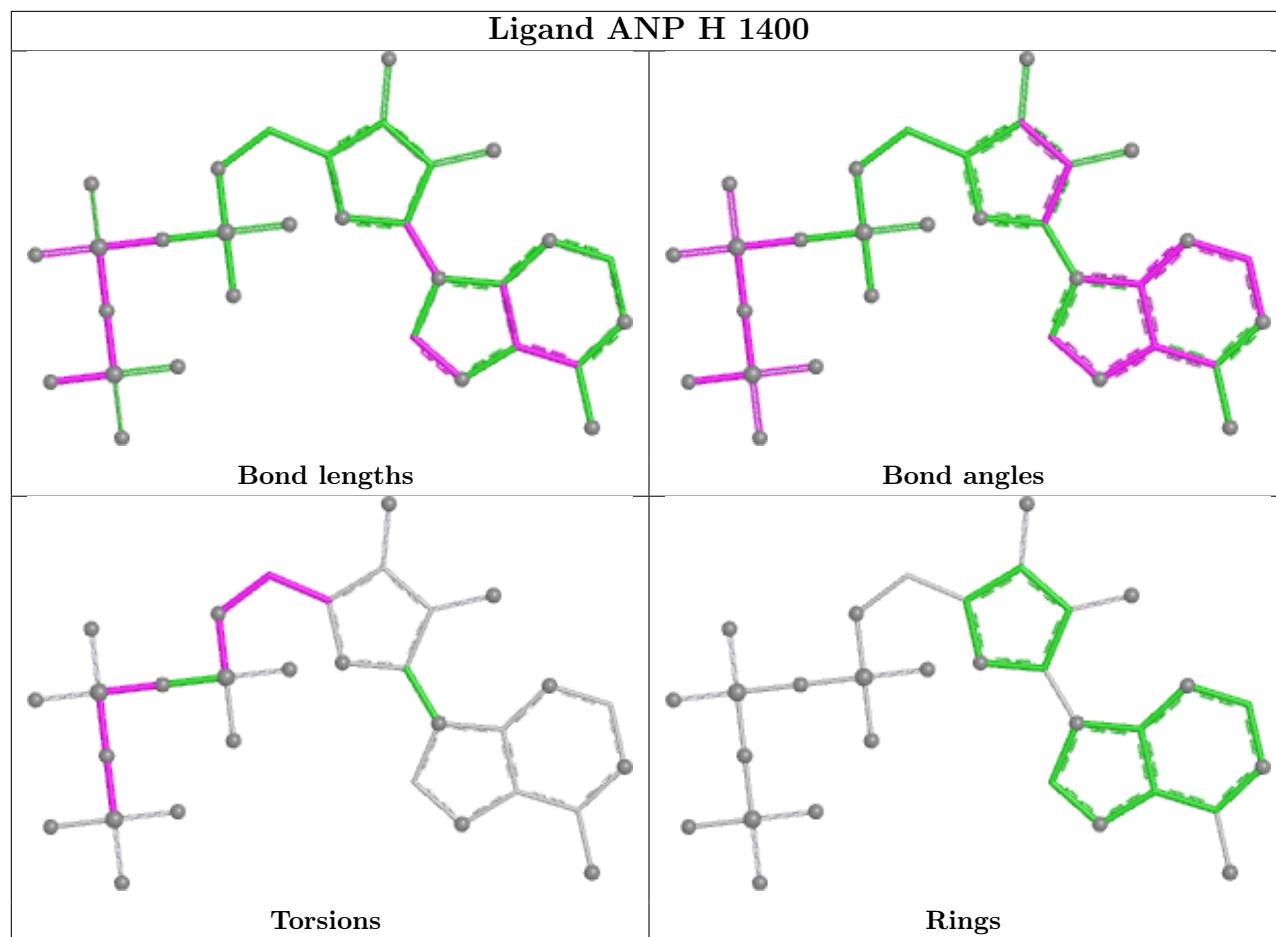
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

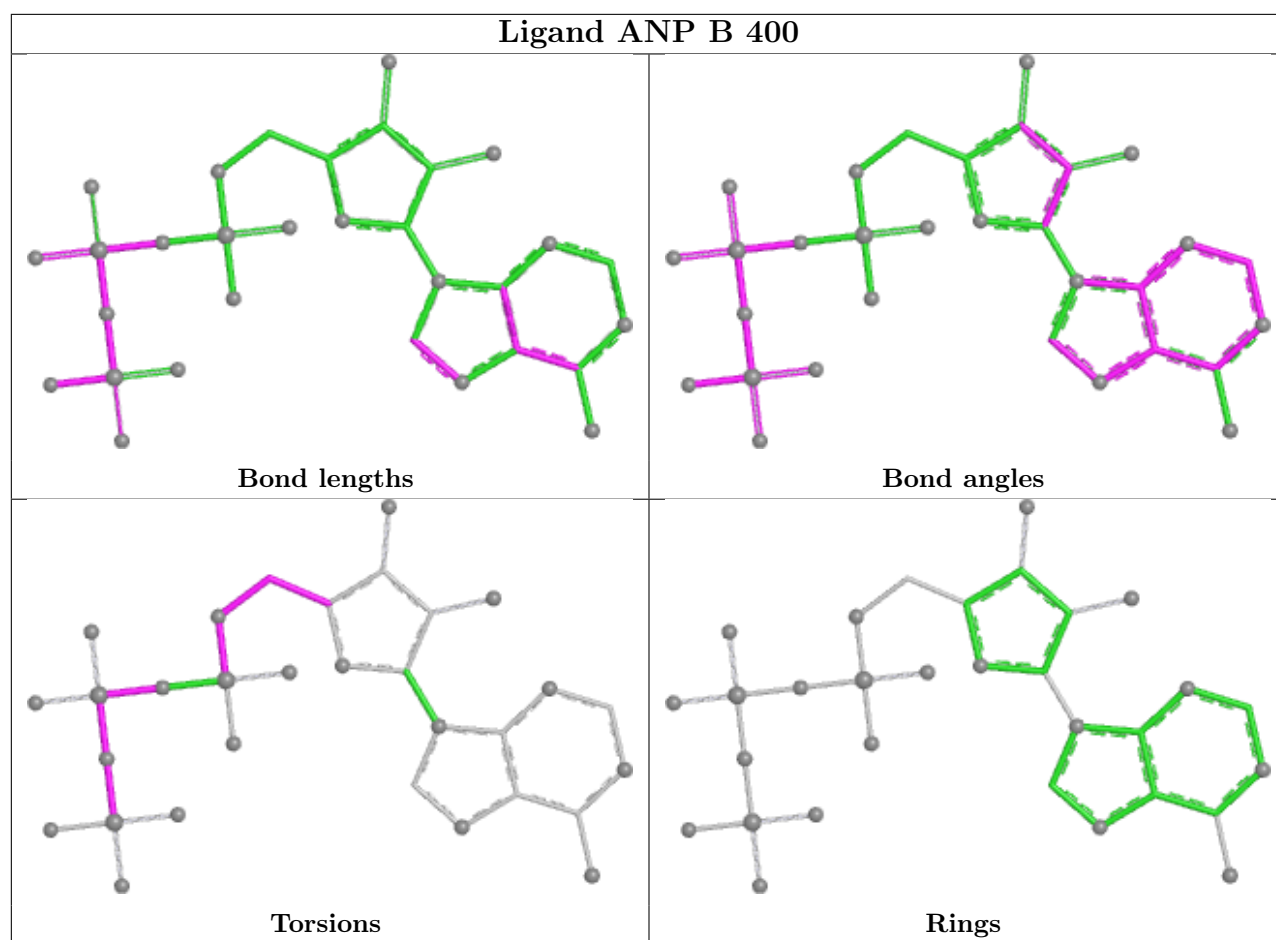


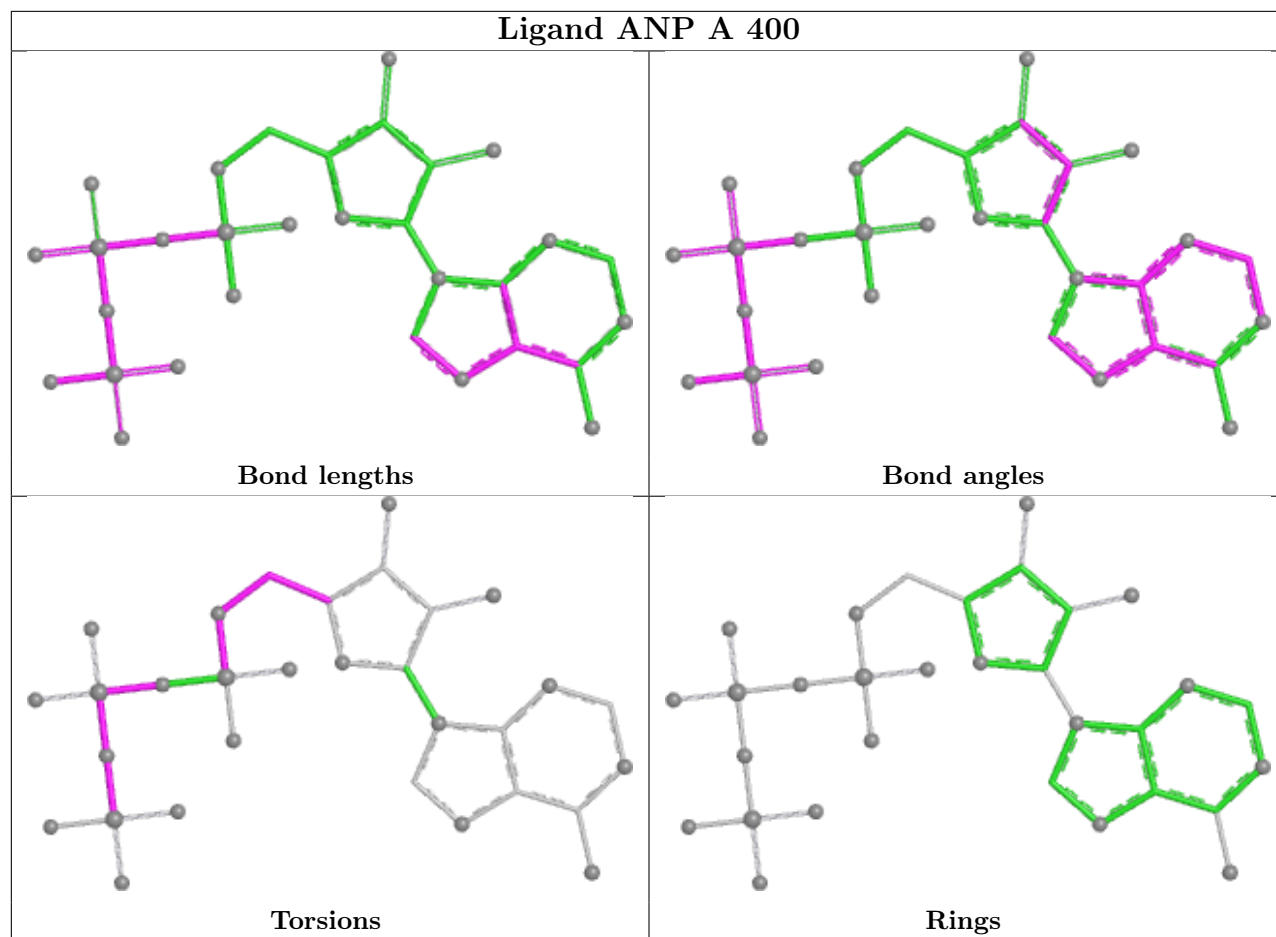


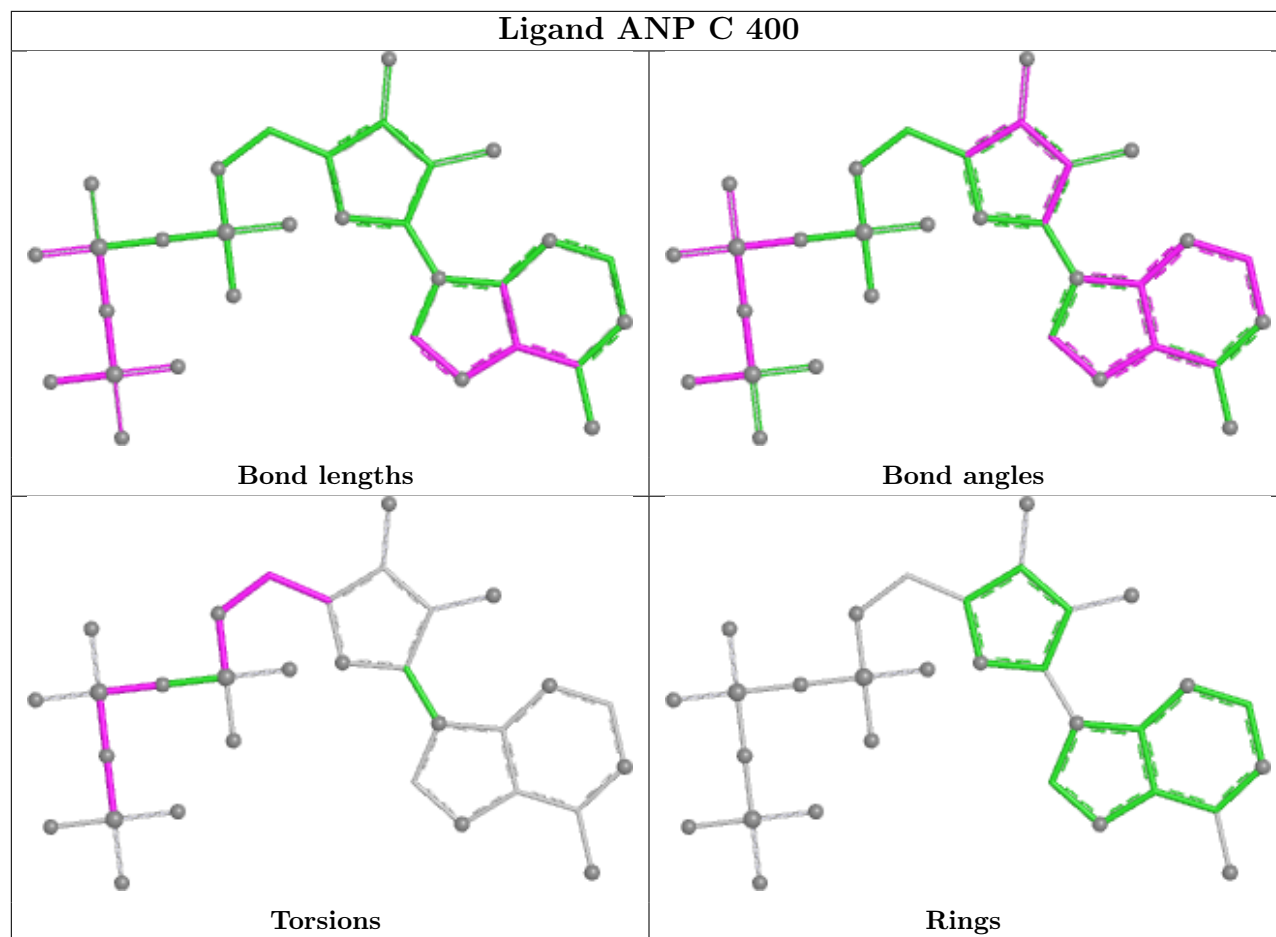


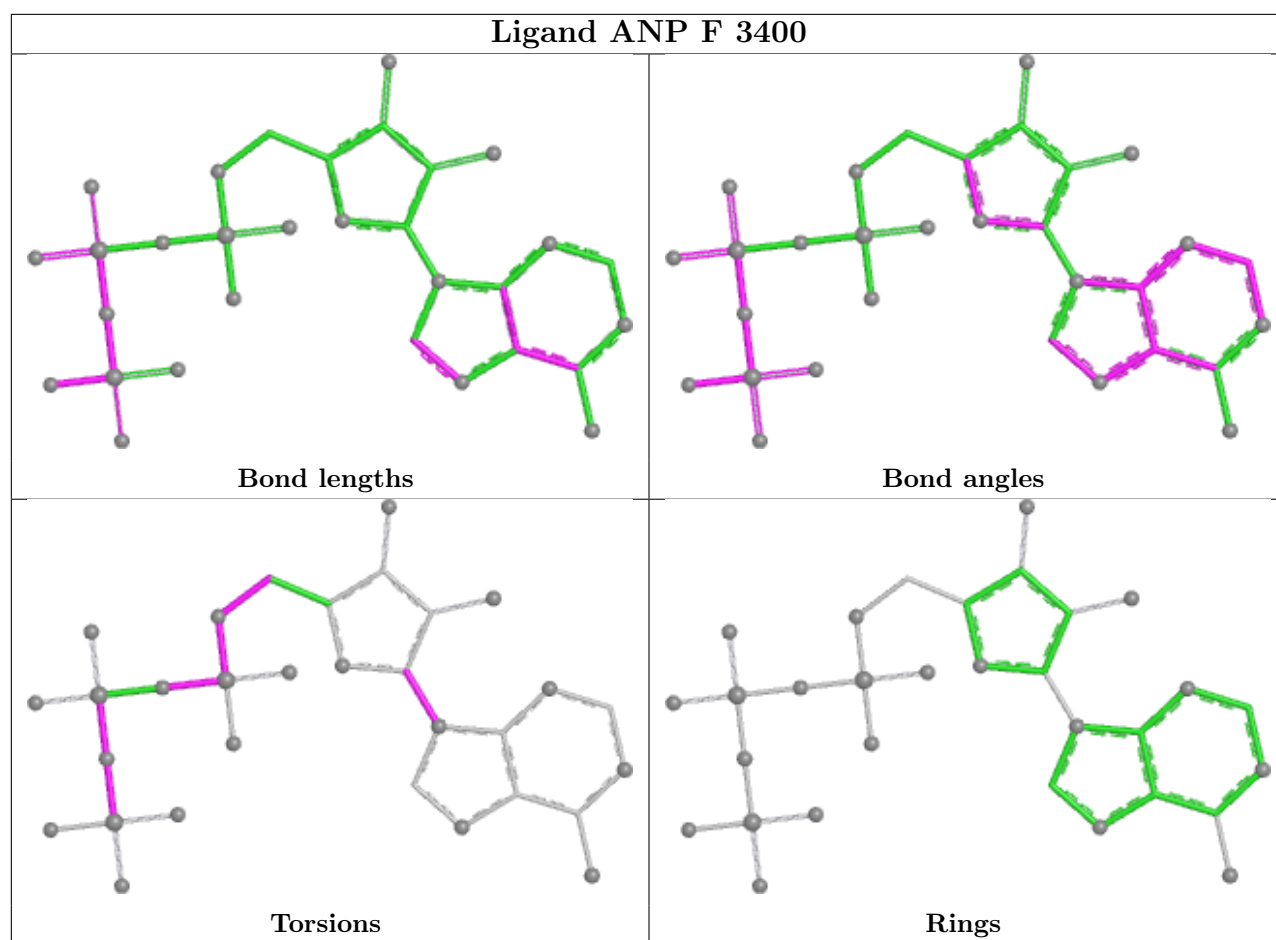


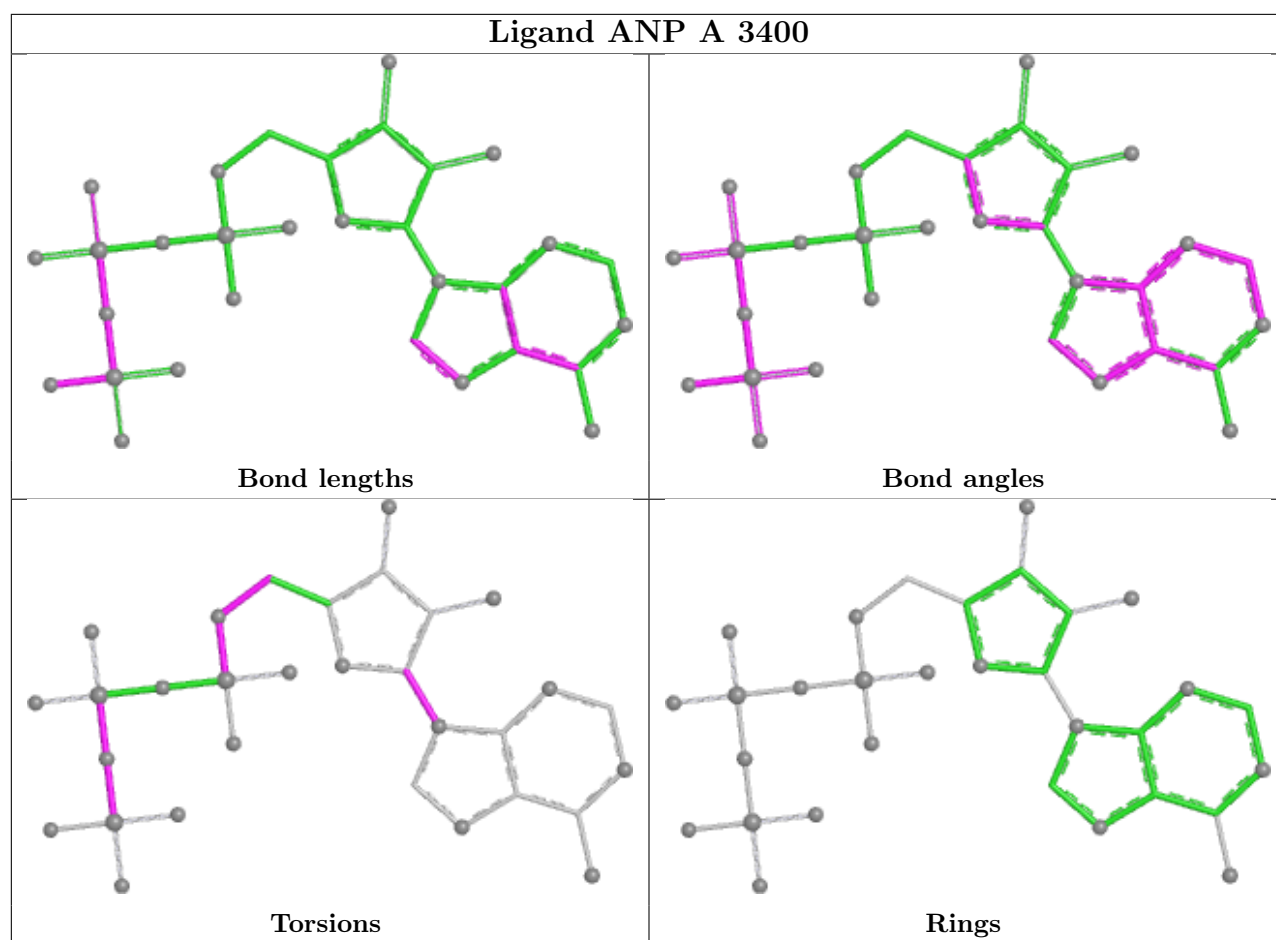


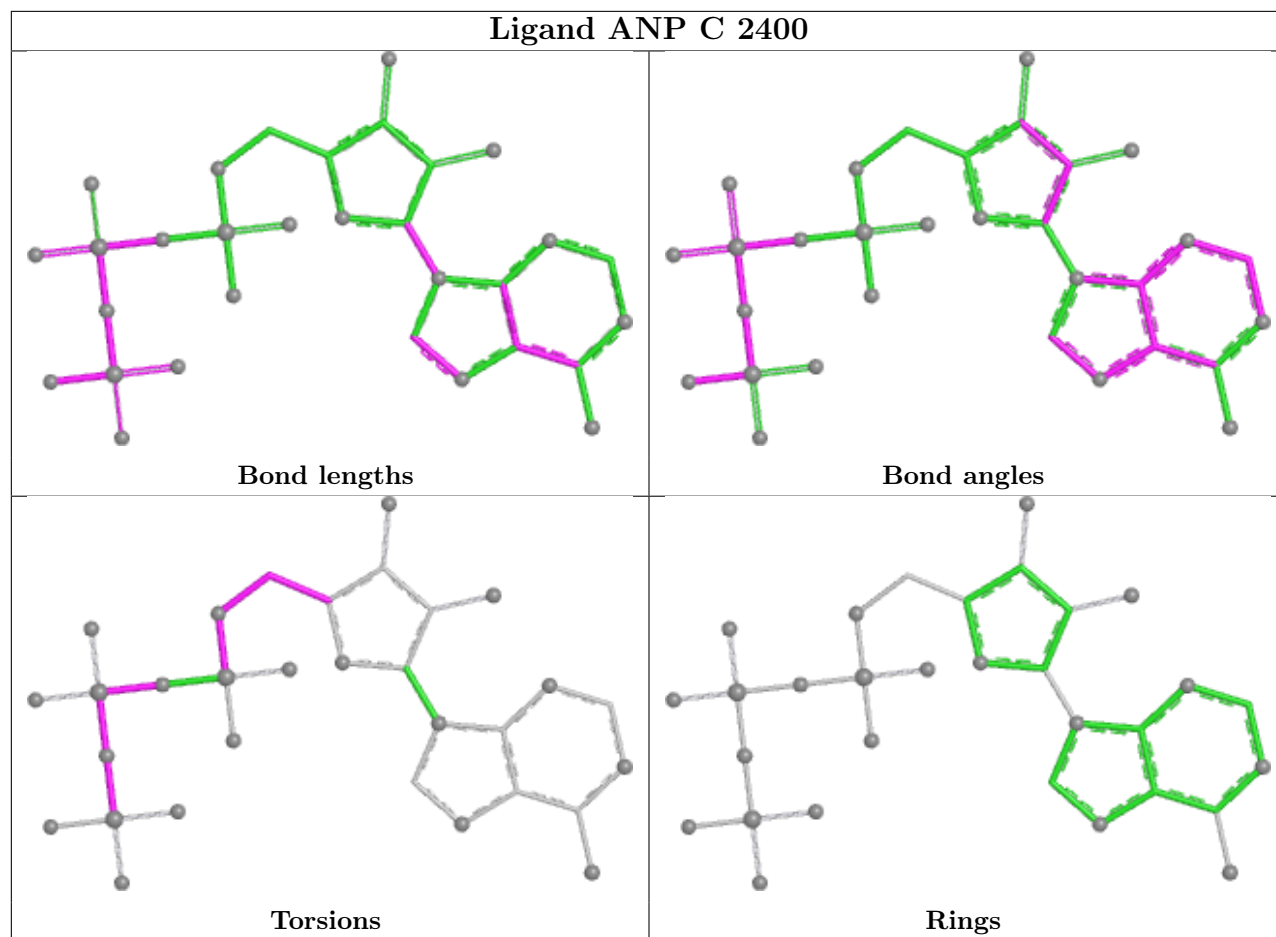


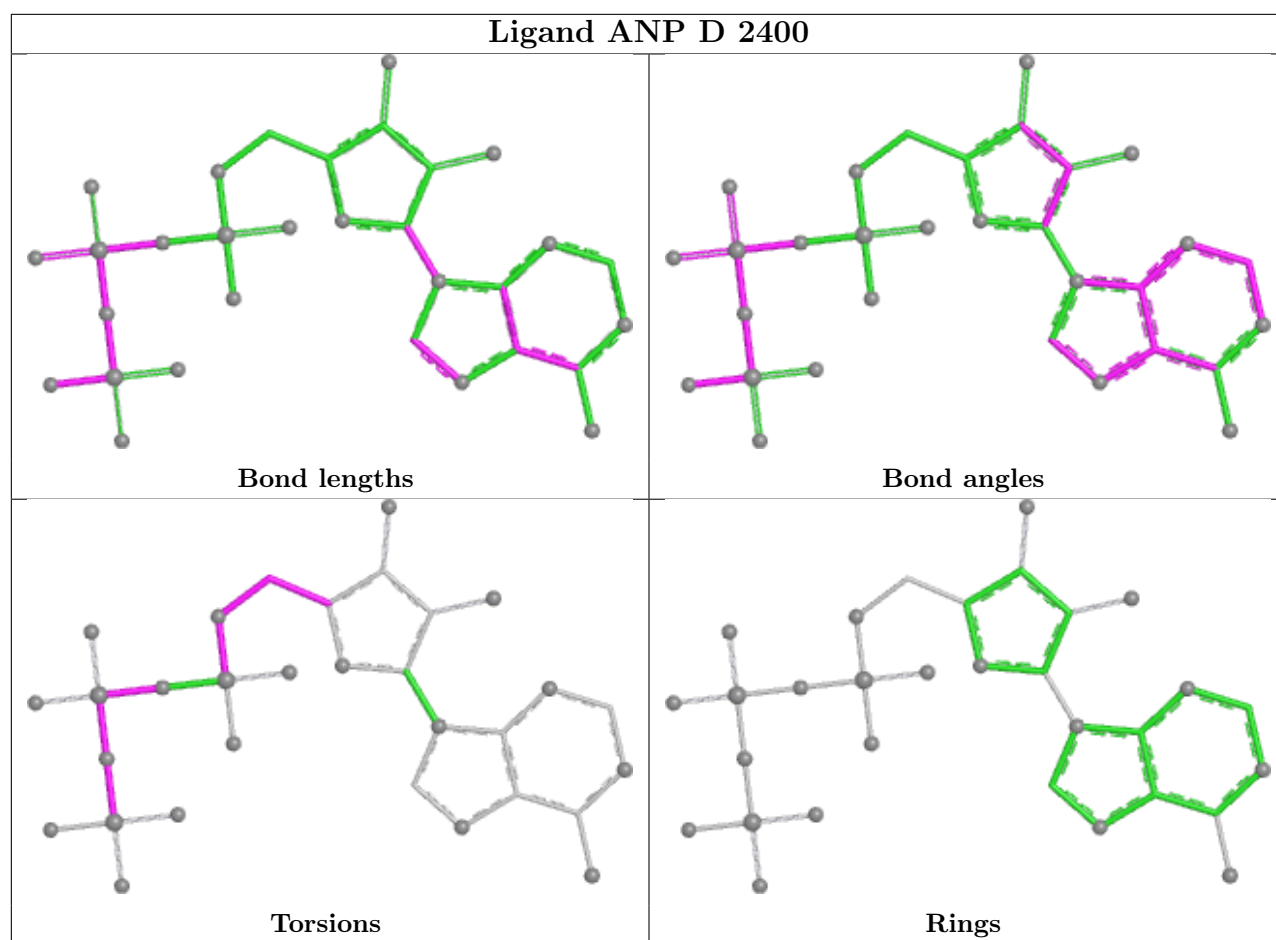


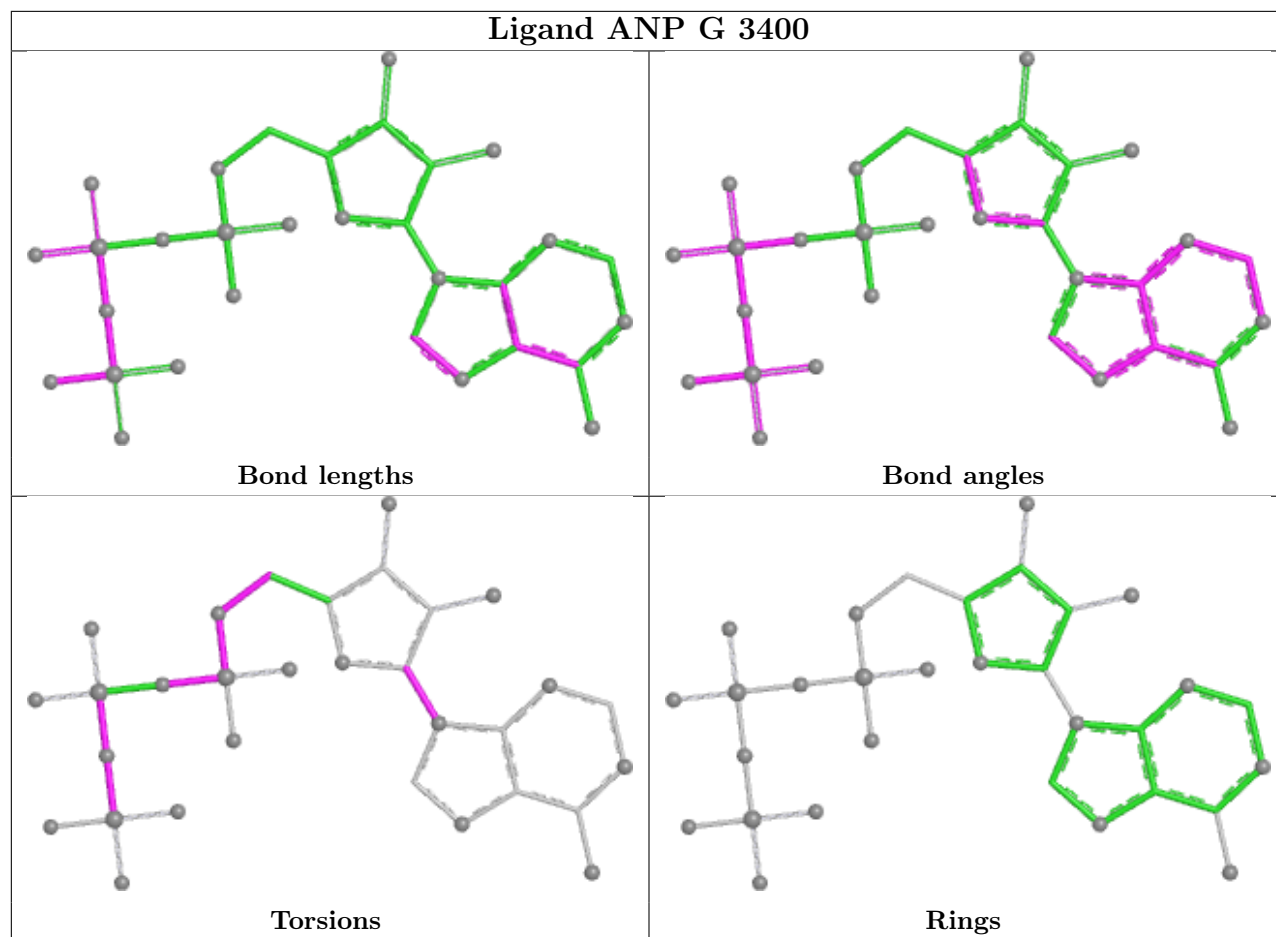


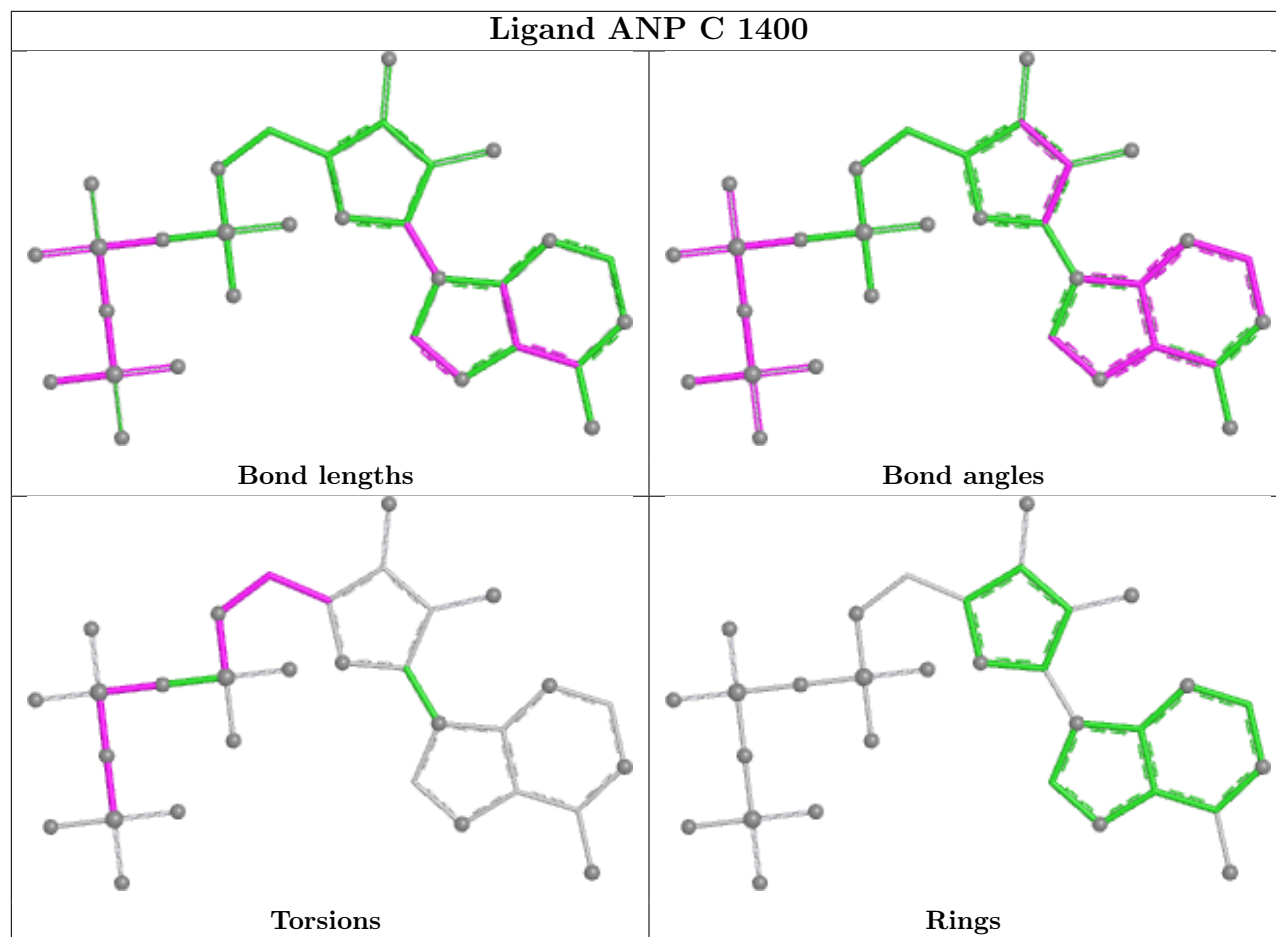


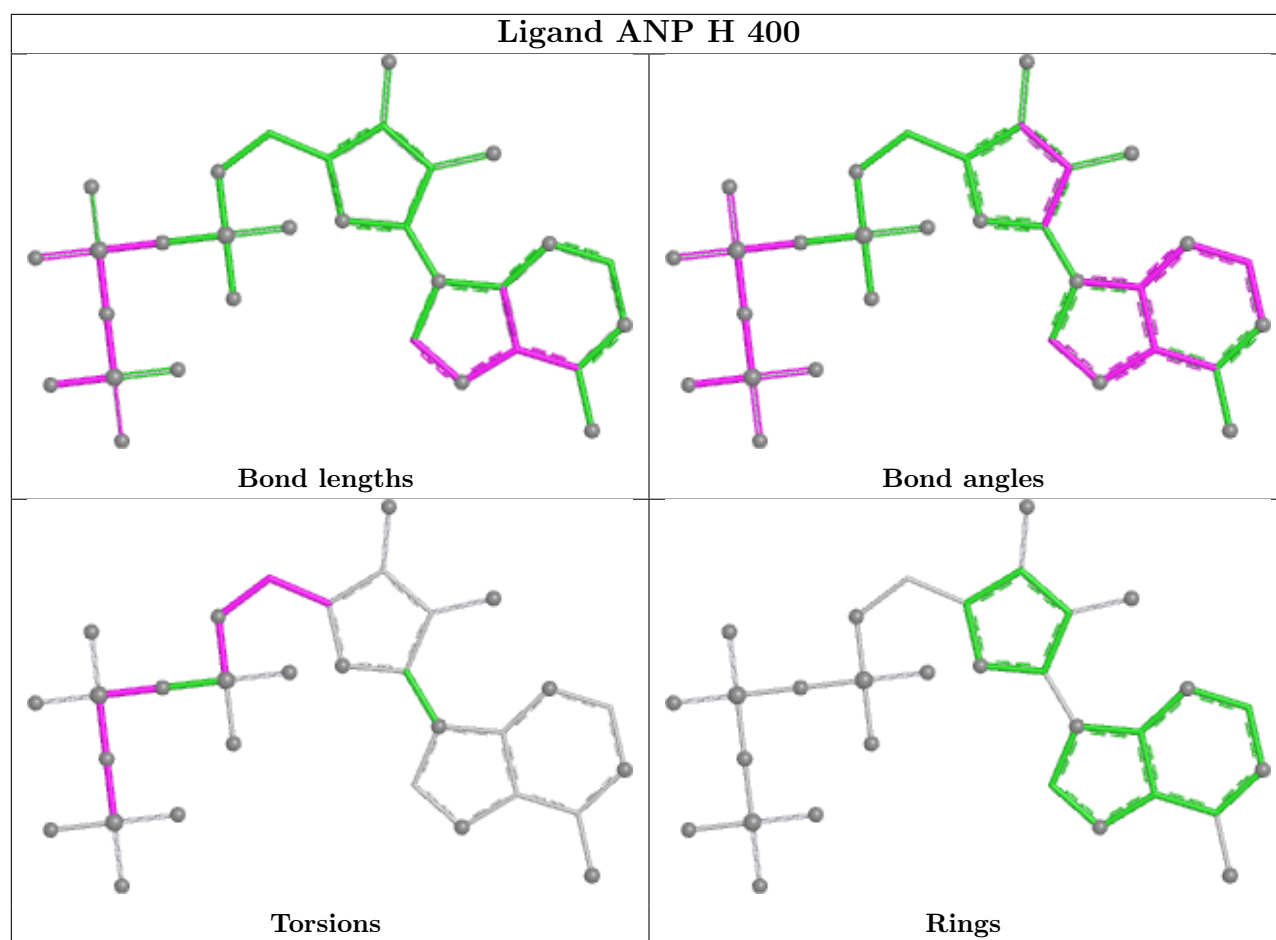


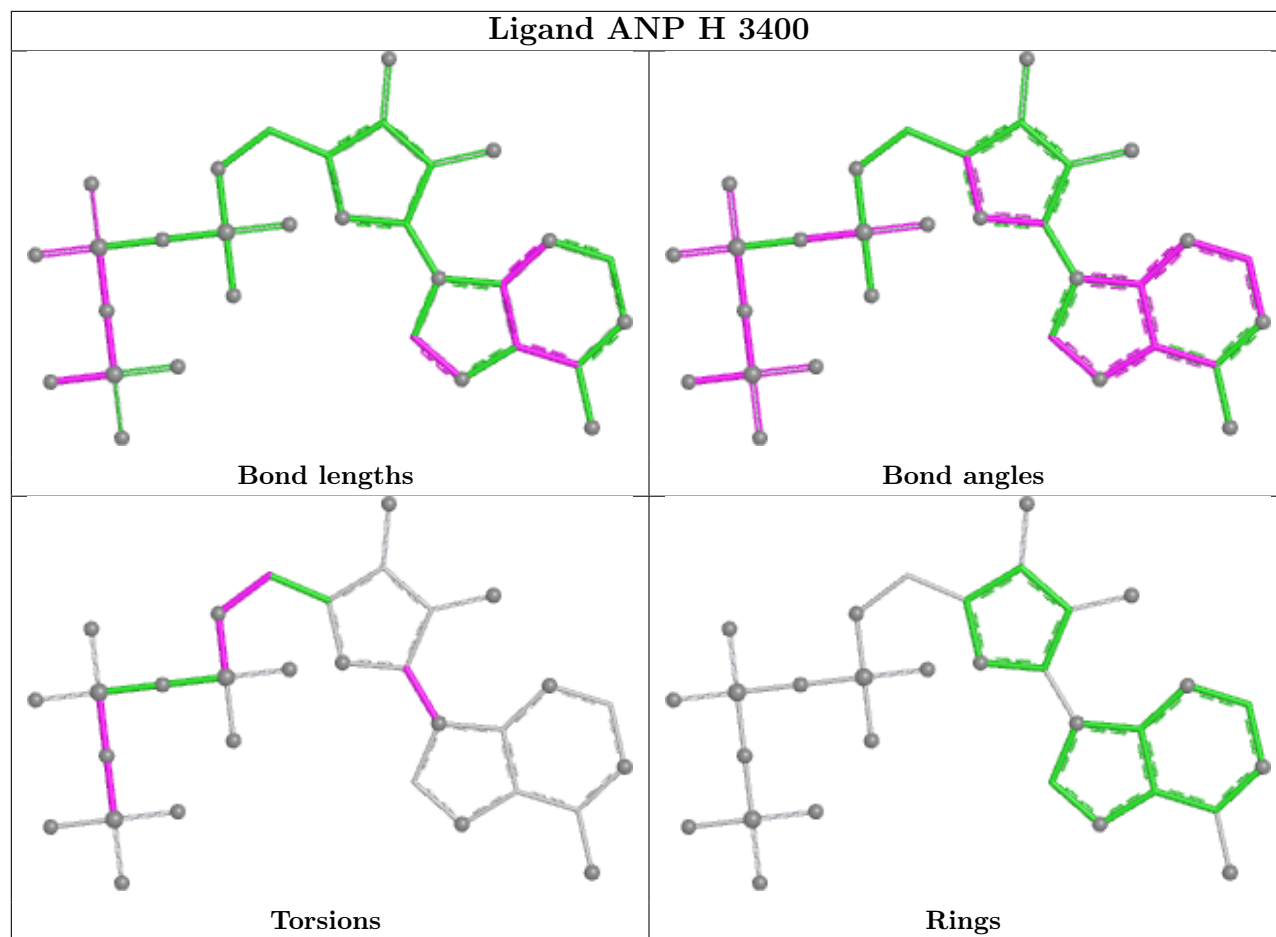


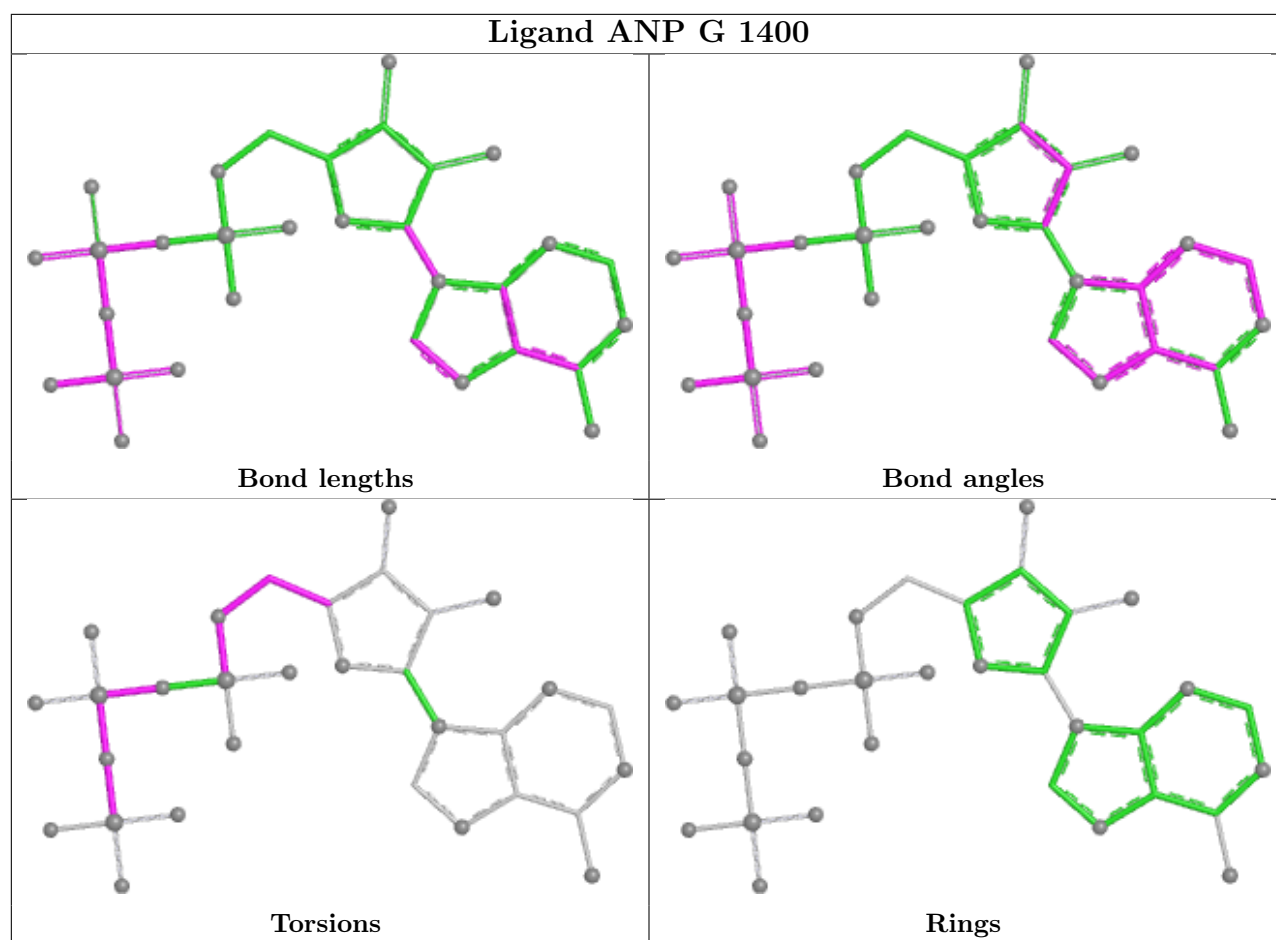


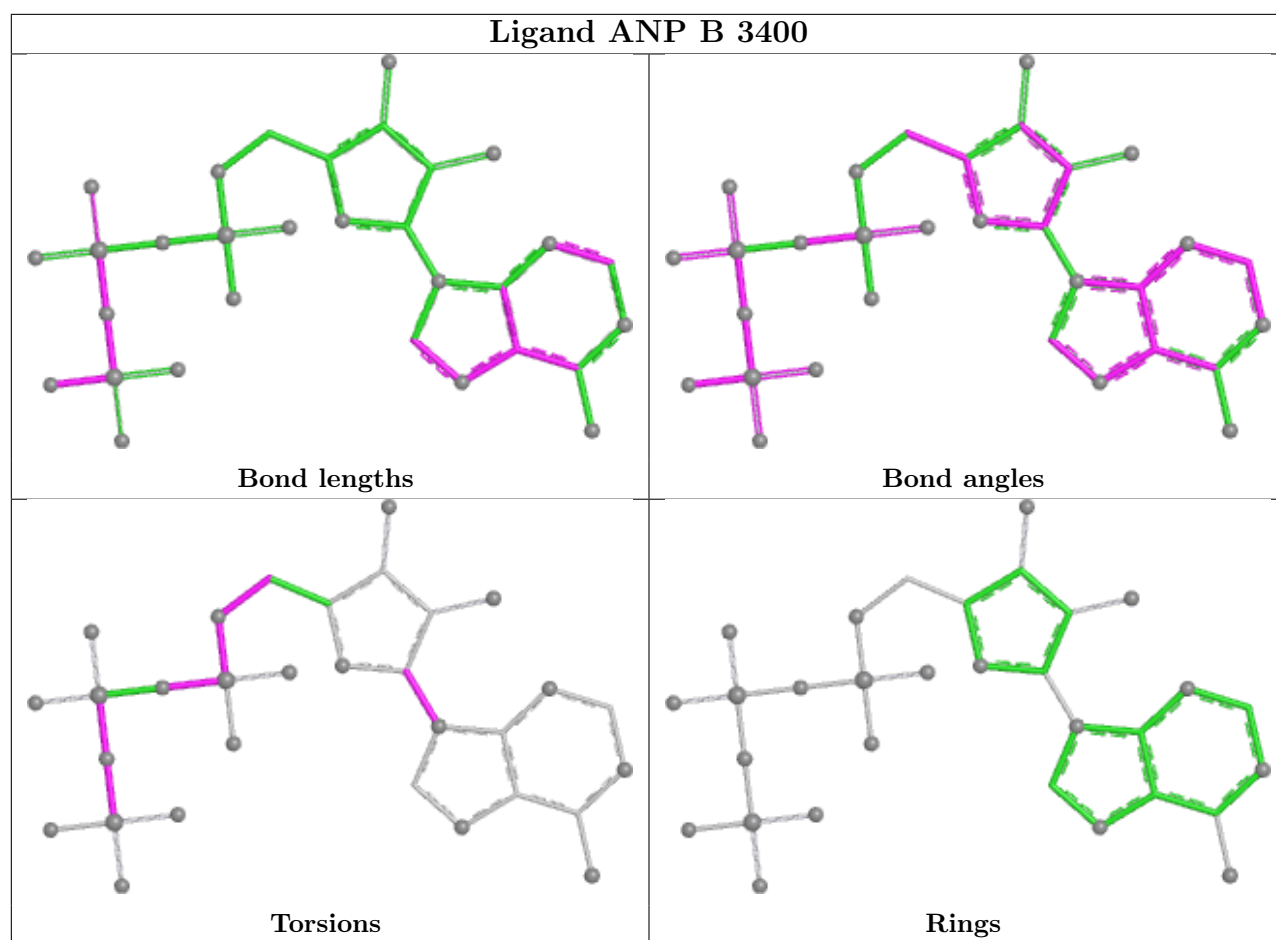


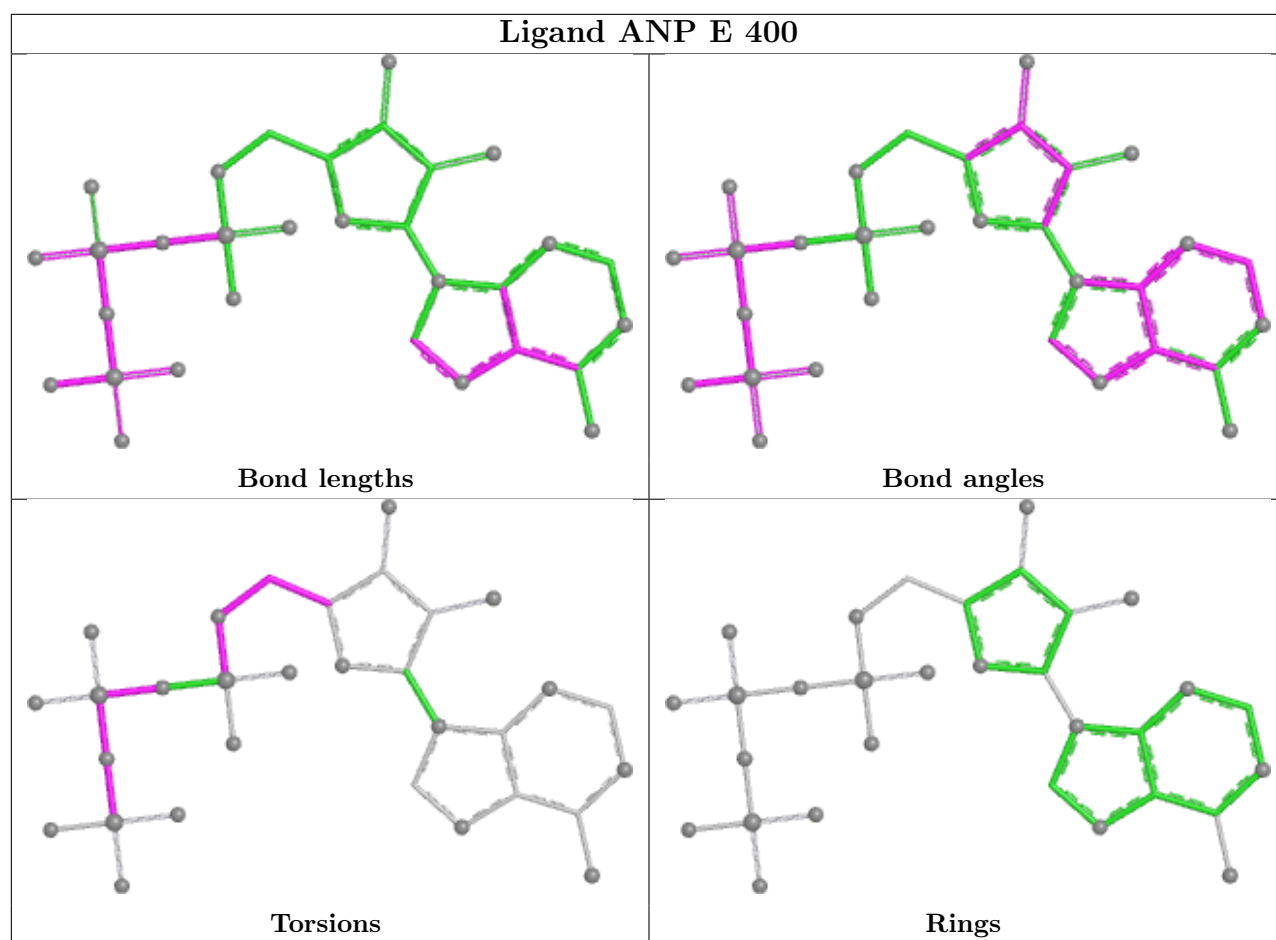


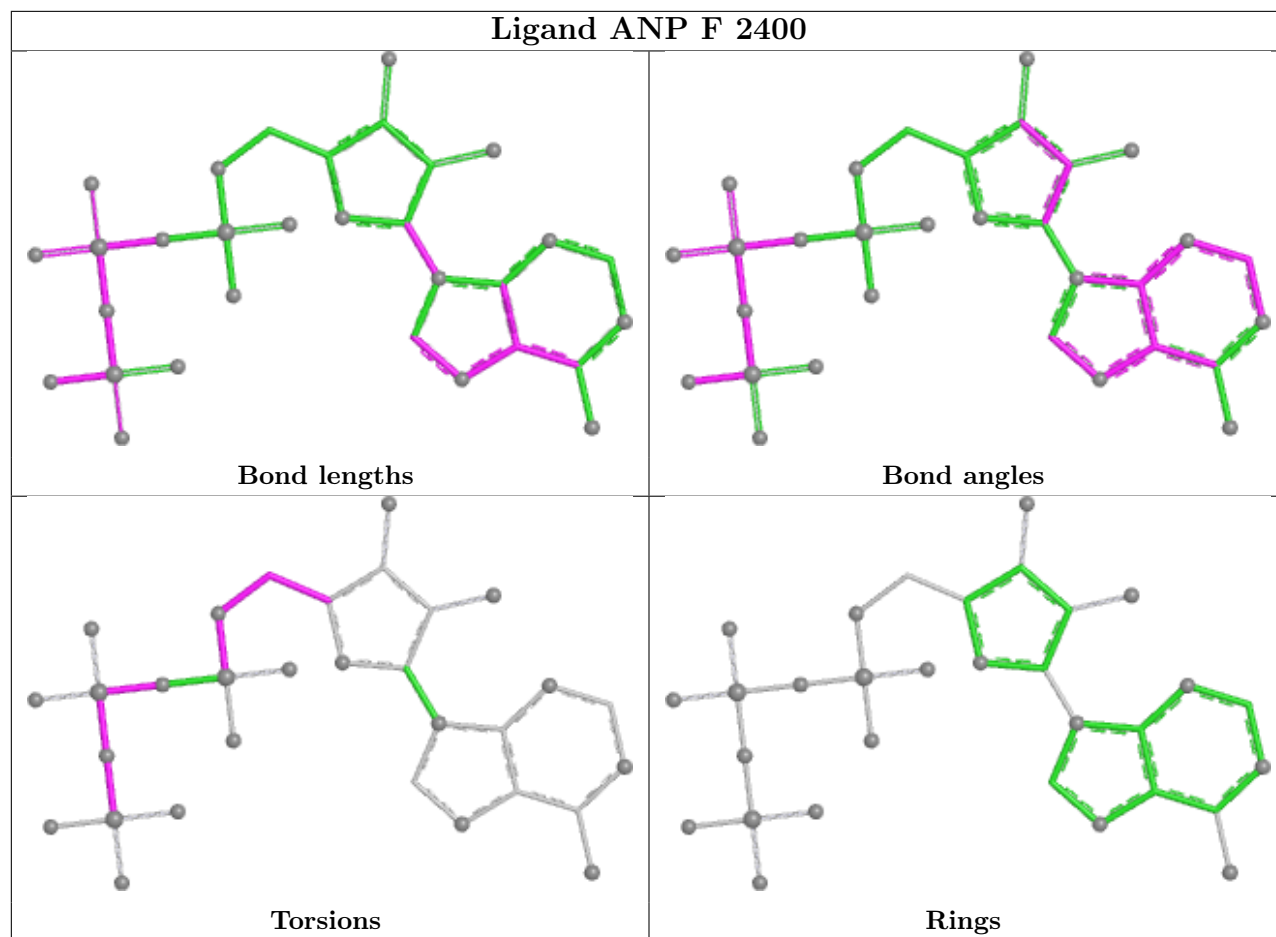


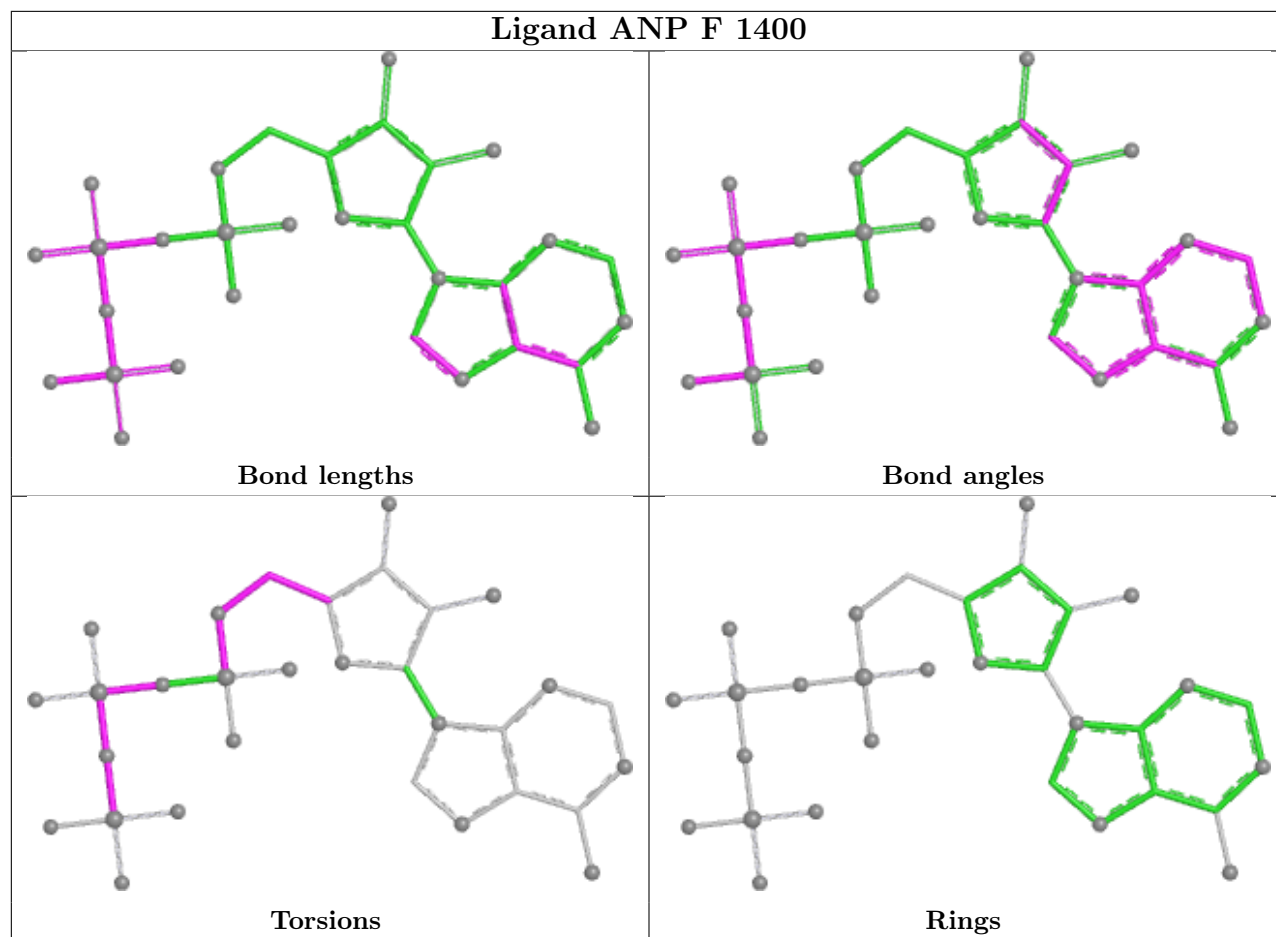


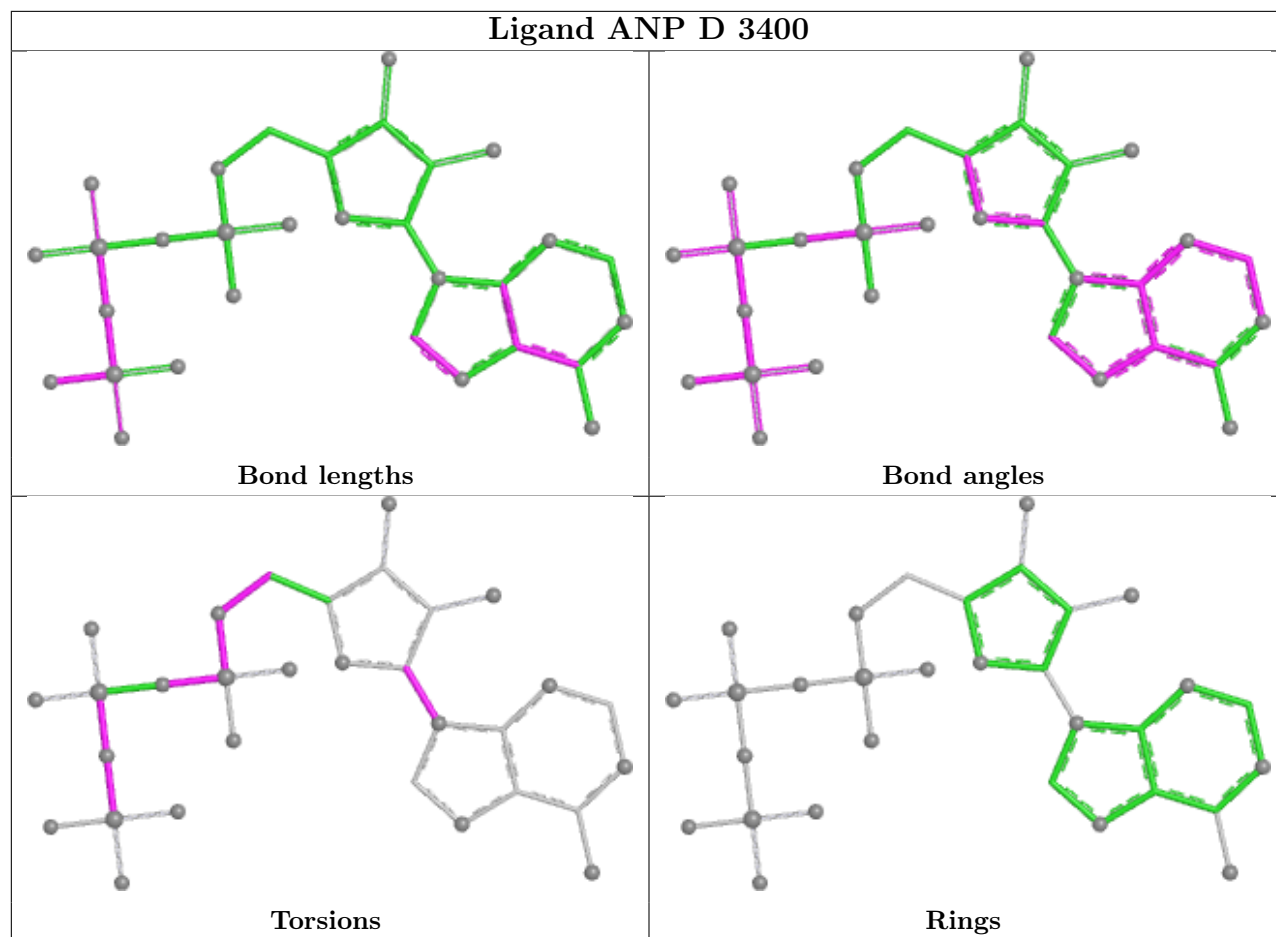


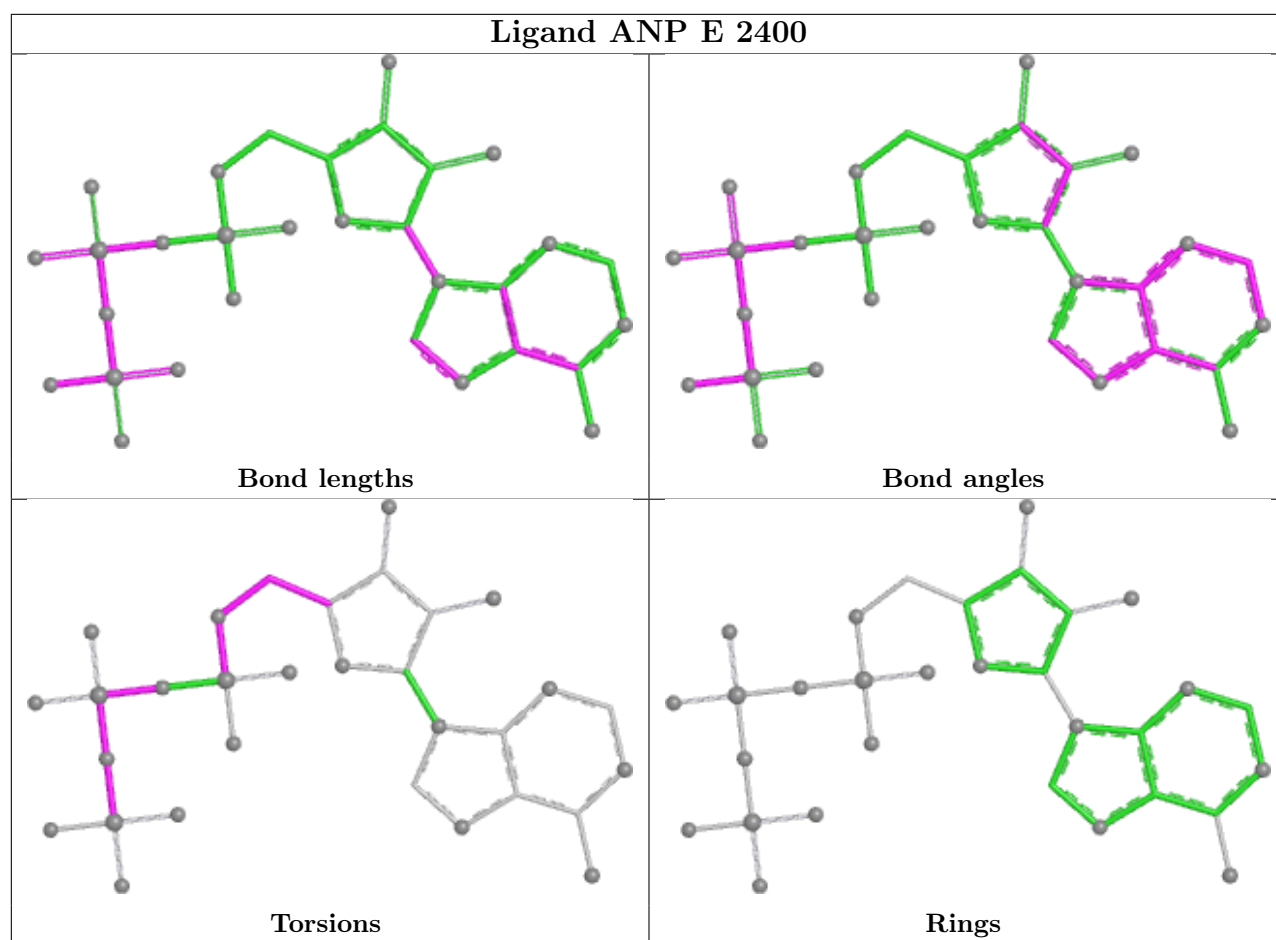


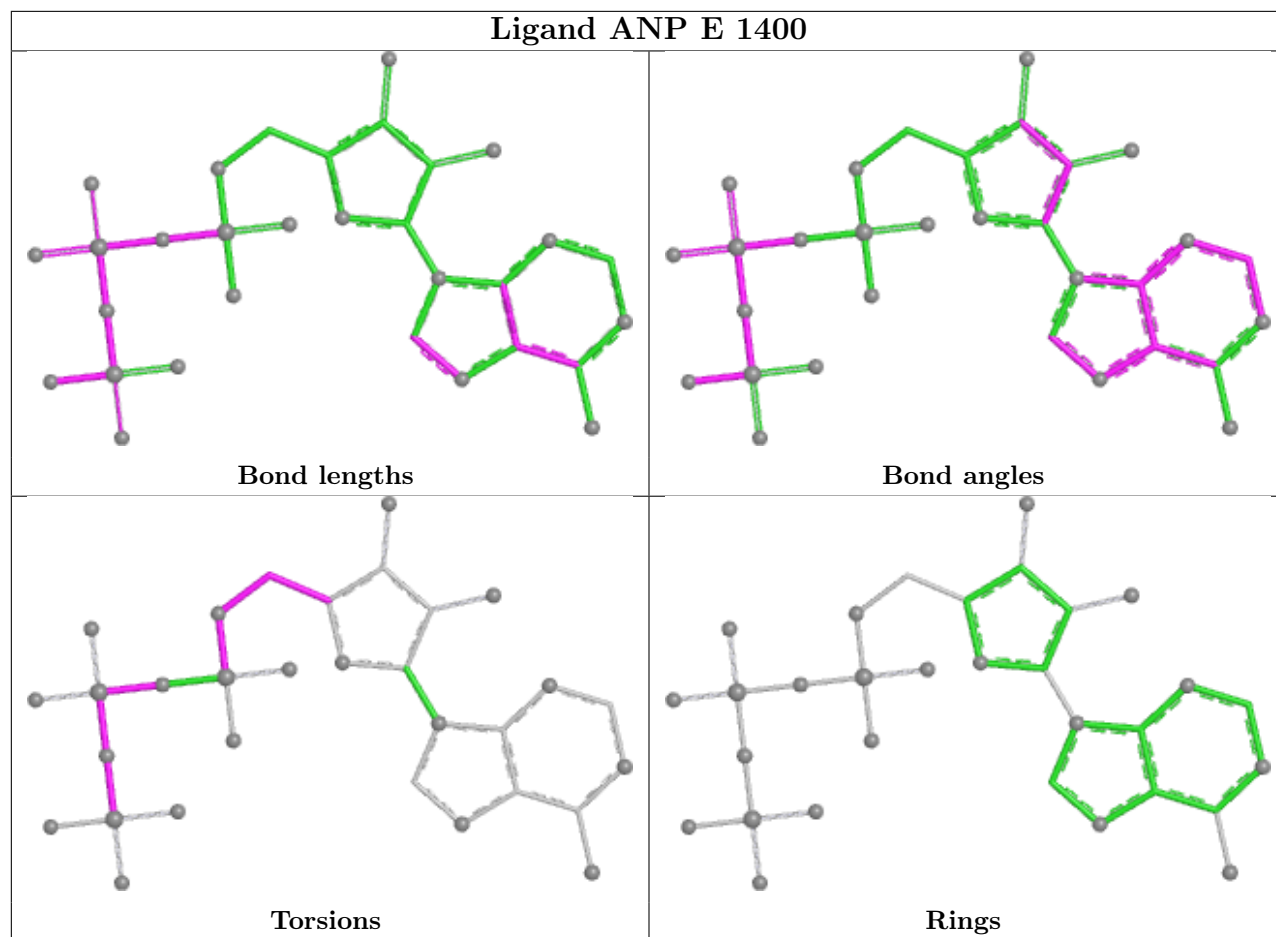


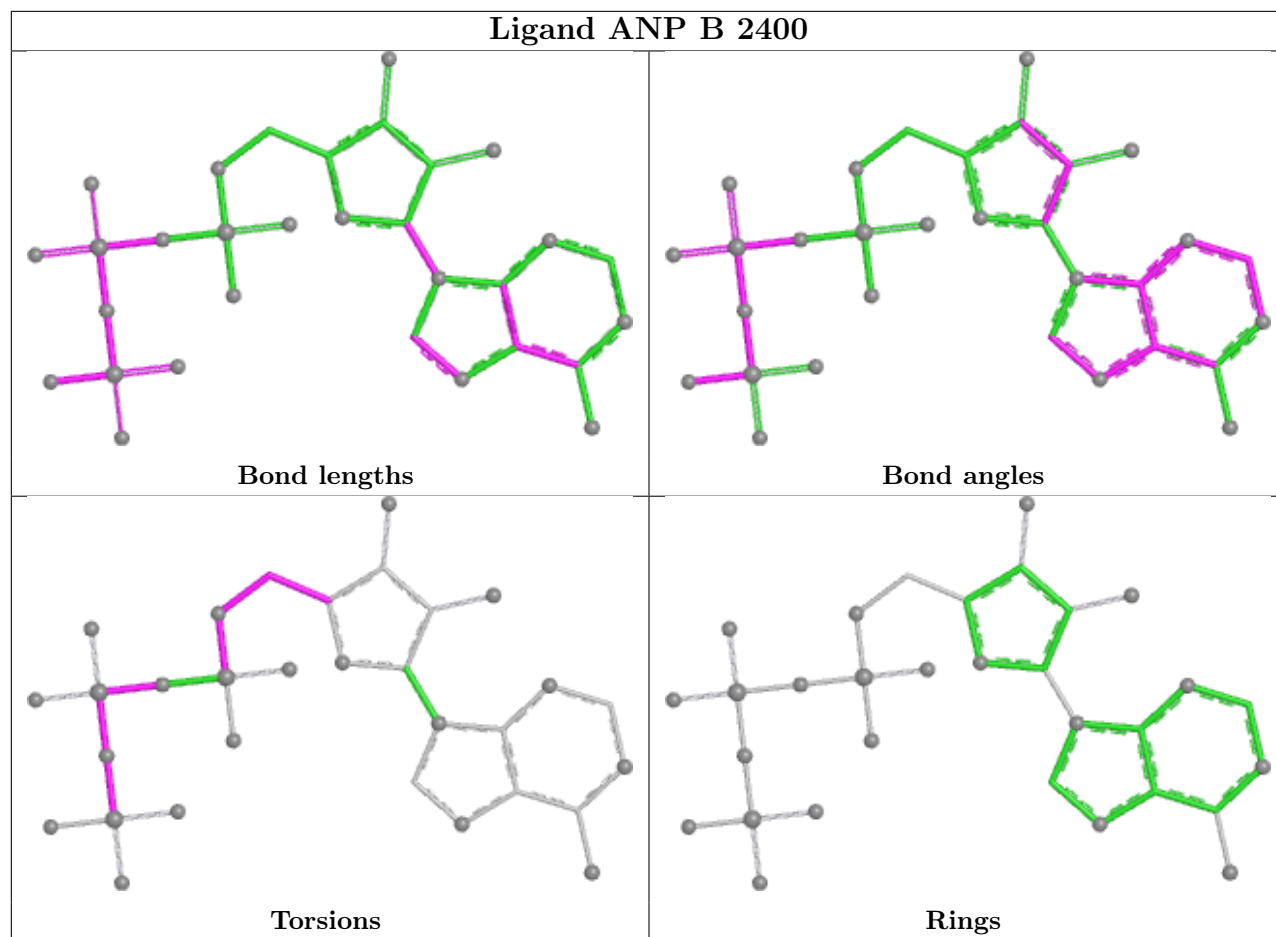


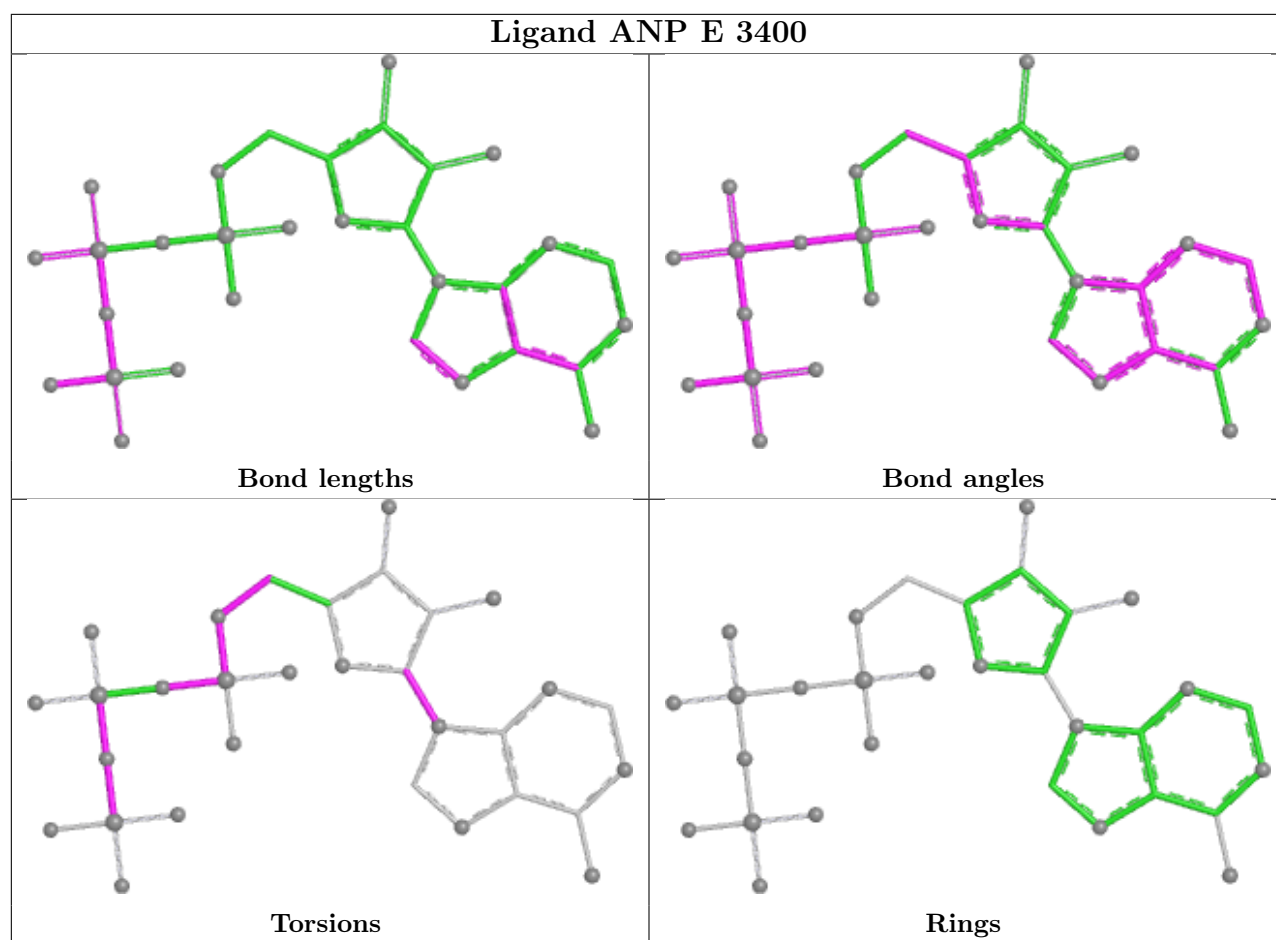


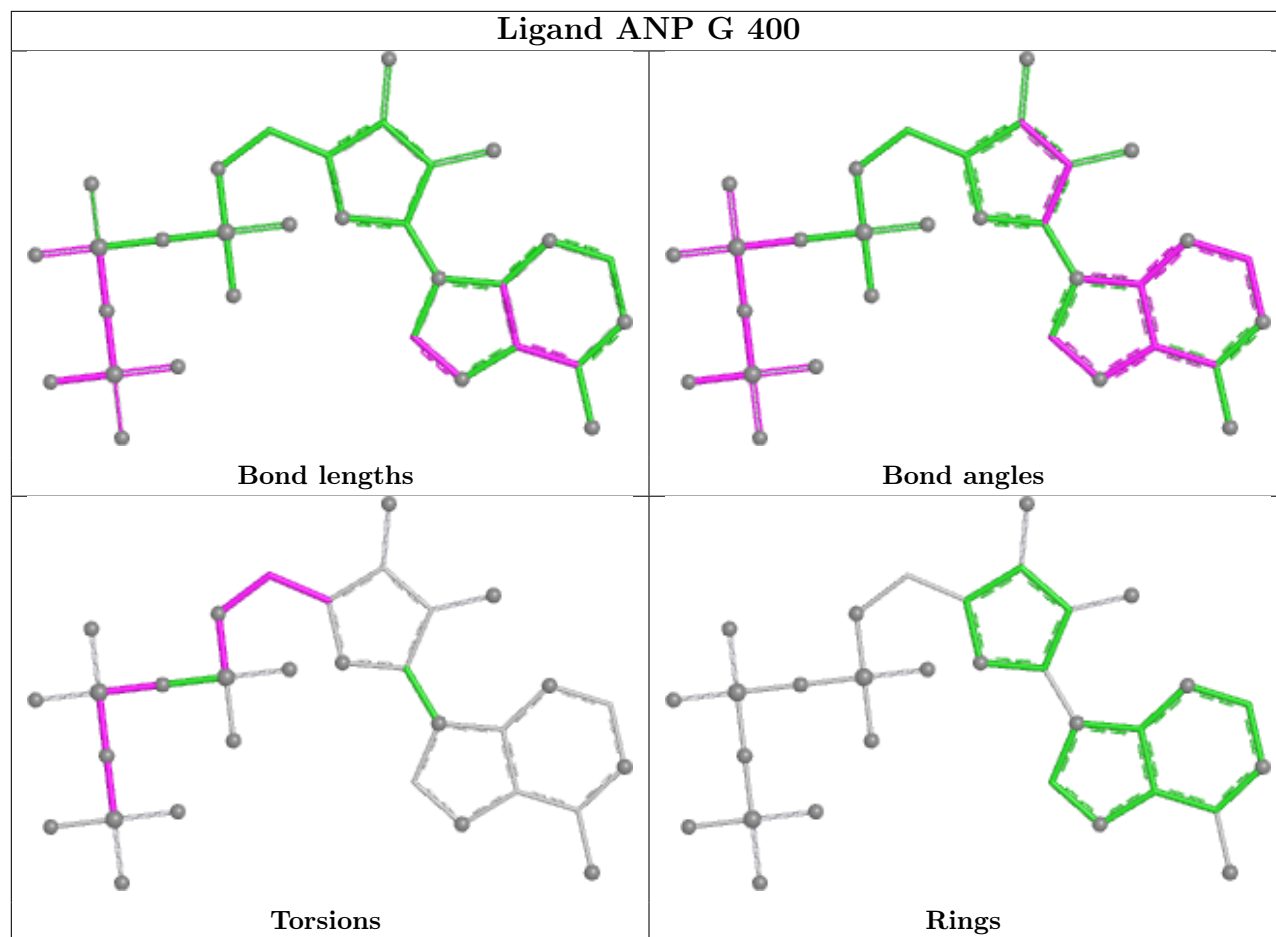


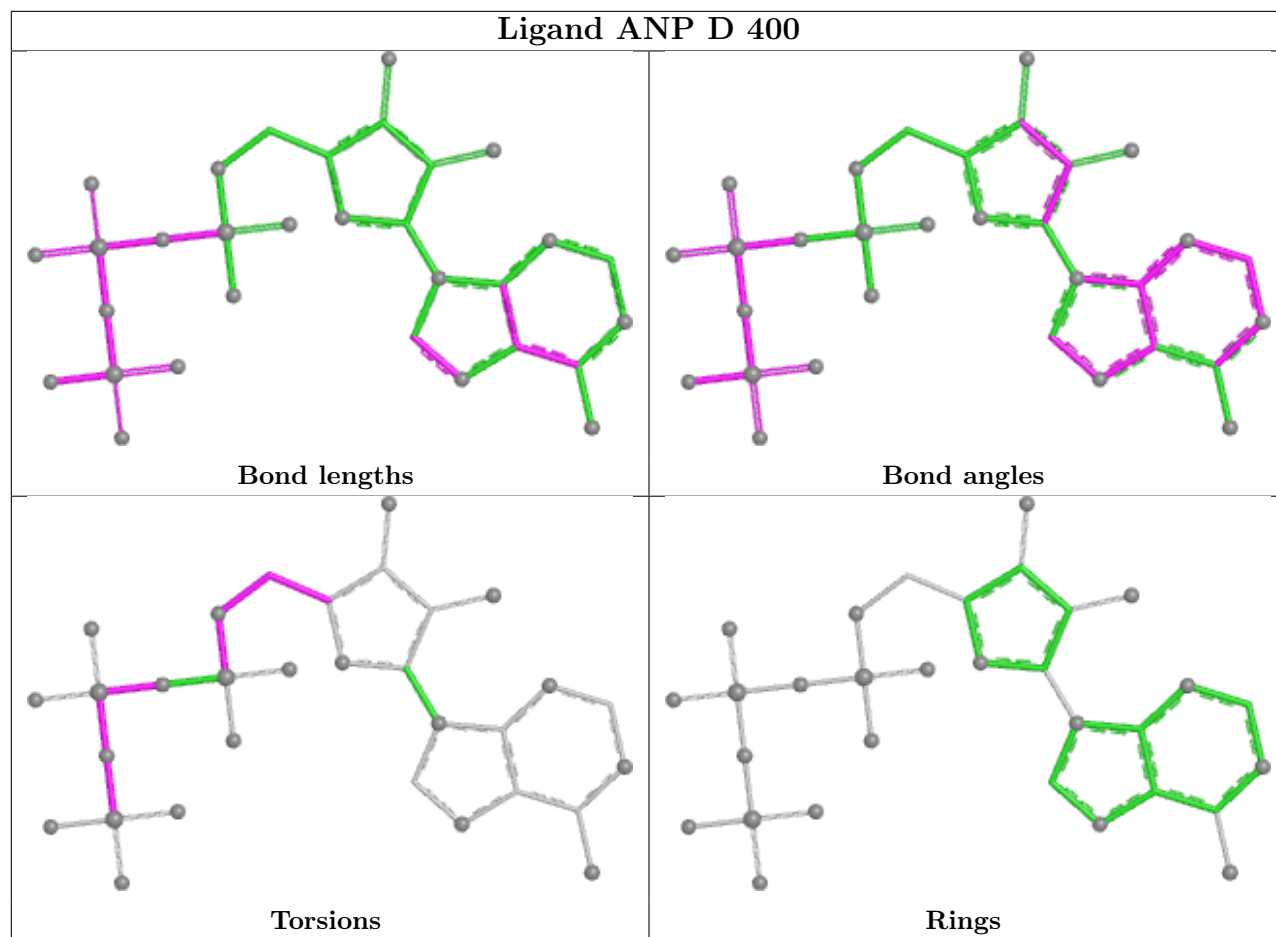


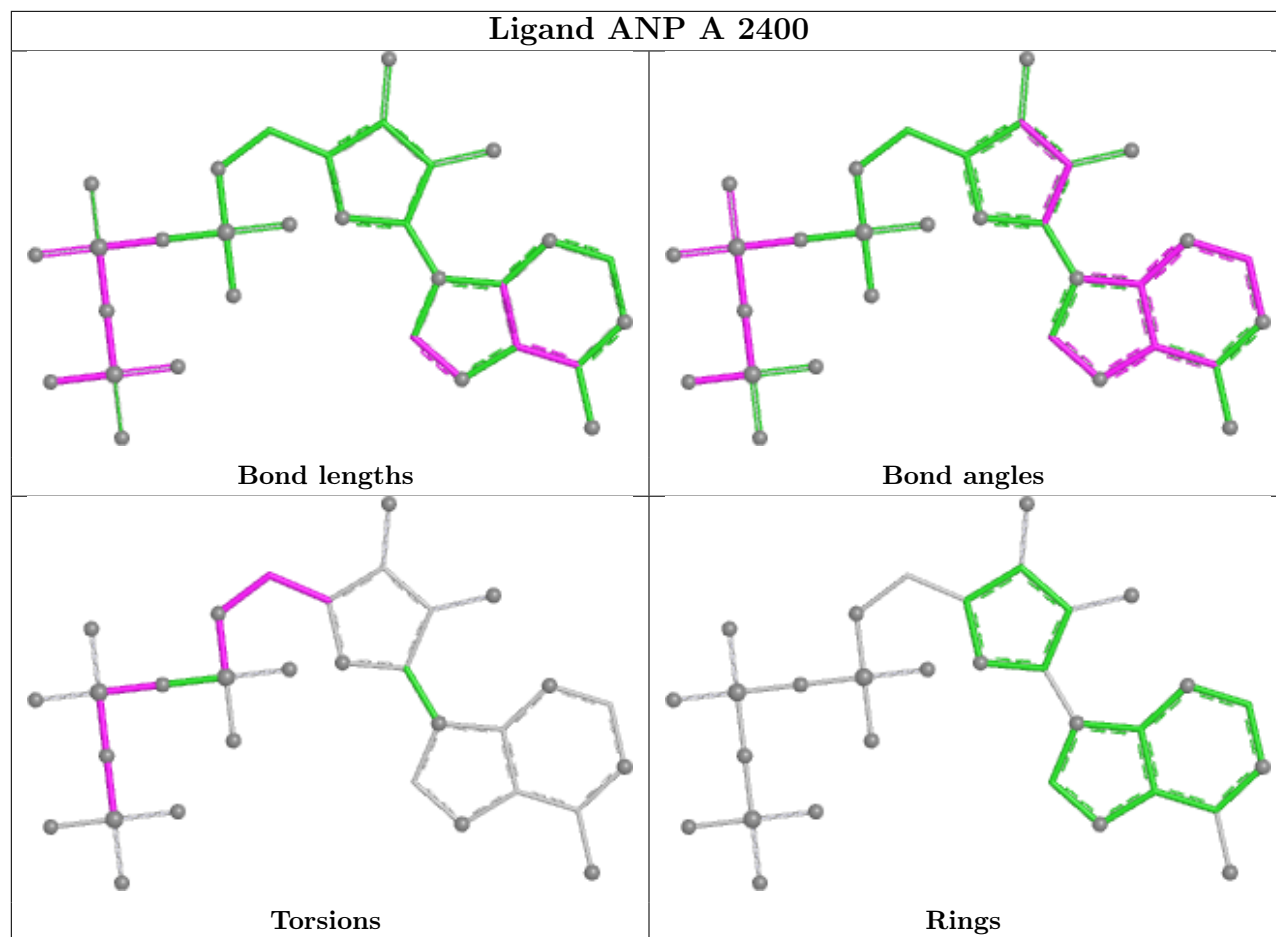


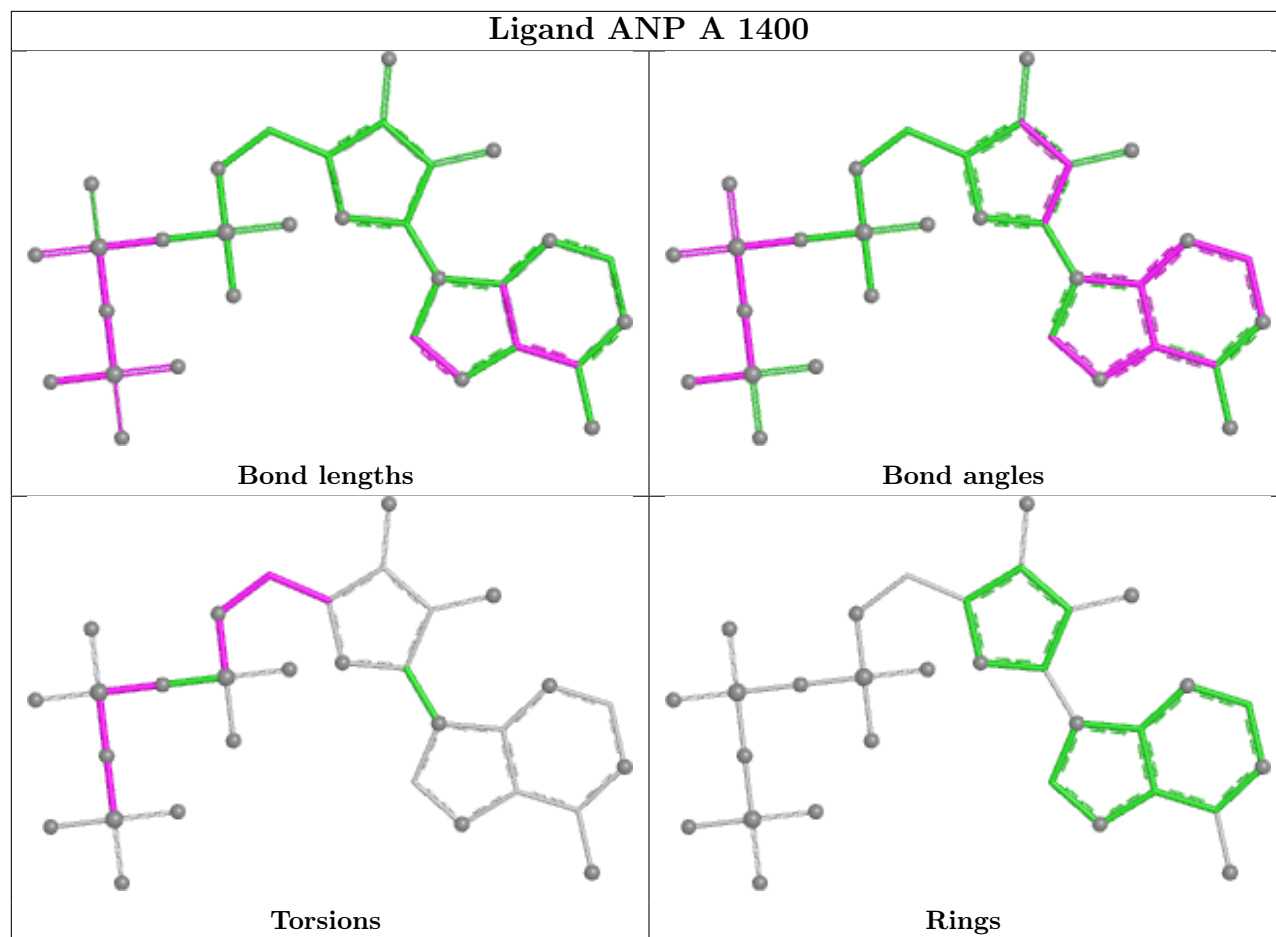


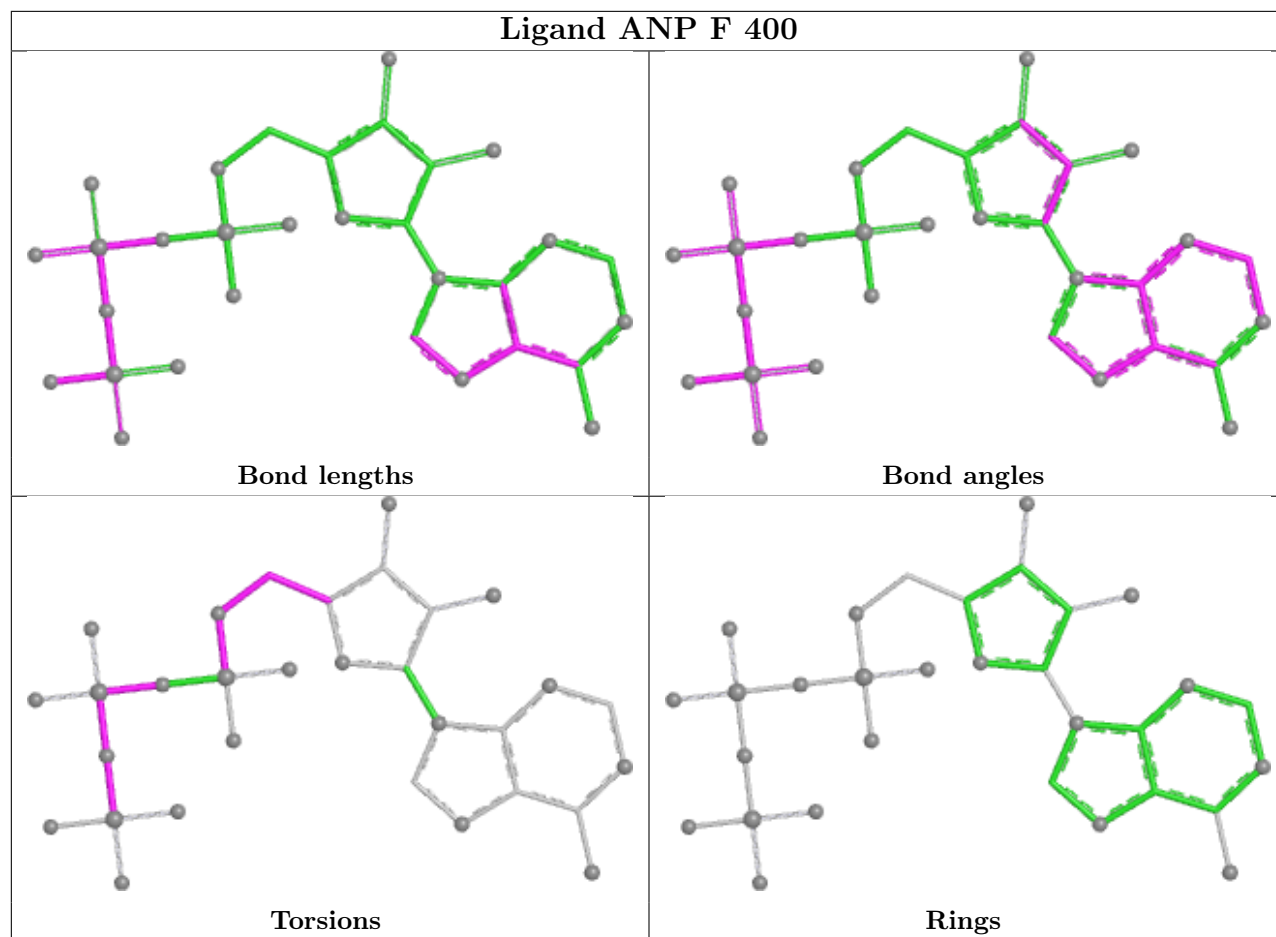


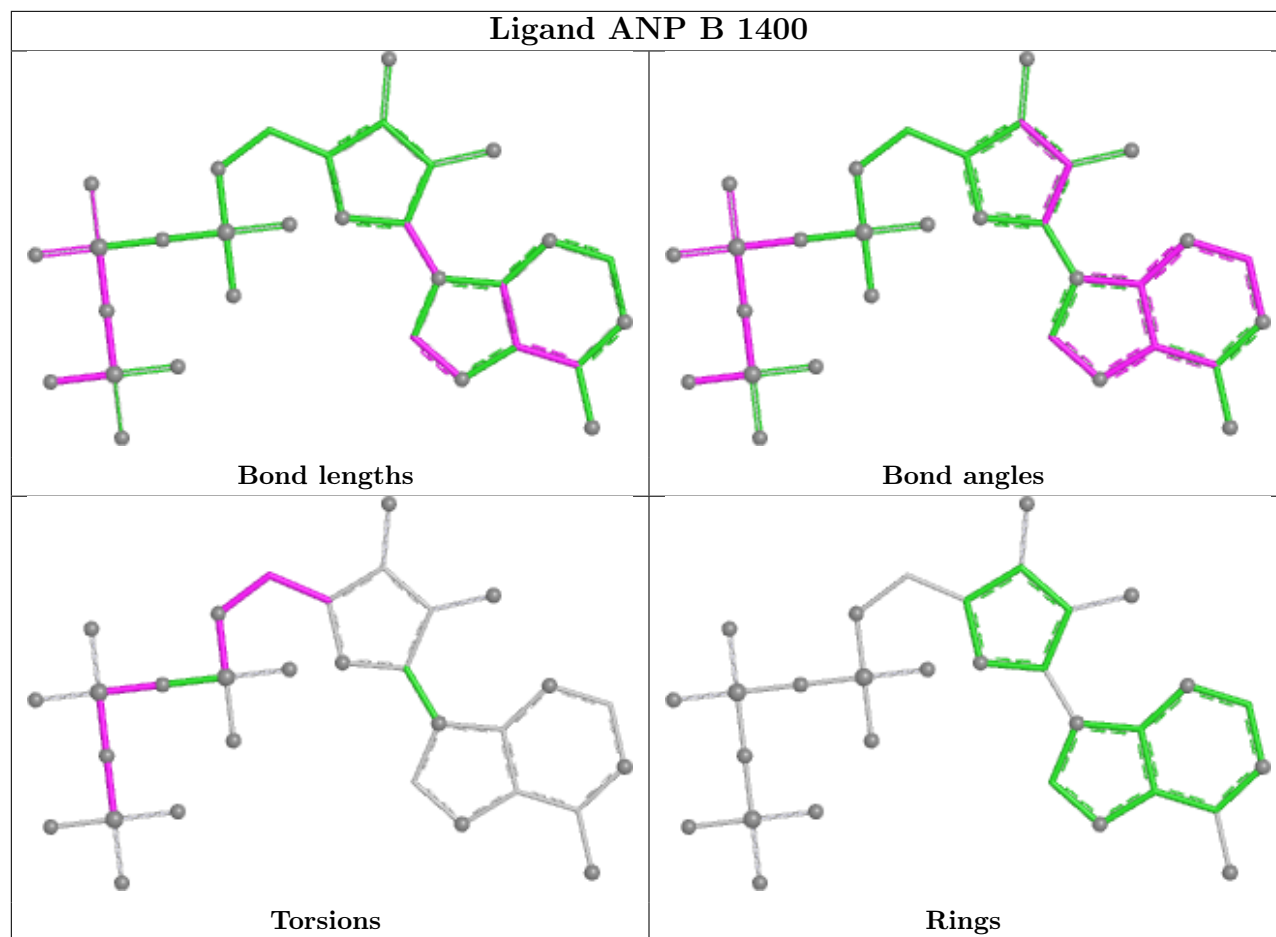












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.14	6 (0%) 87 75	181, 217, 253, 285	0
1	B	1163/1357 (85%)	-0.22	2 (0%) 91 83	175, 217, 254, 286	0
1	C	1175/1357 (86%)	-0.09	4 (0%) 90 80	187, 216, 253, 284	0
1	D	1175/1357 (86%)	-0.21	2 (0%) 91 83	181, 218, 256, 286	0
1	E	1165/1357 (85%)	-0.16	5 (0%) 88 77	186, 218, 255, 288	0
1	F	1175/1357 (86%)	-0.15	2 (0%) 91 83	185, 217, 255, 285	0
1	G	1167/1357 (85%)	-0.13	5 (0%) 88 77	185, 216, 254, 291	0
1	H	1173/1357 (86%)	-0.18	3 (0%) 90 80	186, 218, 255, 288	0
All	All	9383/10856 (86%)	-0.16	29 (0%) 90 80	175, 217, 255, 291	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ALA	4.1
1	H	2251	ILE	4.1
1	D	3251	ILE	3.9
1	G	2083	ALA	3.5
1	A	1053	ALA	3.2

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 ⓘ

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	0.27	0.20	215,215,215,215	0
2	MG	F	1701	1/1	0.62	0.33	175,175,175,175	0
2	MG	F	701	1/1	0.63	0.26	189,189,189,189	0
2	MG	D	701	1/1	0.65	0.32	261,261,261,261	0
2	MG	D	1701	1/1	0.68	0.30	212,212,212,212	0
2	MG	H	1701	1/1	0.69	0.25	188,188,188,188	0
2	MG	E	701	1/1	0.74	0.22	204,204,204,204	0
3	ANP	E	2400	31/31	0.75	0.11	307,317,320,320	0
2	MG	H	701	1/1	0.76	0.19	200,200,200,200	0
2	MG	C	701	1/1	0.78	0.17	177,177,177,177	0
3	ANP	C	1400	31/31	0.78	0.11	288,291,293,294	0
2	MG	A	701	1/1	0.78	0.14	143,143,143,143	0
2	MG	B	701	1/1	0.80	0.16	184,184,184,184	0
3	ANP	A	2400	31/31	0.80	0.13	308,311,315,315	0
3	ANP	H	1400	31/31	0.80	0.12	296,299,304,304	0
3	ANP	E	1400	31/31	0.81	0.11	287,293,296,296	0
2	MG	H	3701	1/1	0.81	0.15	121,121,121,121	0
3	ANP	F	1400	31/31	0.81	0.11	271,280,286,286	0
3	ANP	D	400	31/31	0.81	0.10	263,273,274,274	0
2	MG	E	3701	1/1	0.82	0.16	131,131,131,131	0
2	MG	E	1701	1/1	0.83	0.17	190,190,190,190	0
3	ANP	D	2400	31/31	0.83	0.10	305,310,315,315	0
2	MG	E	2701	1/1	0.84	0.20	228,228,228,228	0
3	ANP	G	1400	31/31	0.84	0.12	279,285,289,290	0
3	ANP	G	2400	31/31	0.84	0.12	303,308,315,315	0
2	MG	C	3701	1/1	0.84	0.11	140,140,140,140	0
2	MG	G	1701	1/1	0.85	0.21	191,191,191,191	0
3	ANP	A	1400	31/31	0.85	0.11	267,280,283,283	0
2	MG	B	2701	1/1	0.85	0.29	238,238,238,238	0
3	ANP	B	1400	31/31	0.85	0.10	275,286,290,290	0
2	MG	B	1701	1/1	0.85	0.21	214,214,214,214	0
2	MG	H	2701	1/1	0.85	0.28	271,271,271,271	0
3	ANP	D	1400	31/31	0.85	0.09	287,290,294,294	0
3	ANP	B	400	31/31	0.87	0.09	242,255,259,260	0
3	ANP	C	2400	31/31	0.87	0.09	296,309,314,315	0
3	ANP	F	2400	31/31	0.87	0.11	286,303,310,310	0
3	ANP	H	2400	31/31	0.87	0.10	298,312,316,316	0

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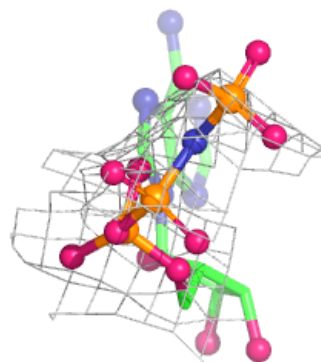
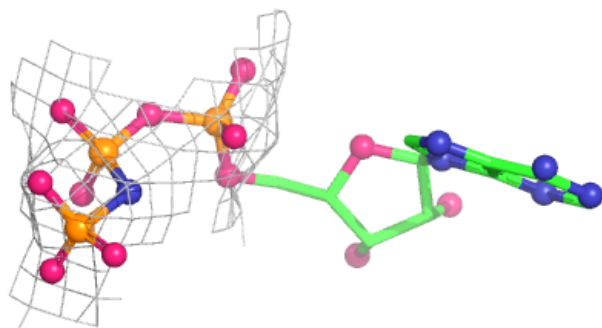
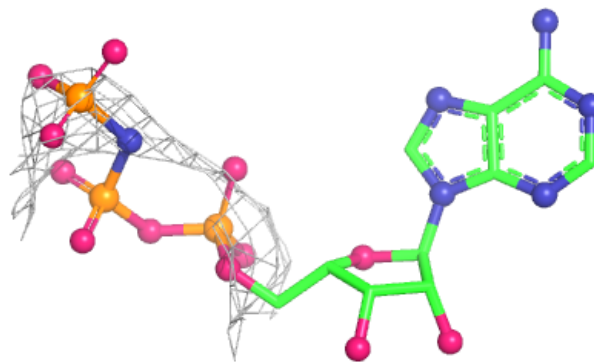
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	H	400	31/31	0.88	0.08	254,263,265,265	0
3	ANP	F	400	31/31	0.89	0.09	243,257,263,263	0
3	ANP	G	400	31/31	0.90	0.09	253,262,264,265	0
2	MG	G	2701	1/1	0.90	0.24	192,192,192,192	0
3	ANP	A	400	31/31	0.90	0.09	246,250,255,256	0
3	ANP	H	3400	31/31	0.90	0.08	180,187,196,197	0
3	ANP	B	2400	31/31	0.91	0.10	306,312,314,314	0
2	MG	D	2701	1/1	0.91	0.39	237,237,237,237	0
3	ANP	E	400	31/31	0.92	0.07	256,261,264,265	0
2	MG	A	1701	1/1	0.92	0.13	181,181,181,181	0
3	ANP	D	3400	31/31	0.92	0.08	149,170,188,189	0
3	ANP	G	3400	31/31	0.92	0.08	153,176,191,192	0
3	ANP	C	3400	31/31	0.93	0.07	176,190,200,200	0
3	ANP	C	400	31/31	0.93	0.07	226,245,250,250	0
3	ANP	E	3400	31/31	0.93	0.07	163,180,187,187	0
3	ANP	F	3400	31/31	0.93	0.08	148,171,183,183	0
2	MG	D	3701	1/1	0.94	0.14	108,108,108,108	0
2	MG	F	2701	1/1	0.94	0.25	232,232,232,232	0
3	ANP	A	3400	31/31	0.94	0.06	152,165,180,181	0
2	MG	B	3701	1/1	0.95	0.11	69,69,69,69	0
2	MG	A	3701	1/1	0.95	0.04	116,116,116,116	0
2	MG	C	1701	1/1	0.95	0.10	132,132,132,132	0
2	MG	C	2701	1/1	0.95	0.17	211,211,211,211	0
2	MG	A	2701	1/1	0.95	0.15	247,247,247,247	0
3	ANP	B	3400	31/31	0.95	0.06	143,159,176,178	0
2	MG	G	3701	1/1	0.96	0.06	100,100,100,100	0
2	MG	F	3701	1/1	0.97	0.06	77,77,77,77	0

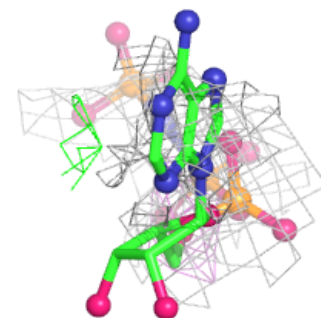
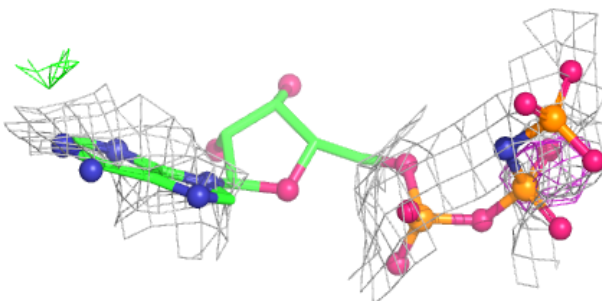
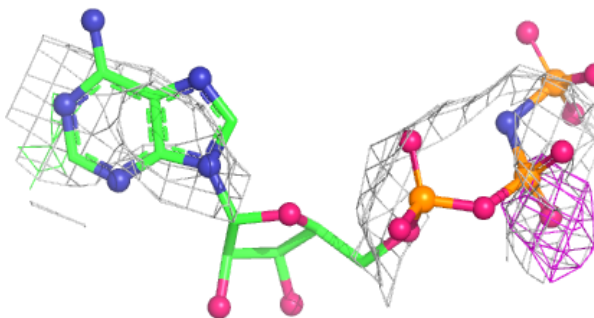
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP 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)

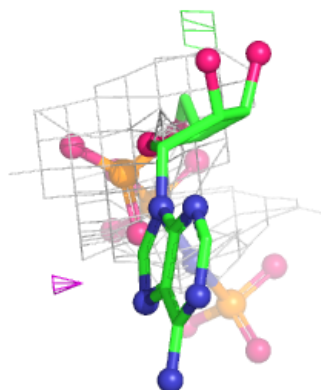
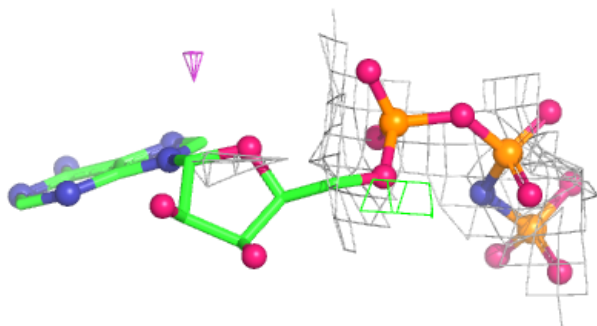
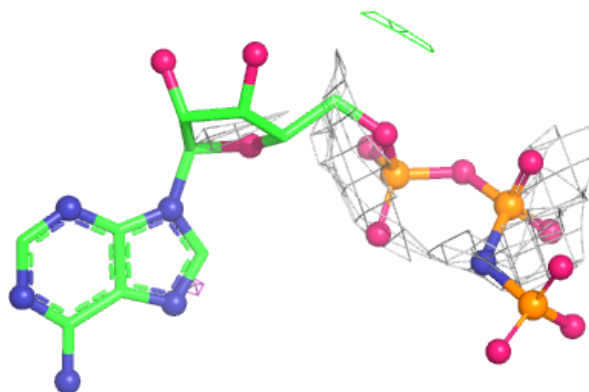
**Electron density around ANP C 1400:**

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

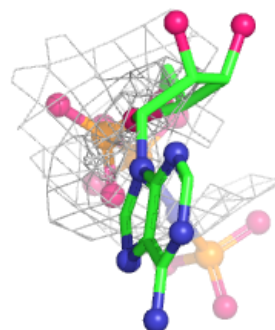
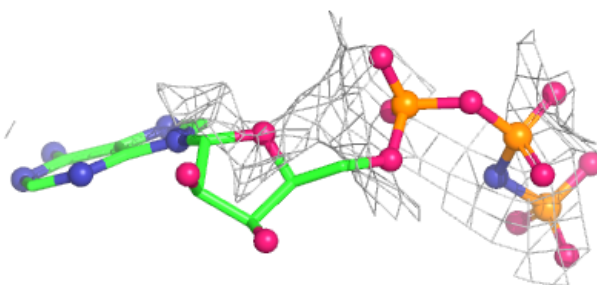
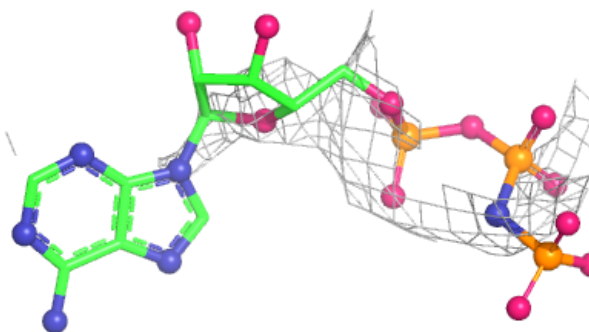


Electron density around ANP A 2400:

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

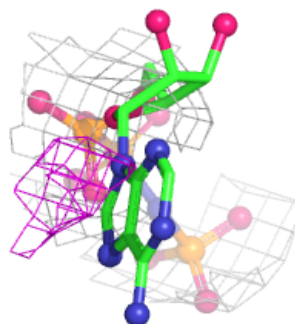
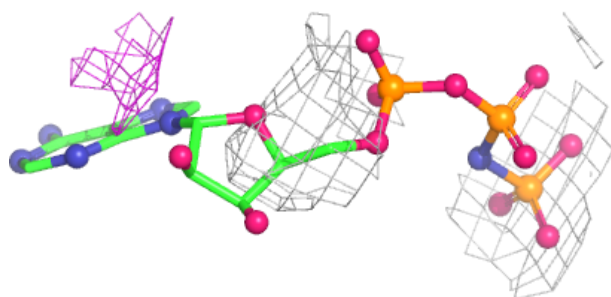
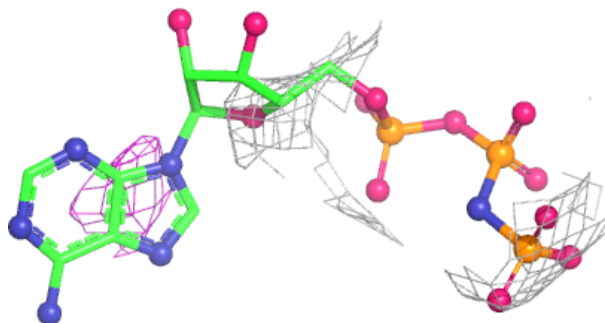
**Electron density around ANP H 1400:**

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

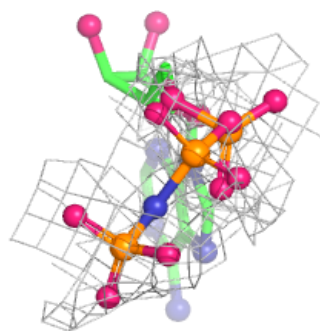
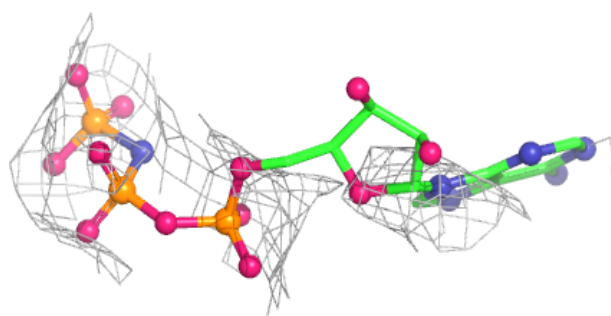
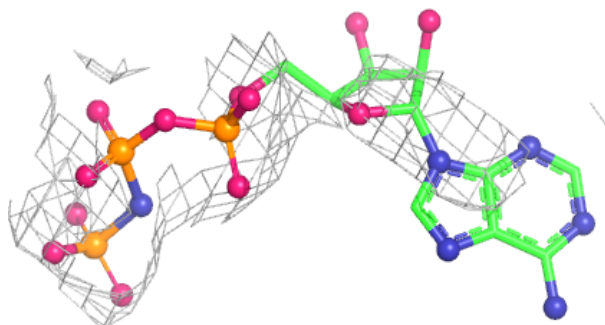


Electron density around ANP E 1400:

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

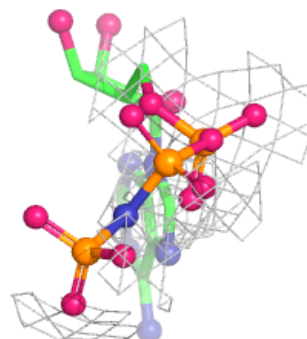
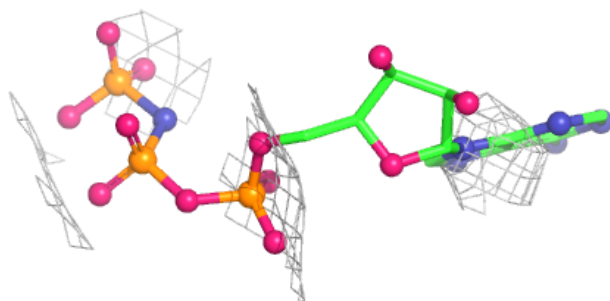
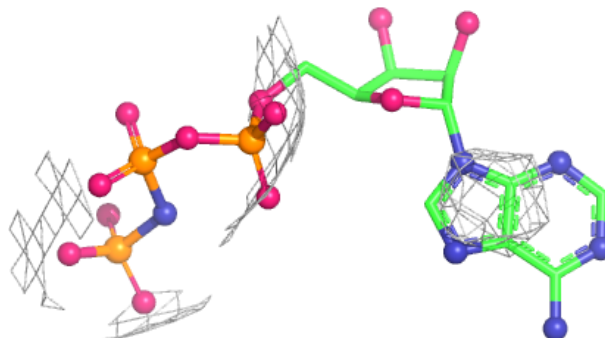
**Electron density around ANP F 1400:**

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

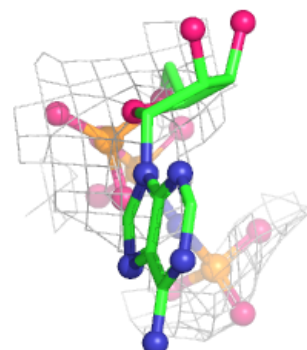
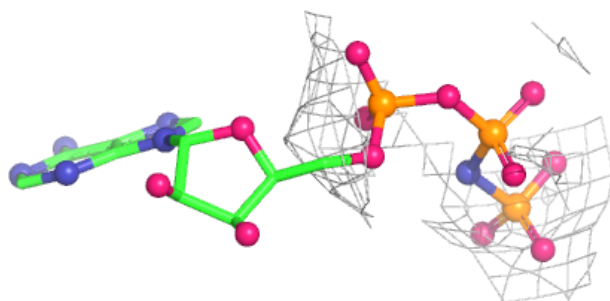
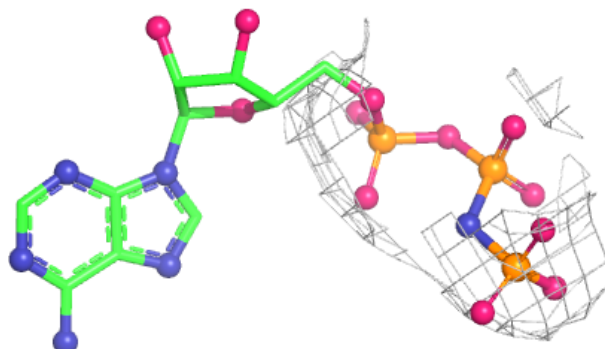


Electron density around ANP D 400:

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

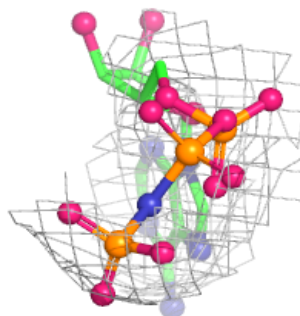
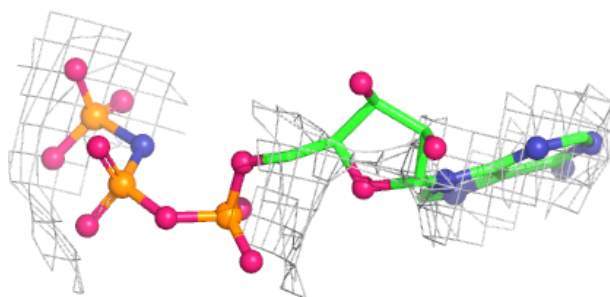
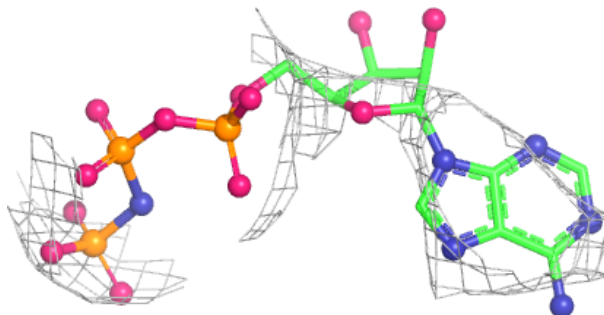
**Electron density around ANP D 2400:**

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

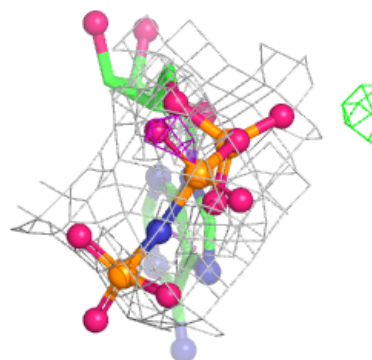
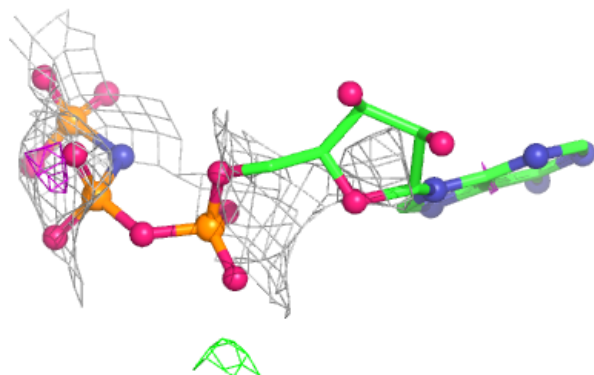
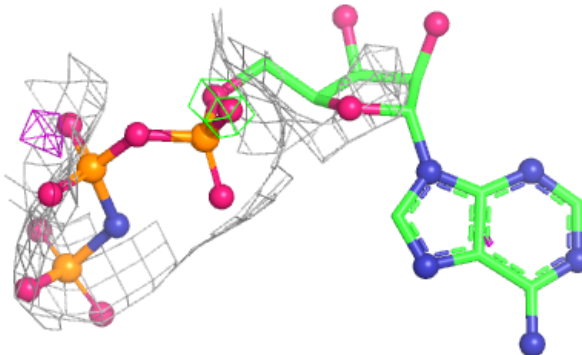


Electron density around ANP G 1400:

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

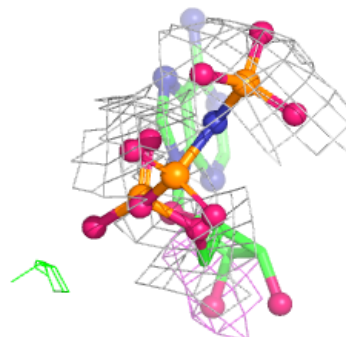
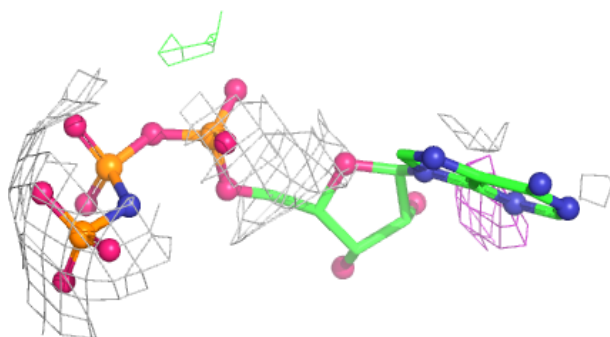
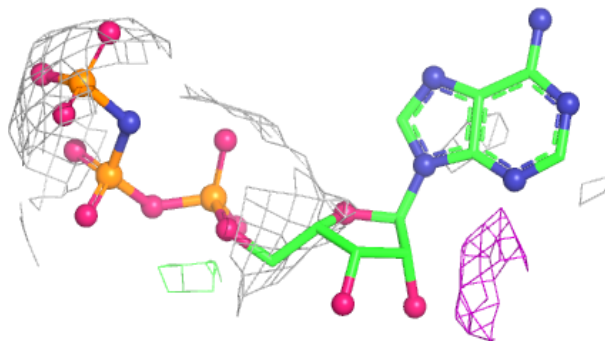
**Electron density around ANP G 2400:**

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

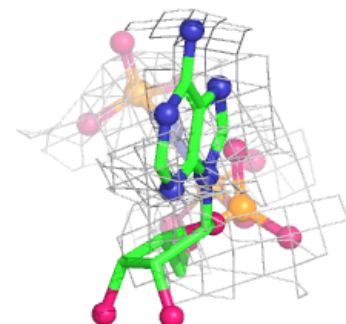
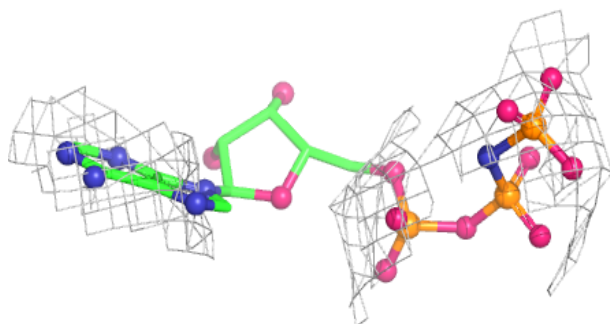
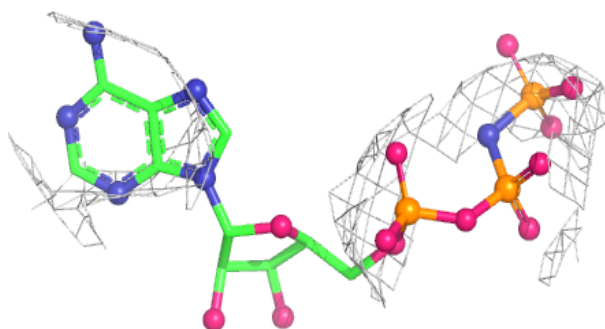


Electron density around ANP A 1400:

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

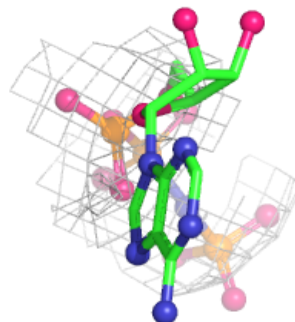
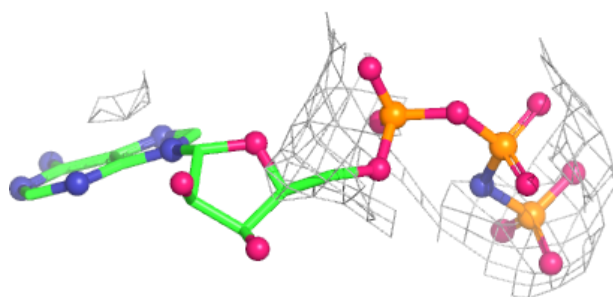
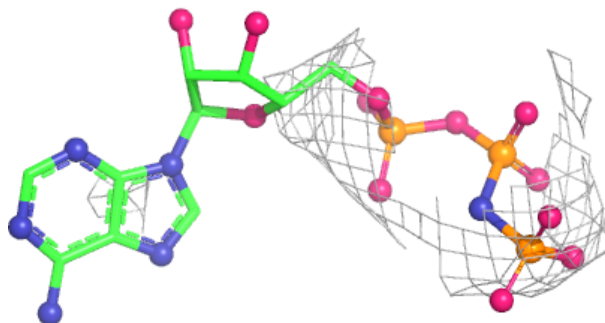
**Electron density around ANP B 1400:**

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

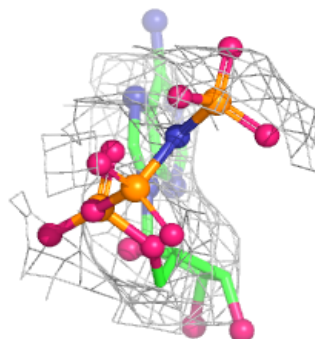
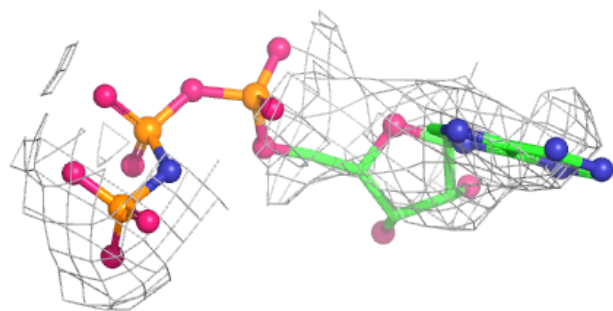
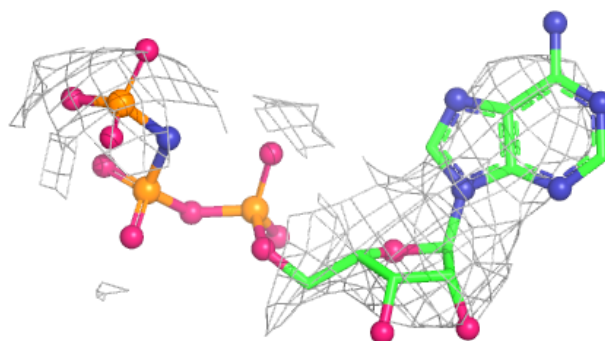


Electron density around ANP D 1400:

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

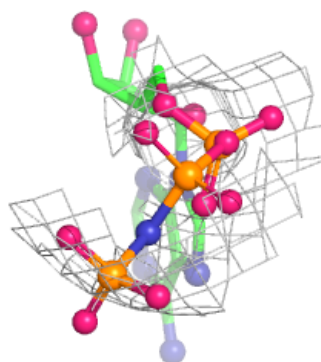
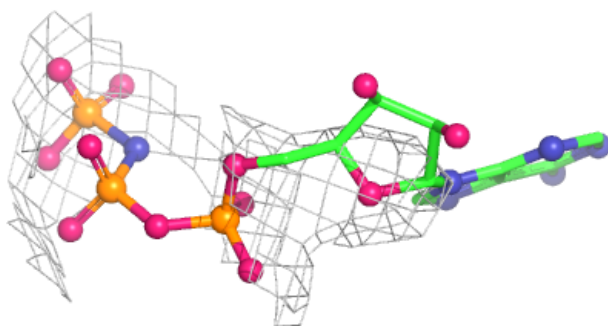
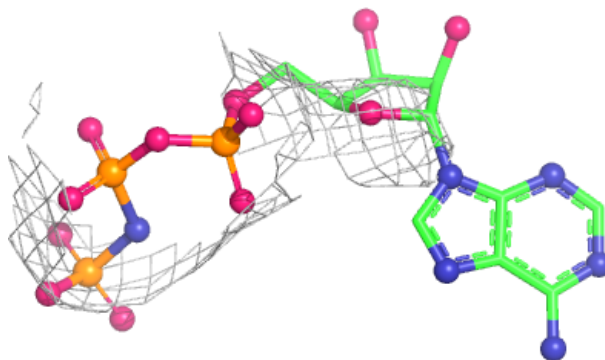
**Electron density around ANP B 400:**

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

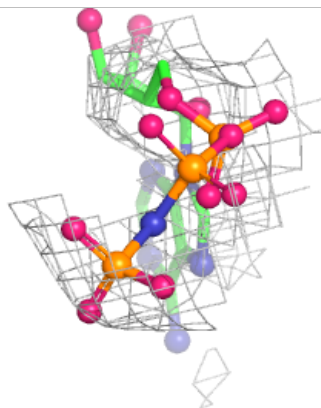
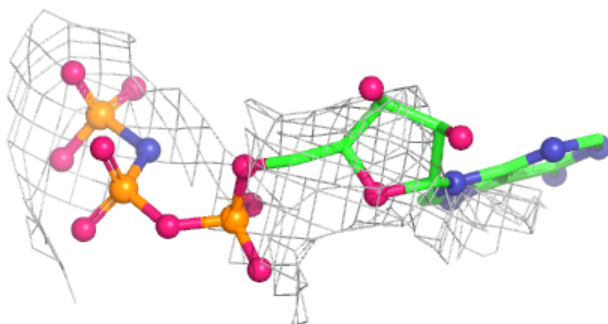
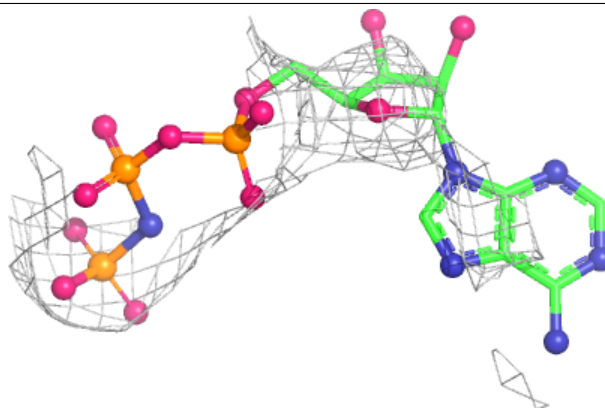


Electron density around ANP C 2400:

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

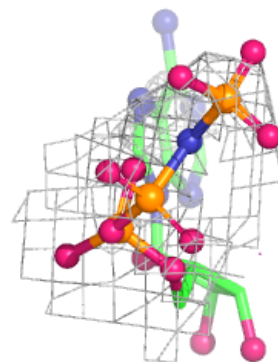
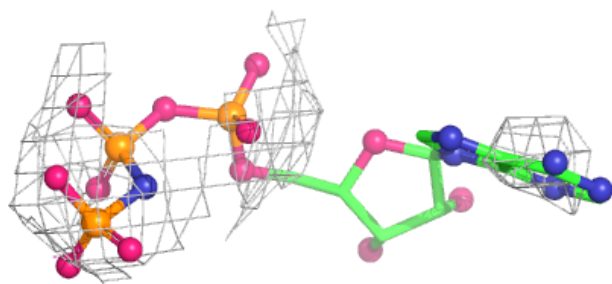
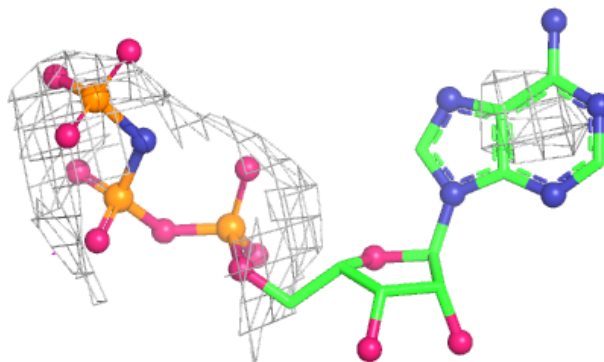
**Electron density around ANP F 2400:**

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

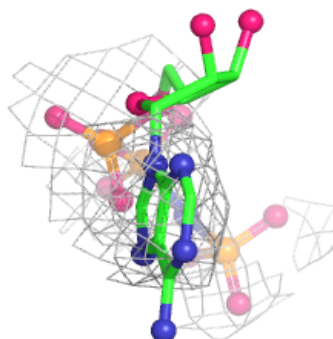
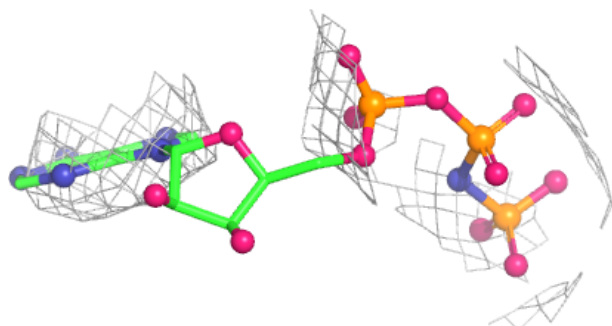
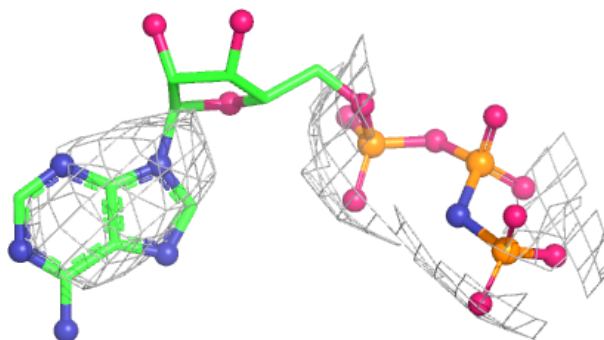


Electron density around ANP H 2400:

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

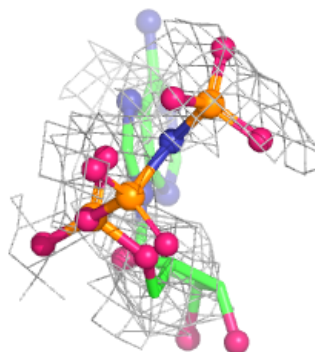
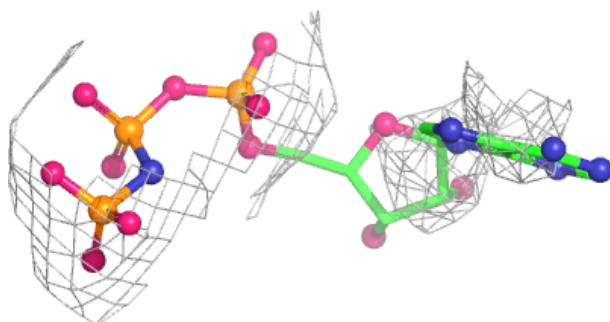
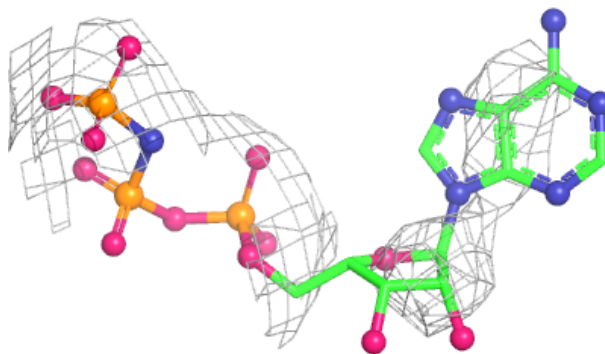
**Electron density around ANP H 400:**

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

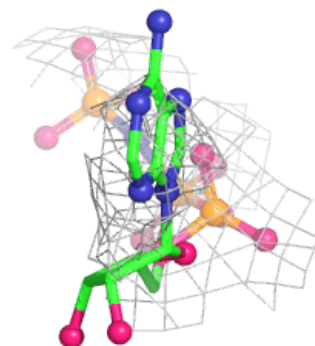
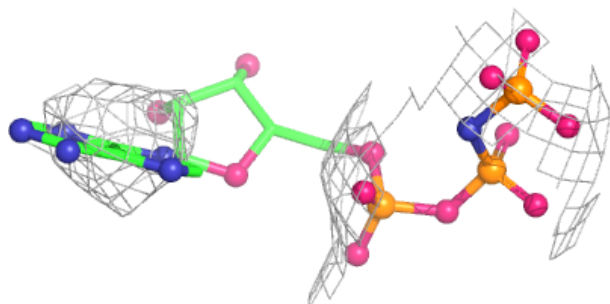
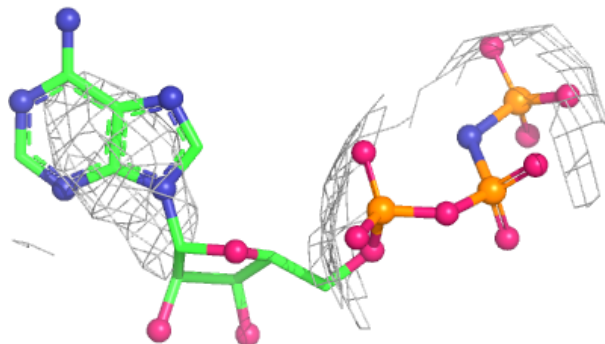


Electron density around ANP F 400:

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

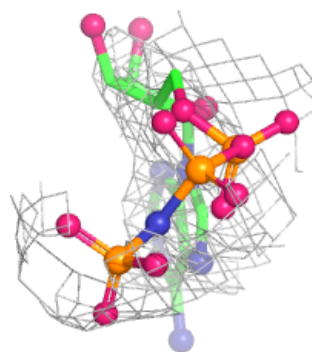
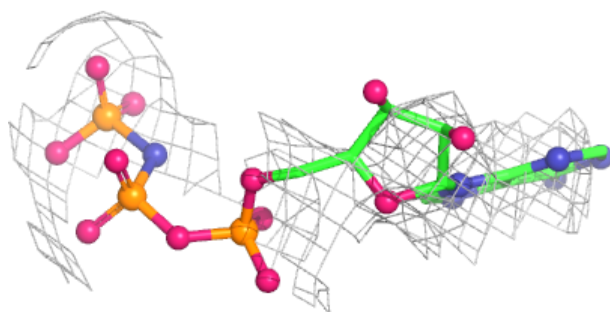
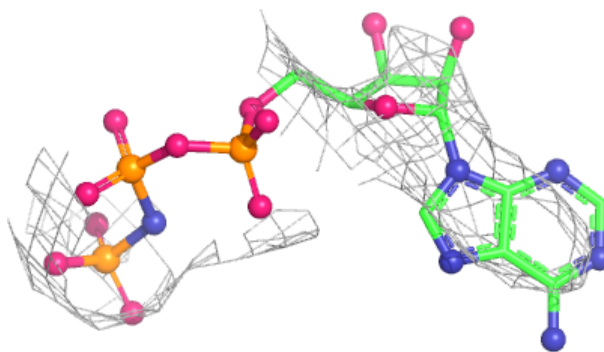
**Electron density around ANP G 400:**

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

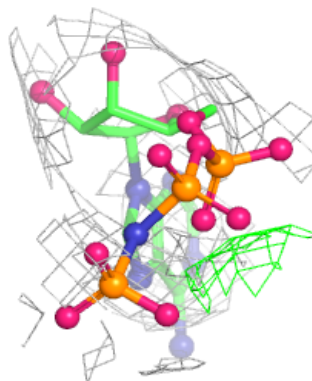
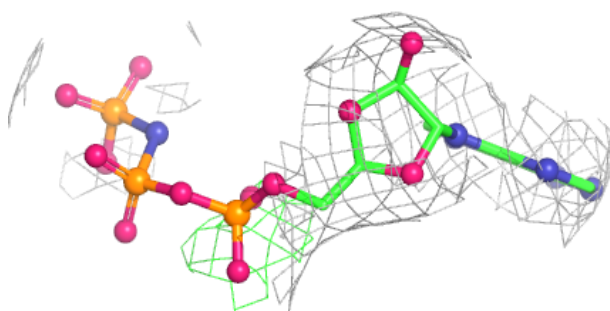
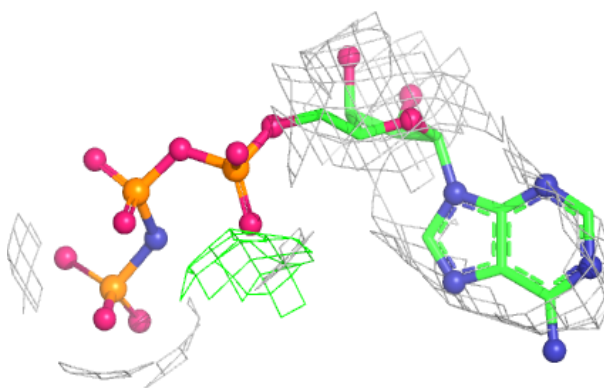


Electron density around ANP A 400:

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

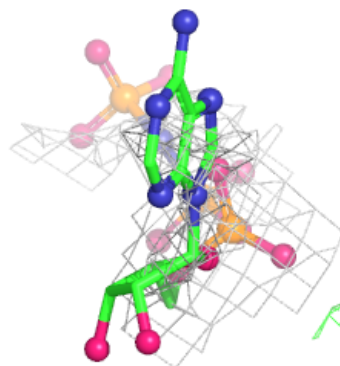
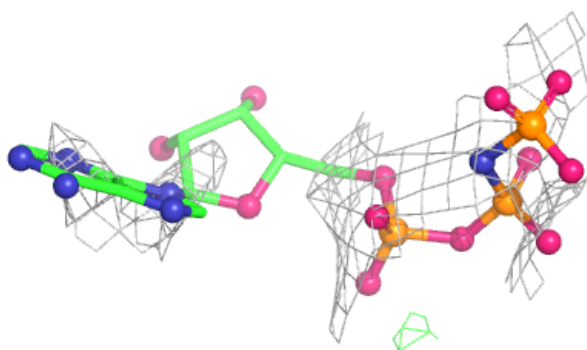
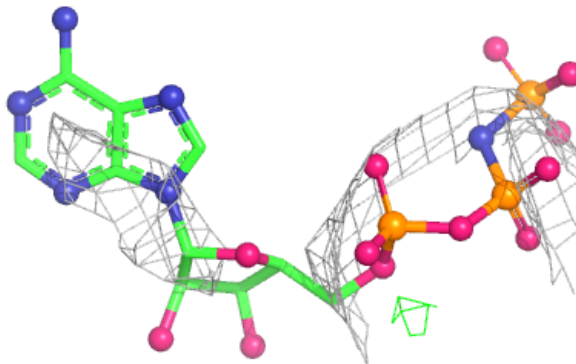
**Electron density around ANP H 3400:**

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

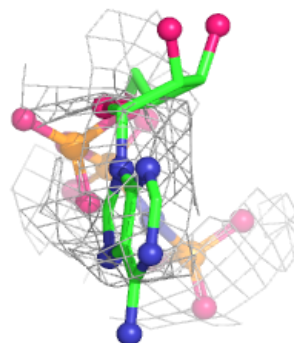
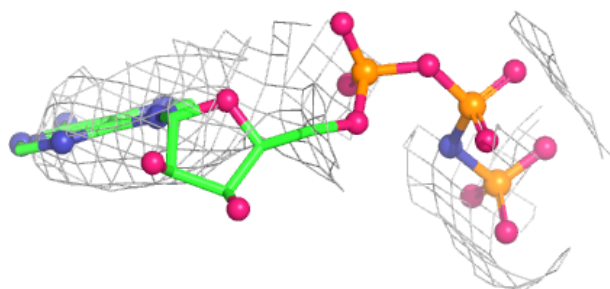
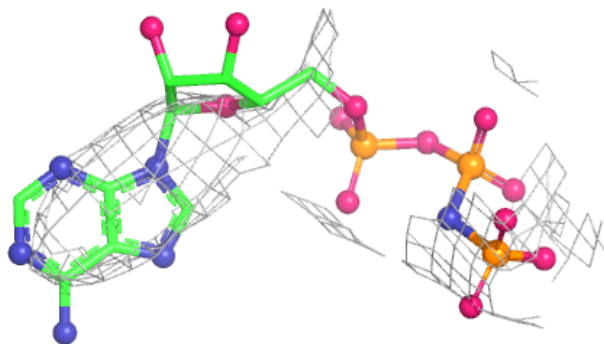


Electron density around ANP B 2400:

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

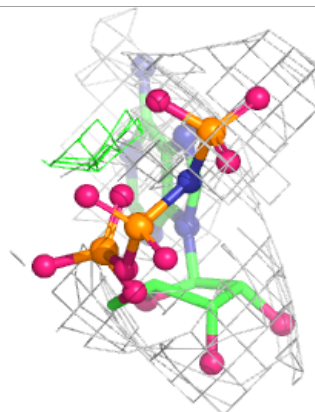
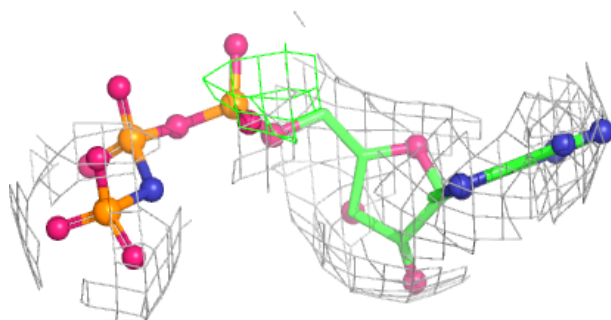
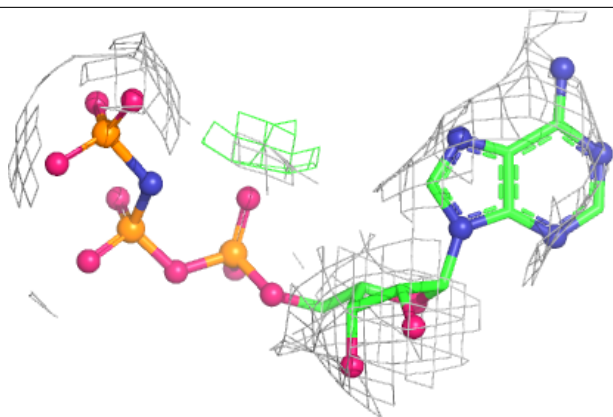
**Electron density around ANP E 400:**

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

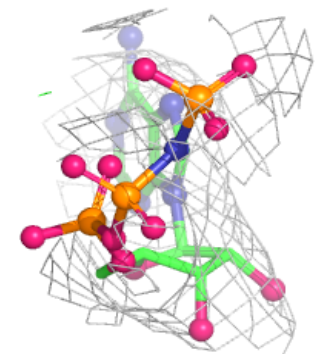
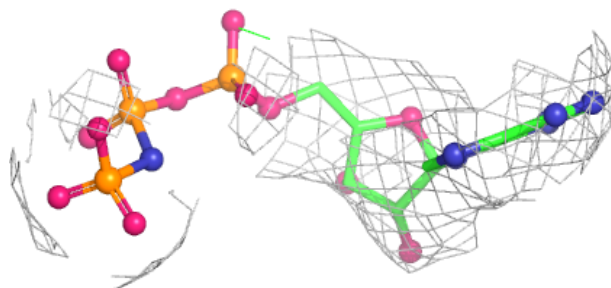
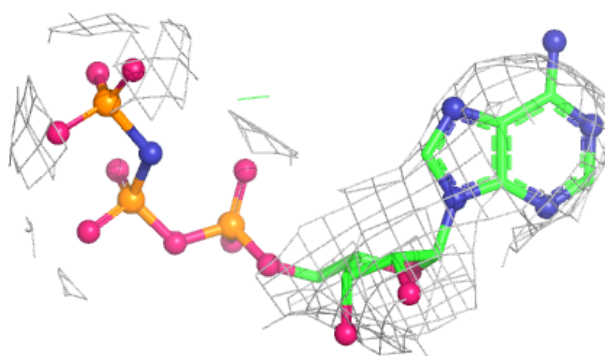


Electron density around ANP D 3400:

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

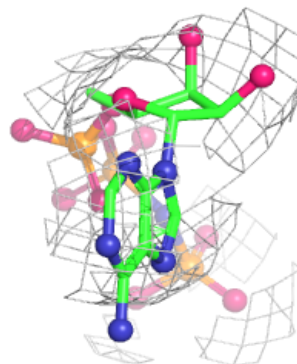
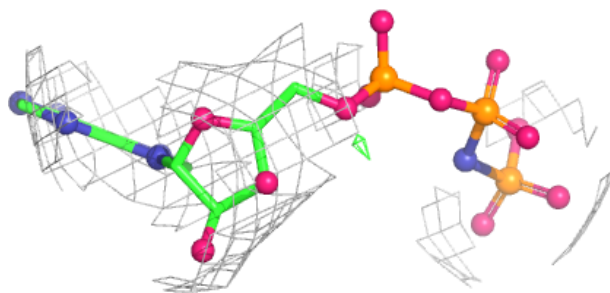
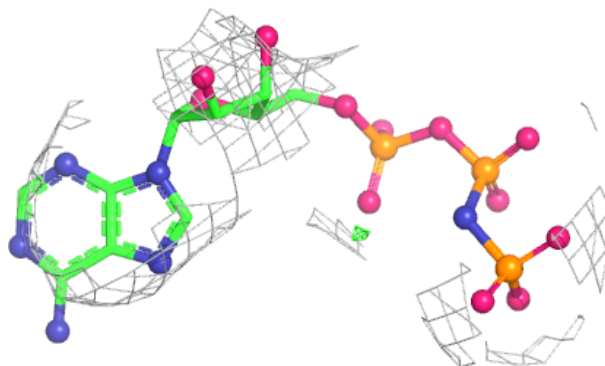
**Electron density around ANP G 3400:**

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

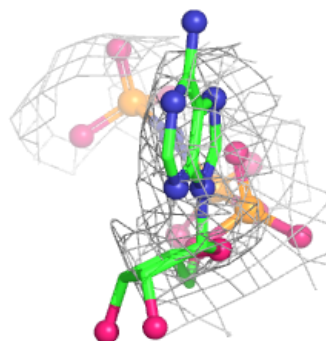
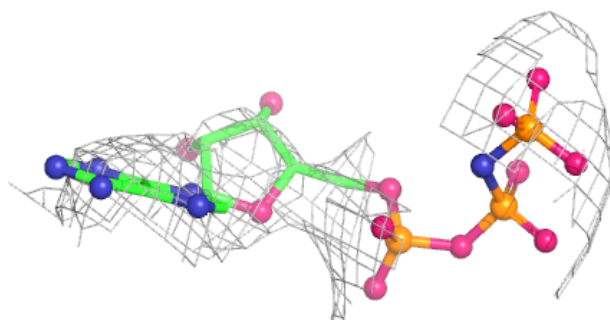
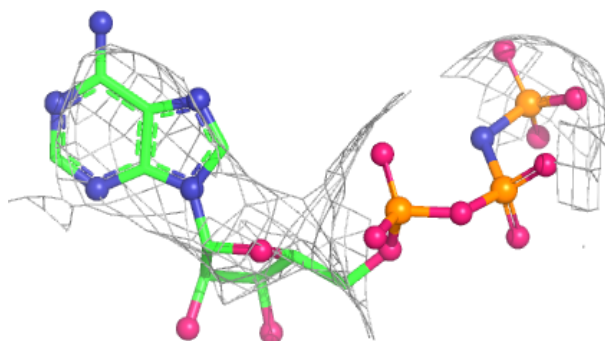


Electron density around ANP C 3400:

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

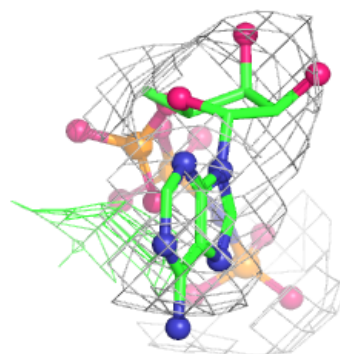
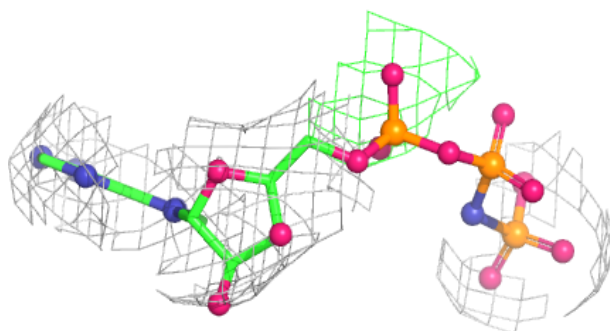
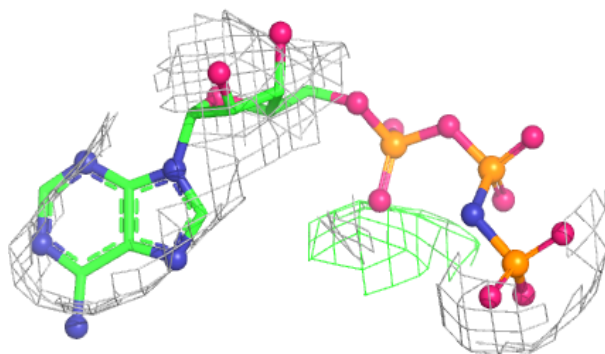
**Electron density around ANP C 400:**

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

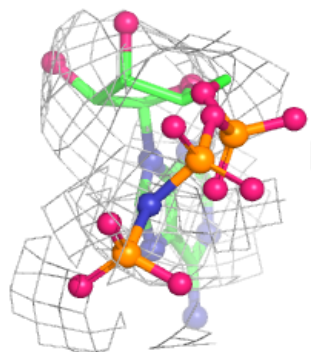
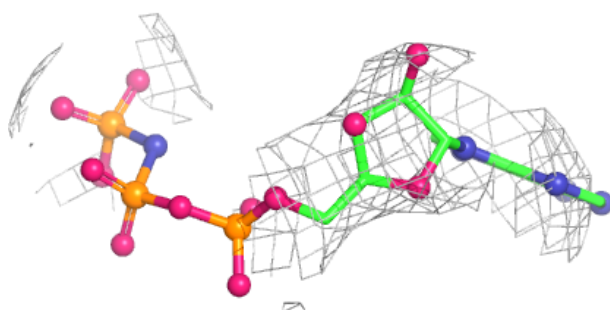
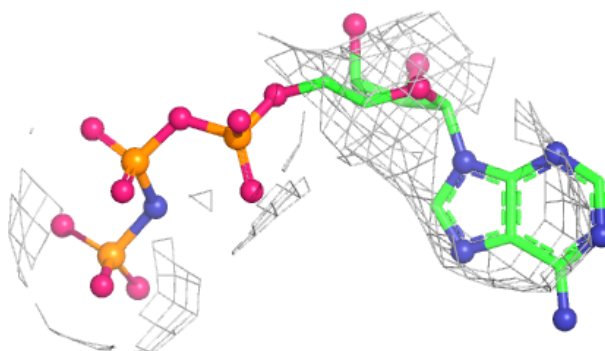


Electron density around ANP E 3400:

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

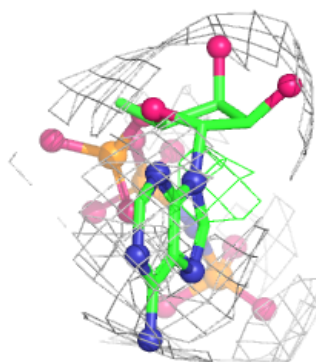
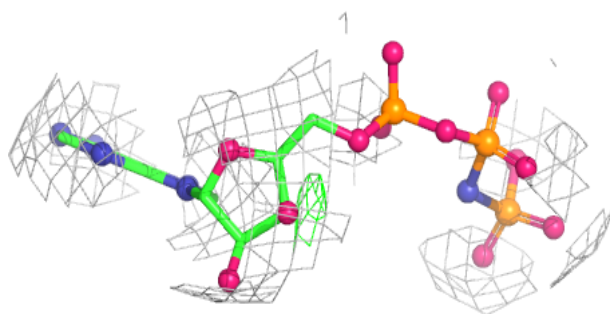
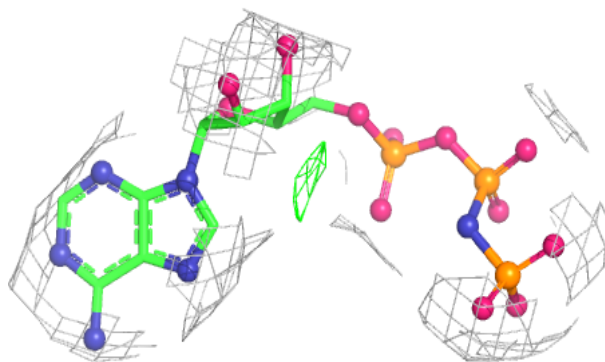
**Electron density around ANP F 3400:**

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

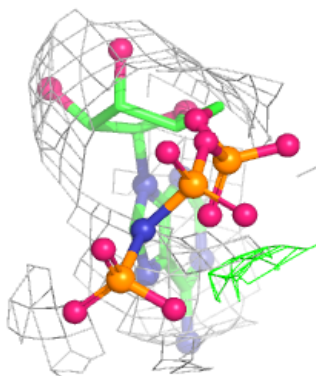
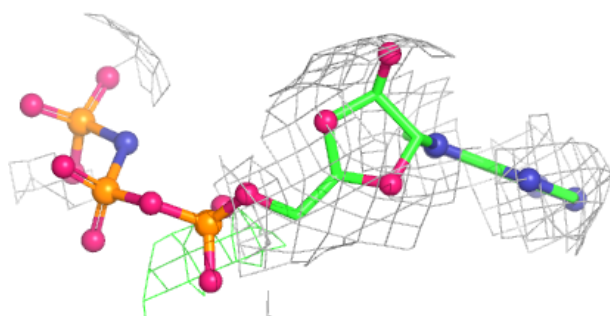
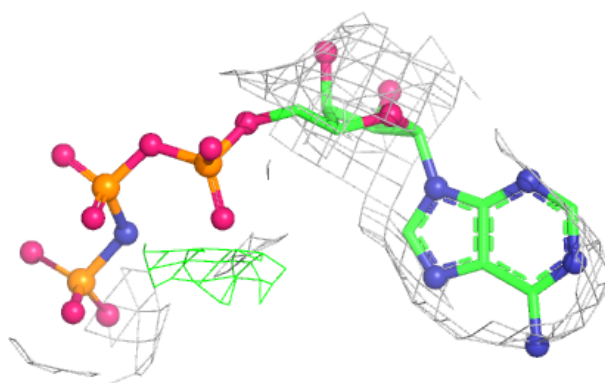


Electron density around ANP A 3400:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.