wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 06:44 am BST

PDB ID	:	6TUG
Title	:	Enterococcus italicus Csm6 bound to cyclic hexa-2'-fluoro-hexa-dAMP
Authors	:	Garcia-Doval, C.; Jinek, M.
Deposited on	:	2020-01-07
Resolution	:	2.42 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 (i) symbol.

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

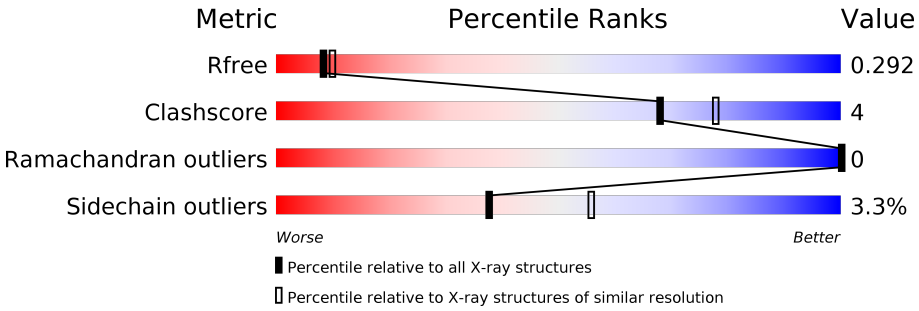
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	433	84% 9% • 6%
1	B	433	84% 11% •
1	C	433	85% 9% 6%
1	D	433	84% 10% 6%
1	E	433	82% 12% 6%
1	F	433	86% 9% •
1	G	433	83% 11% 6%

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Mol	Chain	Length	Quality of chain
1	H	433	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 55331 atoms, of which 27236 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 CRISPR system endoribonuclease Csm6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	408	Total	C	H	N	O	S	0	0	0
			6733	2147	3351	579	640	16			
1	B	415	Total	C	H	N	O	S	0	0	0
			6858	2185	3418	588	650	17			
1	C	408	Total	C	H	N	O	S	0	0	0
			6733	2147	3351	579	640	16			
1	D	406	Total	C	H	N	O	S	0	0	0
			6716	2140	3348	576	636	16			
1	E	409	Total	C	H	N	O	S	0	0	0
			6755	2153	3364	581	641	16			
1	F	415	Total	C	H	N	O	S	0	0	0
			6852	2183	3414	588	651	16			
1	G	407	Total	C	H	N	O	S	0	0	0
			6718	2143	3344	577	638	16			
1	H	414	Total	C	H	N	O	S	0	0	0
			6833	2177	3406	584	649	17			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP E6LHV2
A	-1	ASN	-	expression tag	UNP E6LHV2
A	0	ALA	-	expression tag	UNP E6LHV2
B	-2	SER	-	expression tag	UNP E6LHV2
B	-1	ASN	-	expression tag	UNP E6LHV2
B	0	ALA	-	expression tag	UNP E6LHV2
C	-2	SER	-	expression tag	UNP E6LHV2
C	-1	ASN	-	expression tag	UNP E6LHV2
C	0	ALA	-	expression tag	UNP E6LHV2
D	-2	SER	-	expression tag	UNP E6LHV2
D	-1	ASN	-	expression tag	UNP E6LHV2
D	0	ALA	-	expression tag	UNP E6LHV2
E	-2	SER	-	expression tag	UNP E6LHV2

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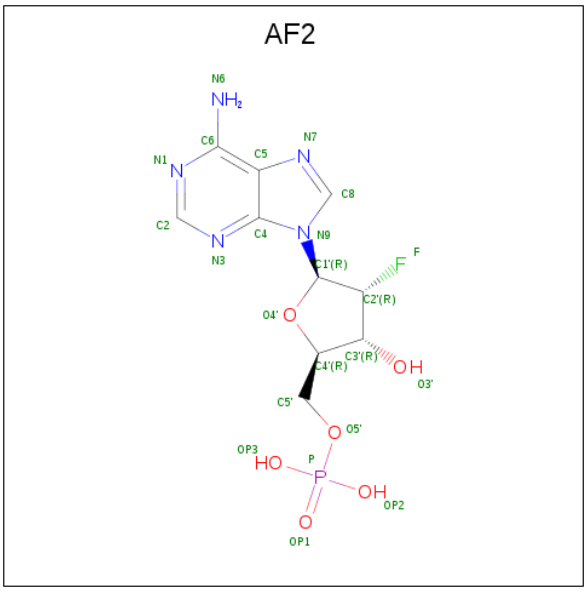
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP E6LHV2
E	0	ALA	-	expression tag	UNP E6LHV2
F	-2	SER	-	expression tag	UNP E6LHV2
F	-1	ASN	-	expression tag	UNP E6LHV2
F	0	ALA	-	expression tag	UNP E6LHV2
G	-2	SER	-	expression tag	UNP E6LHV2
G	-1	ASN	-	expression tag	UNP E6LHV2
G	0	ALA	-	expression tag	UNP E6LHV2
H	-2	SER	-	expression tag	UNP E6LHV2
H	-1	ASN	-	expression tag	UNP E6LHV2
H	0	ALA	-	expression tag	UNP E6LHV2

- Molecule 2 is 2'-deoxy-2'-fluoroadenosine 5'-(dihydrogen phosphate) (three-letter code: AF2) (formula: $C_{10}H_{13}FN_5O_6P$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	A	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	A	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	B	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	B	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		

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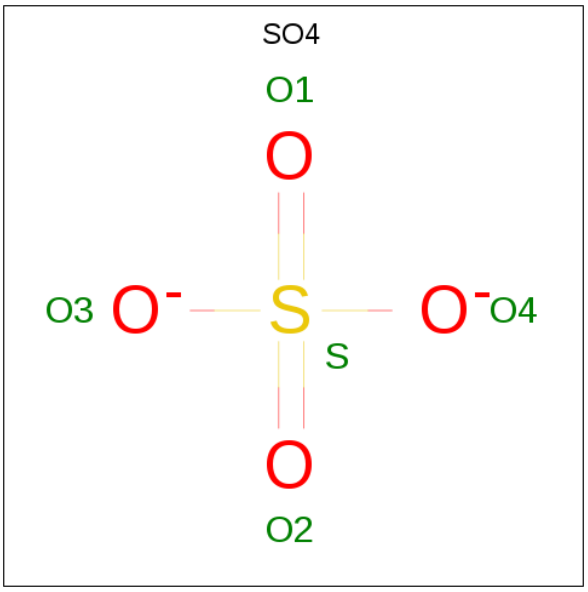
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	B	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	C	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	C	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	C	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	D	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	D	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	D	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	E	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	E	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	E	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	F	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	F	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	F	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	G	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	G	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	G	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	H	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	H	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		
2	H	1	Total	C	F	H	N	O	P	0	0
			32	10	1	10	5	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

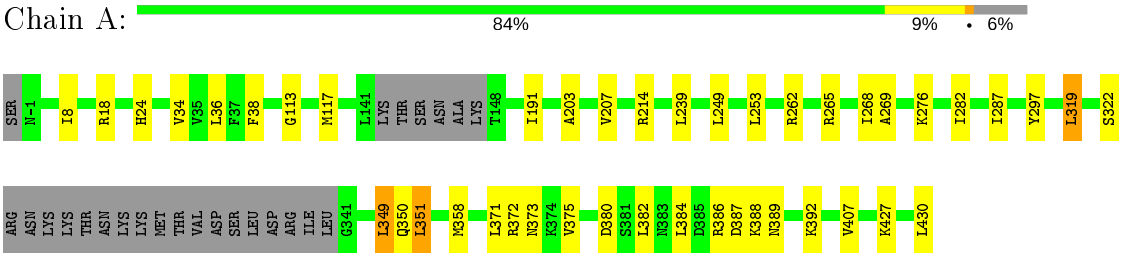
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	39	Total O 39 39	0	0
4	C	42	Total O 42 42	0	0
4	D	43	Total O 43 43	0	0
4	E	39	Total O 39 39	0	0
4	F	44	Total O 44 44	0	0
4	G	45	Total O 45 45	0	0
4	H	47	Total O 47 47	0	0

3 Residue-property plots (i)

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. 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. 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.

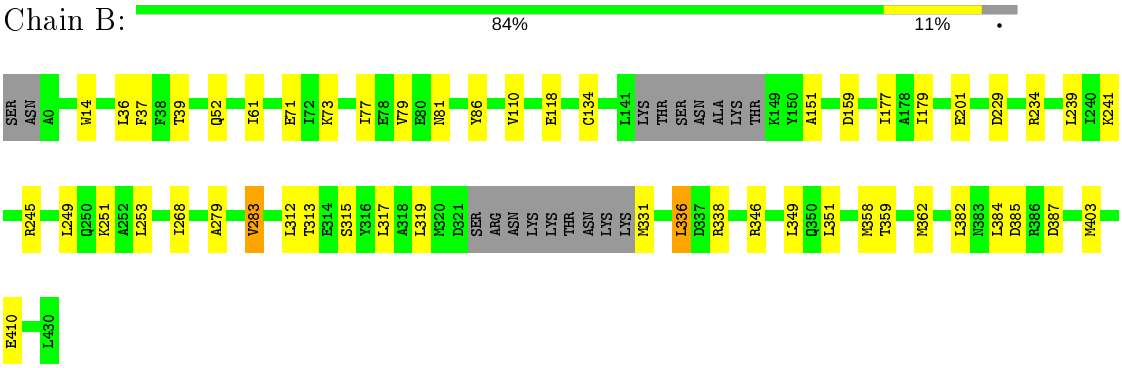
- Molecule 1: CRISPR system endoribonuclease Csm6

Chain A:



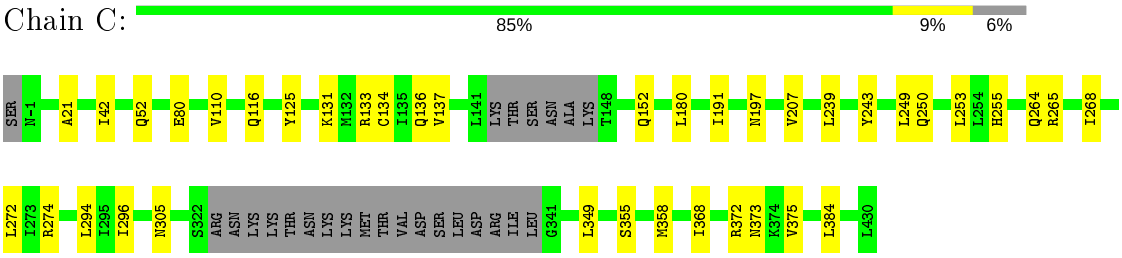
- Molecule 1: CRISPR system endoribonuclease Csm6

Chain B:



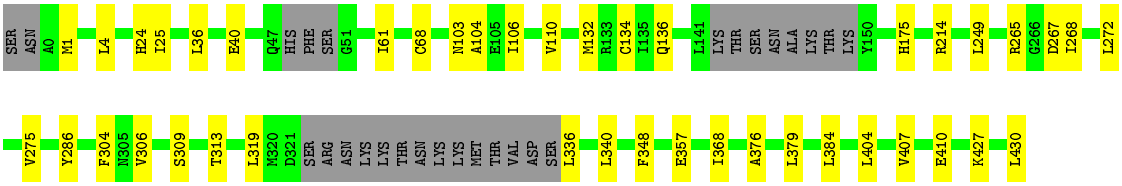
- Molecule 1: CRISPR system endoribonuclease Csm6

Chain C:



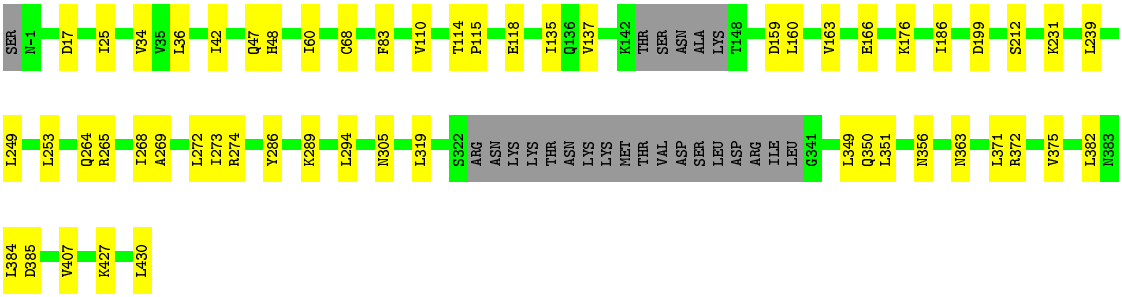
- Molecule 1: CRISPR system endoribonuclease Csm6

Chain D:



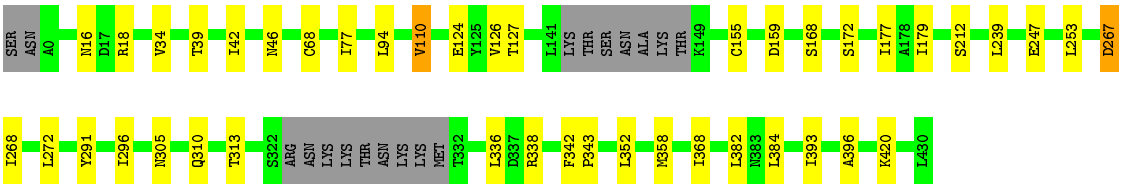
• Molecule 1: CRISPR system endoribonuclease Csm6

Chain E:



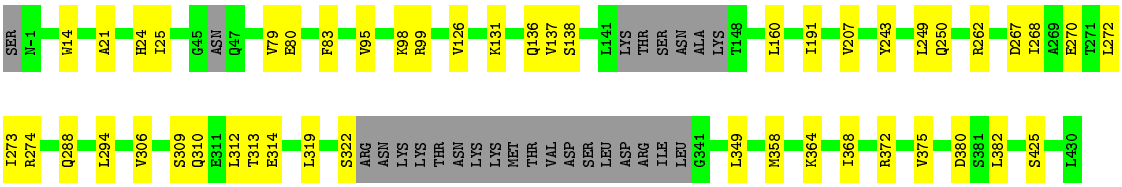
• Molecule 1: CRISPR system endoribonuclease Csm6

Chain F:



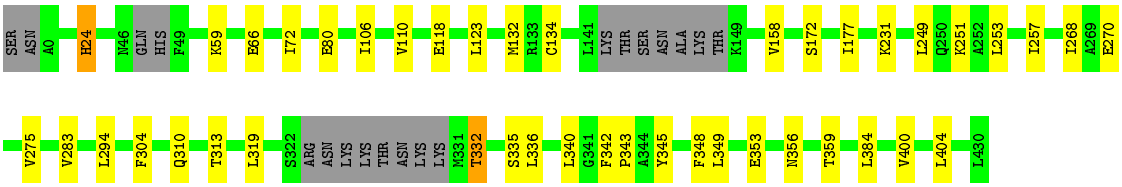
• Molecule 1: CRISPR system endoribonuclease Csm6

Chain G:



• Molecule 1: CRISPR system endoribonuclease Csm6

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	93.60Å 106.69Å 116.79Å 90.03° 90.01° 90.10°	Depositor
Resolution (Å)	48.51 – 2.42 48.51 – 2.42	Depositor EDS
% Data completeness (in resolution range)	90.8 (48.51-2.42) 90.4 (48.51-2.42)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.264 , 0.292 0.264 , 0.292	Depositor DCC
R_{free} test set	7657 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 20.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.437 for h,-k,-l 0.468 for -h,k,-l 0.438 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	55331	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1760e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, AF2

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	0.29	0/3446	0.44	0/4651
1	B	0.29	0/3504	0.45	0/4729
1	C	0.26	0/3446	0.42	0/4651
1	D	0.26	0/3429	0.42	0/4627
1	E	0.26	0/3455	0.42	0/4662
1	F	0.26	0/3502	0.43	0/4727
1	G	0.27	0/3437	0.42	0/4637
1	H	0.27	0/3489	0.45	0/4707
All	All	0.27	0/27708	0.43	0/37391

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3382	3351	3353	22	0
1	B	3440	3418	3419	36	0
1	C	3382	3351	3353	24	0
1	D	3368	3348	3350	25	0
1	E	3391	3364	3366	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3438	3414	3415	27	0
1	G	3374	3344	3346	27	0
1	H	3427	3406	3408	26	0
2	A	66	30	30	1	0
2	B	66	30	30	0	0
2	C	66	30	30	2	0
2	D	66	30	30	1	0
2	E	66	30	30	2	0
2	F	66	30	30	1	0
2	G	66	30	30	1	0
2	H	66	30	30	1	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	F	5	0	0	0	0
3	G	5	0	0	1	0
4	A	46	0	0	0	0
4	B	39	0	0	0	0
4	C	42	0	0	0	0
4	D	43	0	0	0	0
4	E	39	0	0	0	0
4	F	44	0	0	1	0
4	G	45	0	0	0	0
4	H	47	0	0	0	0
All	All	28095	27236	27250	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 211 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:THR:HG22	1:B:77:ILE:HD12	1.52	0.92
1:E:319:LEU:HD11	1:E:351:LEU:HD21	1.57	0.85
1:C:21:ALA:HA	1:C:137:VAL:HG21	1.58	0.83
1:B:268:ILE:HG21	1:B:384:LEU:HD21	1.75	0.69
1:G:294:LEU:HD23	1:G:294:LEU:O	1.94	0.67

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/433 (93%)	395 (98%)	7 (2%)	0	100	100
1	B	409/433 (94%)	399 (98%)	10 (2%)	0	100	100
1	C	402/433 (93%)	398 (99%)	4 (1%)	0	100	100
1	D	398/433 (92%)	392 (98%)	6 (2%)	0	100	100
1	E	403/433 (93%)	400 (99%)	3 (1%)	0	100	100
1	F	409/433 (94%)	401 (98%)	8 (2%)	0	100	100
1	G	399/433 (92%)	396 (99%)	3 (1%)	0	100	100
1	H	406/433 (94%)	404 (100%)	2 (0%)	0	100	100
All	All	3228/3464 (93%)	3185 (99%)	43 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	377/401 (94%)	362 (96%)	15 (4%)	31	48
1	B	384/401 (96%)	373 (97%)	11 (3%)	42	61
1	C	377/401 (94%)	368 (98%)	9 (2%)	49	67
1	D	375/401 (94%)	367 (98%)	8 (2%)	53	71
1	E	378/401 (94%)	363 (96%)	15 (4%)	31	48
1	F	384/401 (96%)	370 (96%)	14 (4%)	35	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	376/401 (94%)	362 (96%)	14 (4%)	34 51
1	H	383/401 (96%)	370 (97%)	13 (3%)	37 54
All	All	3034/3208 (95%)	2935 (97%)	99 (3%)	38 56

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	47	GLN
1	E	356	ASN
1	H	270	GLU
1	E	166	GLU
1	E	274	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	AF2	B	503	2	18,24,25	4.45	11 (61%)	18,35,38	2.53	7 (38%)
2	AF2	A	503	2	18,24,25	4.69	10 (55%)	18,35,38	3.07	5 (27%)
2	AF2	C	503	2	18,24,25	4.75	10 (55%)	18,35,38	2.97	5 (27%)
2	AF2	H	503	2	18,24,25	4.48	10 (55%)	18,35,38	2.72	5 (27%)
2	AF2	F	501	2	18,24,25	4.59	10 (55%)	18,35,38	2.85	6 (33%)
2	AF2	G	501	2	18,24,25	4.45	10 (55%)	18,35,38	2.73	5 (27%)
3	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.05	0
2	AF2	A	502	2	18,24,25	4.54	10 (55%)	18,35,38	2.66	6 (33%)
2	AF2	H	501	2	18,24,25	4.62	10 (55%)	18,35,38	2.86	5 (27%)
3	SO4	F	504	-	4,4,4	0.13	0	6,6,6	0.05	0
2	AF2	F	503	2	18,24,25	4.49	10 (55%)	18,35,38	2.66	4 (22%)
2	AF2	G	503	2	18,24,25	4.73	10 (55%)	18,35,38	3.07	5 (27%)
2	AF2	B	502	2	18,24,25	4.72	10 (55%)	18,35,38	3.06	6 (33%)
2	AF2	H	502	2	18,24,25	4.73	10 (55%)	18,35,38	3.06	5 (27%)
3	SO4	G	504	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.05	0
2	AF2	C	502	2	18,24,25	4.61	10 (55%)	18,35,38	2.72	6 (33%)
2	AF2	D	503	2	18,24,25	4.47	10 (55%)	18,35,38	2.66	4 (22%)
2	AF2	E	503	2	18,24,25	4.96	11 (61%)	18,35,38	2.50	4 (22%)
2	AF2	D	501	2	18,24,25	4.59	10 (55%)	18,35,38	2.84	5 (27%)
2	AF2	B	501	2	18,24,25	4.56	10 (55%)	18,35,38	2.72	5 (27%)
2	AF2	E	501	2	18,24,25	4.44	10 (55%)	18,35,38	2.81	5 (27%)
2	AF2	C	501	2	18,24,25	4.47	10 (55%)	18,35,38	2.72	5 (27%)
2	AF2	D	502	2	18,24,25	4.71	10 (55%)	18,35,38	3.04	5 (27%)
2	AF2	F	502	2	18,24,25	4.66	10 (55%)	18,35,38	3.04	5 (27%)
2	AF2	E	502	2	18,24,25	4.54	11 (61%)	18,35,38	2.68	6 (33%)
2	AF2	A	501	2	18,24,25	4.44	10 (55%)	18,35,38	2.70	5 (27%)
2	AF2	G	502	2	18,24,25	4.64	10 (55%)	18,35,38	2.70	6 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AF2	B	503	2	-	2/3/25/26	0/3/3/3
2	AF2	A	503	2	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AF2	C	503	2	-	0/3/25/26	0/3/3/3
2	AF2	H	503	2	-	2/3/25/26	0/3/3/3
2	AF2	F	501	2	-	2/3/25/26	0/3/3/3
2	AF2	G	501	2	-	2/3/25/26	0/3/3/3
2	AF2	A	502	2	-	2/3/25/26	0/3/3/3
2	AF2	H	501	2	-	2/3/25/26	0/3/3/3
2	AF2	F	503	2	-	2/3/25/26	0/3/3/3
2	AF2	G	503	2	-	0/3/25/26	0/3/3/3
2	AF2	B	502	2	-	0/3/25/26	0/3/3/3
2	AF2	H	502	2	-	0/3/25/26	0/3/3/3
2	AF2	C	502	2	-	2/3/25/26	0/3/3/3
2	AF2	D	503	2	-	2/3/25/26	0/3/3/3
2	AF2	E	503	2	-	0/3/25/26	0/3/3/3
2	AF2	D	501	2	-	2/3/25/26	0/3/3/3
2	AF2	B	501	2	-	2/3/25/26	0/3/3/3
2	AF2	E	501	2	-	2/3/25/26	0/3/3/3
2	AF2	C	501	2	-	2/3/25/26	0/3/3/3
2	AF2	D	502	2	-	0/3/25/26	0/3/3/3
2	AF2	F	502	2	-	0/3/25/26	0/3/3/3
2	AF2	E	502	2	-	2/3/25/26	0/3/3/3
2	AF2	A	501	2	-	2/3/25/26	0/3/3/3
2	AF2	G	502	2	-	2/3/25/26	0/3/3/3

The worst 5 of 243 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	503	AF2	C2'-C3'	-15.61	1.31	1.52
2	G	503	AF2	C2'-C3'	-15.32	1.31	1.52
2	C	503	AF2	C2'-C3'	-15.29	1.31	1.52
2	B	502	AF2	C2'-C3'	-15.23	1.31	1.52
2	H	502	AF2	C2'-C3'	-15.19	1.31	1.52

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	AF2	C5-C6-N6	7.67	132.01	120.35
2	H	501	AF2	C5-C6-N6	7.41	131.62	120.35
2	H	502	AF2	C5-C6-N6	7.34	131.51	120.35
2	A	503	AF2	C5-C6-N6	7.33	131.49	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	503	AF2	C5-C6-N6	7.32	131.47	120.35

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	503	AF2	C3'-C4'-C5'-O5'
2	F	503	AF2	C3'-C4'-C5'-O5'
2	D	501	AF2	O4'-C4'-C5'-O5'
2	B	501	AF2	O4'-C4'-C5'-O5'
2	E	501	AF2	O4'-C4'-C5'-O5'

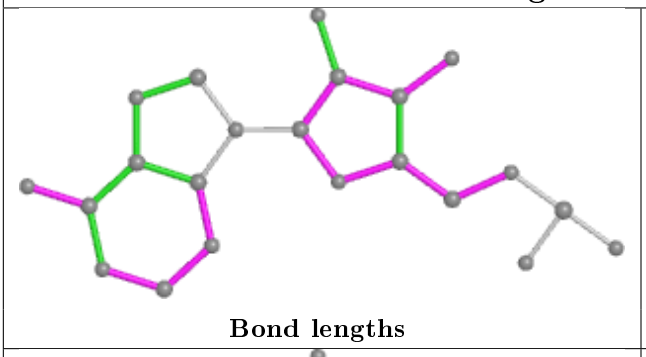
There are no ring outliers.

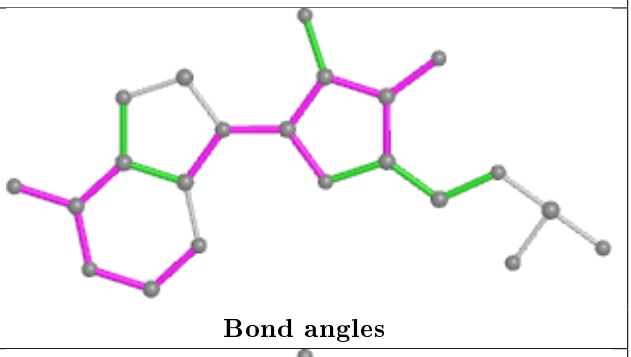
10 monomers are involved in 11 short contacts:

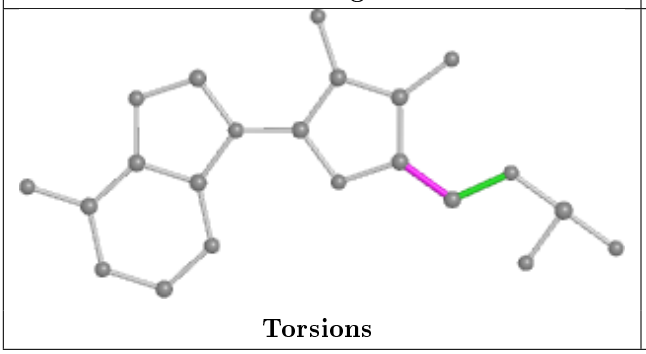
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	503	AF2	1	0
2	G	501	AF2	1	0
3	C	504	SO4	1	0
2	F	503	AF2	1	0
3	G	504	SO4	1	0
2	D	503	AF2	1	0
2	E	503	AF2	1	0
2	E	501	AF2	1	0
2	C	501	AF2	2	0
2	A	501	AF2	1	0

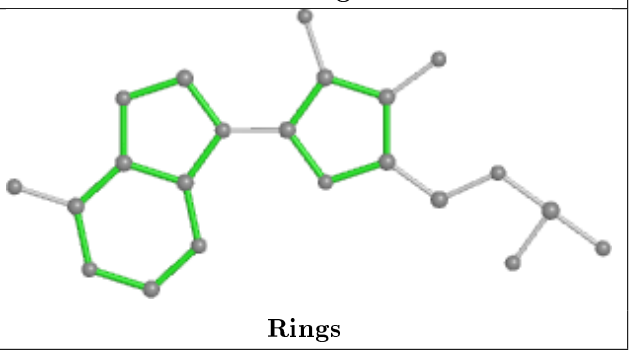
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AF2 B 503

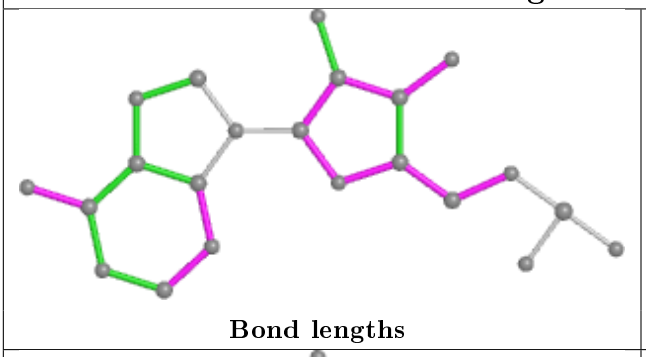

Bond lengths


Bond angles


Torsions


Rings

Ligand AF2 A 503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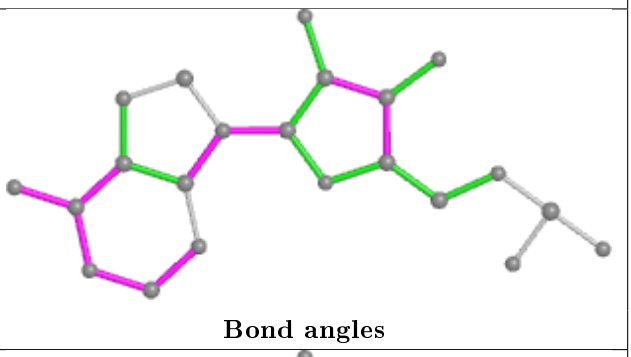
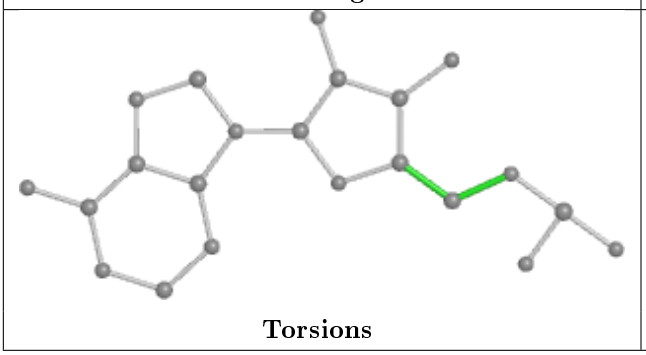
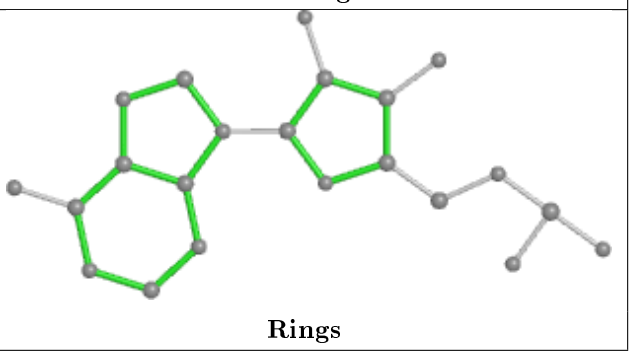
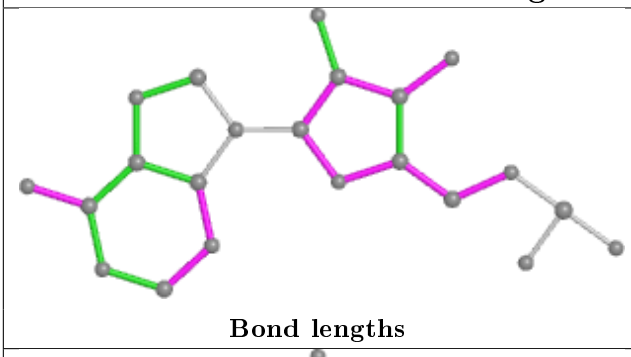

Bond angles


Torsions


Rings

Ligand AF2 C 503



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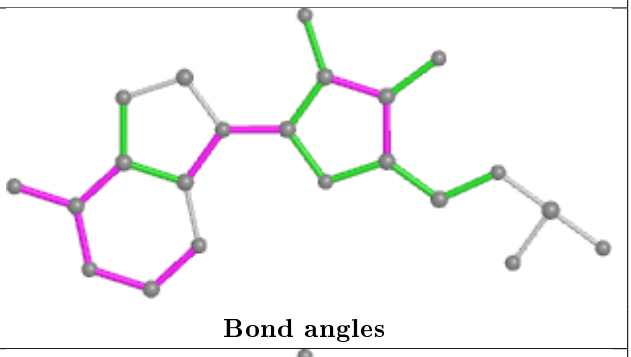
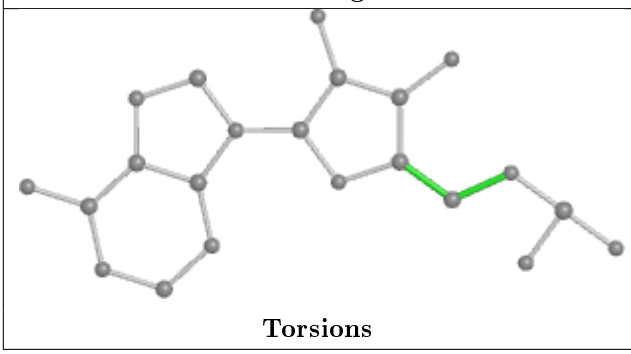
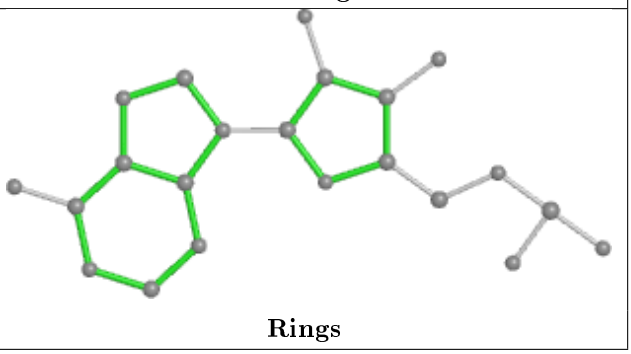


Bond angles

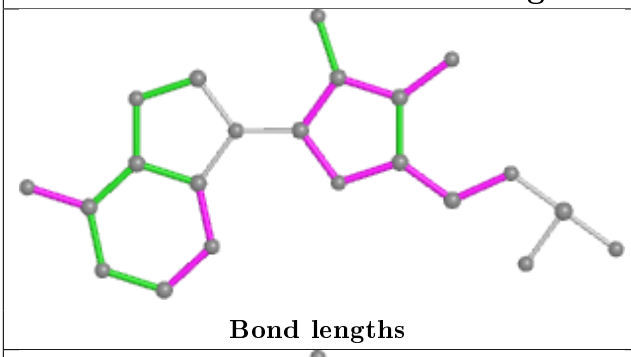


Torsions



Rings

Ligand AF2 H 503



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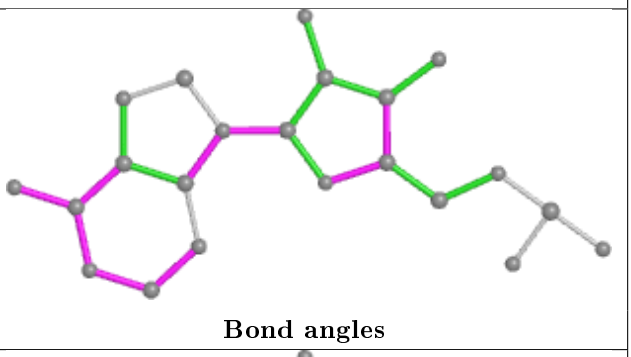
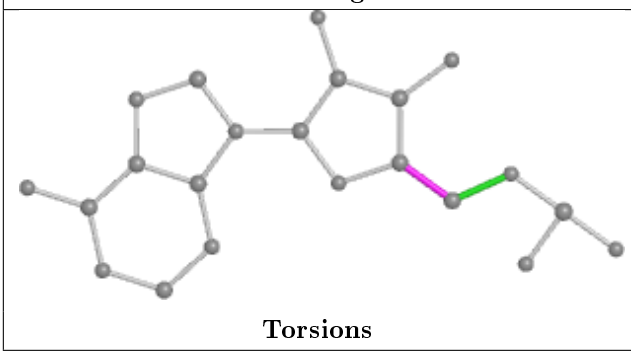
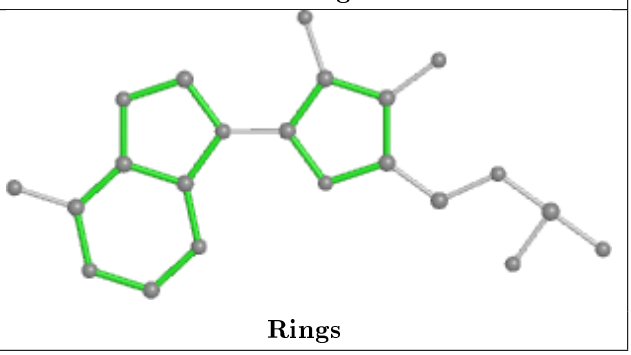


Bond angles

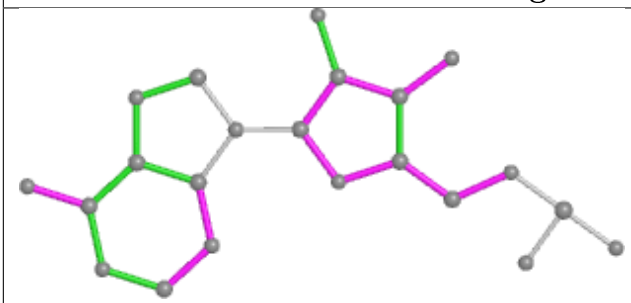


Torsions

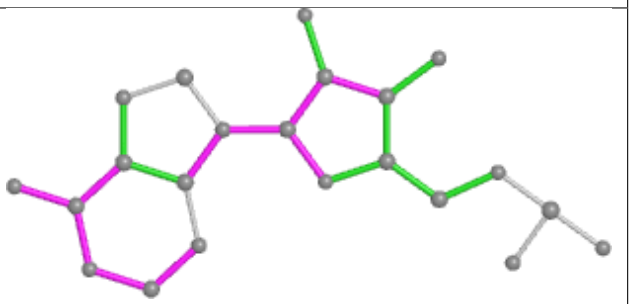


Rings

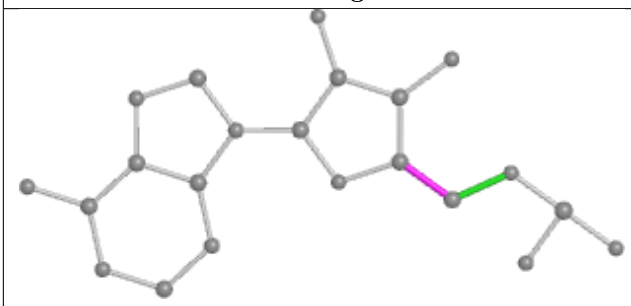
Ligand AF2 F 501



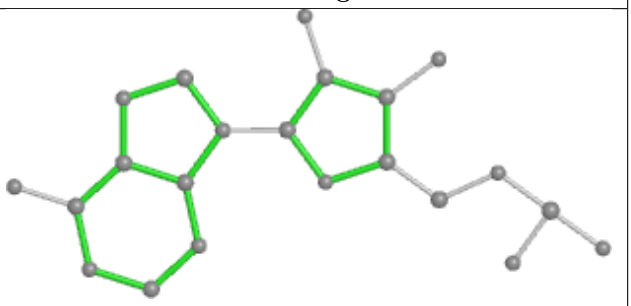
Bond lengths



Bond angles

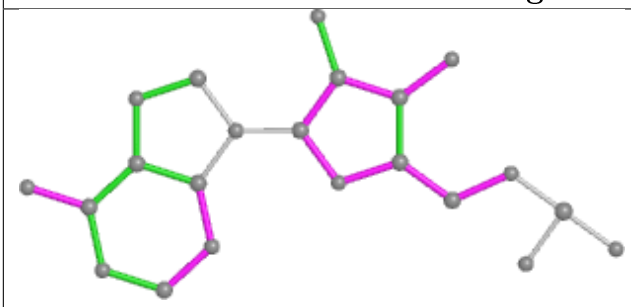


Torsions



Rings

Ligand AF2 G 501



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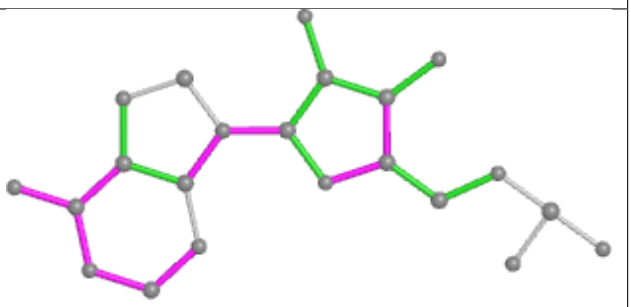
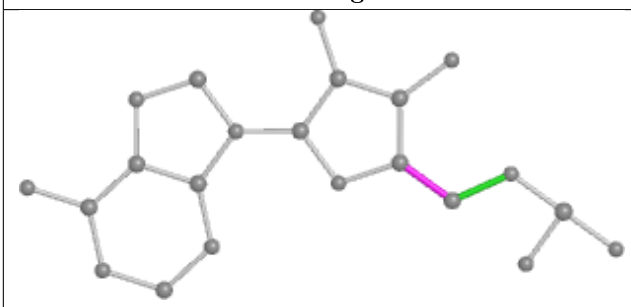


Bond angles



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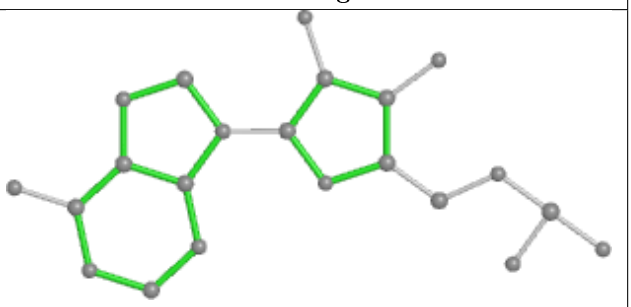
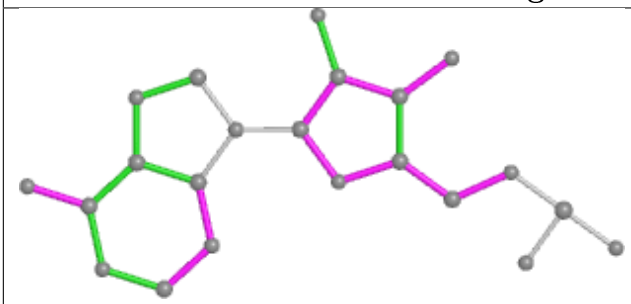


Rings

Ligand AF2 A 502



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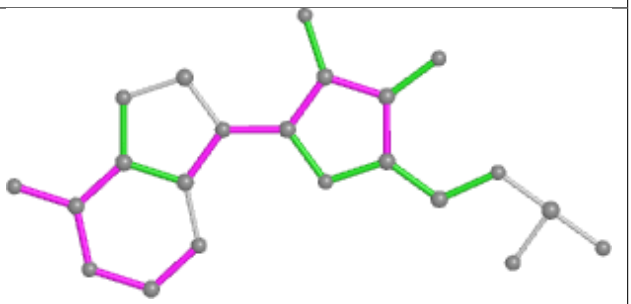

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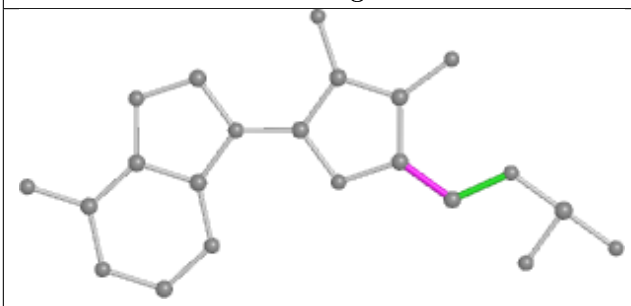

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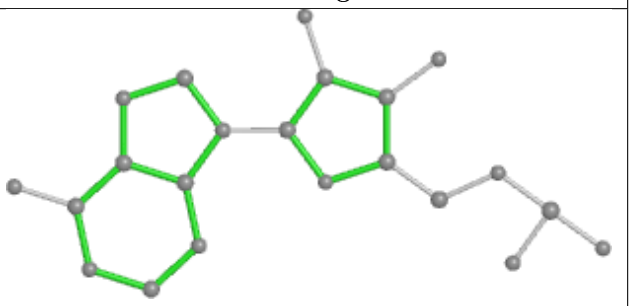
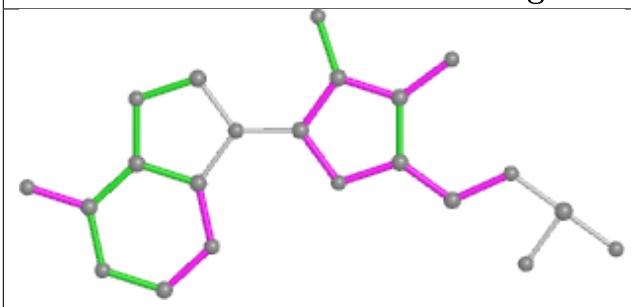


Rings

Ligand AF2 H 501



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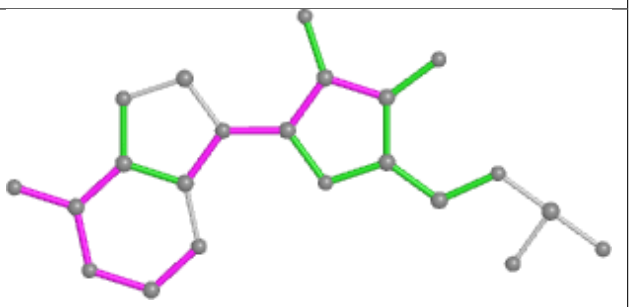
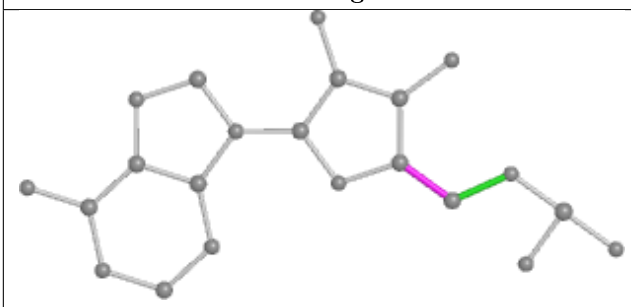
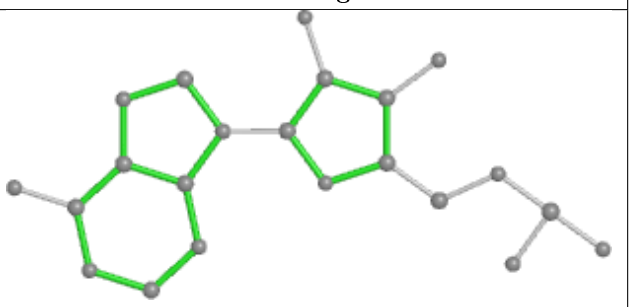


Bond angles

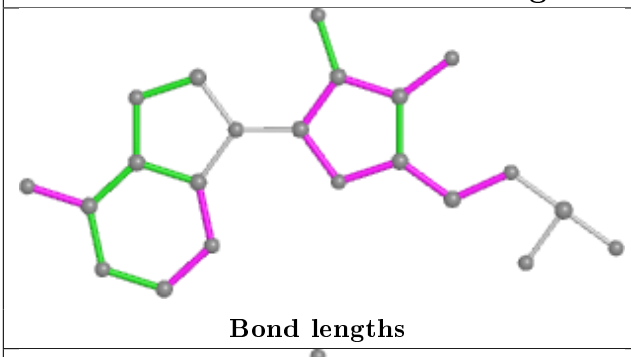


Torsions

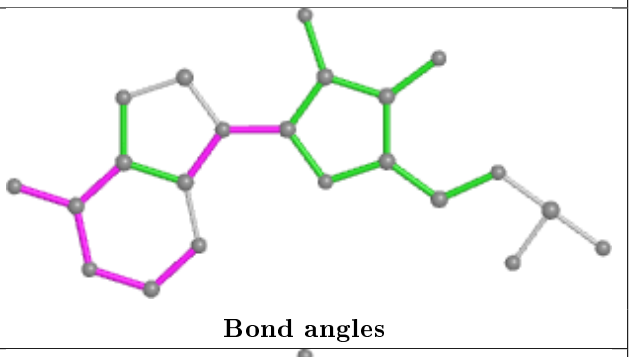


Rings

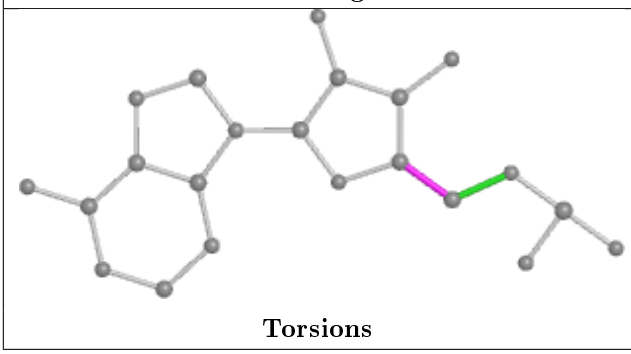
Ligand AF2 F 503



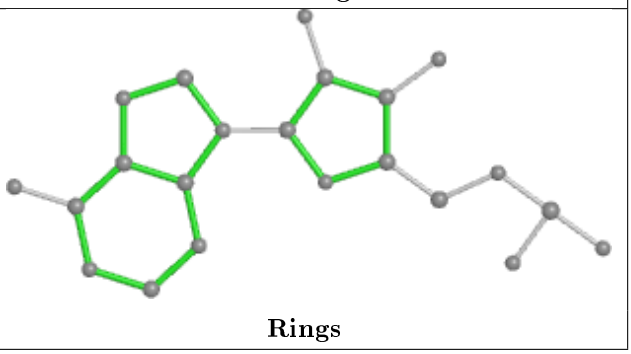
Bond lengths



Bond angles

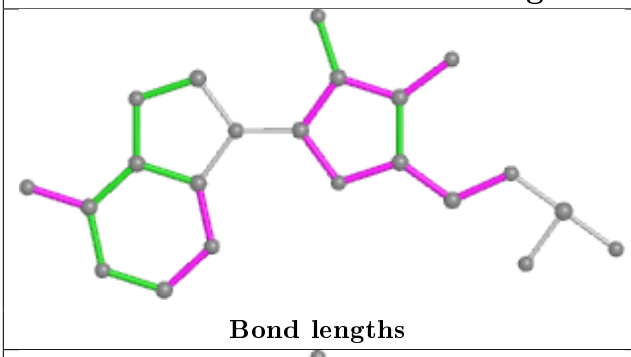


Torsions



Rings

Ligand AF2 G 503



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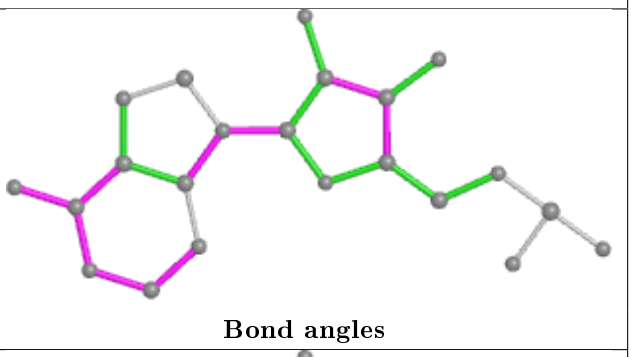
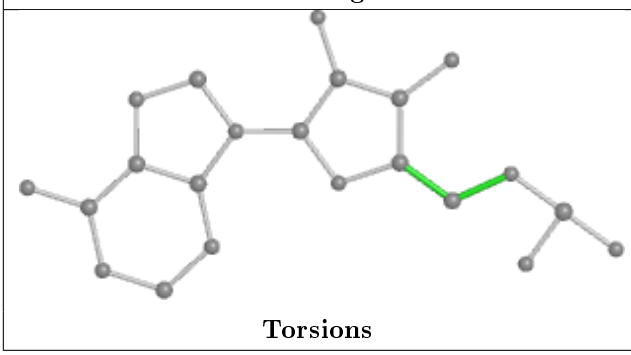


Bond angles



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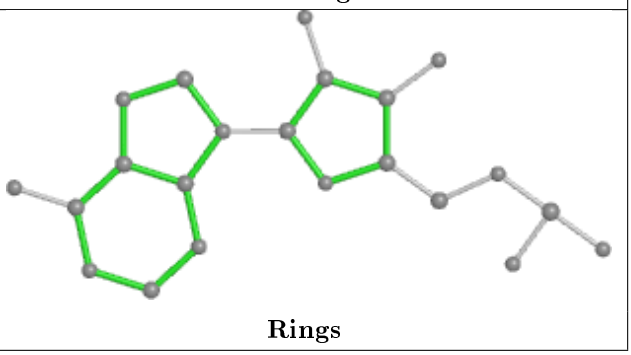
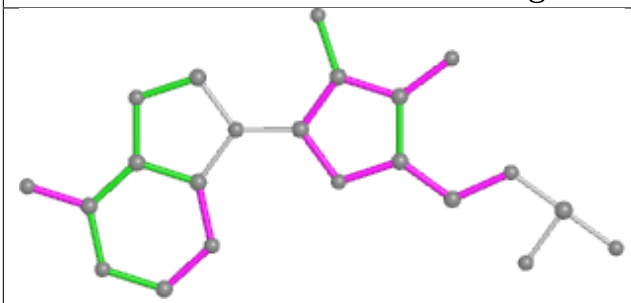


Rings

Ligand AF2 B 502



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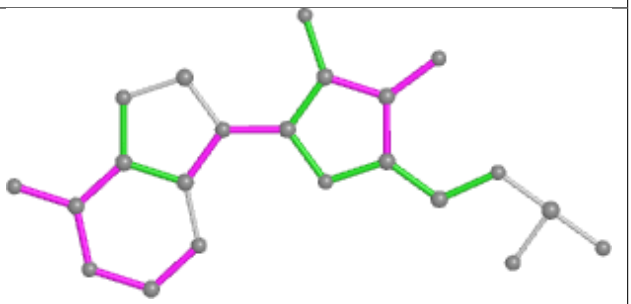

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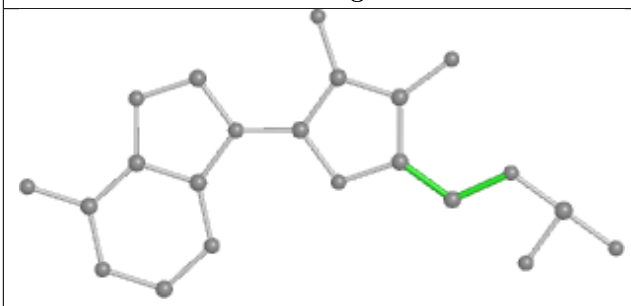

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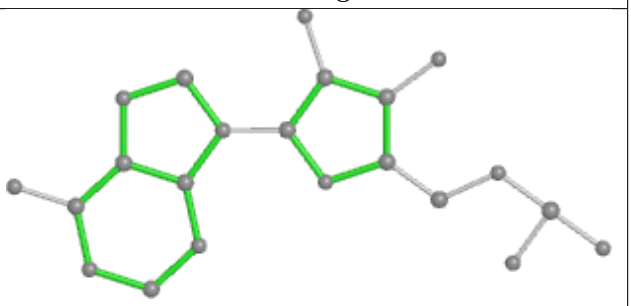
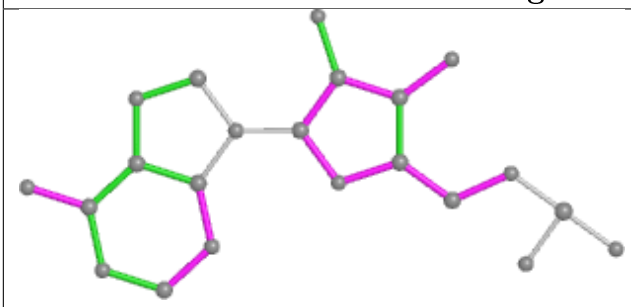


Rings

Ligand AF2 H 502



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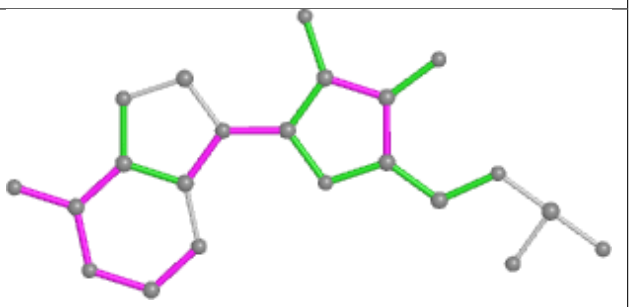

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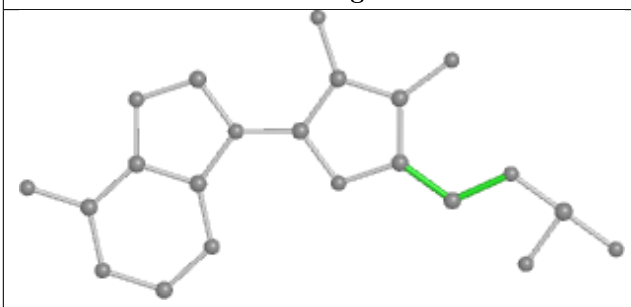

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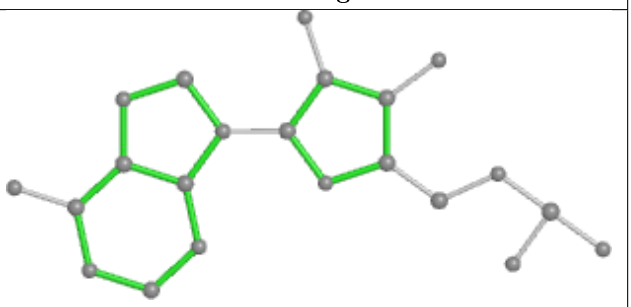
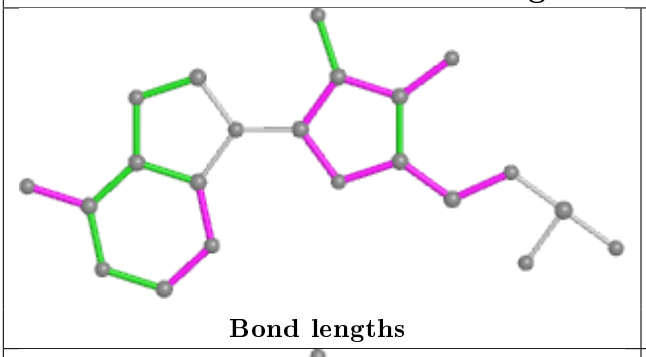


Rings

Ligand AF2 C 502



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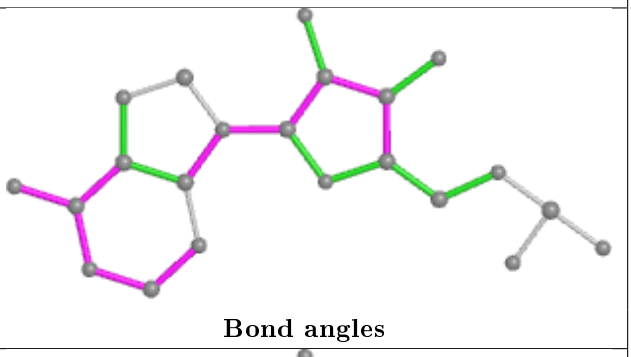

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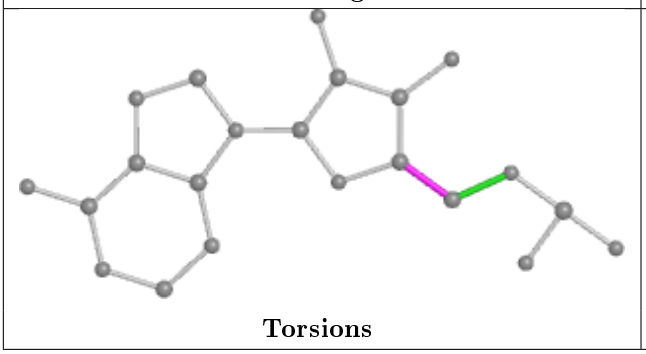

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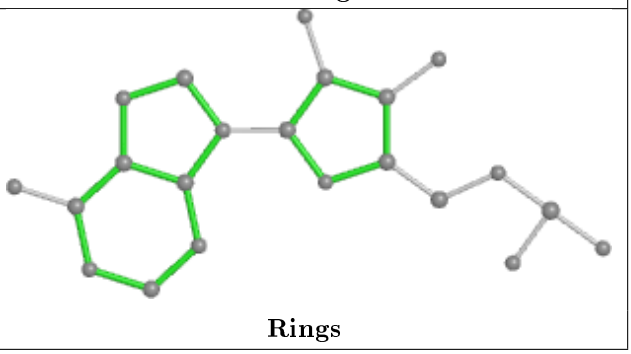
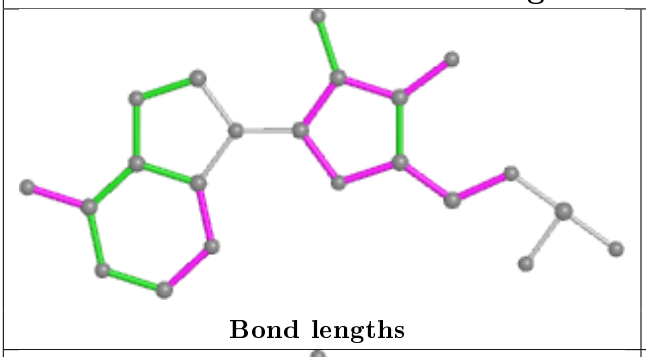


Rings

Ligand AF2 D 503



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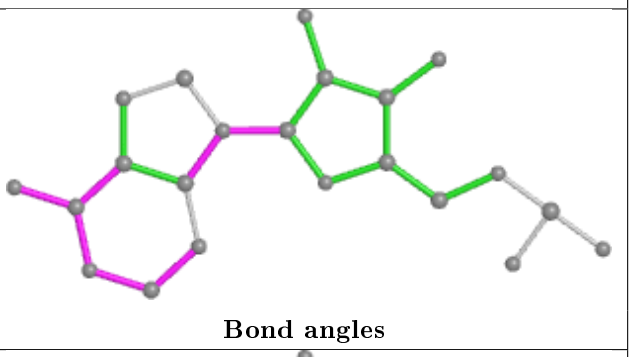

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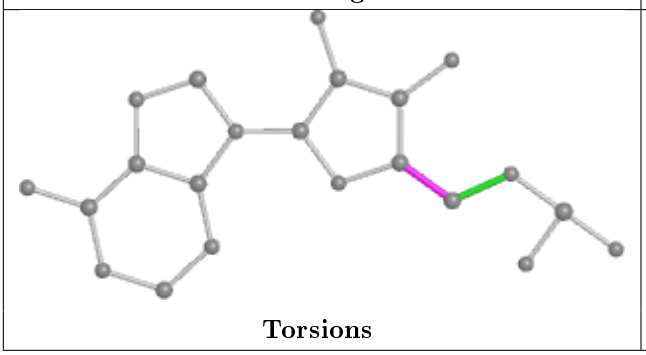

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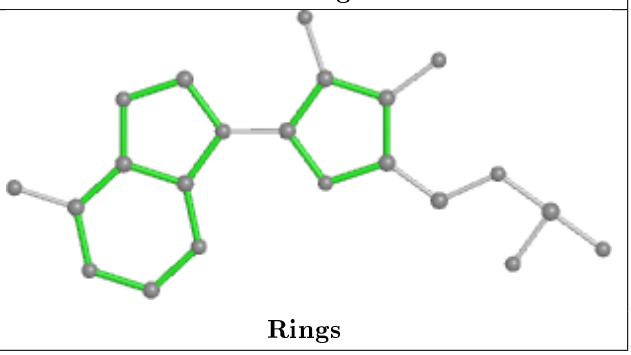
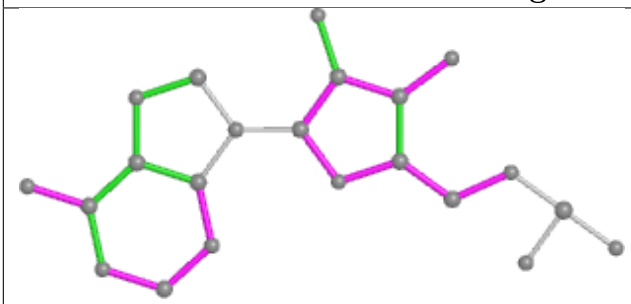


Rings

Ligand AF2 E 503



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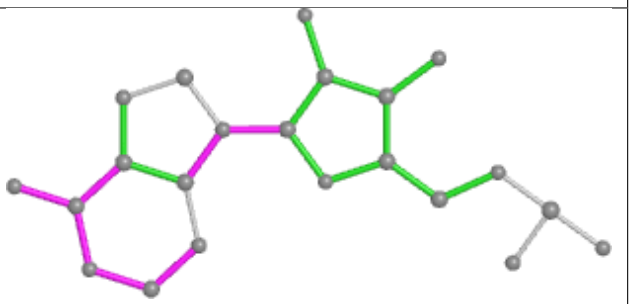

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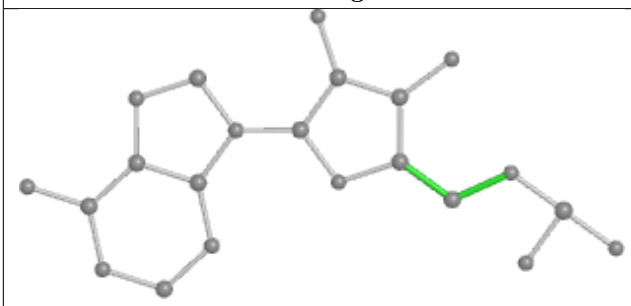

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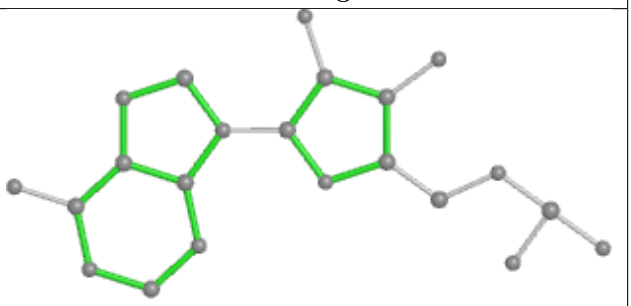
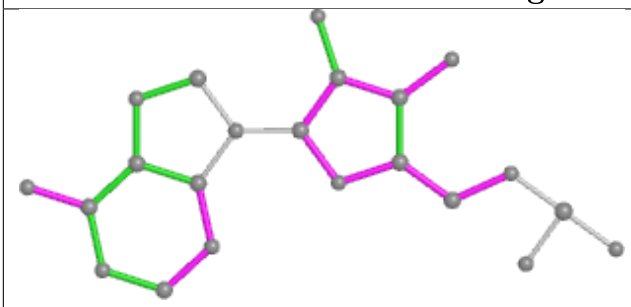


Rings

Ligand AF2 D 501



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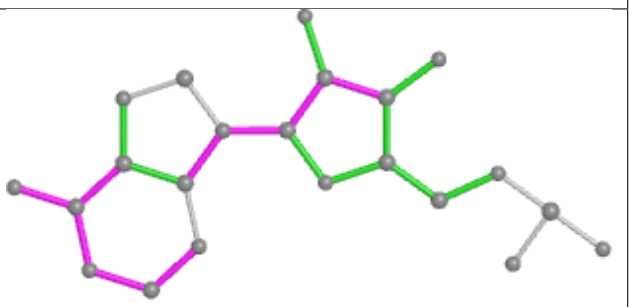

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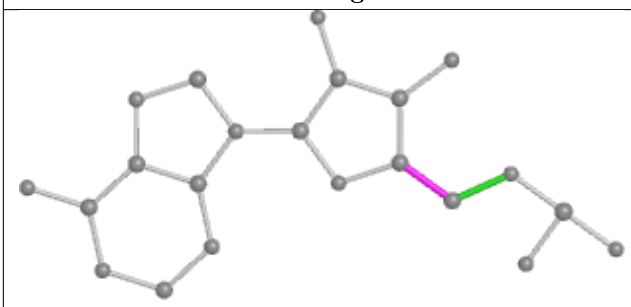

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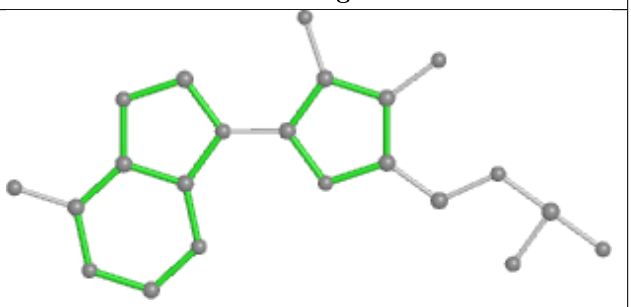
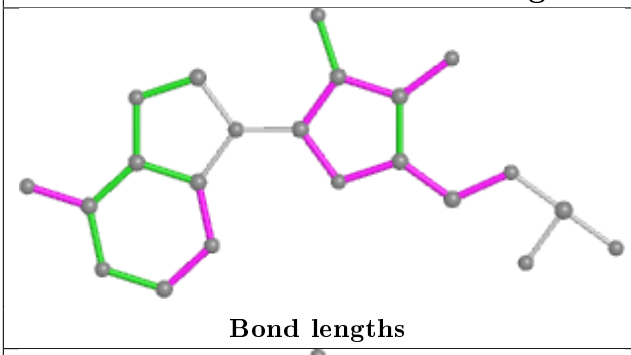


Rings

Ligand AF2 B 501



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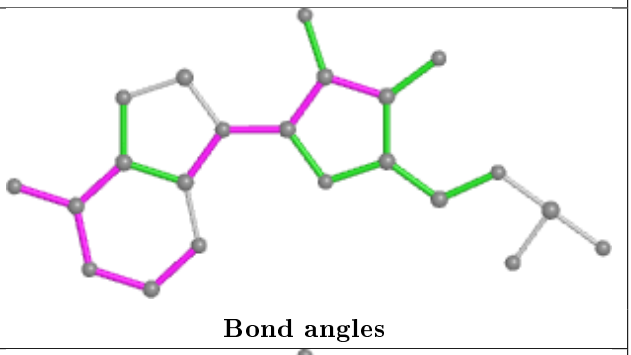

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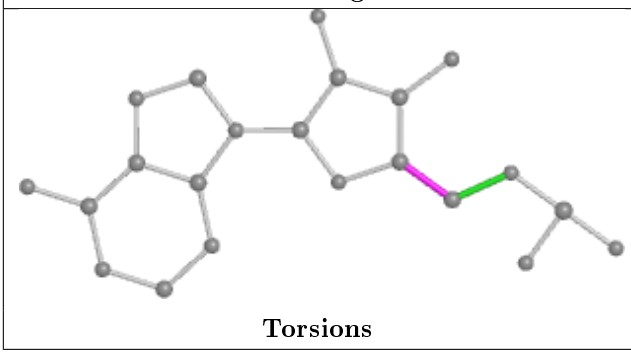

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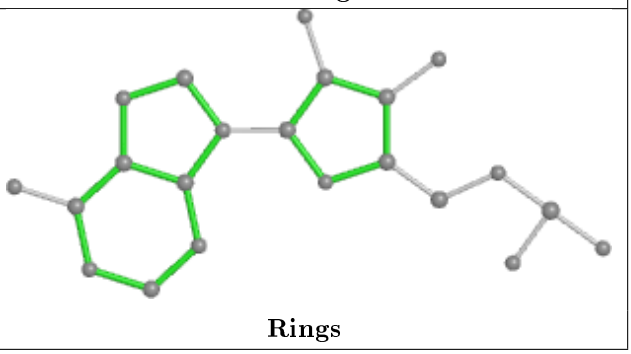
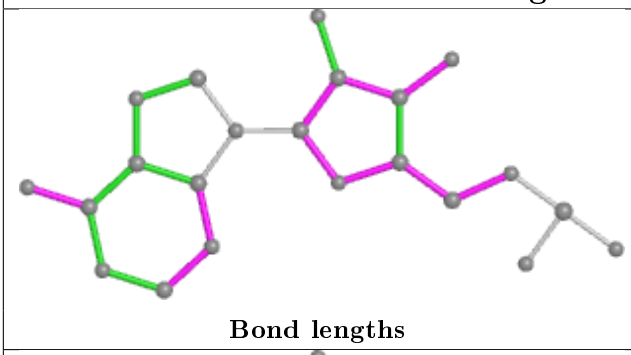


Rings

Ligand AF2 E 501



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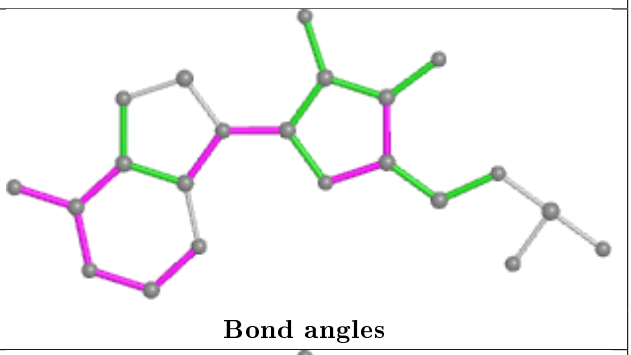

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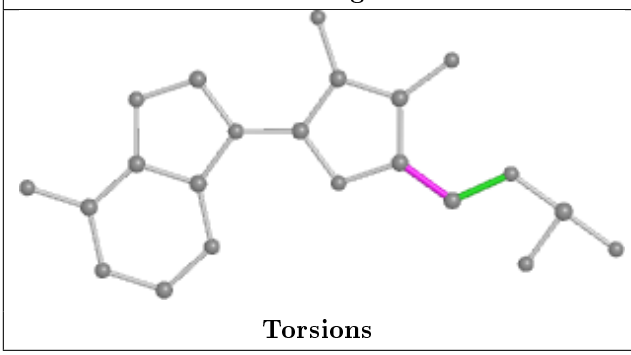

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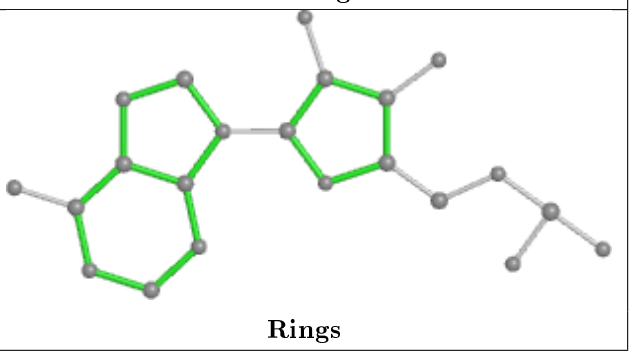
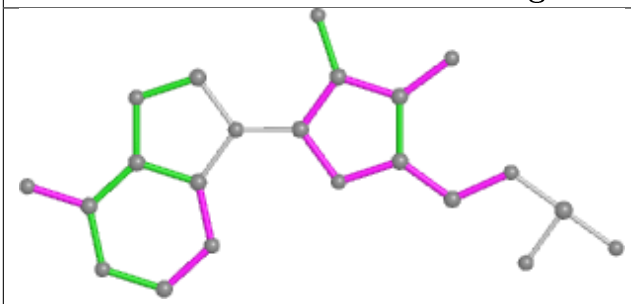


Rings

Ligand AF2 C 501



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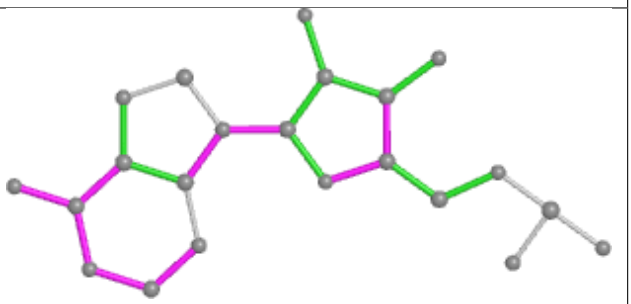
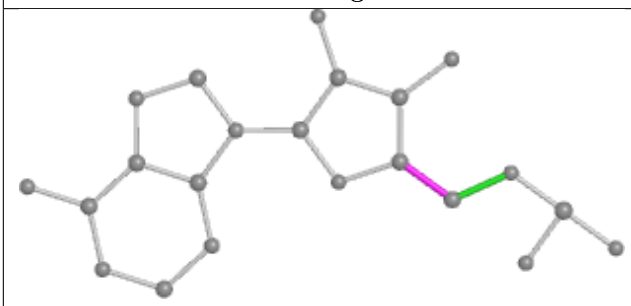


Bond angles



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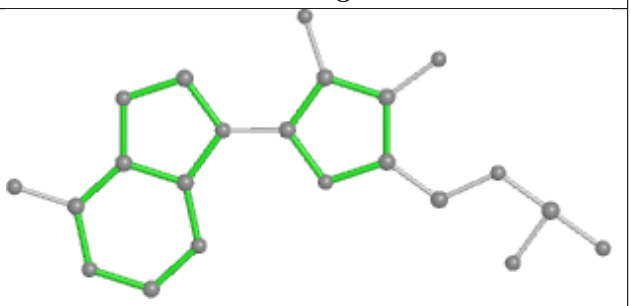
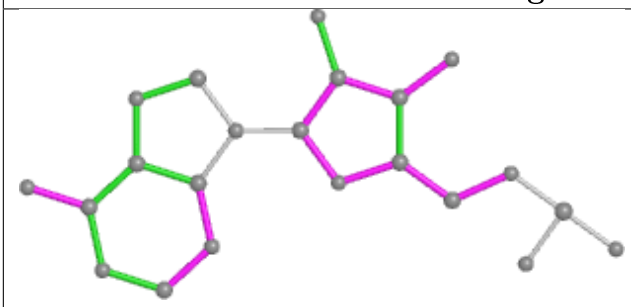


Rings

Ligand AF2 D 502



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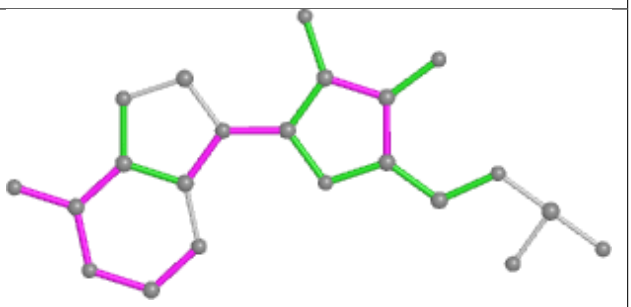

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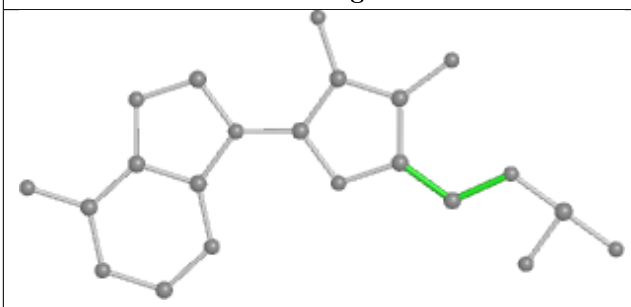

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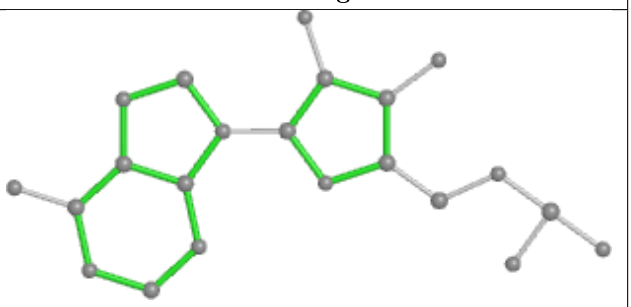
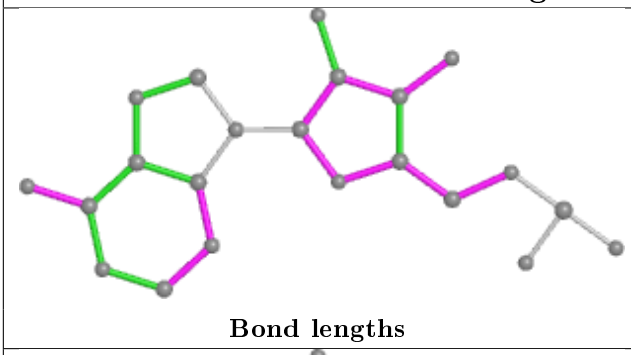


Rings

Ligand AF2 F 502



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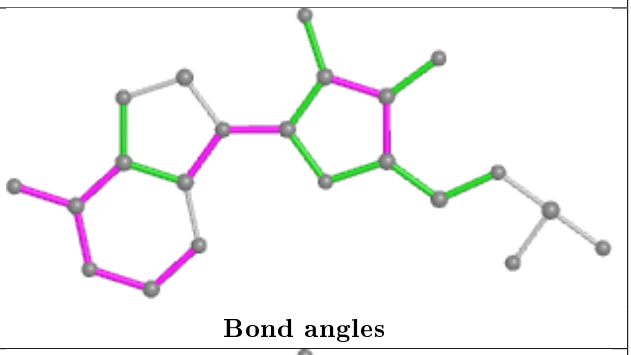
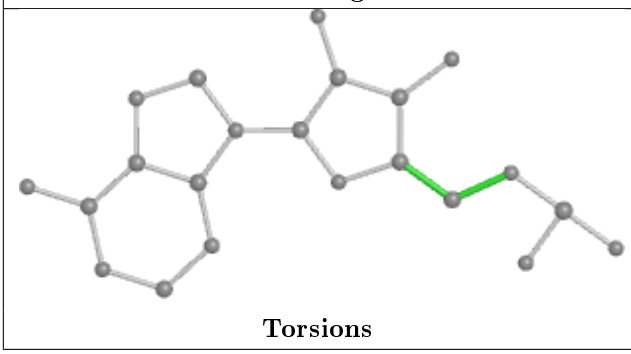


Bond angles



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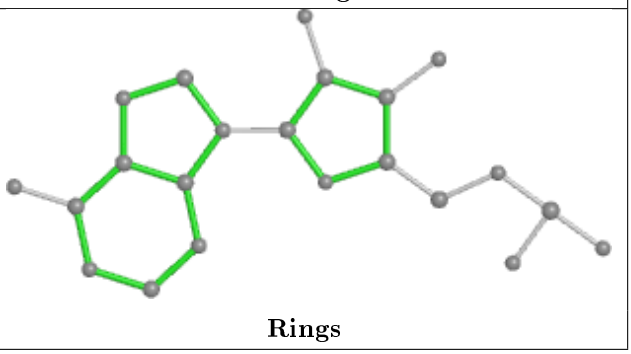
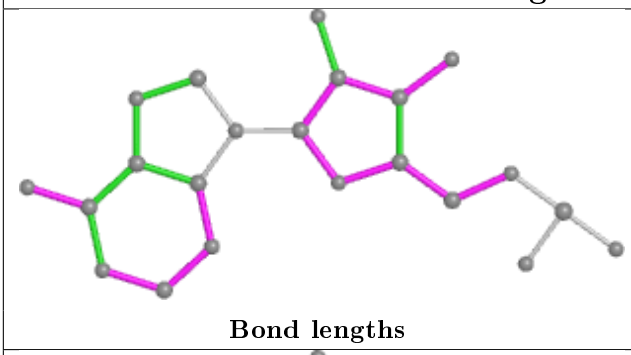
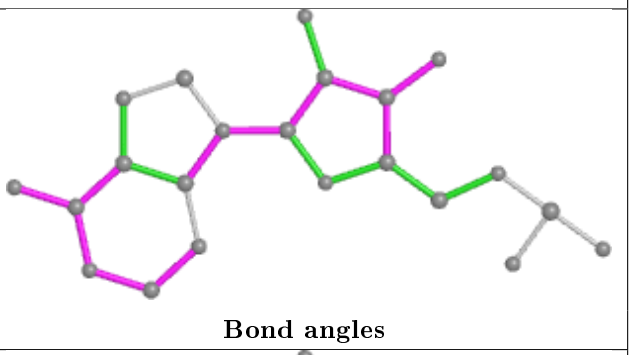


Rings

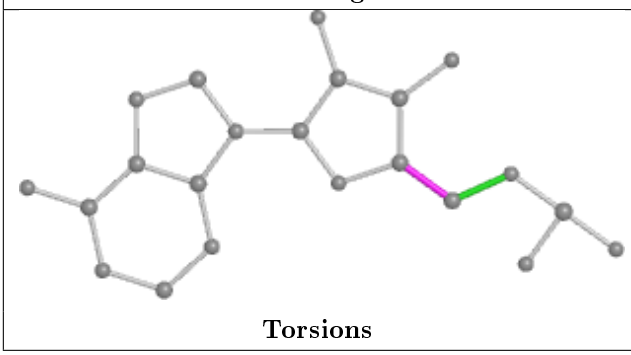
Ligand AF2 E 502



Bond lengths



Bond angles



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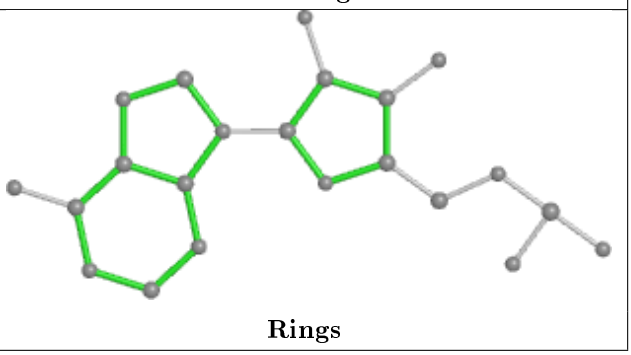
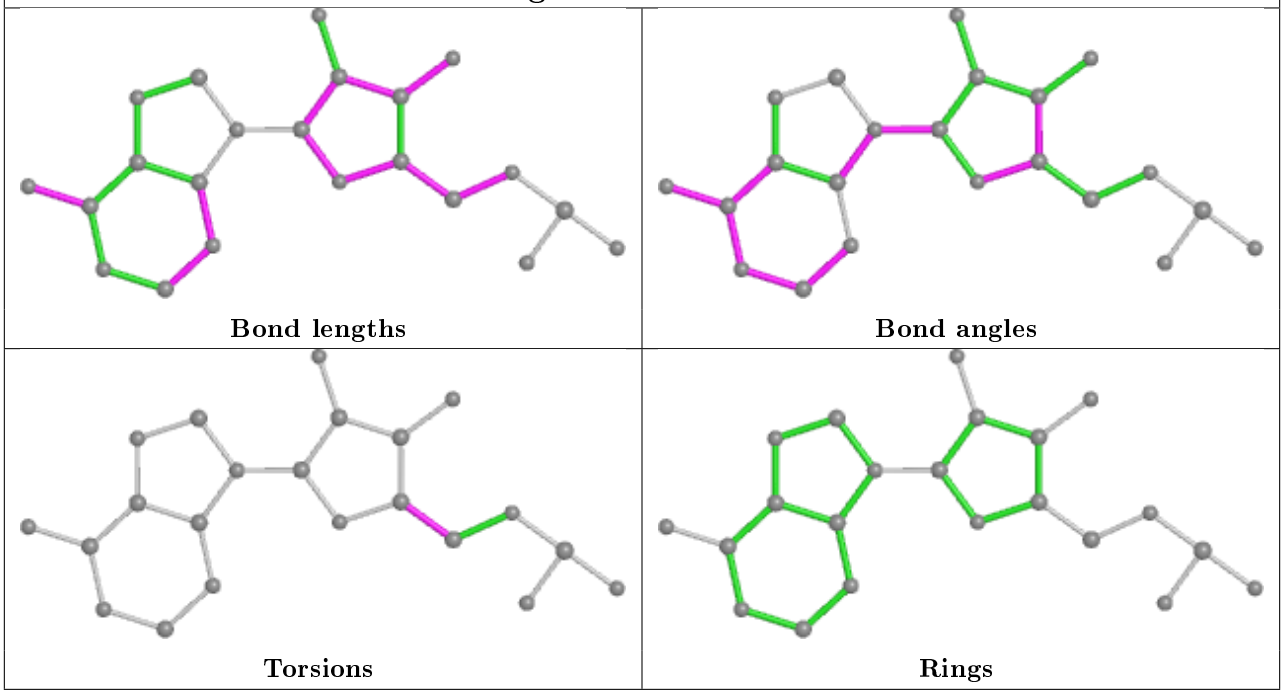
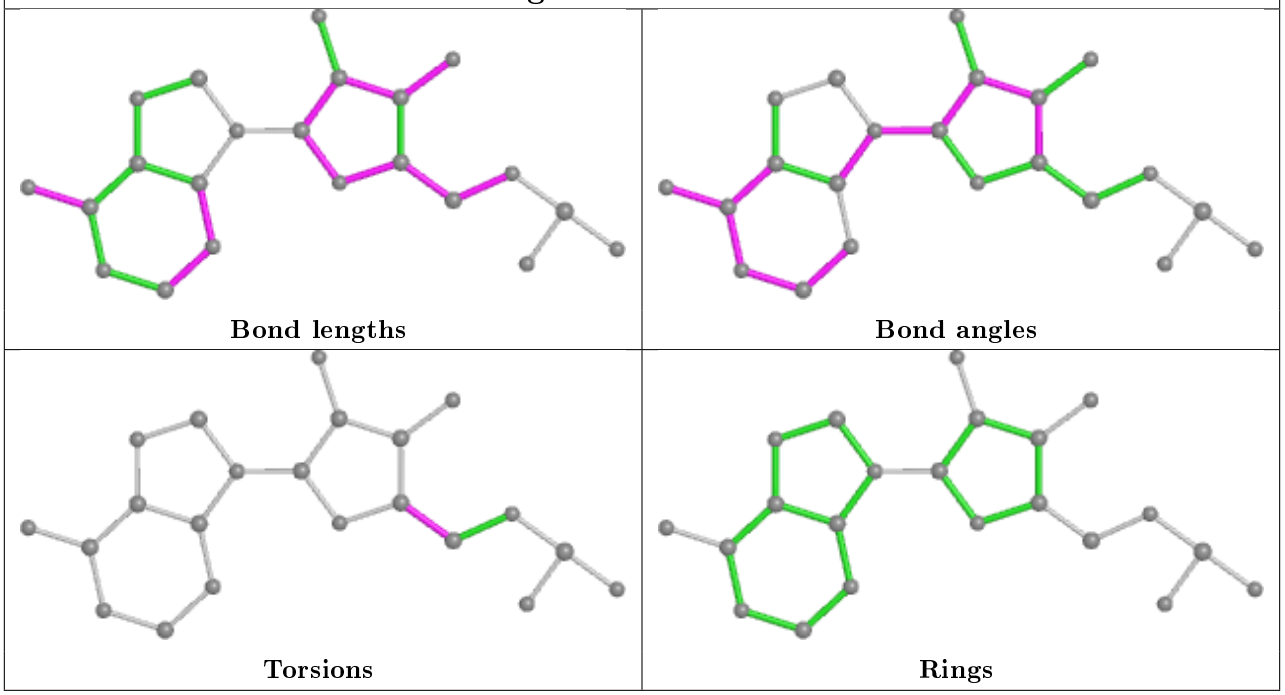


Rings

Ligand AF2 A 501



Ligand AF2 G 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

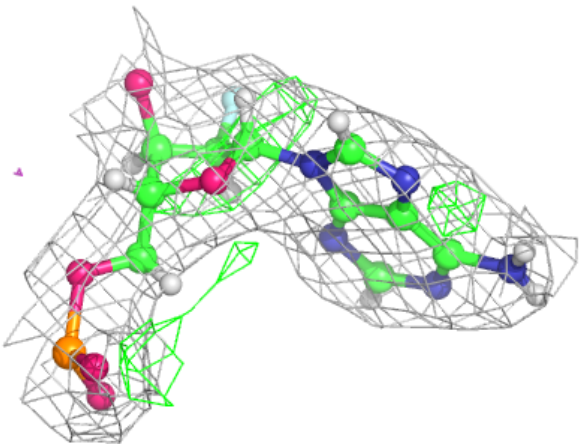
6.4 Ligands

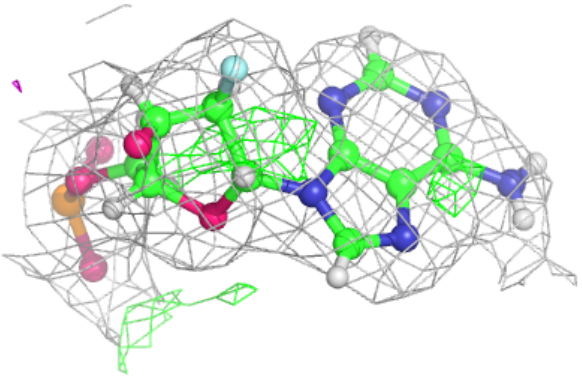
Unable to reproduce the depositors R factor - this section is therefore empty.

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 AF2 B 503:

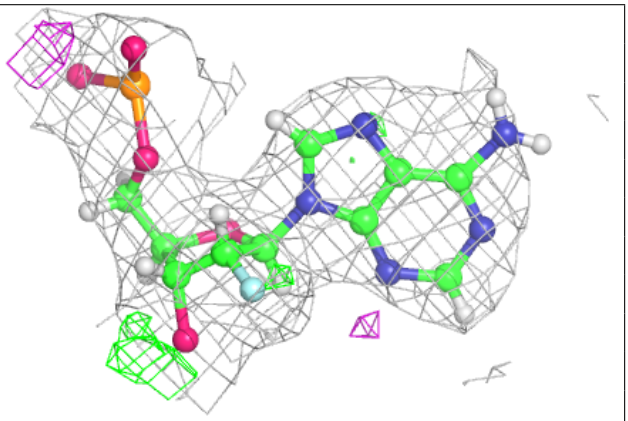
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

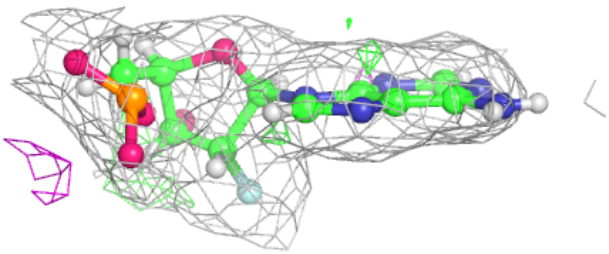


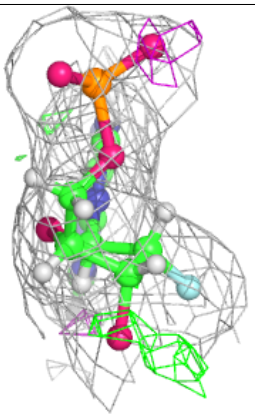


Electron density around AF2 A 503:

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

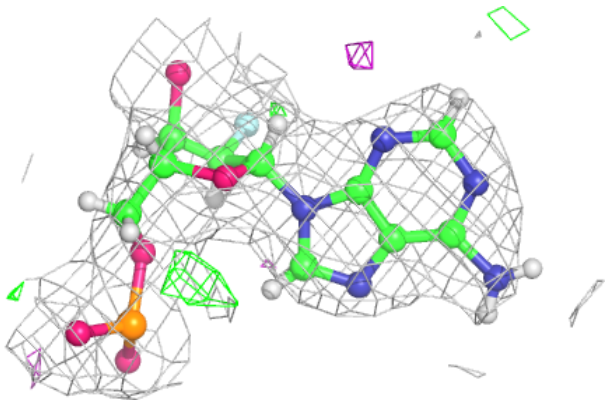


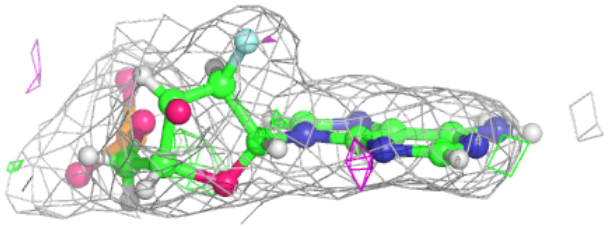


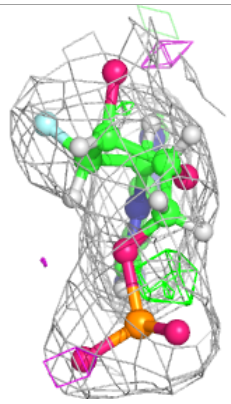


Electron density around AF2 C 503:

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

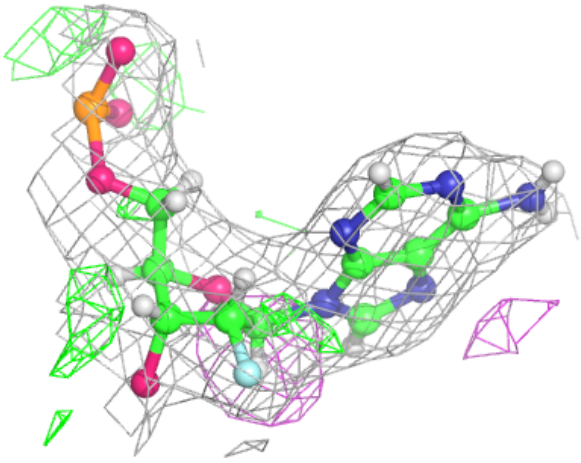


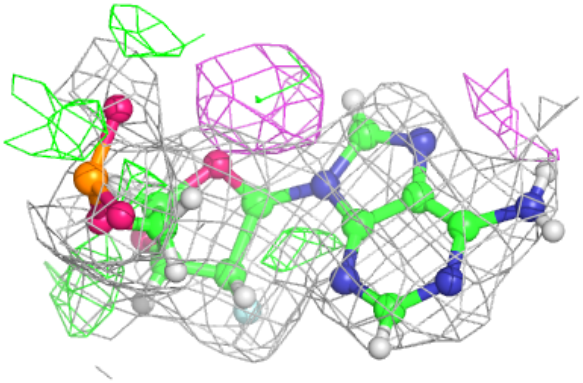


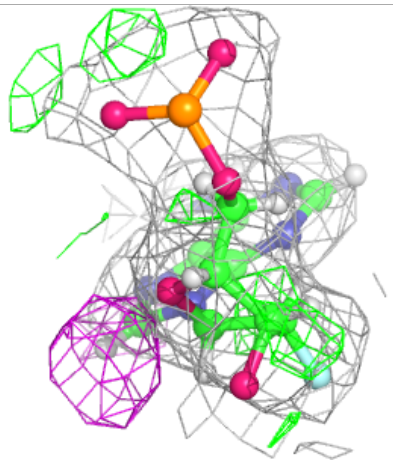


Electron density around AF2 H 503:

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

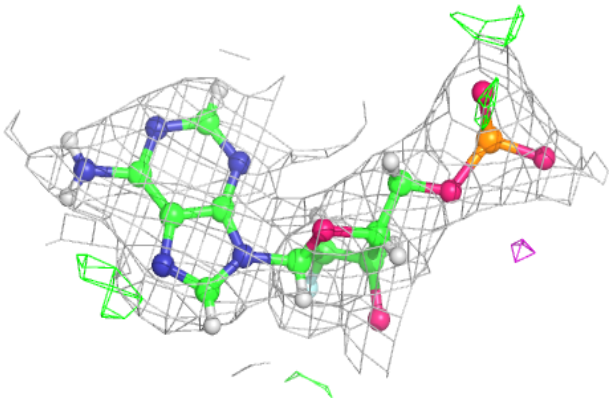


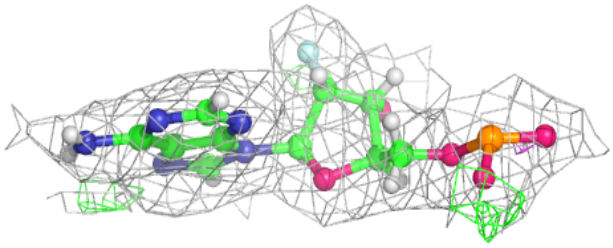


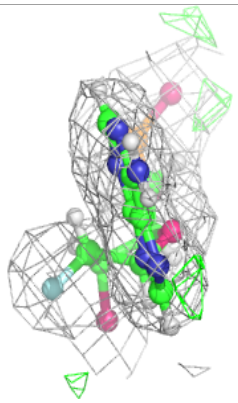


Electron density around AF2 F 501:

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

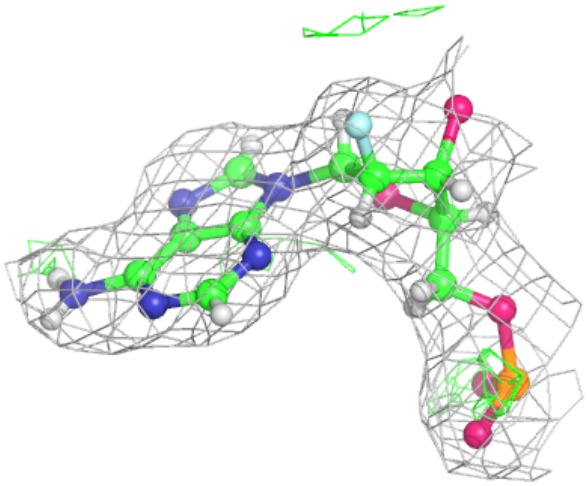


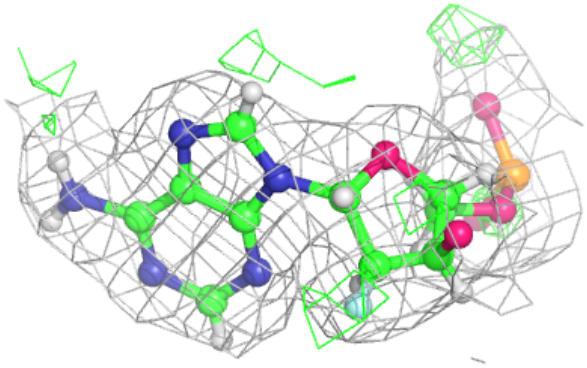


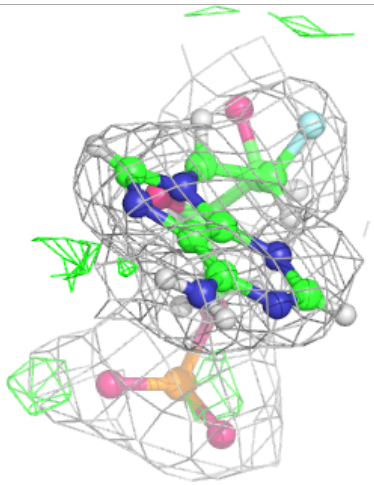


Electron density around AF2 G 501:

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

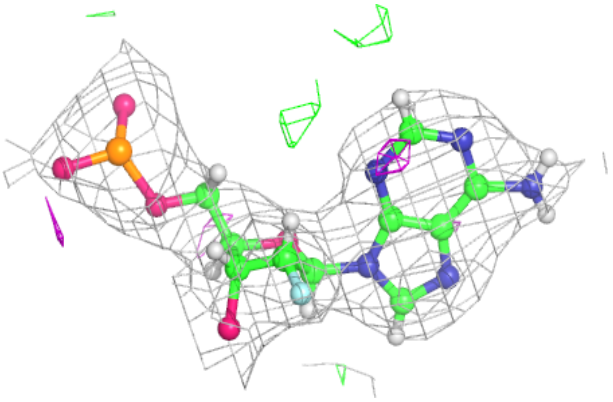


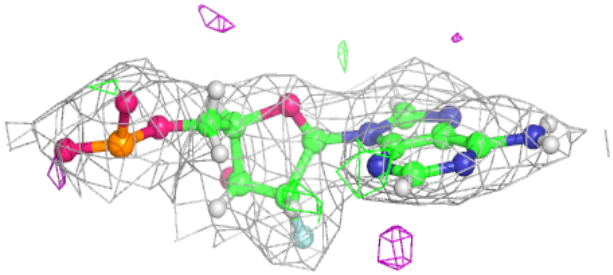


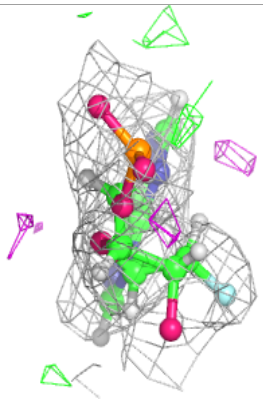


Electron density around AF2 A 502:

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

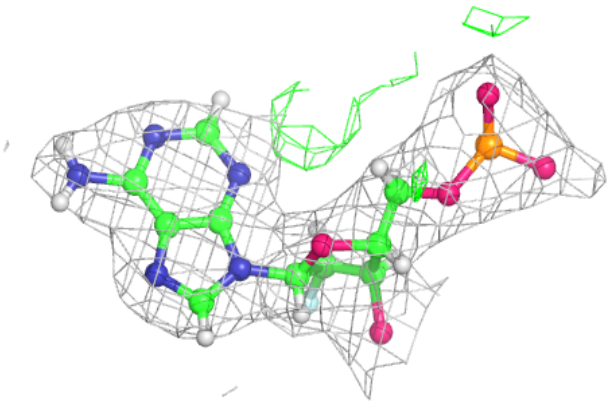


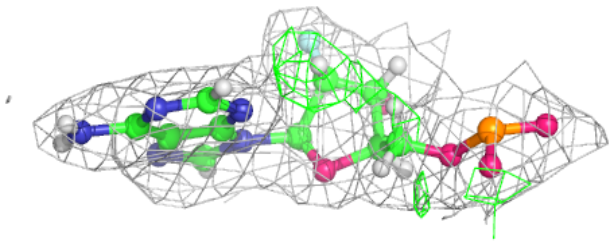




Electron density around AF2 H 501:

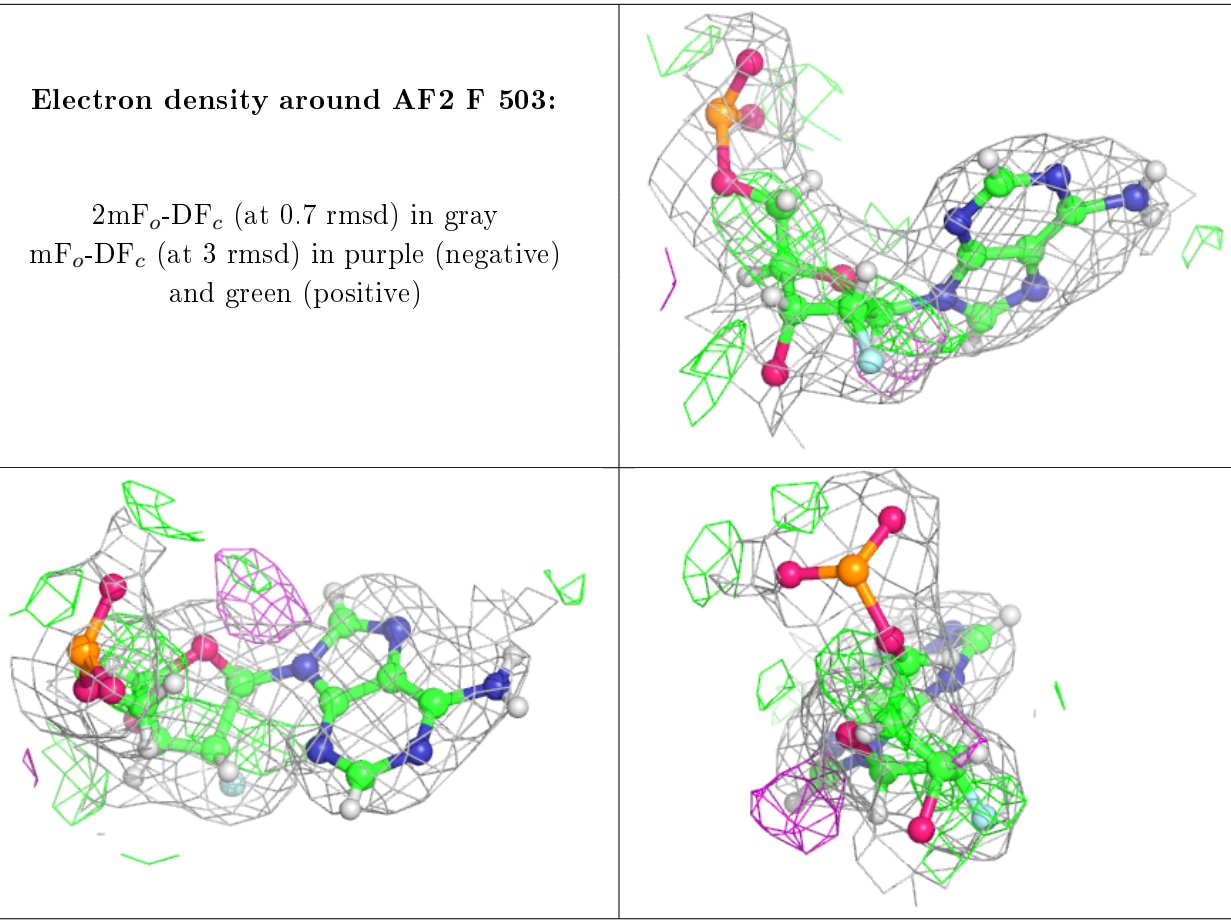
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





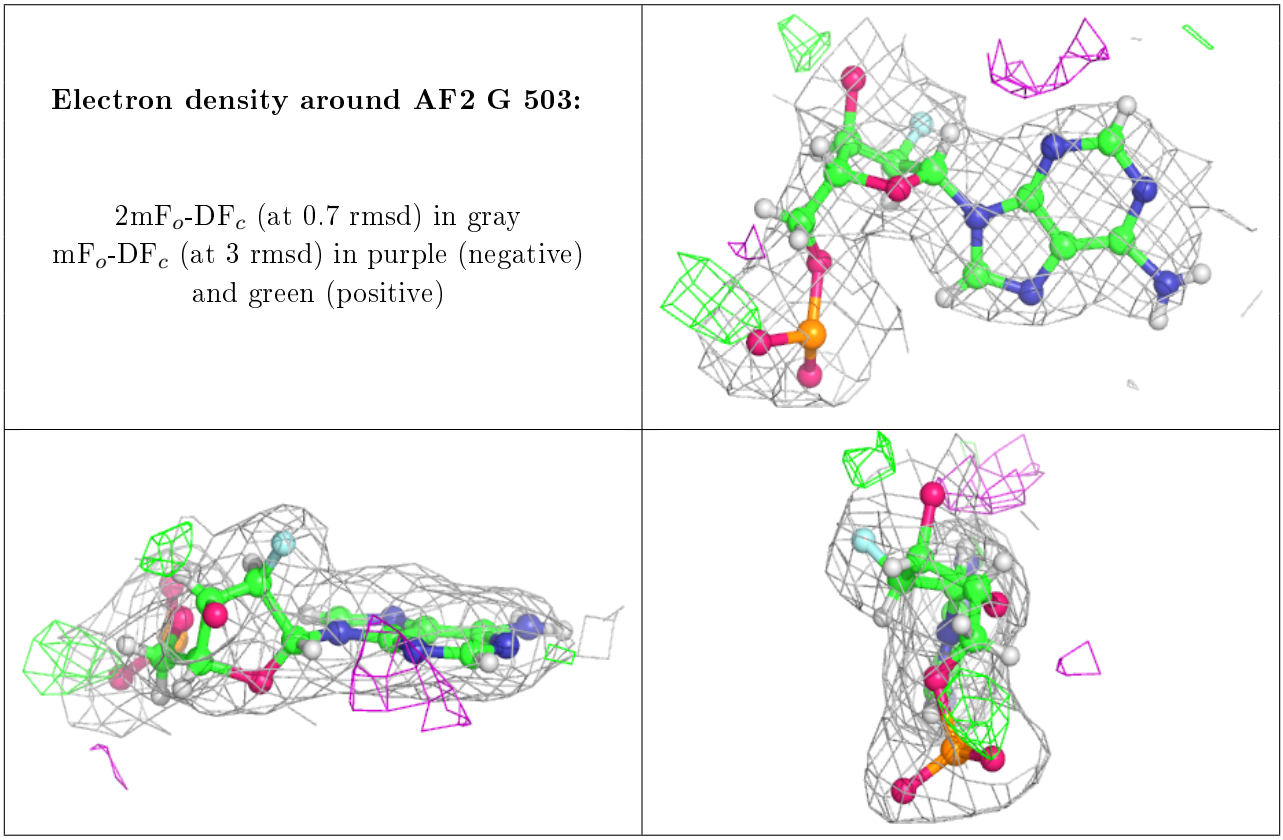
Electron density around AF2 F 503:

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



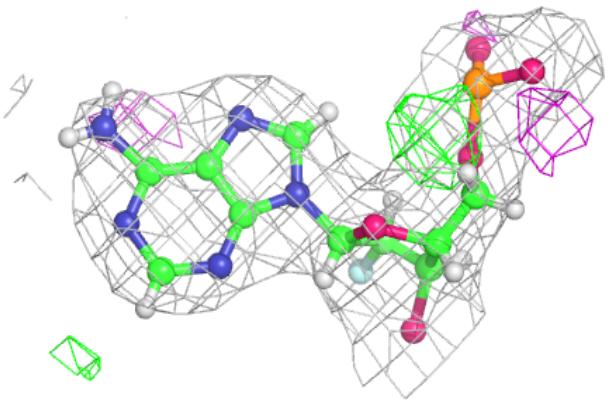
Electron density around AF2 G 503:

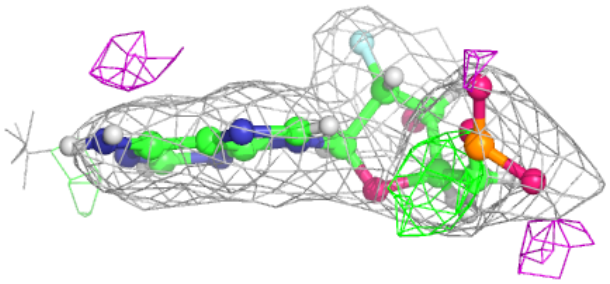
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

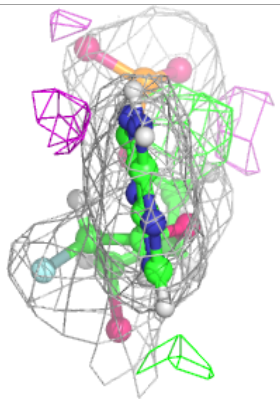


Electron density around AF2 B 502:

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

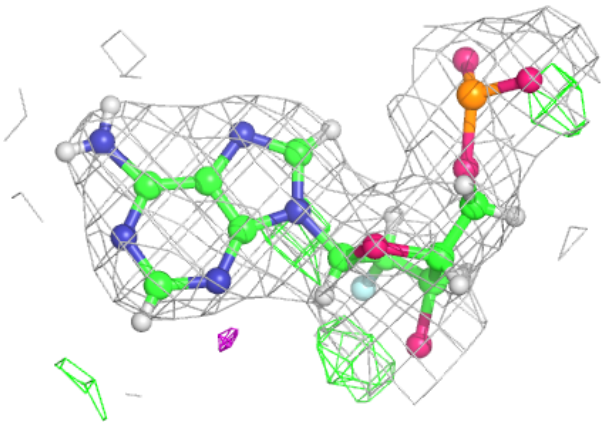


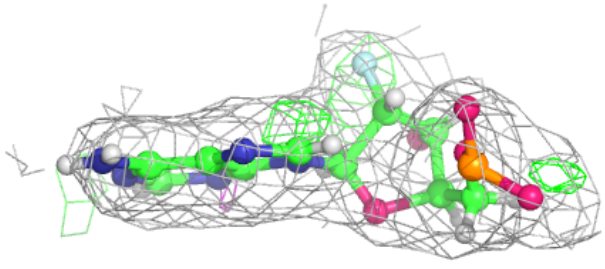


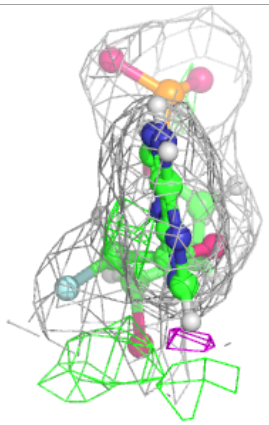


Electron density around AF2 H 502:

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

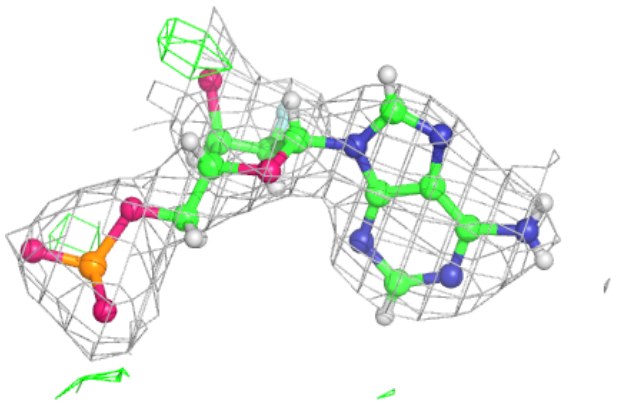


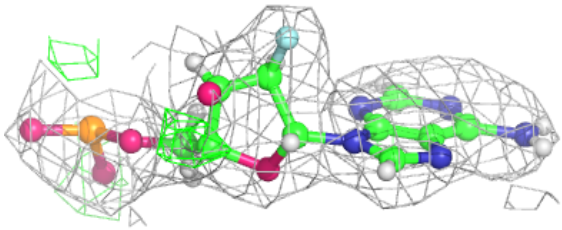


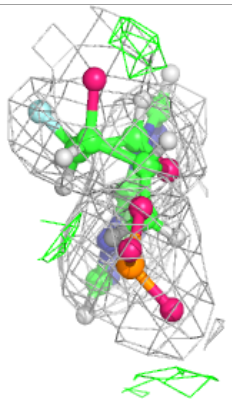


Electron density around AF2 C 502:

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

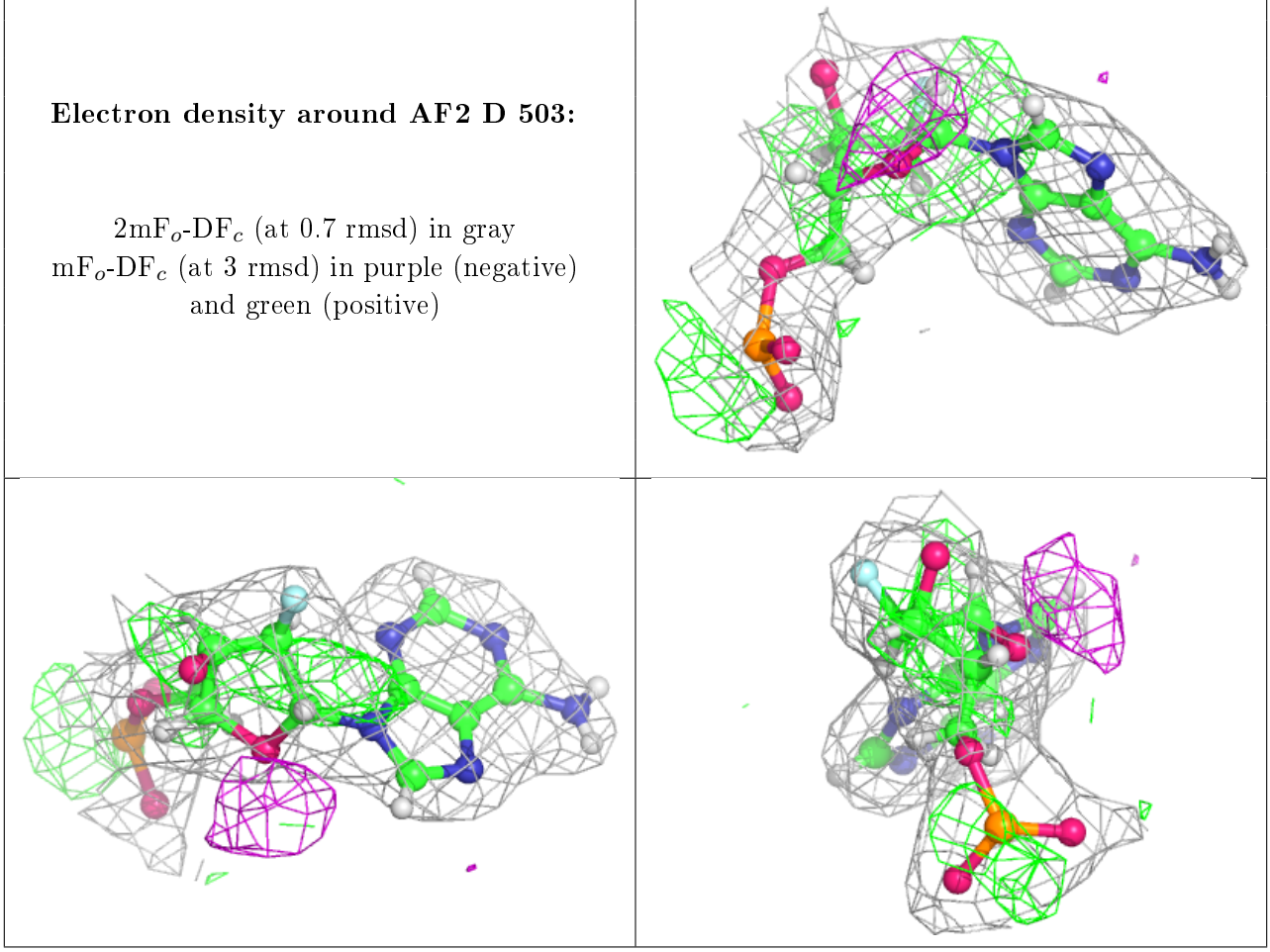






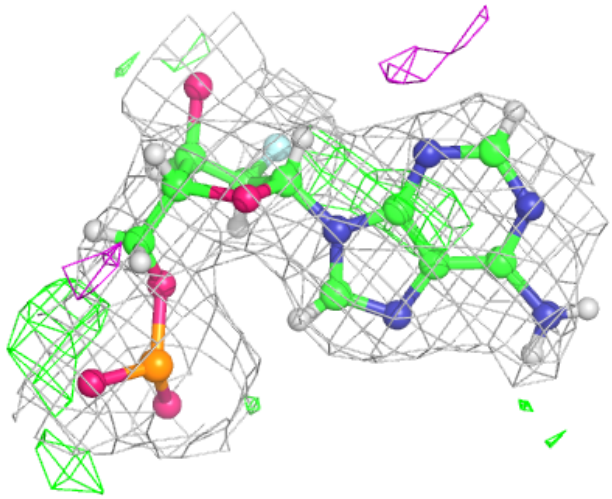
Electron density around AF2 D 503:

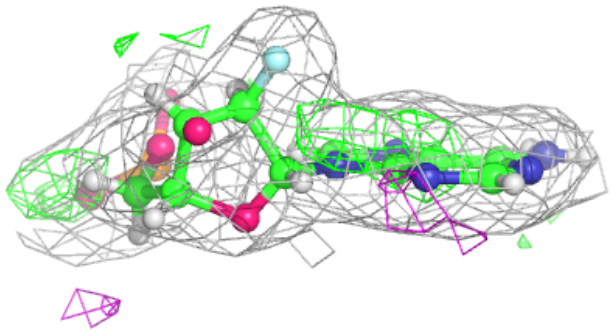
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

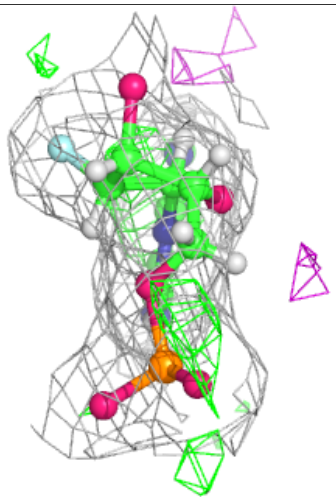


Electron density around AF2 E 503:

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

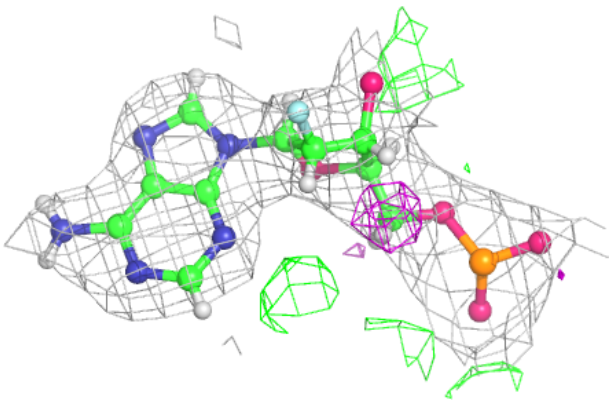


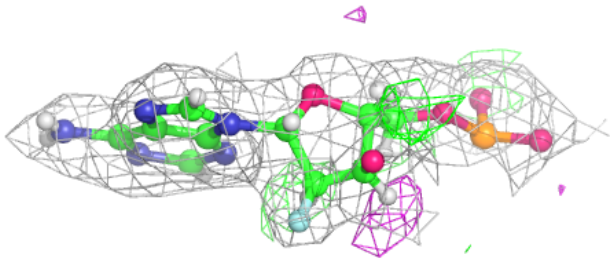


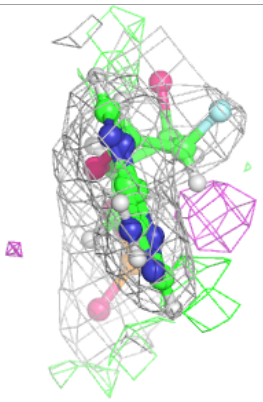


Electron density around AF2 D 501:

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

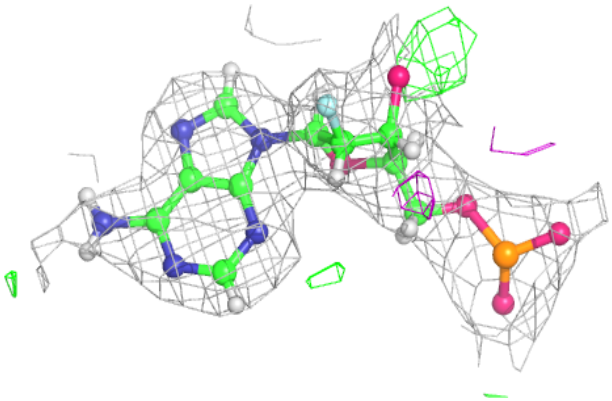


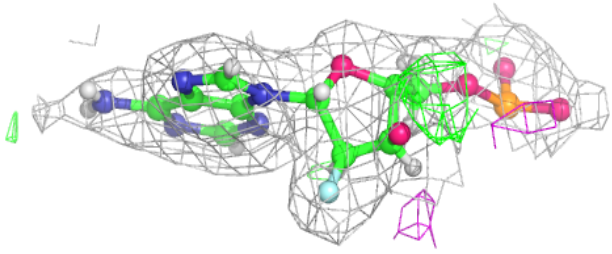


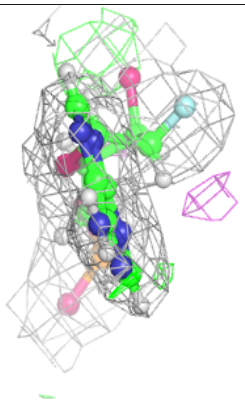


Electron density around AF2 B 501:

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

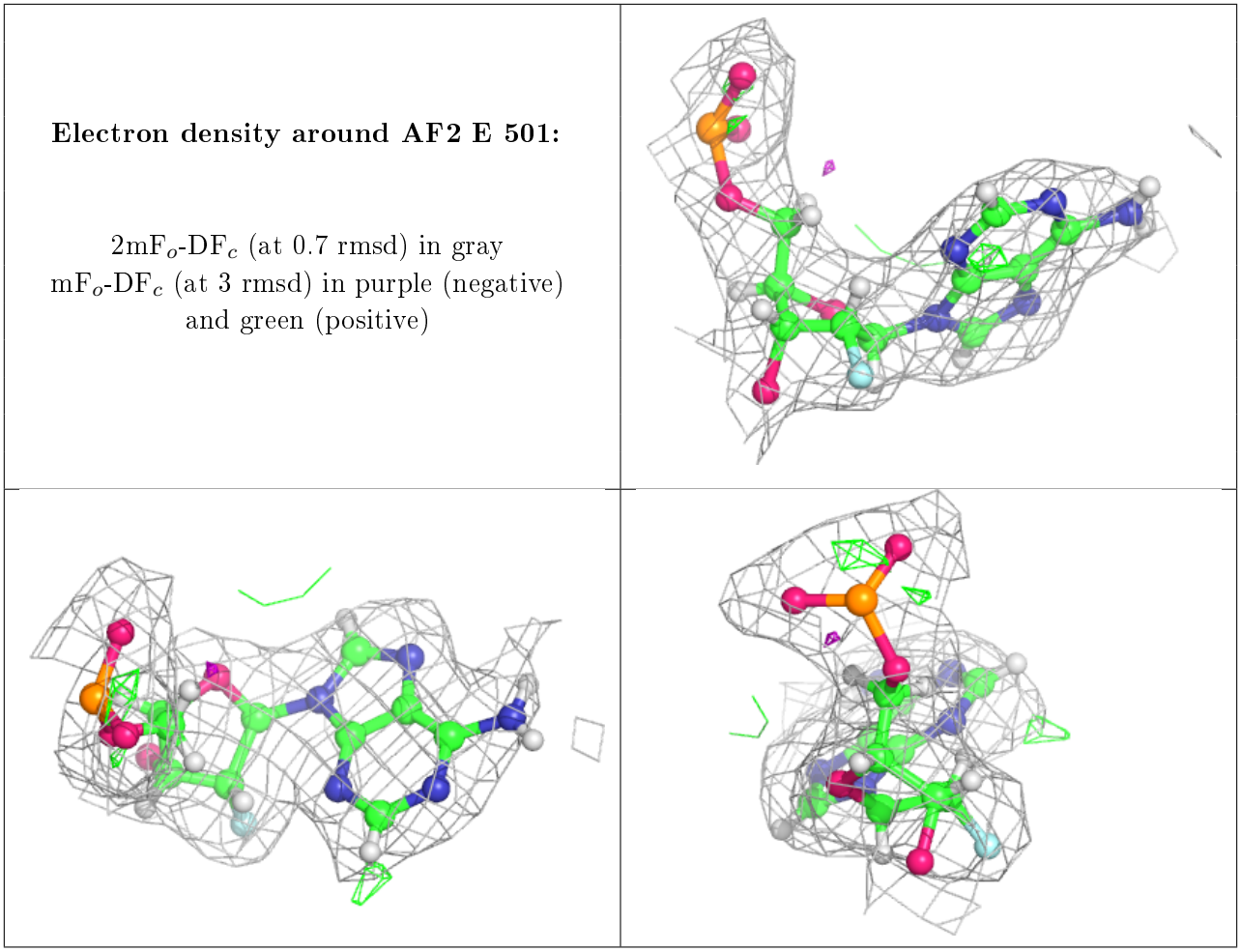






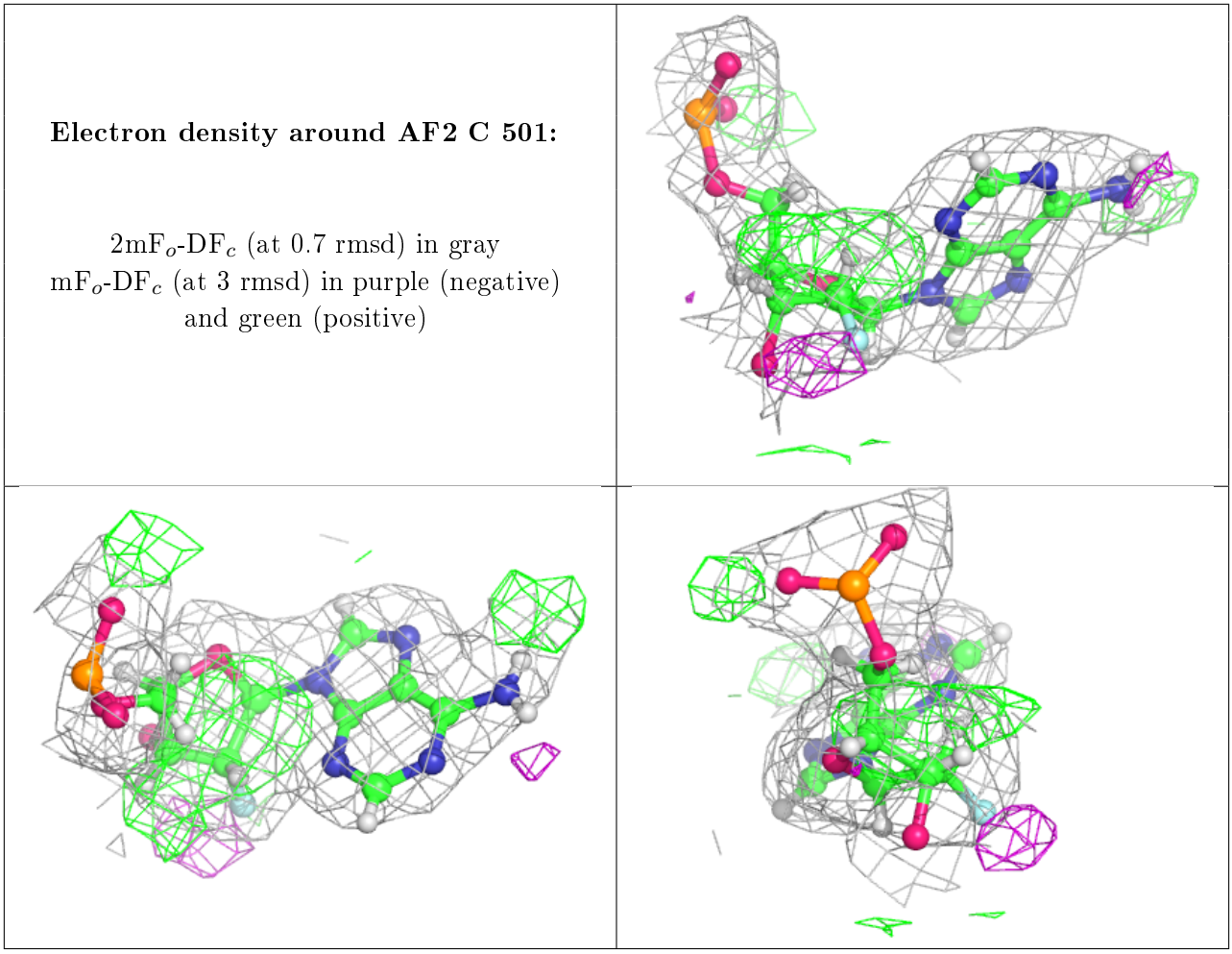
Electron density around AF2 E 501:

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



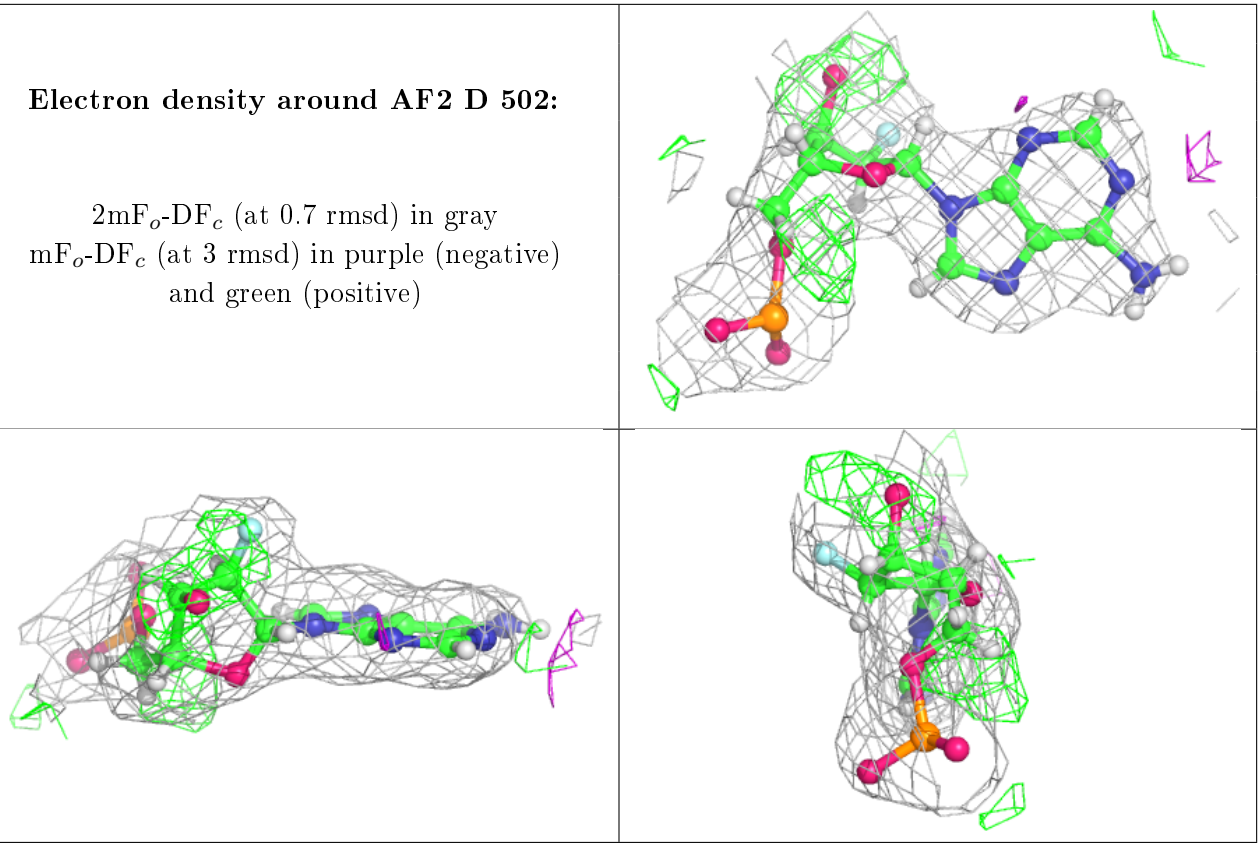
Electron density around AF2 C 501:

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



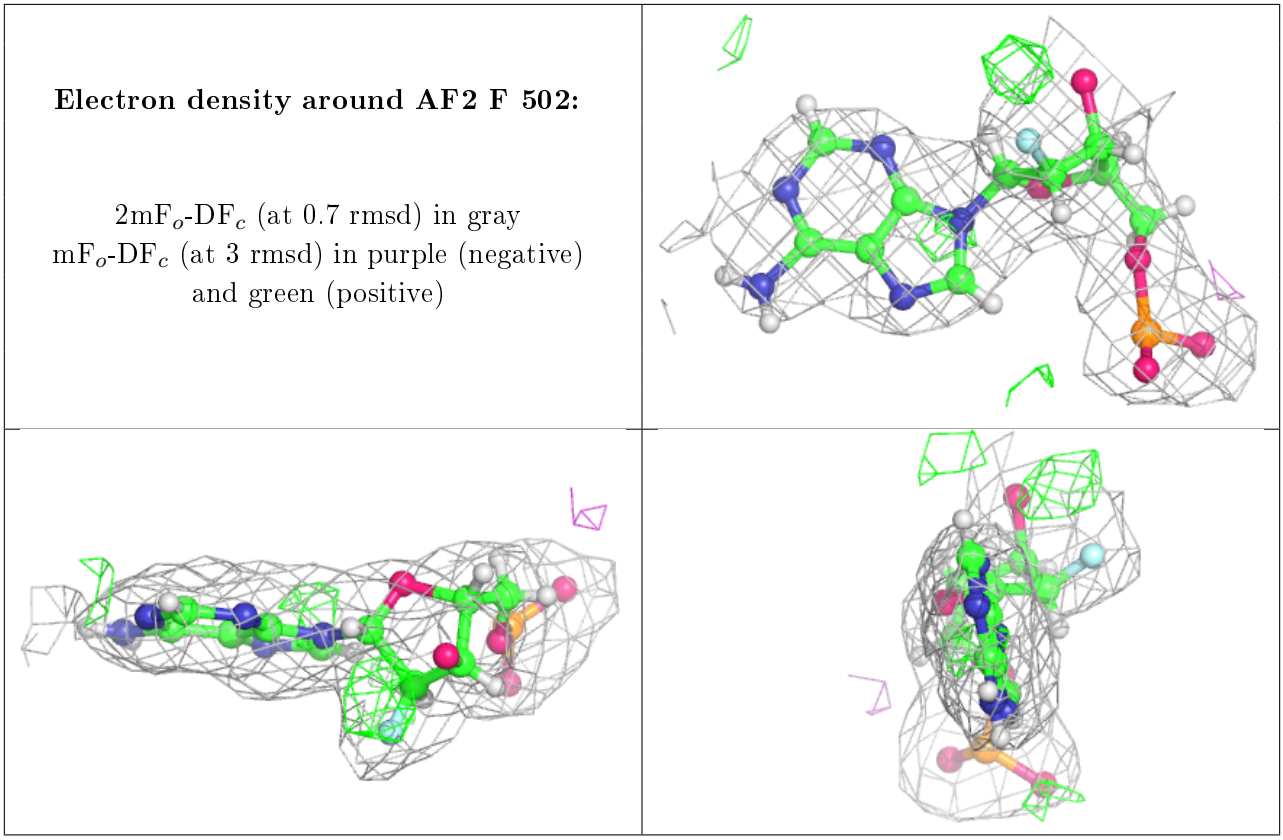
Electron density around AF2 D 502:

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



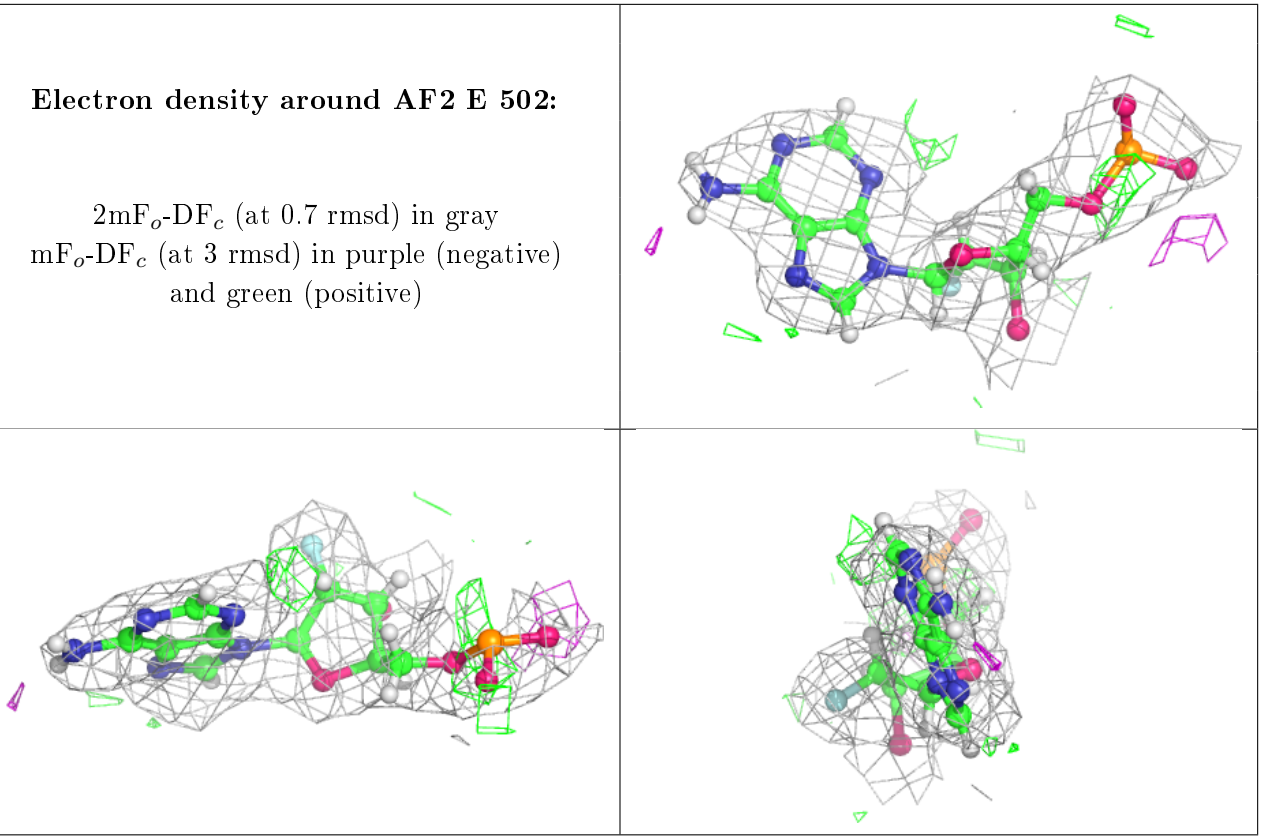
Electron density around AF2 F 502:

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



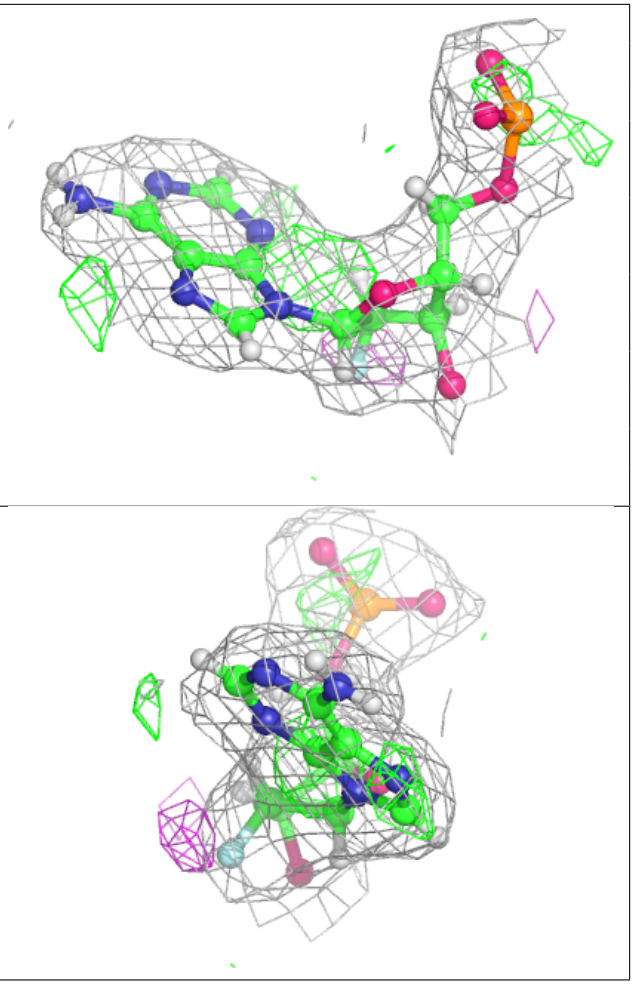
Electron density around AF2 E 502:

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



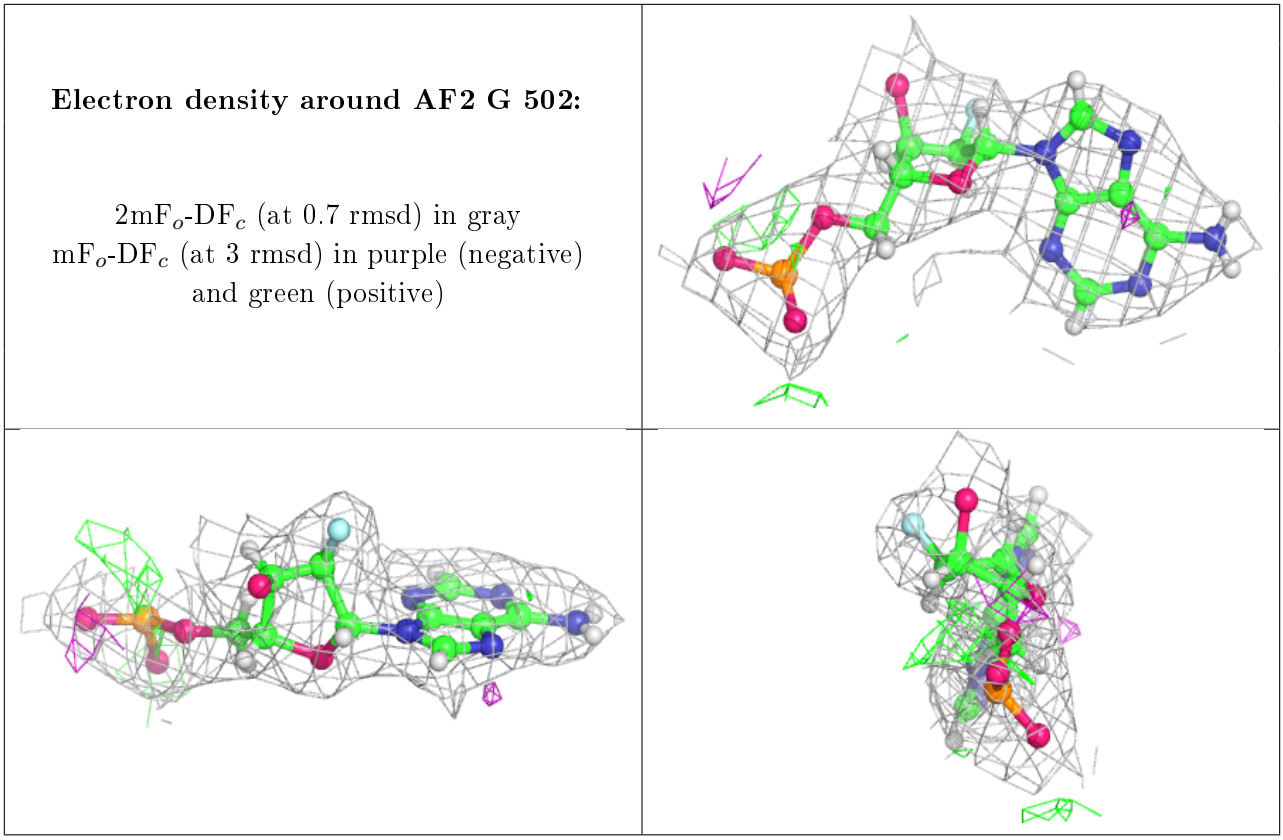
Electron density around AF2 A 501:

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



Electron density around AF2 G 502:

$2mF_o$-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

Unable to reproduce the depositors R factor - this section is therefore empty.