wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 10:31 PM EDT

PDB ID	:	6CI9
Title	:	RMM microcompartment-associated aminopropanol dehydrogenase NADP + aminoacetone holo-structure
Authors	:	Mallette, E.; Kimber, M.S.
Deposited on	:	2018-02-23
Resolution	:	1.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

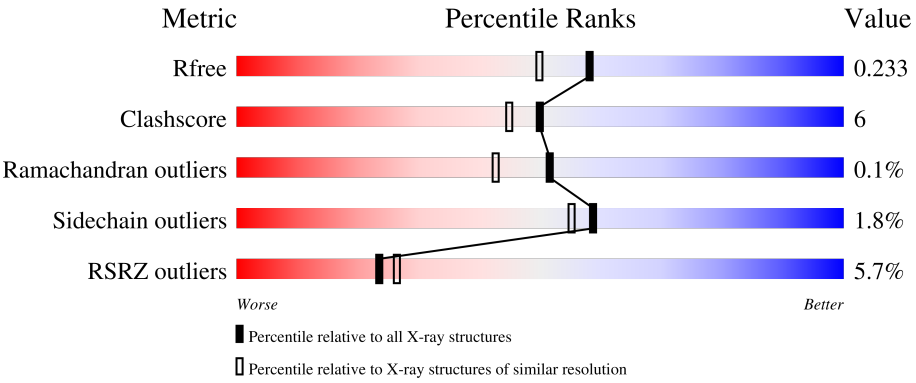
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	259	5% 90% 8% ·
1	B	259	6% 83% 15% ·
1	C	259	5% 87% 12% ·
1	D	259	3% 85% 15% ·
1	E	259	2% 88% 11% ·

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Mol	Chain	Length	Quality of chain
1	F	259	4% 91% 7%
1	G	259	7% 89% 10%
1	H	259	% 89% 9%
1	I	259	5% 92% 8%
1	J	259	8% 90% 9%
1	K	259	11% 81% 16%
1	L	259	5% 88% 9%
1	M	259	11% 89% 10%
1	N	259	4% 81% 16%
1	O	259	4% 86% 11%
1	P	259	8% 91% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 33083 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.

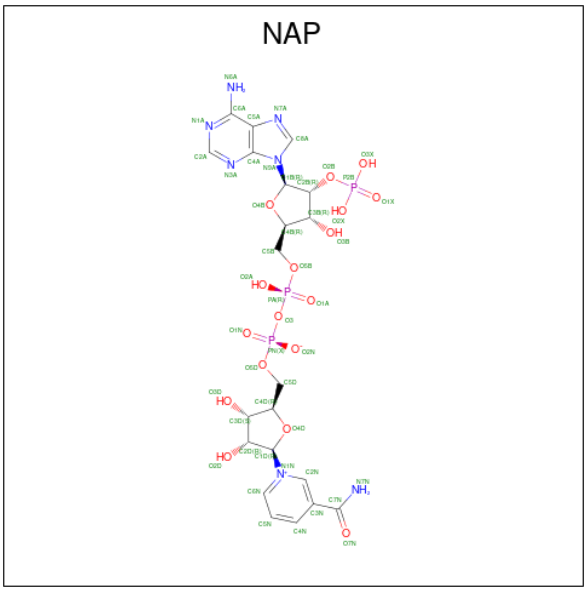
- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1862	1156	328	372	6			
1	B	255	Total	C	N	O	S	0	0	0
			1856	1153	327	370	6			
1	C	258	Total	C	N	O	S	0	0	0
			1875	1165	330	374	6			
1	D	259	Total	C	N	O	S	0	0	0
			1880	1168	331	375	6			
1	E	255	Total	C	N	O	S	0	0	0
			1854	1150	327	371	6			
1	F	254	Total	C	N	O	S	0	0	0
			1848	1147	326	369	6			
1	G	256	Total	C	N	O	S	0	0	0
			1862	1156	328	372	6			
1	H	253	Total	C	N	O	S	0	0	0
			1838	1141	323	368	6			
1	I	258	Total	C	N	O	S	0	0	0
			1874	1165	330	373	6			
1	J	257	Total	C	N	O	S	0	0	0
			1869	1162	329	372	6			
1	K	255	Total	C	N	O	S	0	0	0
			1854	1150	327	371	6			
1	L	253	Total	C	N	O	S	0	0	0
			1838	1141	323	368	6			
1	M	256	Total	C	N	O	S	0	0	0
			1862	1156	328	372	6			
1	N	254	Total	C	N	O	S	0	0	0
			1848	1147	326	369	6			
1	O	253	Total	C	N	O	S	0	0	0
			1838	1141	323	368	6			
1	P	255	Total	C	N	O	S	0	0	0
			1854	1150	327	371	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0QP46
A	0	HIS	-	expression tag	UNP A0QP46
B	-1	SER	-	expression tag	UNP A0QP46
B	0	HIS	-	expression tag	UNP A0QP46
C	-1	SER	-	expression tag	UNP A0QP46
C	0	HIS	-	expression tag	UNP A0QP46
D	-1	SER	-	expression tag	UNP A0QP46
D	0	HIS	-	expression tag	UNP A0QP46
E	-1	SER	-	expression tag	UNP A0QP46
E	0	HIS	-	expression tag	UNP A0QP46
F	-1	SER	-	expression tag	UNP A0QP46
F	0	HIS	-	expression tag	UNP A0QP46
G	-1	SER	-	expression tag	UNP A0QP46
G	0	HIS	-	expression tag	UNP A0QP46
H	-1	SER	-	expression tag	UNP A0QP46
H	0	HIS	-	expression tag	UNP A0QP46
I	-1	SER	-	expression tag	UNP A0QP46
I	0	HIS	-	expression tag	UNP A0QP46
J	-1	SER	-	expression tag	UNP A0QP46
J	0	HIS	-	expression tag	UNP A0QP46
K	-1	SER	-	expression tag	UNP A0QP46
K	0	HIS	-	expression tag	UNP A0QP46
L	-1	SER	-	expression tag	UNP A0QP46
L	0	HIS	-	expression tag	UNP A0QP46
M	-1	SER	-	expression tag	UNP A0QP46
M	0	HIS	-	expression tag	UNP A0QP46
N	-1	SER	-	expression tag	UNP A0QP46
N	0	HIS	-	expression tag	UNP A0QP46
O	-1	SER	-	expression tag	UNP A0QP46
O	0	HIS	-	expression tag	UNP A0QP46
P	-1	SER	-	expression tag	UNP A0QP46
P	0	HIS	-	expression tag	UNP A0QP46

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	M	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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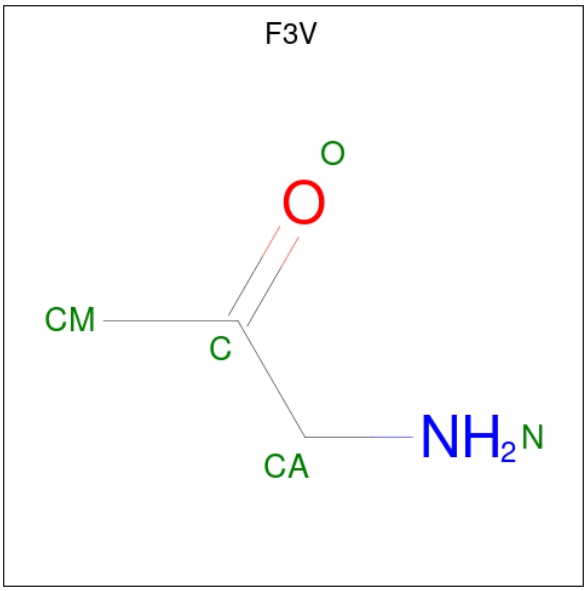
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	O	1	Total C N O P 48 21 7 17 3	0	0
2	P	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 3 is 1-aminopropan-2-one (three-letter code: F3V) (formula: C_3H_7NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 5 3 1 1	0	0
3	B	1	Total C N O 5 3 1 1	0	0
3	C	1	Total C N O 5 3 1 1	0	0
3	D	1	Total C N O 5 3 1 1	0	0
3	E	1	Total C N O 5 3 1 1	0	0
3	F	1	Total C N O 5 3 1 1	0	0
3	G	1	Total C N O 5 3 1 1	0	0
3	H	1	Total C N O 5 3 1 1	0	0
3	I	1	Total C N O 5 3 1 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	N	O	0	0
			5	3	1	1		
3	K	1	Total	C	N	O	0	0
			5	3	1	1		
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	M	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	O	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		
4	I	1	Total	Cl	0	0
			1	1		
4	J	1	Total	Cl	0	0
			1	1		
4	K	1	Total	Cl	0	0
			1	1		
4	L	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total Cl 1 1	0	0
4	N	1	Total Cl 1 1	0	0
4	O	1	Total Cl 1 1	0	0
4	P	1	Total Cl 1 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0
5	L	1	Total Mg 1 1	0	0
5	M	1	Total Mg 1 1	0	0
5	O	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	223	Total O 223 223	0	0
6	B	180	Total O 180 180	0	0
6	C	189	Total O 189 189	0	0
6	D	191	Total O 191 191	0	0
6	E	202	Total O 202 202	0	0

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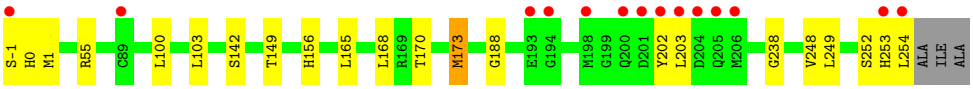
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	203	Total O 203 203	0	0
6	G	186	Total O 186 186	0	0
6	H	209	Total O 209 209	0	0
6	I	106	Total O 106 106	0	0
6	J	113	Total O 113 113	0	0
6	K	96	Total O 96 96	0	0
6	L	123	Total O 123 123	0	0
6	M	111	Total O 111 111	0	0
6	N	118	Total O 118 118	0	0
6	O	132	Total O 132 132	0	0
6	P	116	Total O 116 116	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

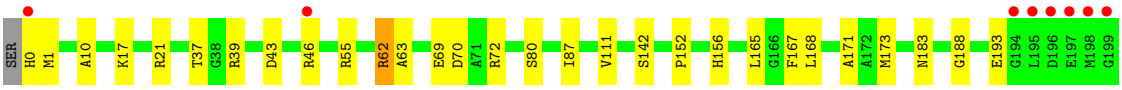
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain A:



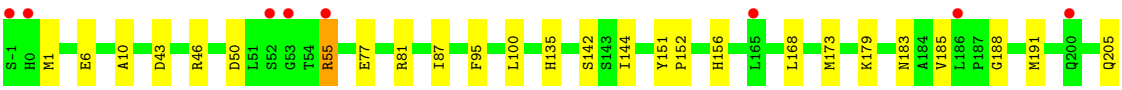
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain B:



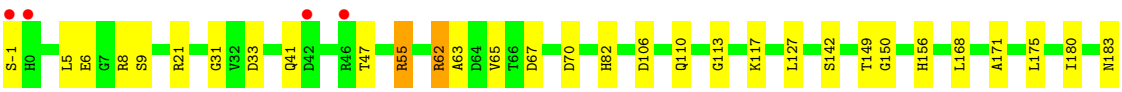
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

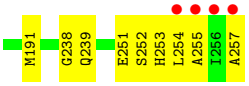
Chain C:



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

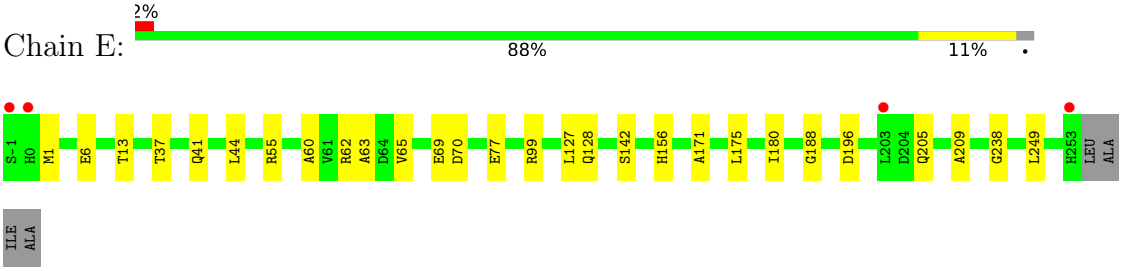
Chain D:





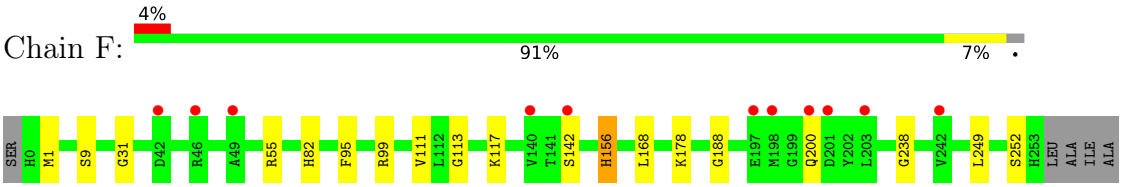
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain E:



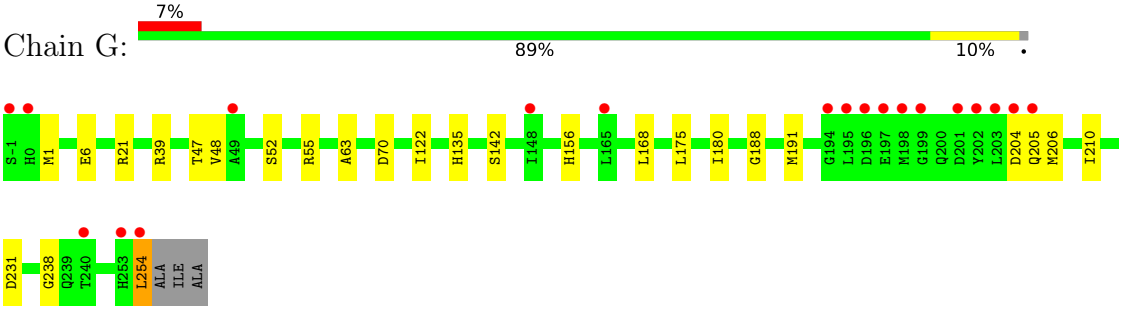
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain F:



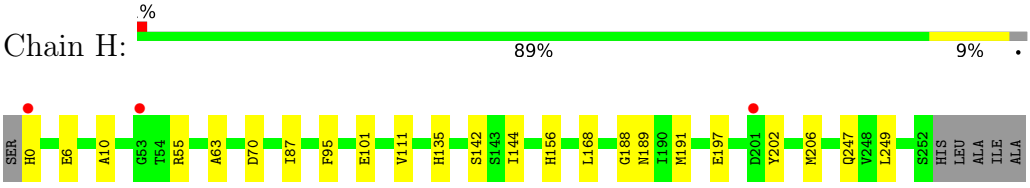
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain G:



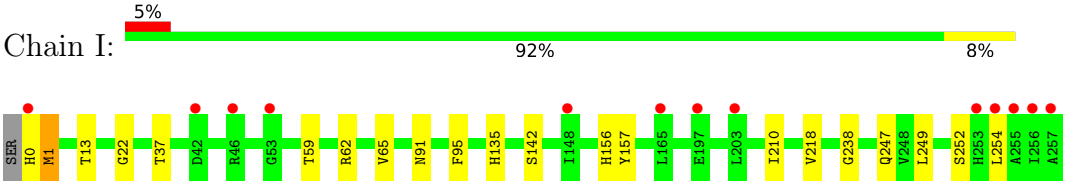
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain H:



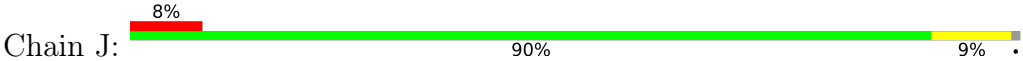
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

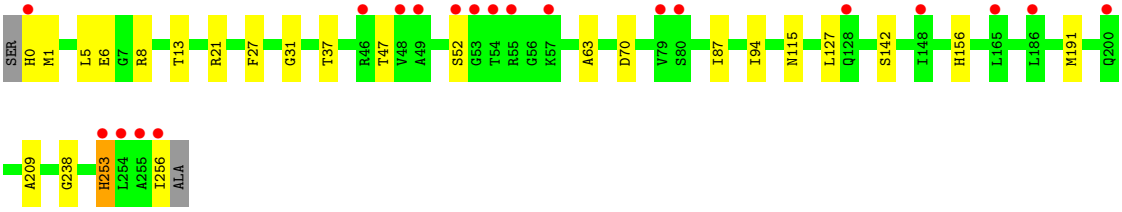
Chain I:



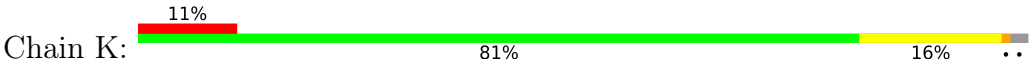
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

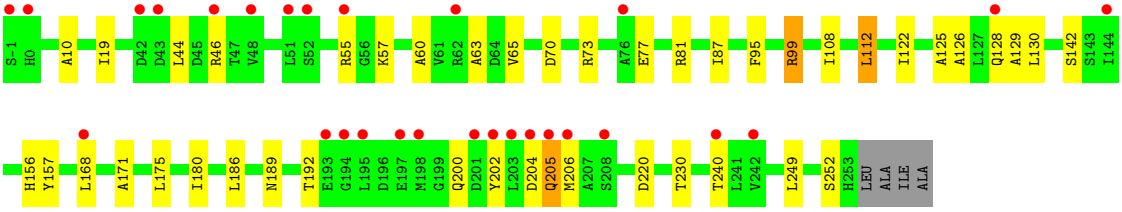
Chain J:



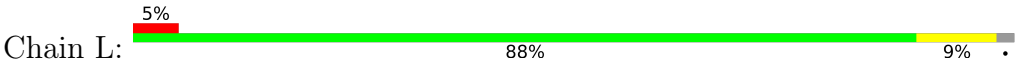


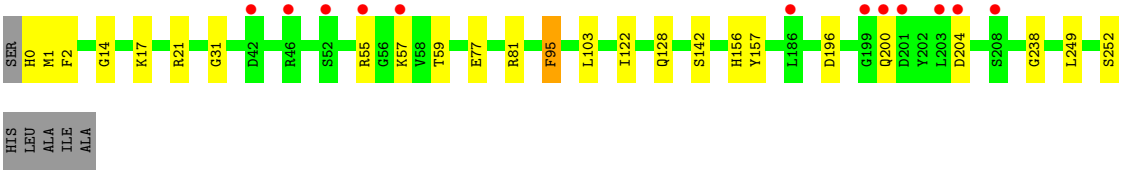
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



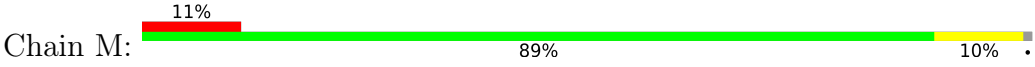


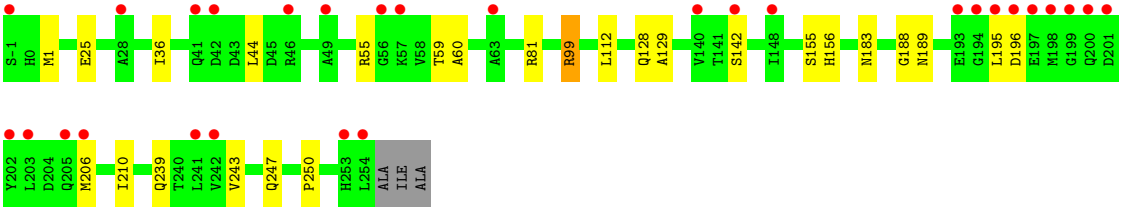
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



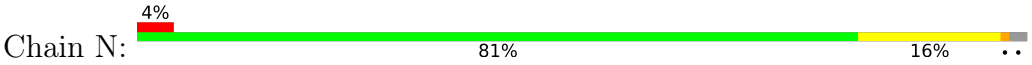


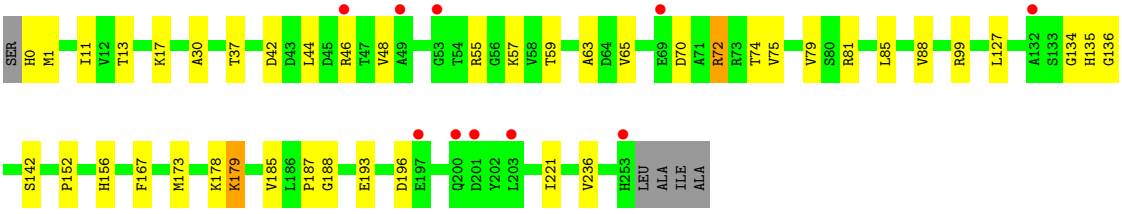
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase





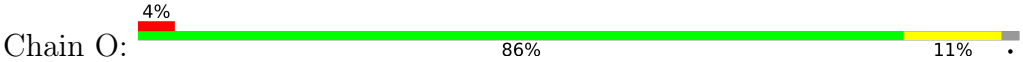
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

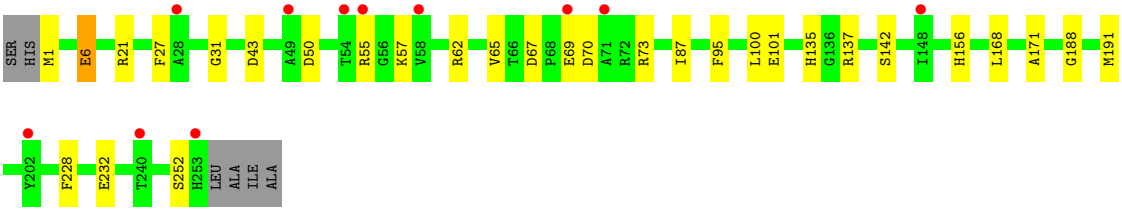




• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

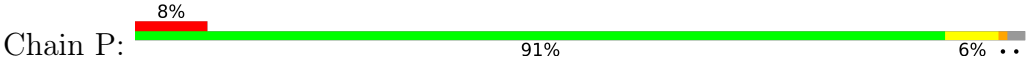
Chain O:

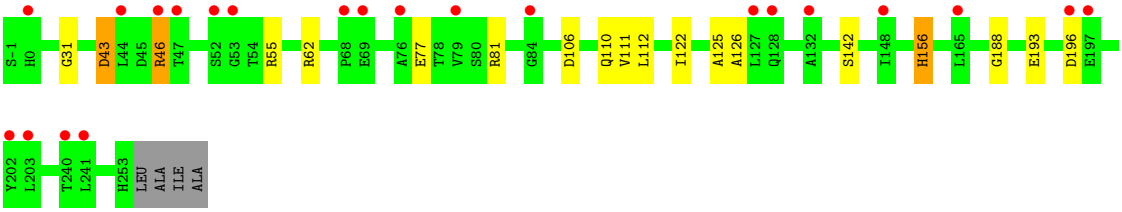




• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.77Å 129.06Å 145.79Å 90.00° 107.88° 90.00°	Depositor
Resolution (Å)	48.49 – 1.90 48.49 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.49-1.90) 81.4 (48.49-1.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.204 , 0.233 0.203 , 0.233	Depositor DCC
R_{free} test set	27768 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33083	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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 47.84 % 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 9.3678e-05. 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: NAP, MG, F3V, CL

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	0.44	0/1889	0.61	1/2568 (0.0%)
1	B	0.41	0/1883	0.58	0/2560
1	C	0.45	0/1902	0.59	1/2586 (0.0%)
1	D	0.42	0/1907	0.59	1/2593 (0.0%)
1	E	0.41	0/1881	0.58	0/2557
1	F	0.42	0/1875	0.58	1/2549 (0.0%)
1	G	0.39	0/1889	0.58	1/2568 (0.0%)
1	H	0.42	0/1864	0.56	1/2534 (0.0%)
1	I	0.32	0/1901	0.52	0/2585
1	J	0.32	0/1896	0.49	0/2578
1	K	0.32	0/1881	0.52	0/2557
1	L	0.31	0/1864	0.51	0/2534
1	M	0.32	0/1889	0.50	0/2568
1	N	0.33	0/1875	0.52	0/2549
1	O	0.32	0/1864	0.50	0/2534
1	P	0.31	0/1881	0.50	0/2557
All	All	0.37	0/30141	0.55	6/40977 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	MET	CG-SD-CE	-7.41	88.35	100.20
1	F	168	LEU	CA-CB-CG	6.33	129.87	115.30
1	D	168	LEU	CA-CB-CG	5.51	127.97	115.30
1	H	168	LEU	CA-CB-CG	5.49	127.92	115.30
1	C	168	LEU	CA-CB-CG	5.43	127.78	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1862	0	1848	22	0
1	B	1856	0	1843	38	0
1	C	1875	0	1864	26	0
1	D	1880	0	1869	37	0
1	E	1854	0	1837	22	0
1	F	1848	0	1832	13	0
1	G	1862	0	1848	20	0
1	H	1838	0	1825	14	0
1	I	1874	0	1864	19	0
1	J	1869	0	1859	19	0
1	K	1854	0	1837	37	0
1	L	1838	0	1825	20	0
1	M	1862	0	1848	23	0
1	N	1848	0	1832	46	0
1	O	1838	0	1825	20	0
1	P	1854	0	1837	13	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
2	E	48	0	25	2	0
2	F	48	0	25	2	0
2	G	48	0	25	2	0
2	H	48	0	25	1	0
2	I	48	0	25	3	0
2	J	48	0	25	1	0
2	K	48	0	25	2	0
2	L	48	0	25	2	0
2	M	48	0	25	2	0
2	N	48	0	25	5	0
2	O	48	0	25	3	0
2	P	48	0	25	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
4	A	2	0	0	1	0
4	B	1	0	0	1	0
4	C	1	0	0	1	0
4	D	1	0	0	1	0
4	E	1	0	0	1	0
4	F	1	0	0	1	0
4	G	1	0	0	1	0
4	H	1	0	0	1	0
4	I	1	0	0	1	0
4	J	1	0	0	1	0
4	K	1	0	0	1	0
4	L	1	0	0	1	0
4	M	1	0	0	1	0
4	N	1	0	0	1	0
4	O	1	0	0	1	0
4	P	1	0	0	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
6	A	223	0	0	6	1
6	B	180	0	0	11	0
6	C	189	0	0	3	2
6	D	191	0	0	10	1
6	E	202	0	0	10	0
6	F	203	0	0	2	1
6	G	186	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	209	0	0	2	1
6	I	106	0	0	5	0
6	J	113	0	0	2	0
6	K	96	0	0	8	0
6	L	123	0	0	6	0
6	M	111	0	0	5	0
6	N	118	0	0	9	0
6	O	132	0	0	4	0
6	P	116	0	0	4	0
All	All	33083	0	29893	352	3

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 6.

The worst 5 of 352 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:N:134:GLY:H	1:N:179:LYS:NZ	1.35	1.23
1:N:134:GLY:N	1:N:179:LYS:NZ	1.94	1.14
1:E:99:ARG:NH1	6:E:401:HOH:O	1.83	1.10
1:N:134:GLY:N	1:N:179:LYS:HZ3	1.50	1.02
1:B:17:LYS:NZ	6:B:401:HOH:O	1.94	1.00

All (3) 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)
6:A:577:HOH:O	6:C:558:HOH:O[2_948]	1.96	0.24
6:C:582:HOH:O	6:D:534:HOH:O[2_958]	2.14	0.06
6:F:470:HOH:O	6:H:566:HOH:O[2_859]	2.16	0.04

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	254/259 (98%)	244 (96%)	10 (4%)	0	100	100
1	B	253/259 (98%)	246 (97%)	7 (3%)	0	100	100
1	C	256/259 (99%)	244 (95%)	11 (4%)	1 (0%)	34	24
1	D	257/259 (99%)	246 (96%)	11 (4%)	0	100	100
1	E	253/259 (98%)	246 (97%)	7 (3%)	0	100	100
1	F	252/259 (97%)	241 (96%)	11 (4%)	0	100	100
1	G	254/259 (98%)	245 (96%)	9 (4%)	0	100	100
1	H	251/259 (97%)	240 (96%)	11 (4%)	0	100	100
1	I	256/259 (99%)	245 (96%)	11 (4%)	0	100	100
1	J	255/259 (98%)	243 (95%)	11 (4%)	1 (0%)	34	24
1	K	253/259 (98%)	243 (96%)	9 (4%)	1 (0%)	34	24
1	L	251/259 (97%)	243 (97%)	8 (3%)	0	100	100
1	M	254/259 (98%)	242 (95%)	12 (5%)	0	100	100
1	N	252/259 (97%)	240 (95%)	12 (5%)	0	100	100
1	O	251/259 (97%)	242 (96%)	9 (4%)	0	100	100
1	P	253/259 (98%)	241 (95%)	12 (5%)	0	100	100
All	All	4055/4144 (98%)	3891 (96%)	161 (4%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	253	HIS
1	K	205	GLN
1	C	253	HIS

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	193/194 (100%)	192 (100%)	1 (0%)	88	89
1	B	192/194 (99%)	190 (99%)	2 (1%)	76	76
1	C	194/194 (100%)	188 (97%)	6 (3%)	40	32
1	D	194/194 (100%)	191 (98%)	3 (2%)	65	62
1	E	192/194 (99%)	190 (99%)	2 (1%)	76	76
1	F	191/194 (98%)	187 (98%)	4 (2%)	53	48
1	G	193/194 (100%)	190 (98%)	3 (2%)	62	60
1	H	190/194 (98%)	187 (98%)	3 (2%)	62	60
1	I	193/194 (100%)	190 (98%)	3 (2%)	62	60
1	J	193/194 (100%)	191 (99%)	2 (1%)	76	76
1	K	192/194 (99%)	187 (97%)	5 (3%)	46	39
1	L	190/194 (98%)	185 (97%)	5 (3%)	46	39
1	M	193/194 (100%)	191 (99%)	2 (1%)	76	76
1	N	191/194 (98%)	186 (97%)	5 (3%)	46	39
1	O	190/194 (98%)	185 (97%)	5 (3%)	46	39
1	P	192/194 (99%)	188 (98%)	4 (2%)	53	48
All	All	3073/3104 (99%)	3018 (98%)	55 (2%)	59	55

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	191	MET
1	L	95	PHE
1	P	156	HIS
1	O	156	HIS
1	K	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	253	HIS
1	H	247	GLN
1	G	135	HIS
1	J	115	ASN
1	C	200	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 25 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	F3V	C	302	-	4,4,4	0.78	0	3,4,4	1.54	1 (33%)
3	F3V	A	302	-	4,4,4	0.70	0	3,4,4	2.15	2 (66%)
3	F3V	F	302	-	4,4,4	0.85	0	3,4,4	1.72	1 (33%)
3	F3V	N	302	-	4,4,4	0.98	0	3,4,4	1.80	1 (33%)
2	NAP	K	301	-	45,52,52	2.75	17 (37%)	56,80,80	1.35	5 (8%)
3	F3V	I	302	-	4,4,4	0.80	0	3,4,4	2.77	2 (66%)
2	NAP	J	301	5	45,52,52	2.72	18 (40%)	56,80,80	1.35	8 (14%)
3	F3V	H	302	-	4,4,4	0.67	0	3,4,4	2.48	2 (66%)
3	F3V	B	302	-	4,4,4	0.78	0	3,4,4	3.01	2 (66%)
3	F3V	P	302	-	4,4,4	0.82	0	3,4,4	2.07	1 (33%)
2	NAP	G	301	-	45,52,52	2.67	16 (35%)	56,80,80	1.28	5 (8%)
2	NAP	A	301	-	45,52,52	2.75	16 (35%)	56,80,80	1.37	6 (10%)
2	NAP	O	301	5	45,52,52	2.61	17 (37%)	56,80,80	1.29	6 (10%)
2	NAP	F	301	-	45,52,52	2.74	16 (35%)	56,80,80	1.41	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	H	301	5	45,52,52	2.57	15 (33%)	56,80,80	1.48	8 (14%)
2	NAP	E	301	-	45,52,52	2.74	17 (37%)	56,80,80	1.41	7 (12%)
2	NAP	I	301	-	45,52,52	2.75	17 (37%)	56,80,80	1.35	7 (12%)
2	NAP	L	301	-	45,52,52	2.75	17 (37%)	56,80,80	1.35	7 (12%)
3	F3V	O	302	-	4,4,4	0.73	0	3,4,4	1.85	1 (33%)
2	NAP	D	301	-	45,52,52	2.70	17 (37%)	56,80,80	1.45	9 (16%)
3	F3V	J	302	-	4,4,4	0.83	0	3,4,4	1.53	1 (33%)
2	NAP	C	301	5	45,52,52	2.50	15 (33%)	56,80,80	1.56	8 (14%)
3	F3V	D	302	-	4,4,4	0.86	0	3,4,4	1.17	0
2	NAP	P	301	-	45,52,52	2.71	16 (35%)	56,80,80	1.33	6 (10%)
3	F3V	M	302	-	4,4,4	0.84	0	3,4,4	2.22	1 (33%)
2	NAP	N	301	-	45,52,52	2.79	16 (35%)	56,80,80	1.45	8 (14%)
3	F3V	K	302	-	4,4,4	0.86	0	3,4,4	2.16	1 (33%)
2	NAP	B	301	-	45,52,52	2.82	15 (33%)	56,80,80	1.33	10 (17%)
3	F3V	G	302	-	4,4,4	0.91	0	3,4,4	1.63	1 (33%)
3	F3V	E	302	-	4,4,4	1.07	0	3,4,4	2.28	2 (66%)
2	NAP	M	301	-	45,52,52	2.82	16 (35%)	56,80,80	1.30	8 (14%)
3	F3V	L	302	-	4,4,4	0.79	0	3,4,4	2.02	1 (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
3	F3V	C	302	-	-	0/1/2/2	-
3	F3V	A	302	-	-	0/1/2/2	-
3	F3V	F	302	-	-	0/1/2/2	-
3	F3V	N	302	-	-	0/1/2/2	-
2	NAP	K	301	-	-	4/31/67/67	0/5/5/5
3	F3V	I	302	-	-	0/1/2/2	-
2	NAP	J	301	5	-	5/31/67/67	0/5/5/5
3	F3V	H	302	-	-	0/1/2/2	-
3	F3V	B	302	-	-	0/1/2/2	-
3	F3V	P	302	-	-	0/1/2/2	-
2	NAP	G	301	-	-	4/31/67/67	0/5/5/5
2	NAP	A	301	-	-	5/31/67/67	0/5/5/5
2	NAP	O	301	5	-	2/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	F	301	-	-	3/31/67/67	0/5/5/5
2	NAP	H	301	5	-	3/31/67/67	0/5/5/5
2	NAP	E	301	-	-	2/31/67/67	0/5/5/5
2	NAP	I	301	-	-	3/31/67/67	0/5/5/5
2	NAP	L	301	-	-	4/31/67/67	0/5/5/5
3	F3V	O	302	-	-	0/1/2/2	-
2	NAP	D	301	-	-	5/31/67/67	0/5/5/5
3	F3V	J	302	-	-	0/1/2/2	-
2	NAP	C	301	5	-	3/31/67/67	0/5/5/5
3	F3V	D	302	-	-	0/1/2/2	-
2	NAP	P	301	-	-	5/31/67/67	0/5/5/5
3	F3V	M	302	-	-	0/1/2/2	-
2	NAP	N	301	-	-	3/31/67/67	0/5/5/5
3	F3V	K	302	-	-	0/1/2/2	-
2	NAP	B	301	-	-	2/31/67/67	0/5/5/5
3	F3V	G	302	-	-	0/1/2/2	-
3	F3V	E	302	-	-	0/1/2/2	-
2	NAP	M	301	-	-	6/31/67/67	0/5/5/5
3	F3V	L	302	-	-	0/1/2/2	-

The worst 5 of 261 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	C7N-N7N	9.26	1.50	1.33
2	G	301	NAP	C7N-N7N	9.01	1.50	1.33
2	N	301	NAP	C7N-N7N	8.87	1.49	1.33
2	J	301	NAP	C7N-N7N	8.86	1.49	1.33
2	M	301	NAP	C7N-N7N	8.85	1.49	1.33

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	NAP	N3A-C2A-N1A	-5.77	119.66	128.68
2	D	301	NAP	N3A-C2A-N1A	-4.49	121.65	128.68
2	A	301	NAP	N3A-C2A-N1A	-4.38	121.83	128.68
2	E	301	NAP	N3A-C2A-N1A	-4.31	121.94	128.68
2	K	301	NAP	N3A-C2A-N1A	-4.26	122.02	128.68

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C2B-O2B-P2B-O1X
2	A	301	NAP	C2B-O2B-P2B-O2X
2	B	301	NAP	C2B-O2B-P2B-O2X
2	C	301	NAP	C2B-O2B-P2B-O1X
2	D	301	NAP	C2B-O2B-P2B-O1X

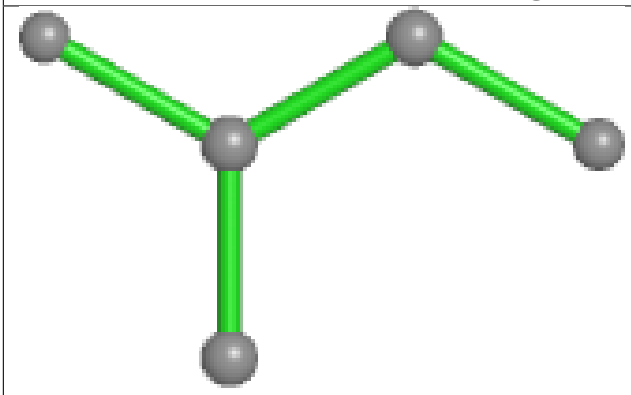
There are no ring outliers.

16 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	301	NAP	2	0
2	J	301	NAP	1	0
2	G	301	NAP	2	0
2	A	301	NAP	2	0
2	O	301	NAP	3	0
2	F	301	NAP	2	0
2	H	301	NAP	1	0
2	E	301	NAP	2	0
2	I	301	NAP	3	0
2	L	301	NAP	2	0
2	D	301	NAP	2	0
2	C	301	NAP	1	0
2	P	301	NAP	2	0
2	N	301	NAP	5	0
2	B	301	NAP	3	0
2	M	301	NAP	2	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 F3V C 302



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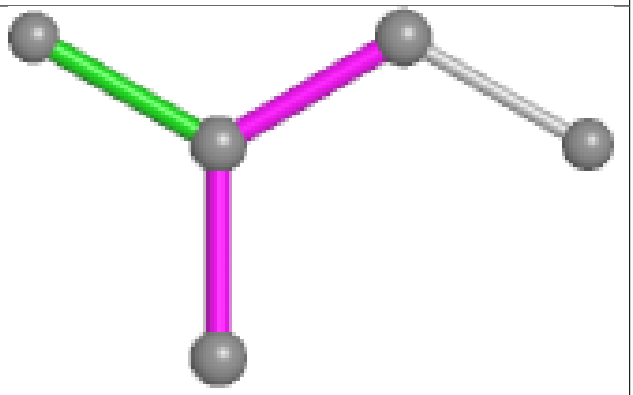
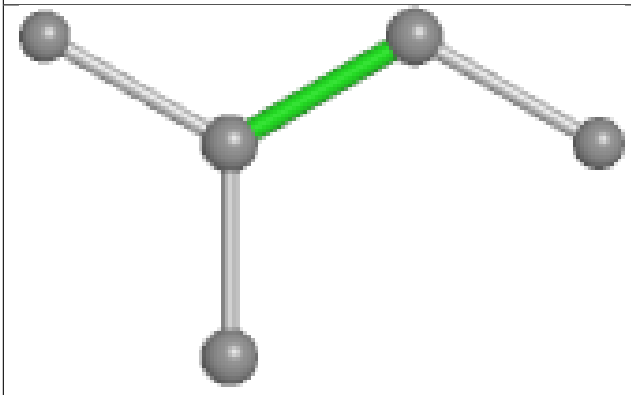
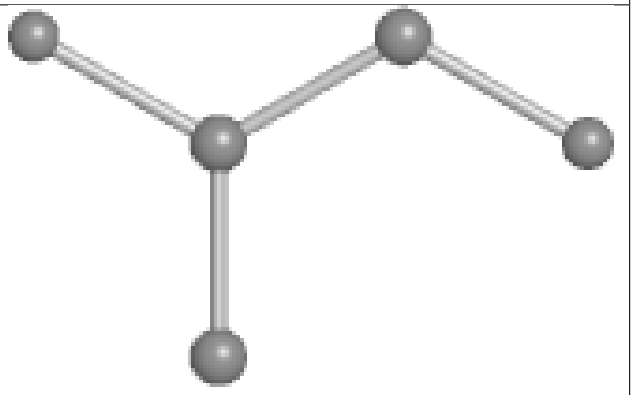


Bond angles

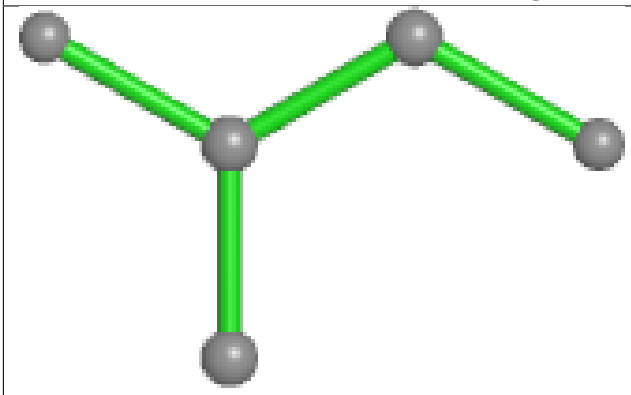


Torsions



Rings

Ligand F3V A 302



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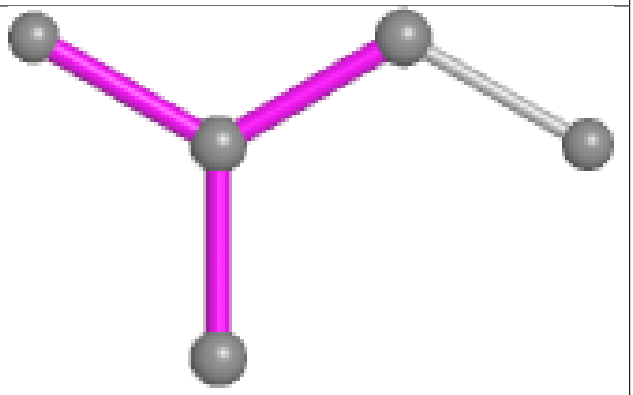

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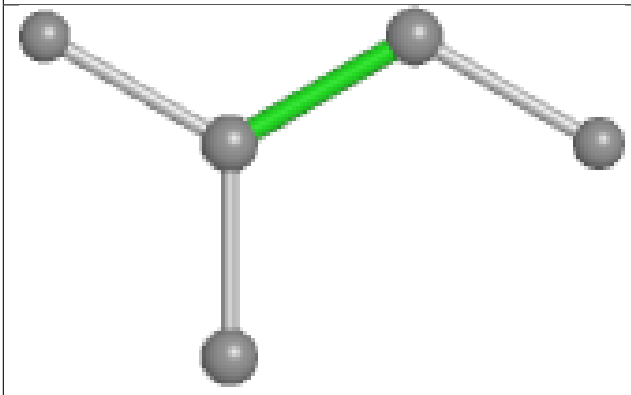

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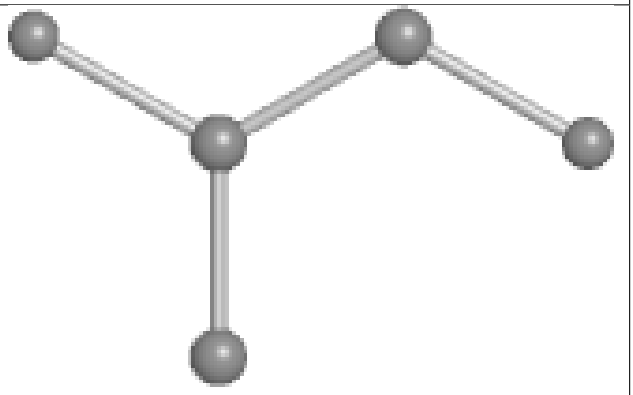
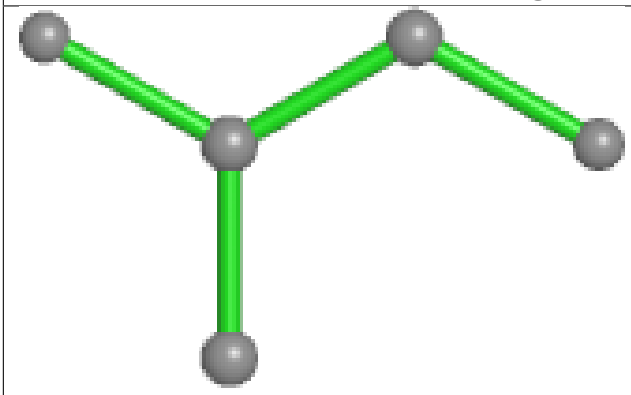


Rings

Ligand F3V F 302



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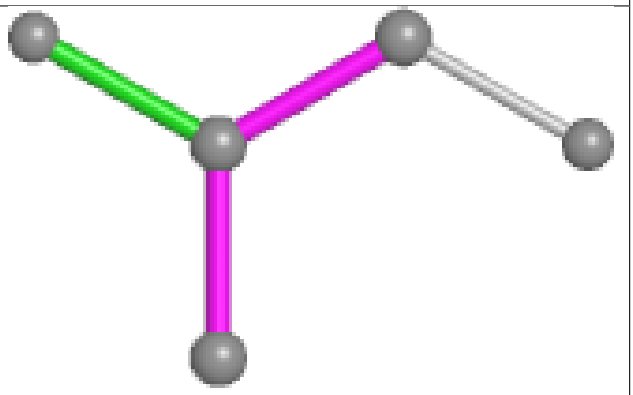

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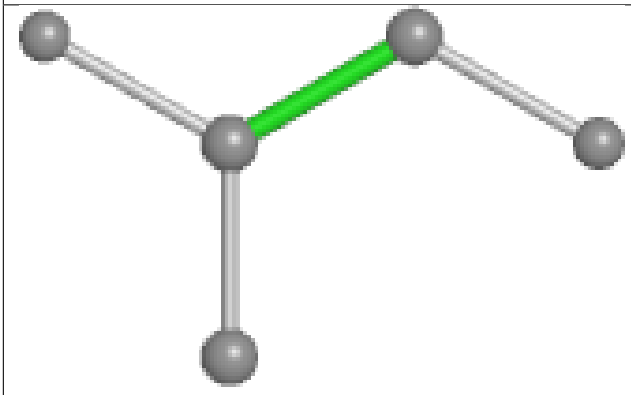

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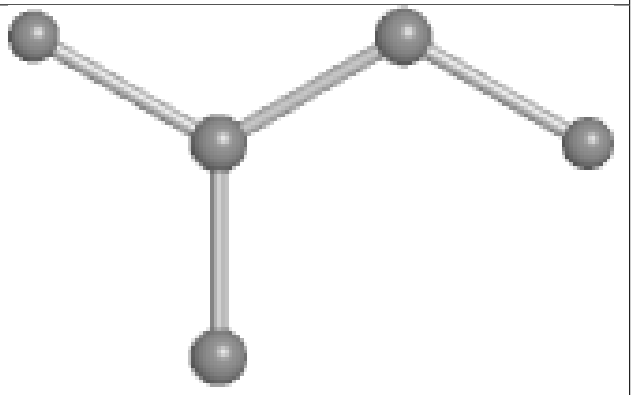

Rings

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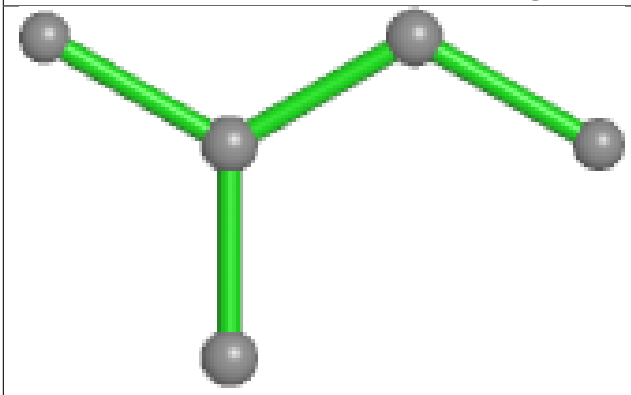

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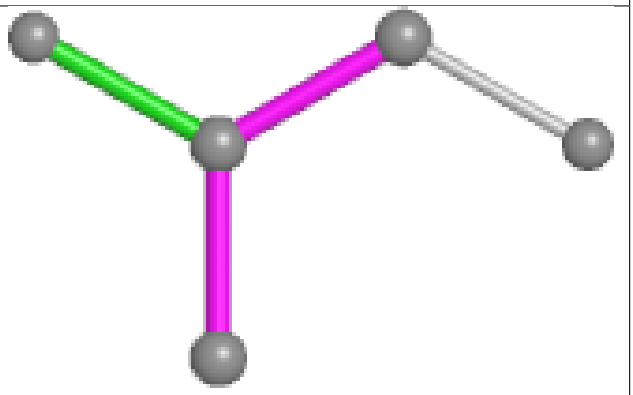

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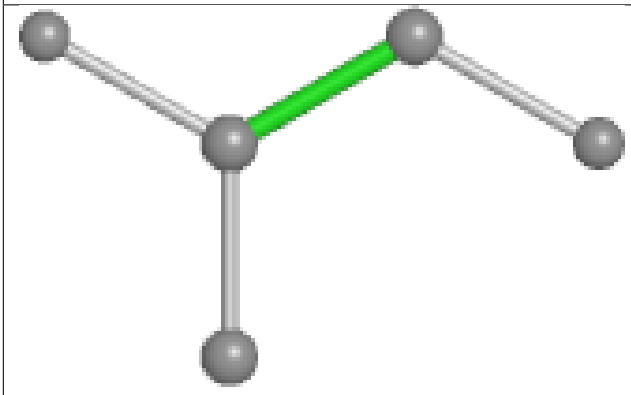

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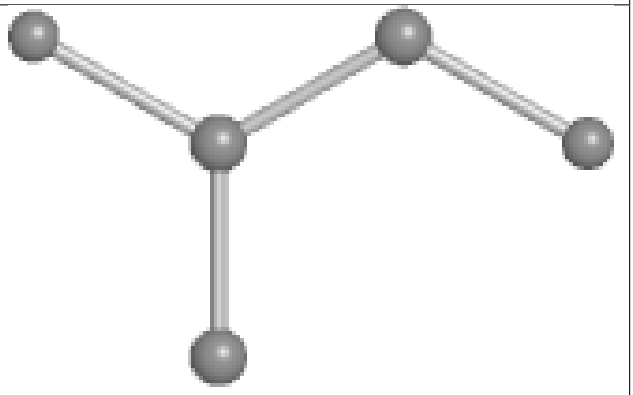
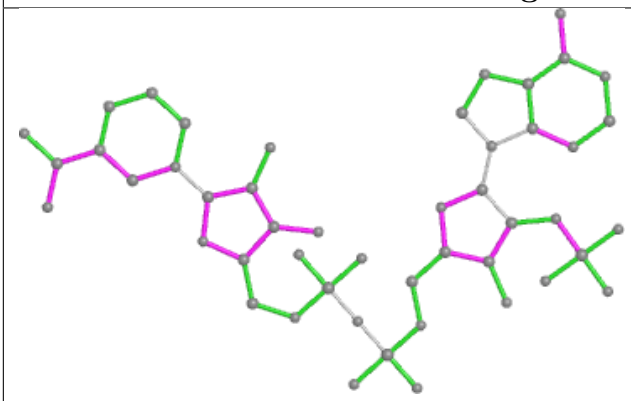


Rings

Ligand NAP K 301



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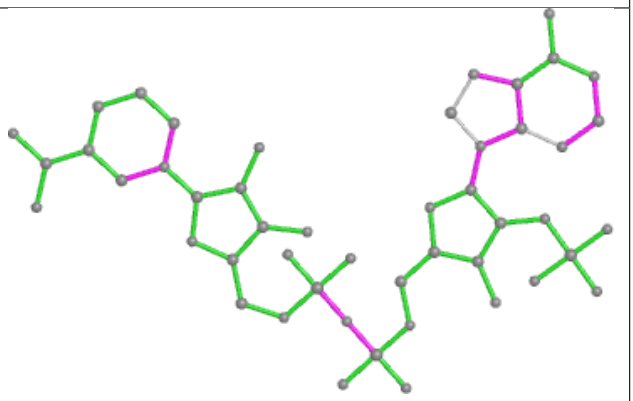

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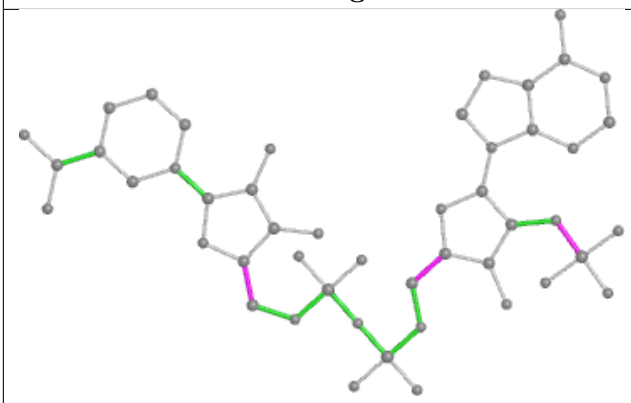

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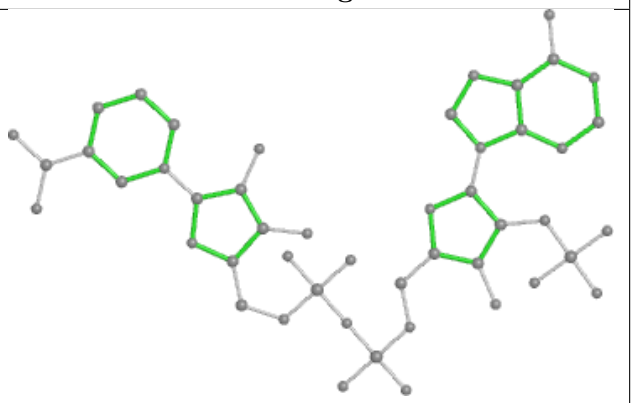

Rings

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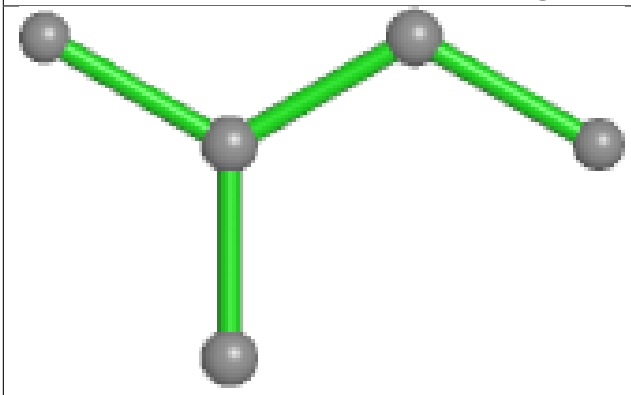

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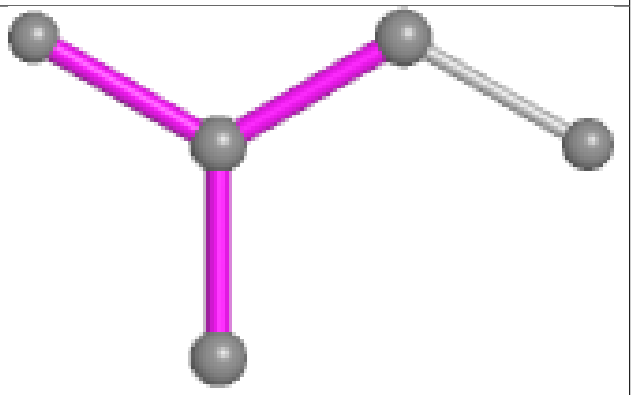

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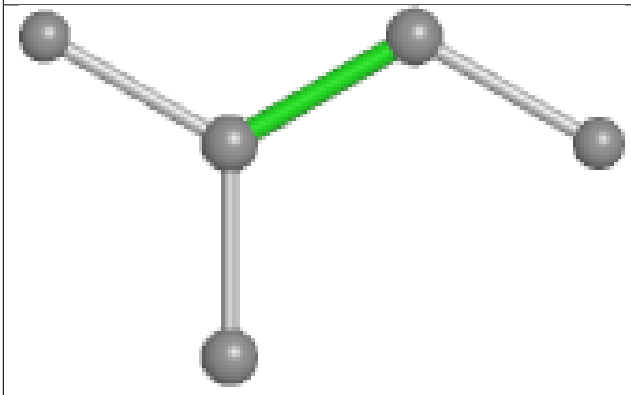

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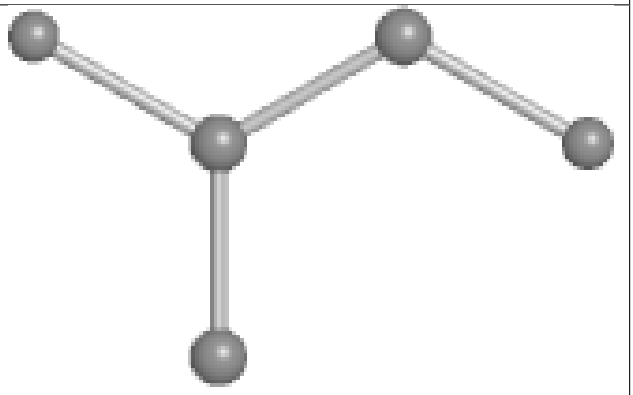

Rings

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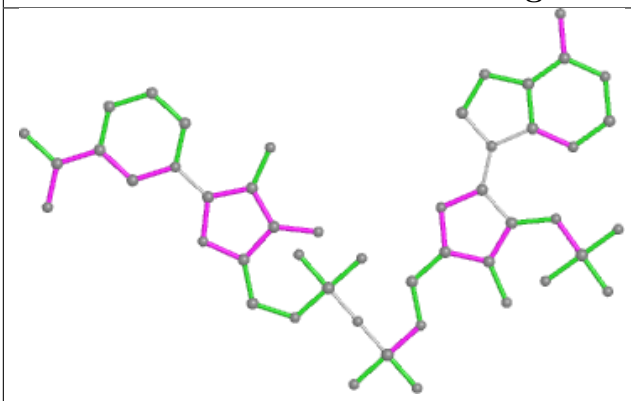

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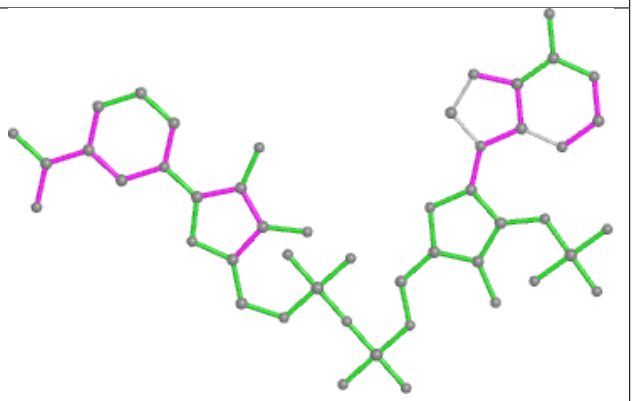

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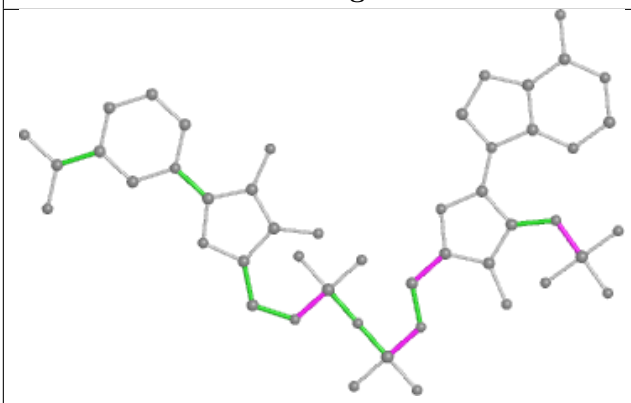

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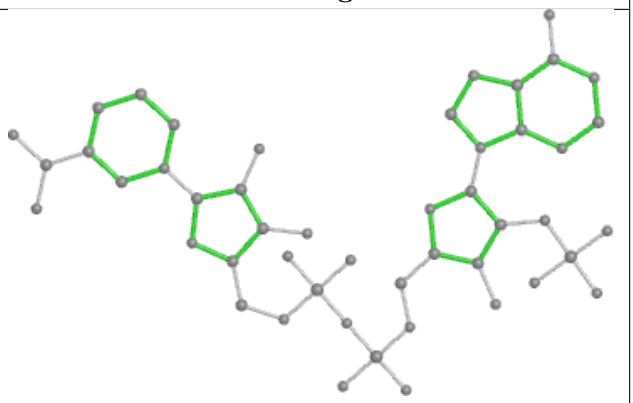

Rings

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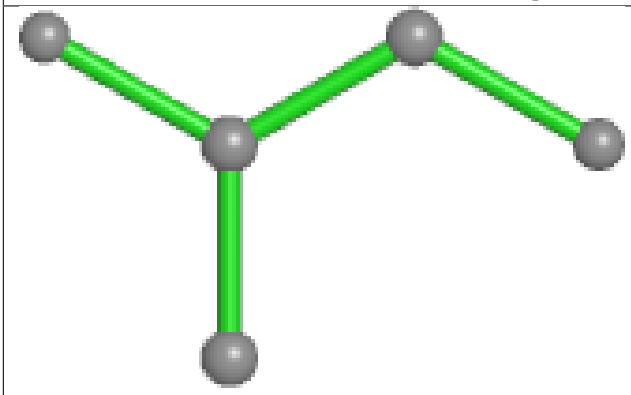

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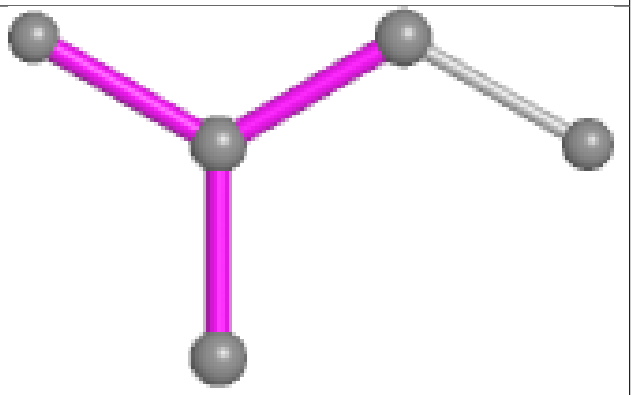

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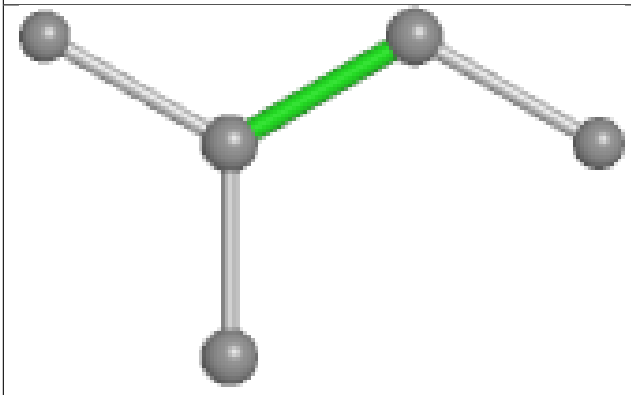

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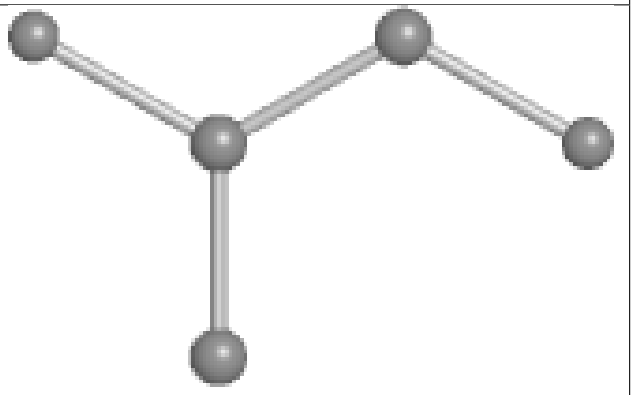
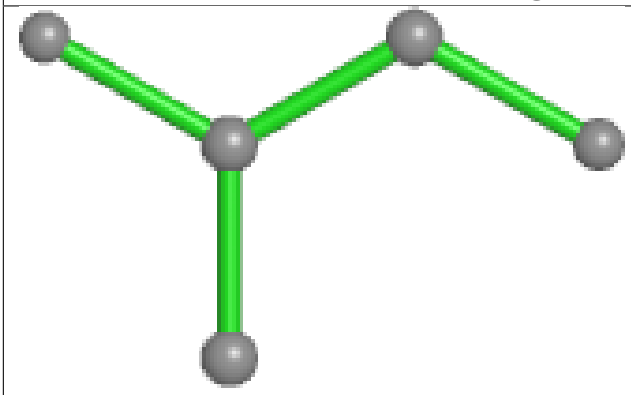


Rings

Ligand F3V B 302



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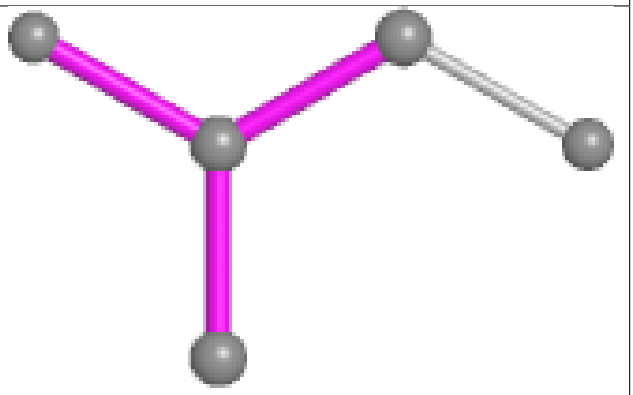

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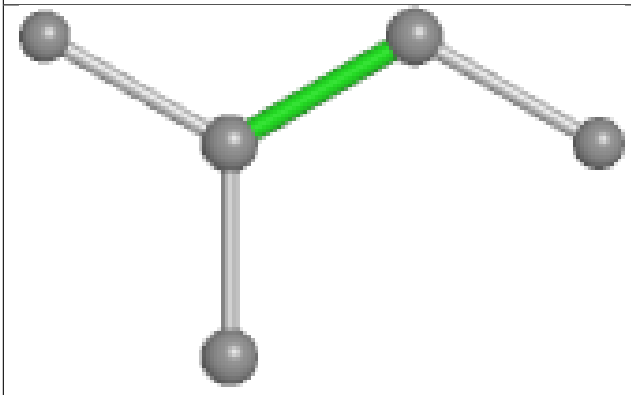

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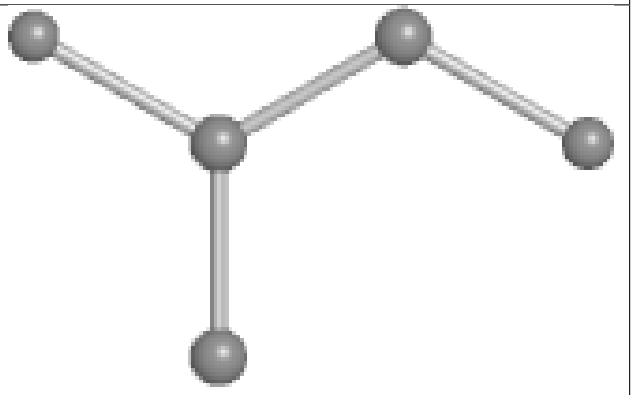

Rings

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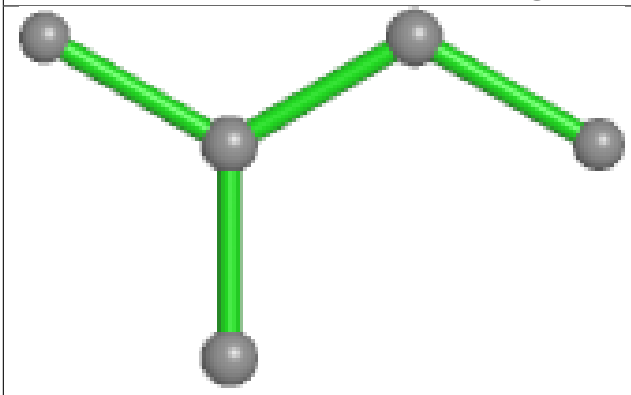

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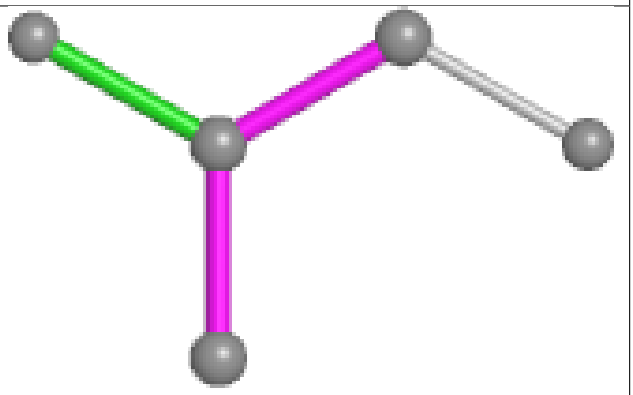

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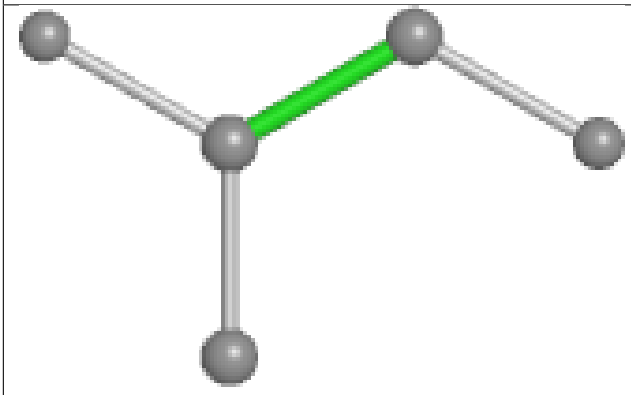

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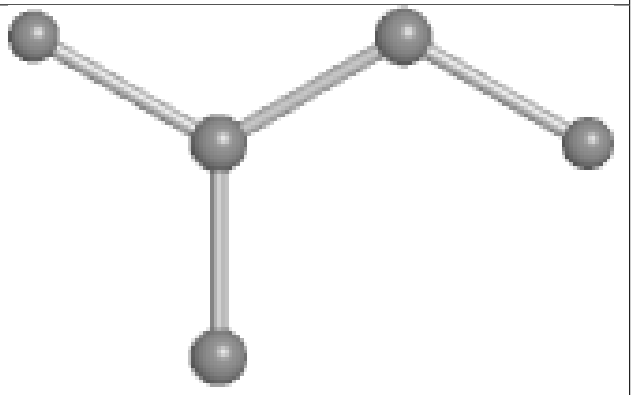
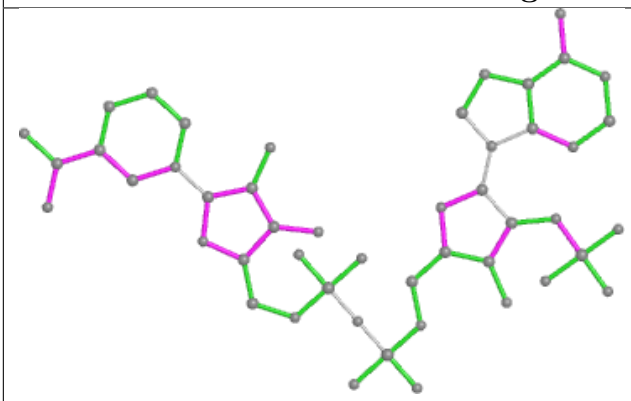


Rings

Ligand NAP G 301



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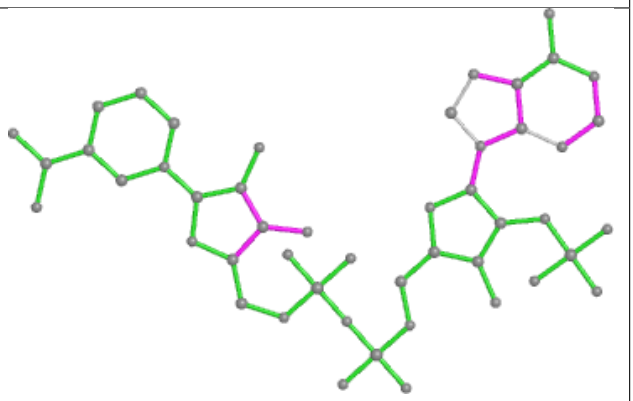

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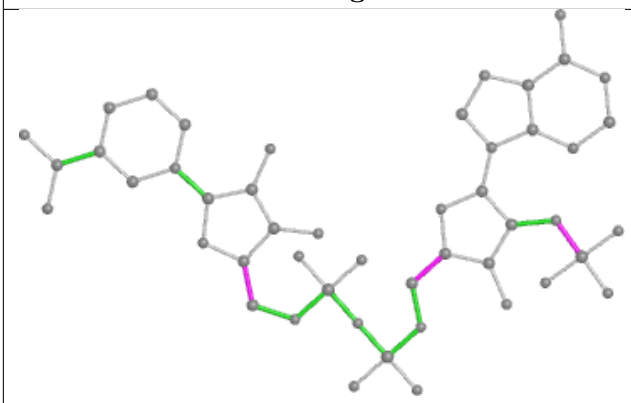

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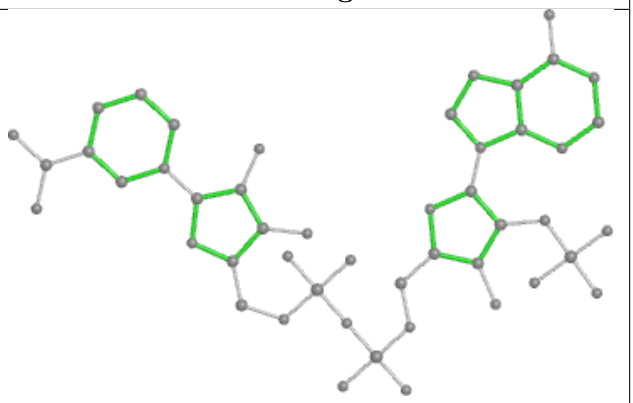
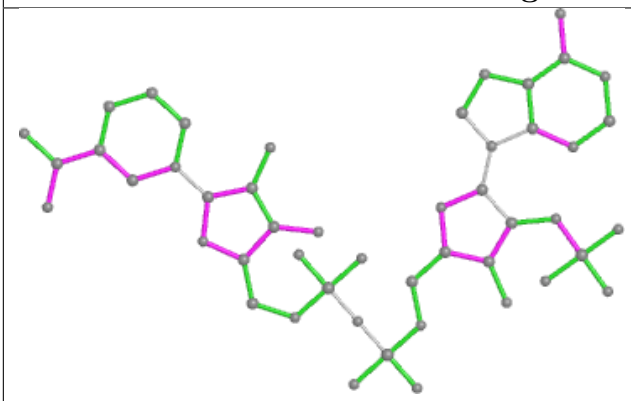


Rings

Ligand NAP A 301



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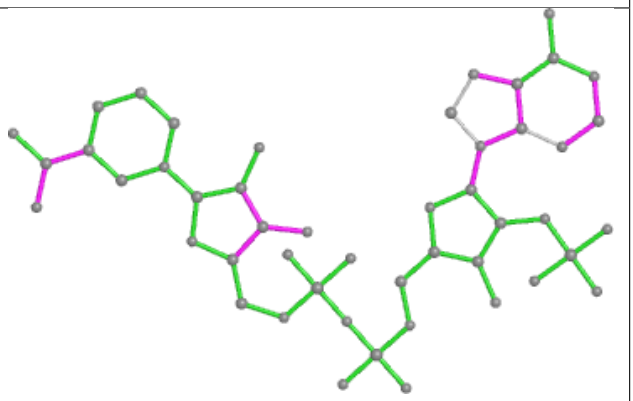
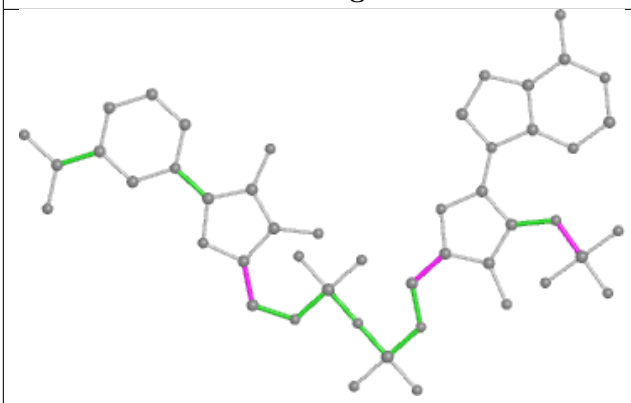
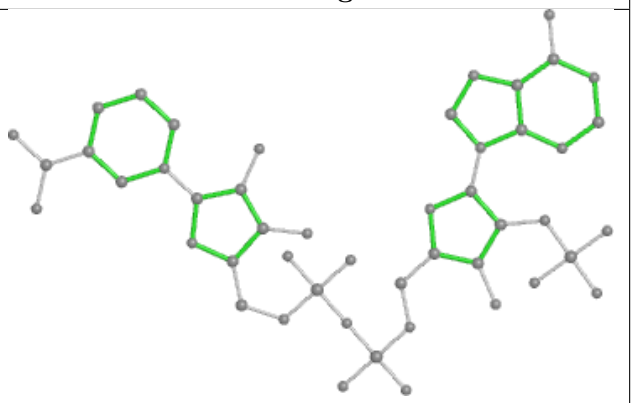


Bond angles

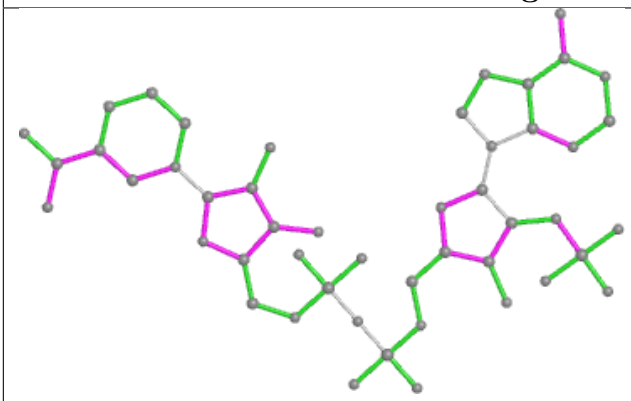


Torsions



Rings

Ligand NAP O 301



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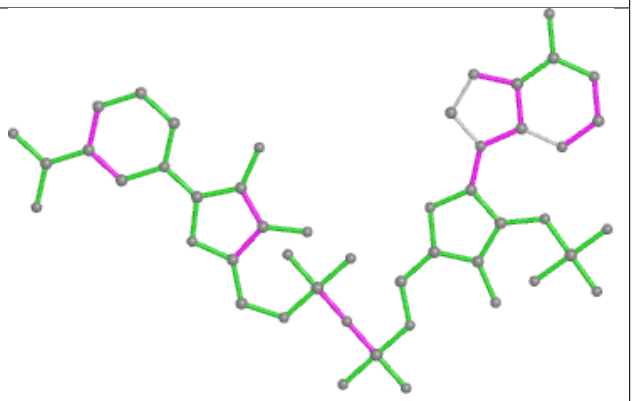

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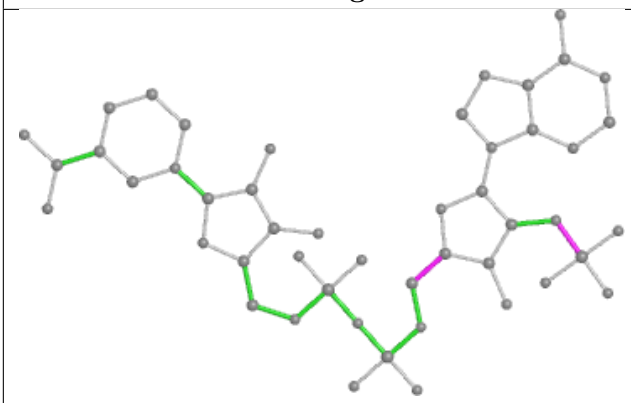

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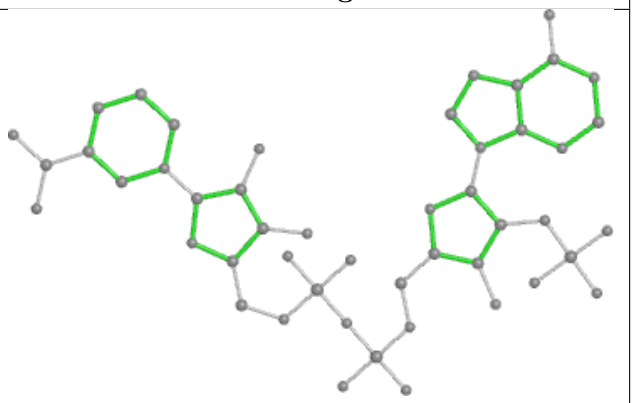
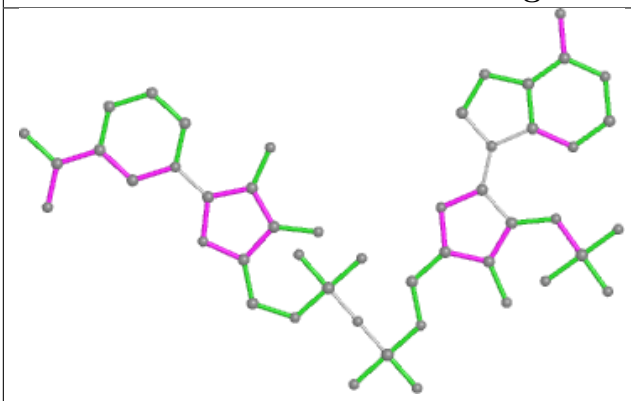


Rings

Ligand NAP F 301



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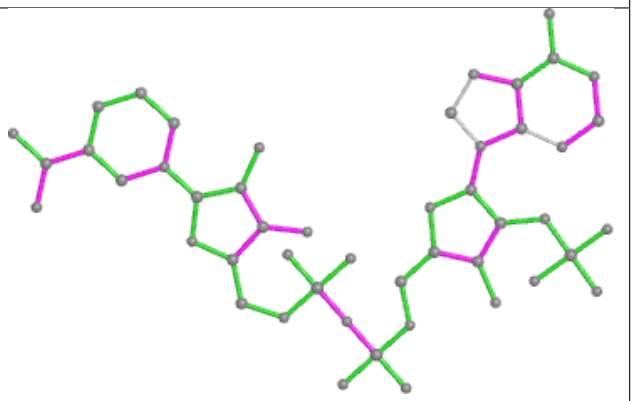

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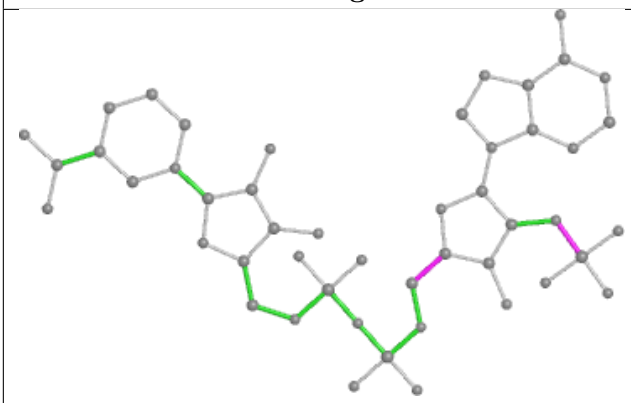

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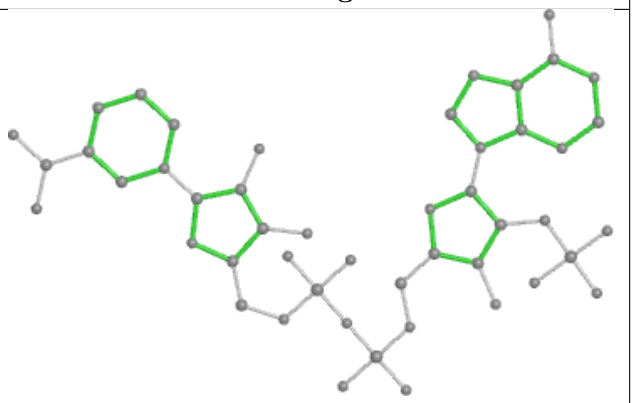

Rings

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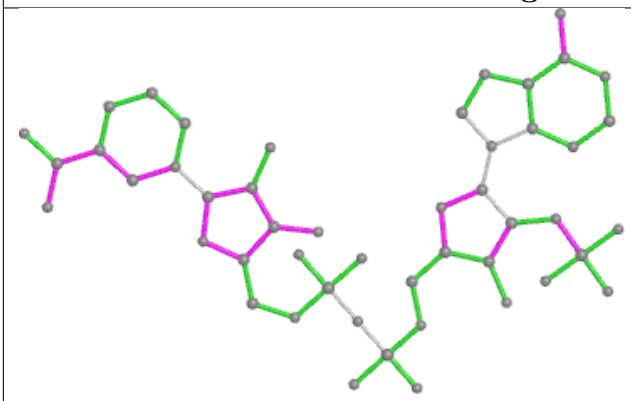

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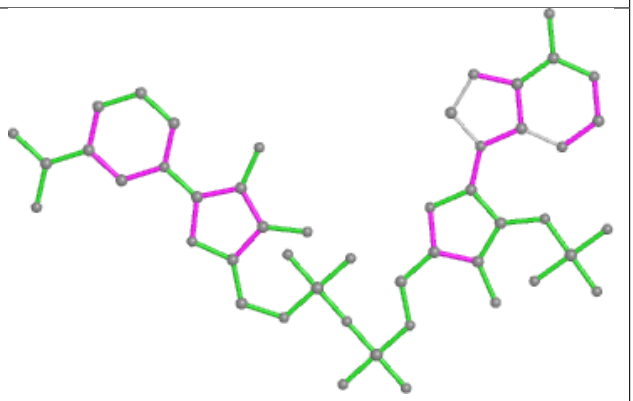

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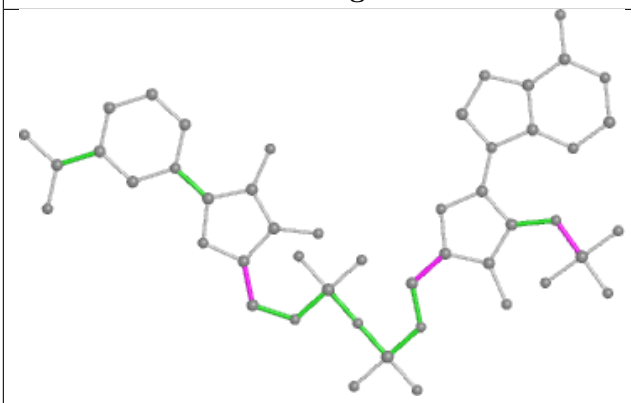

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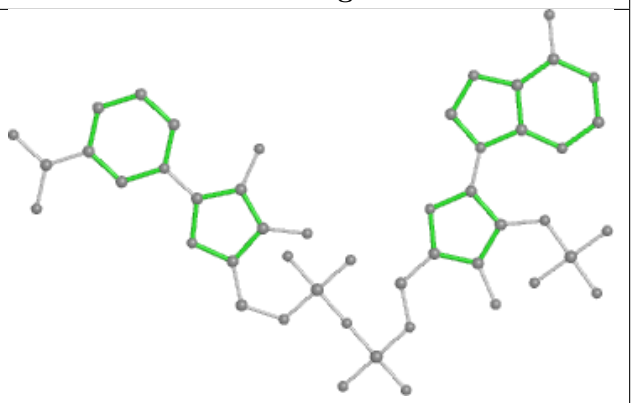
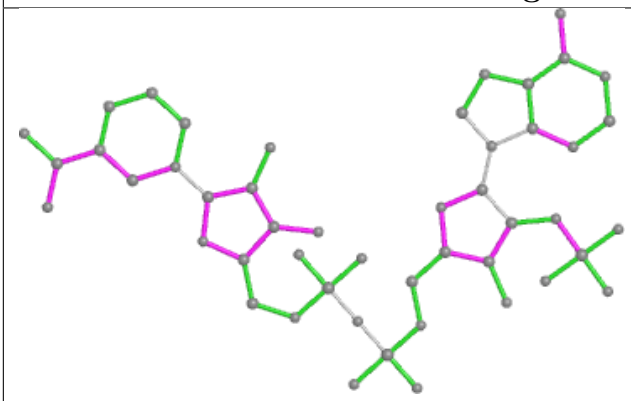


Rings

Ligand NAP E 301



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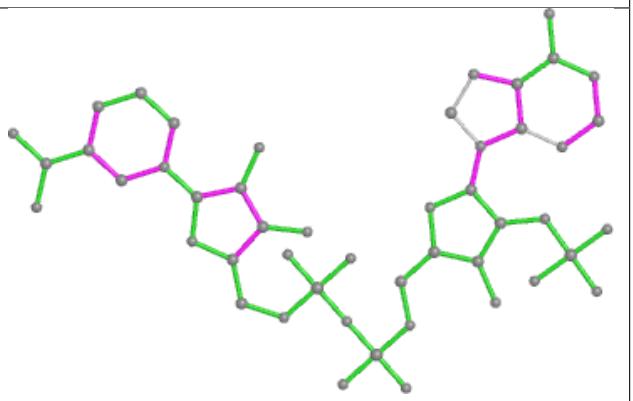

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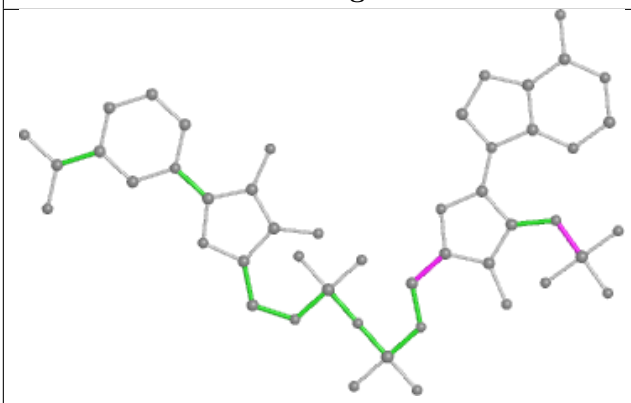

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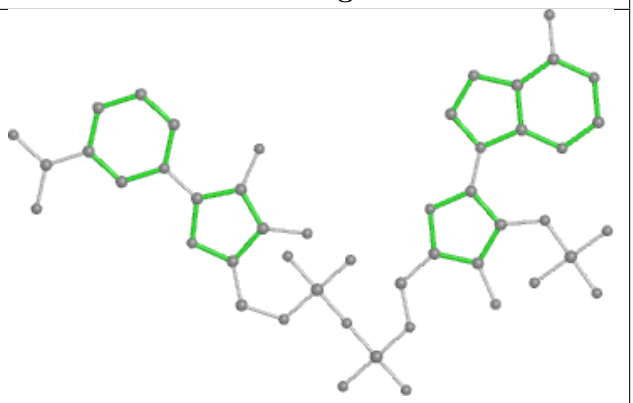
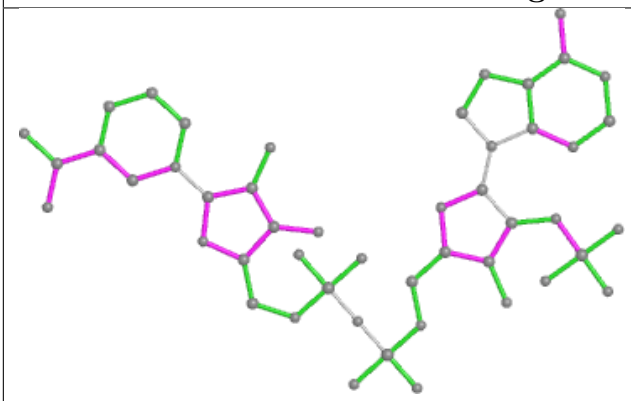


Rings

Ligand NAP I 301



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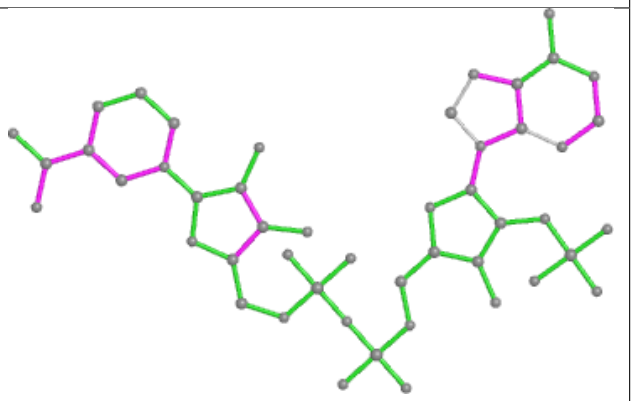

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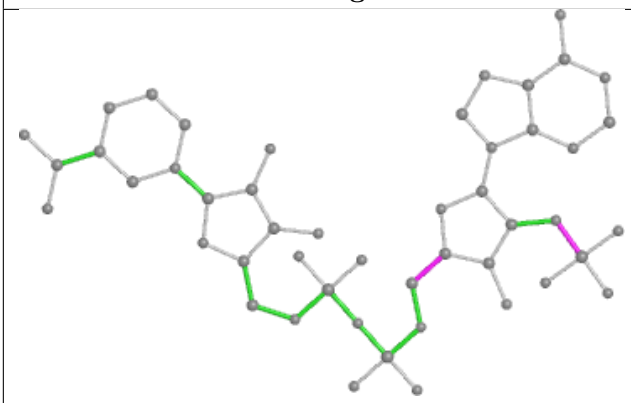

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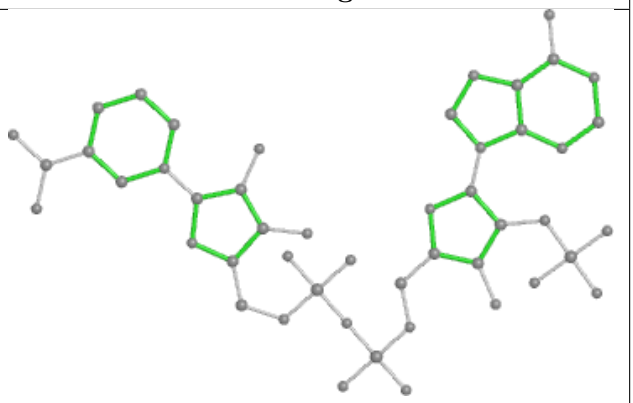
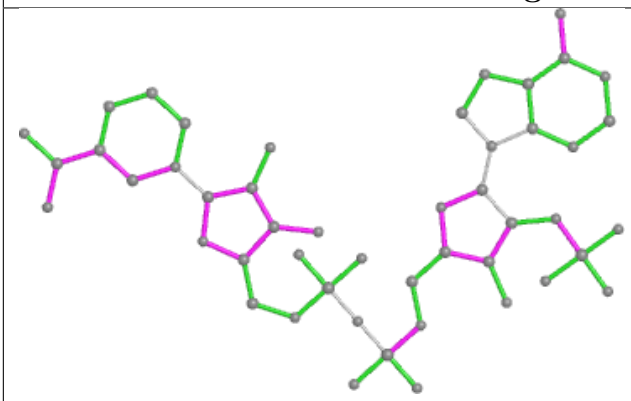


Rings

Ligand NAP L 301



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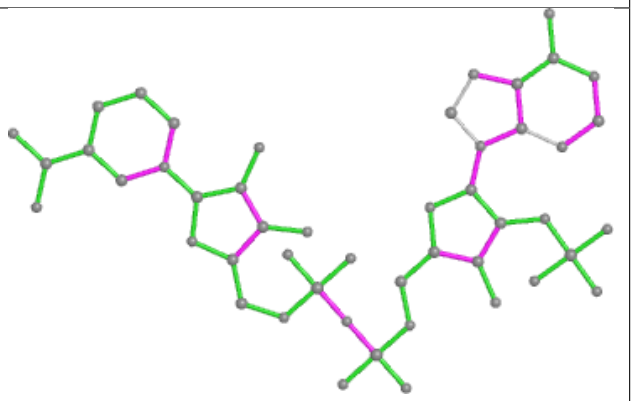

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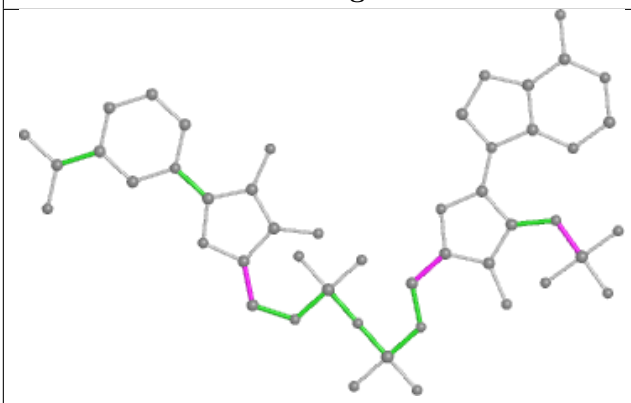

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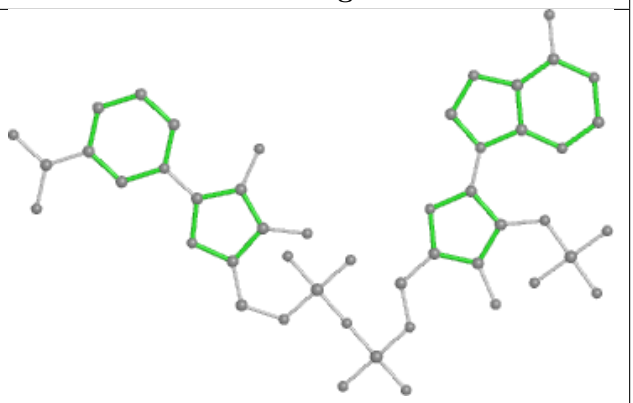
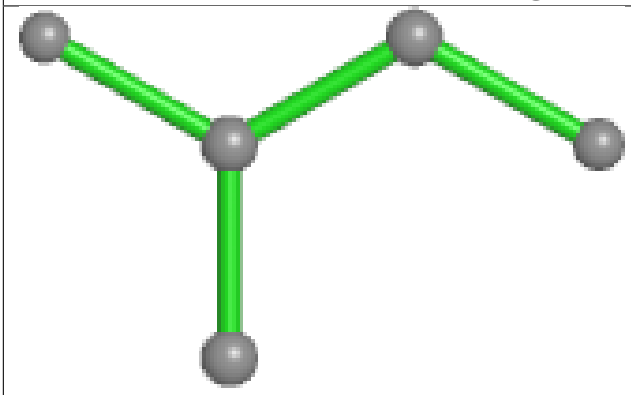


Rings

Ligand F3V O 302



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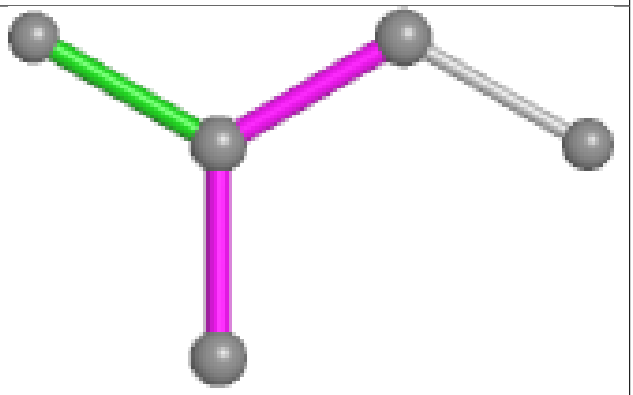

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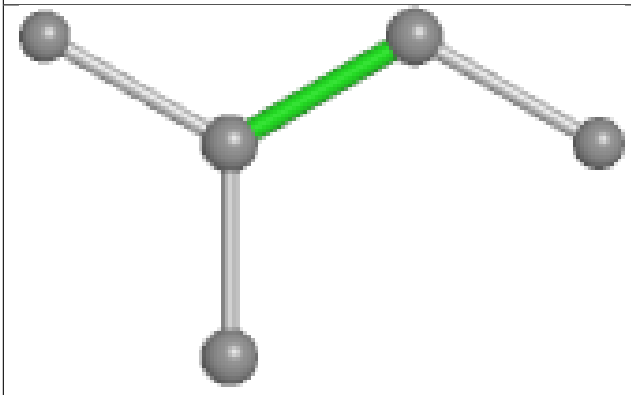

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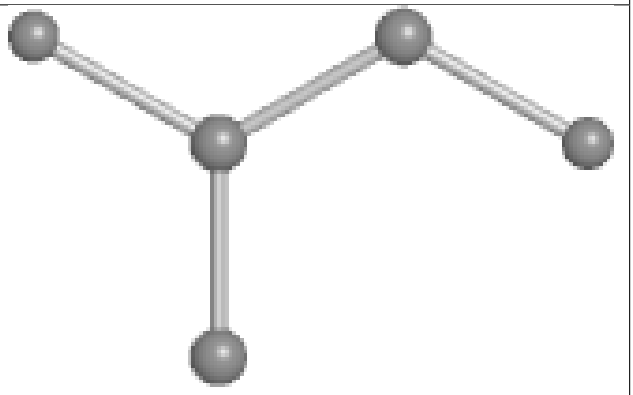

Rings

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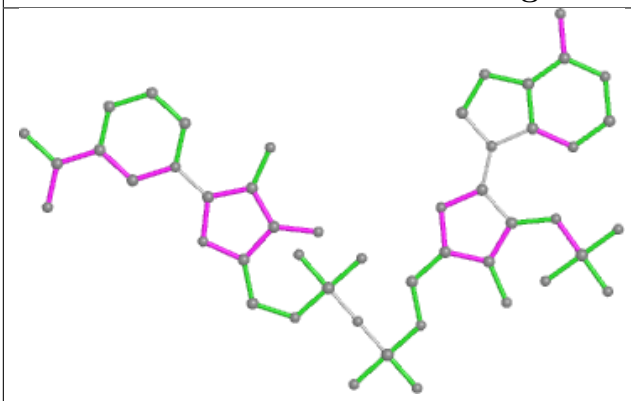

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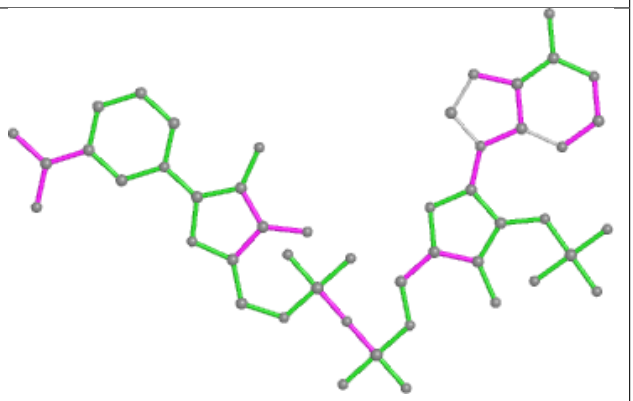

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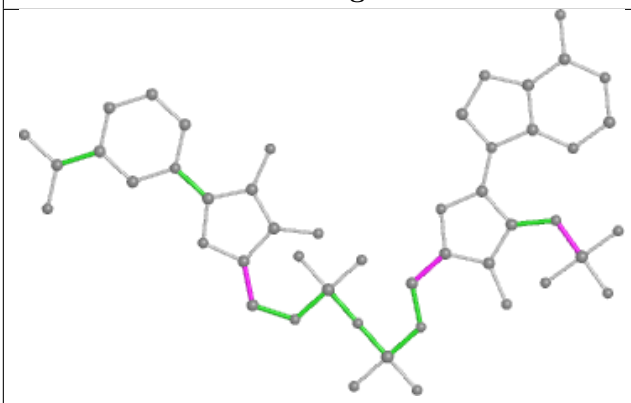

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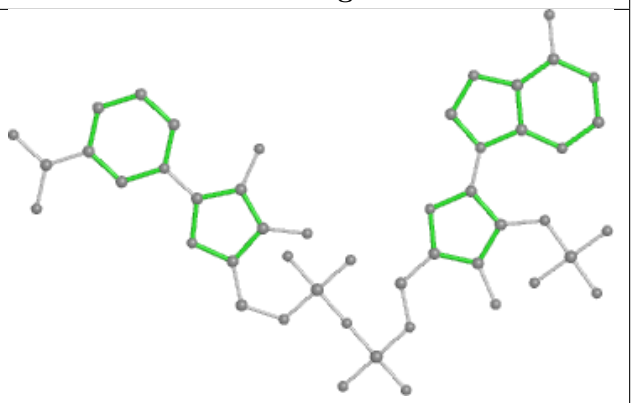
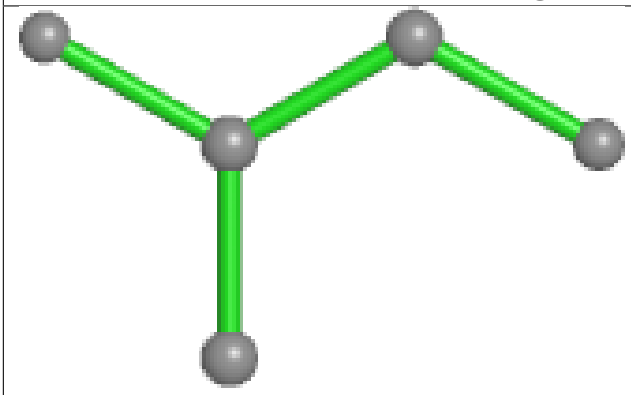


Rings

Ligand F3V J 302



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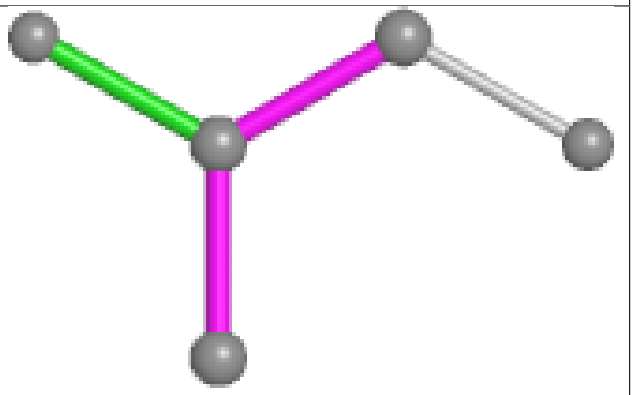

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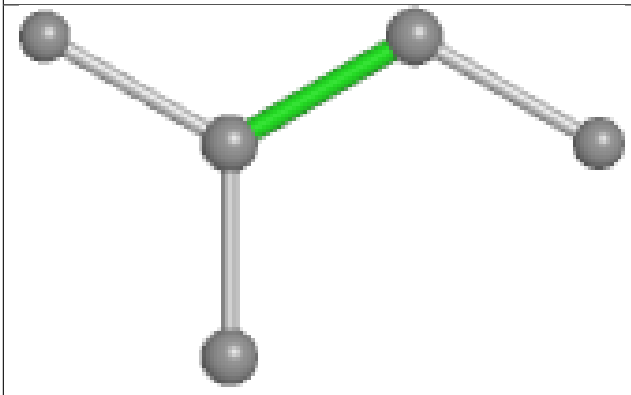

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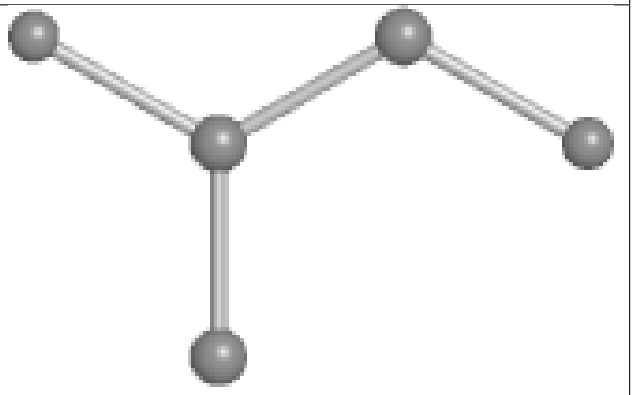
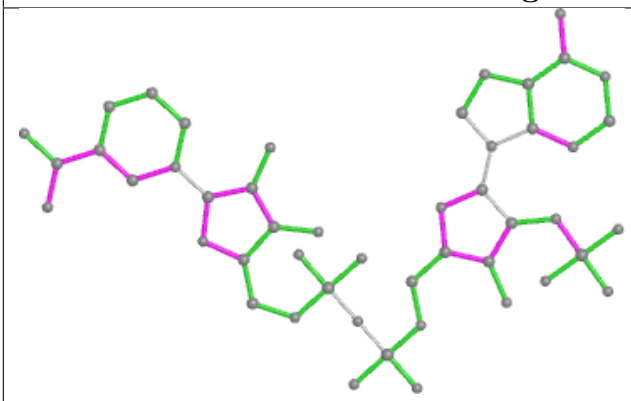


Rings

Ligand NAP C 301



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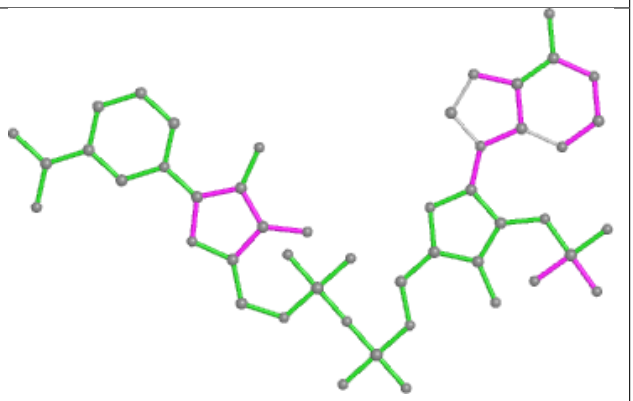

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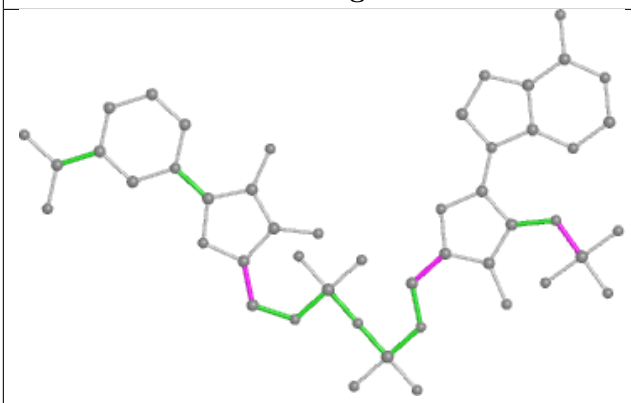

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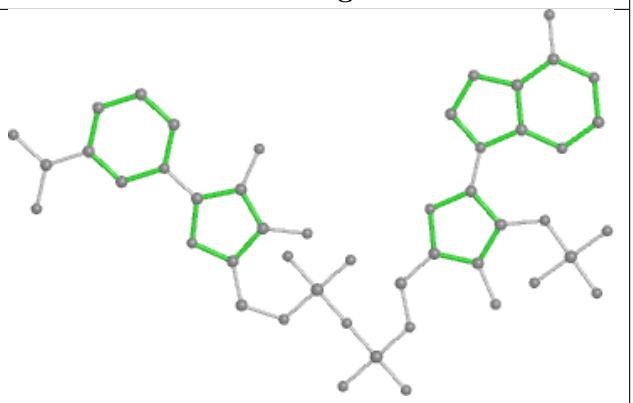
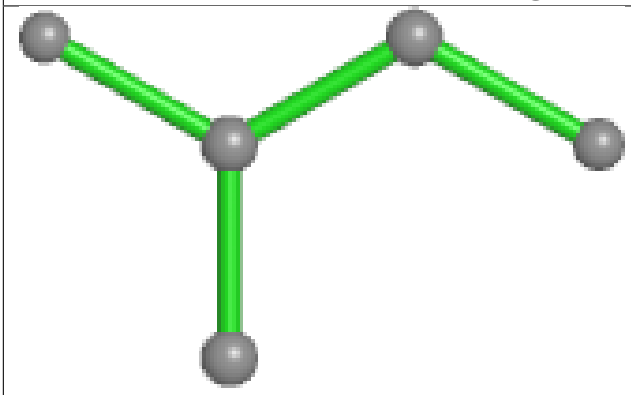


Rings

Ligand F3V D 302



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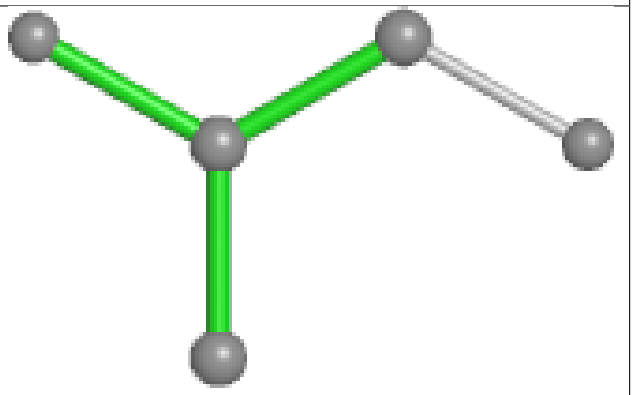

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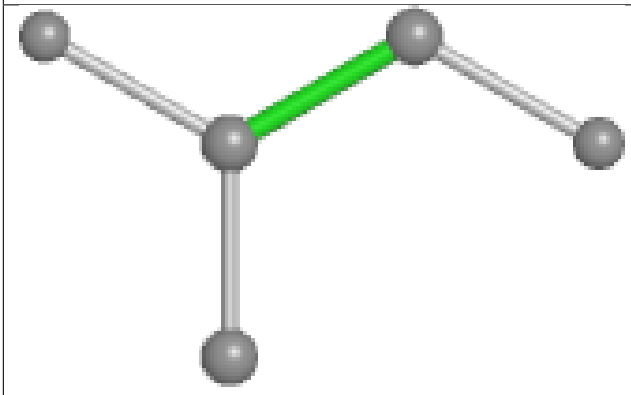

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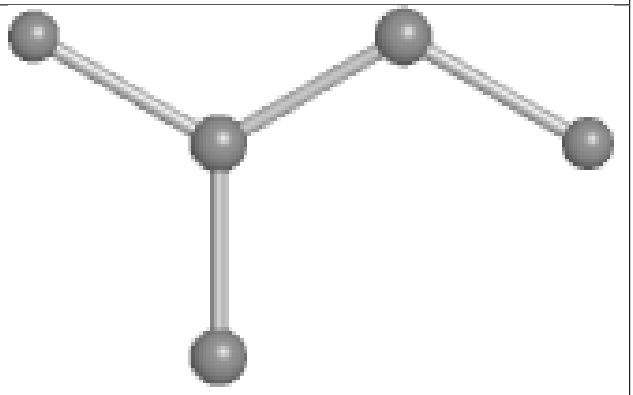
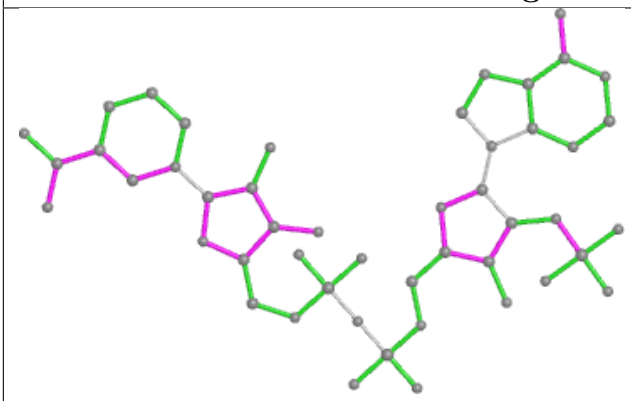


Rings

Ligand NAP P 301



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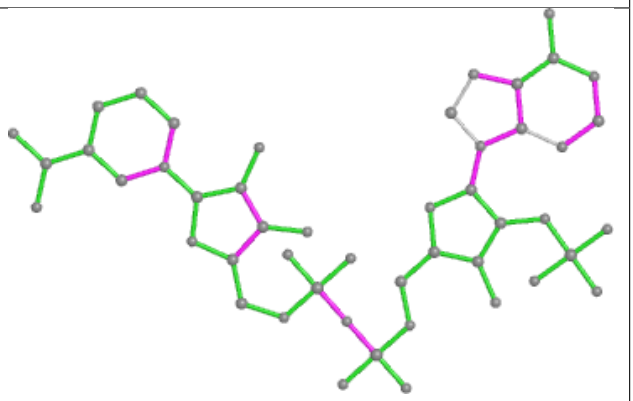

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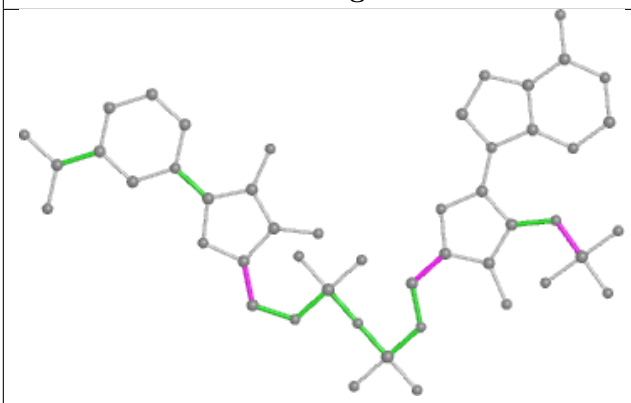

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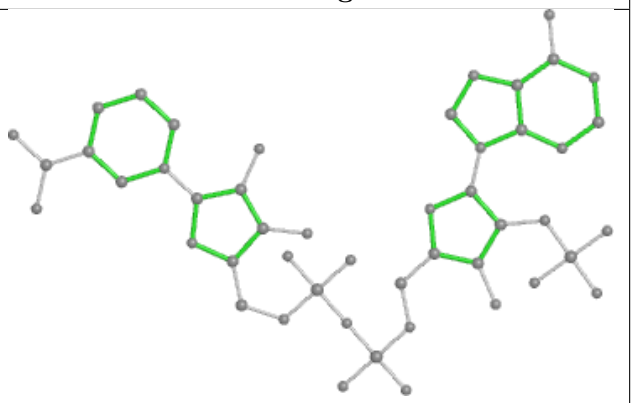
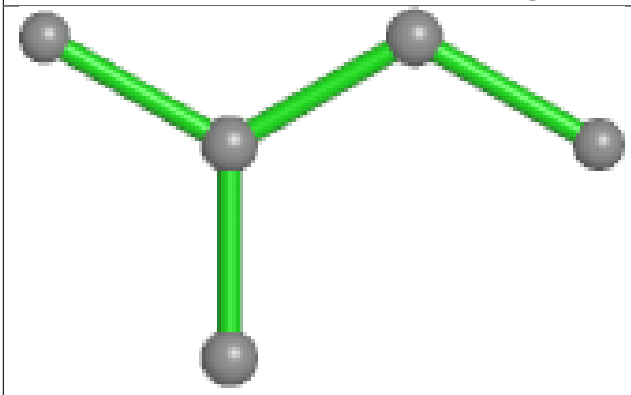


Rings

Ligand F3V M 302



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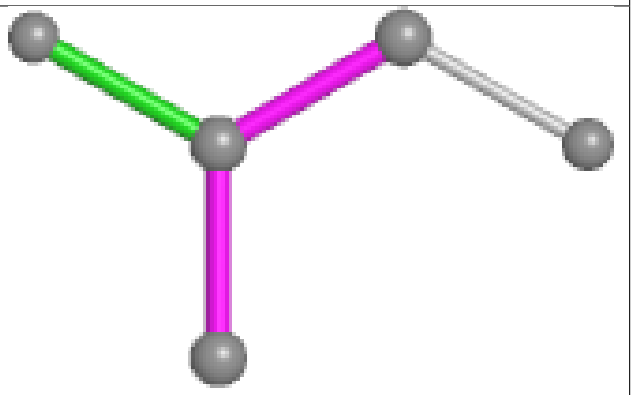

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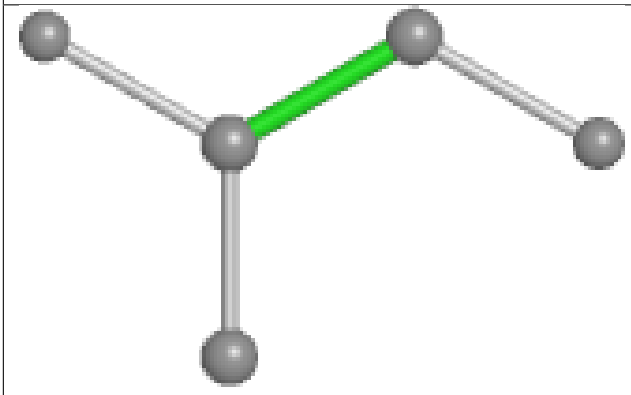

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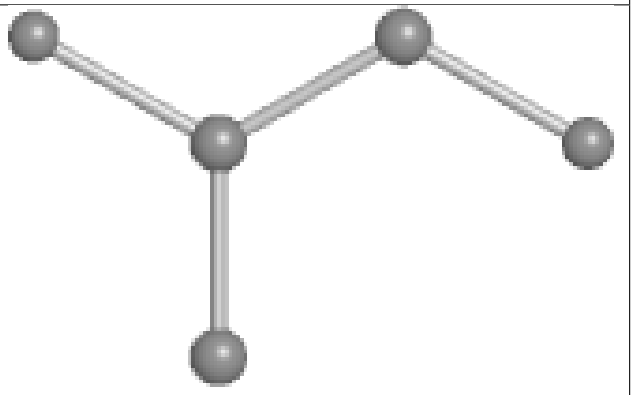
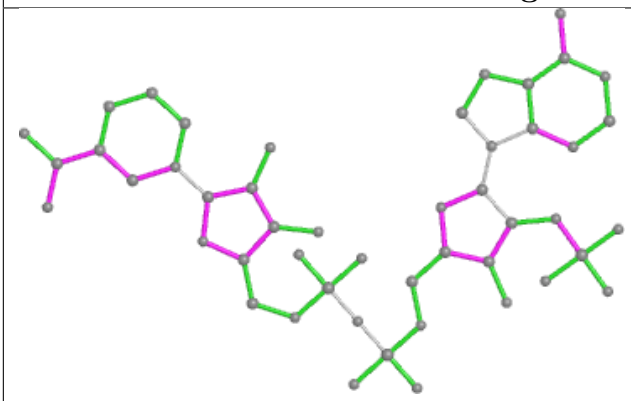
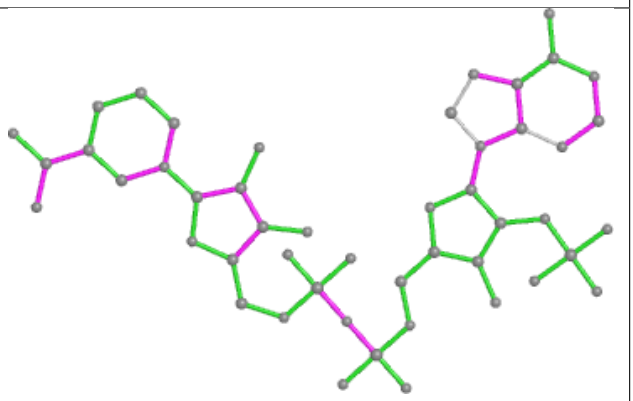


Rings

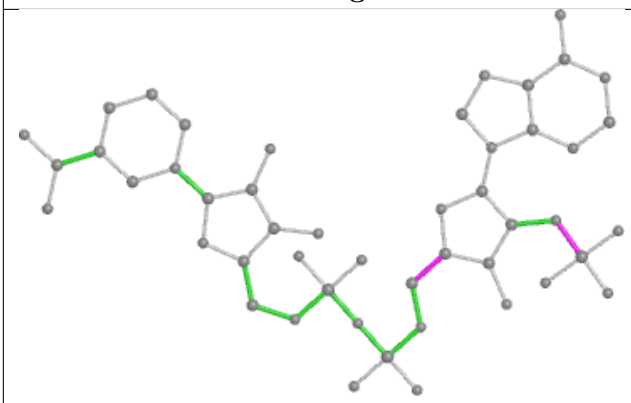
Ligand NAP N 301



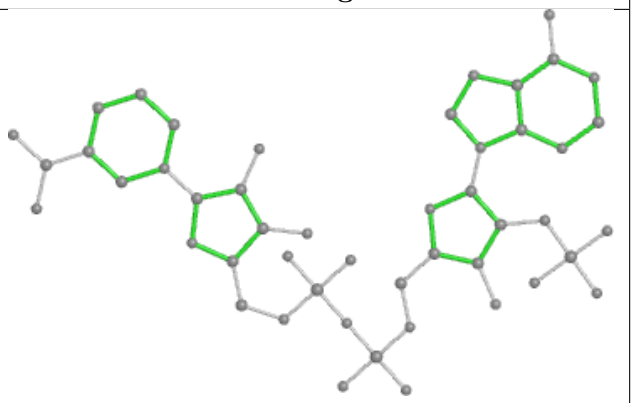
Bond lengths



Bond angles

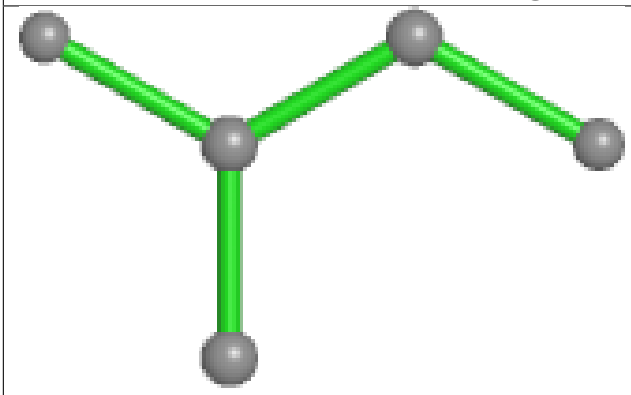


Torsions

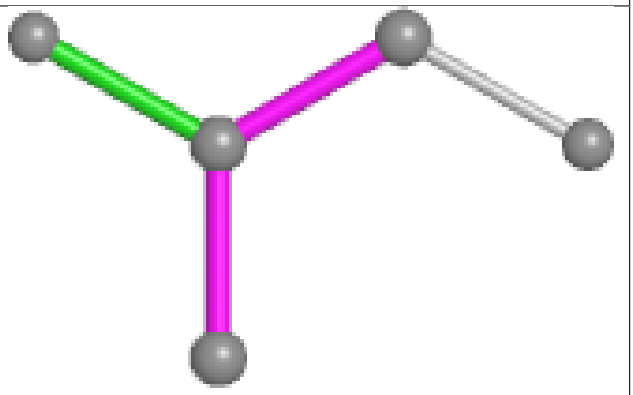


Rings

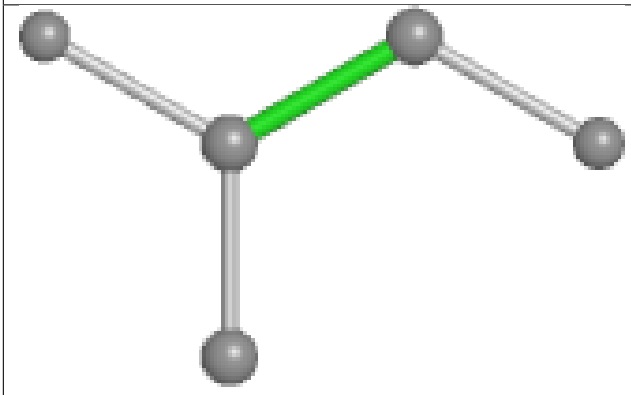
Ligand F3V K 302



Bond lengths



Bond angles



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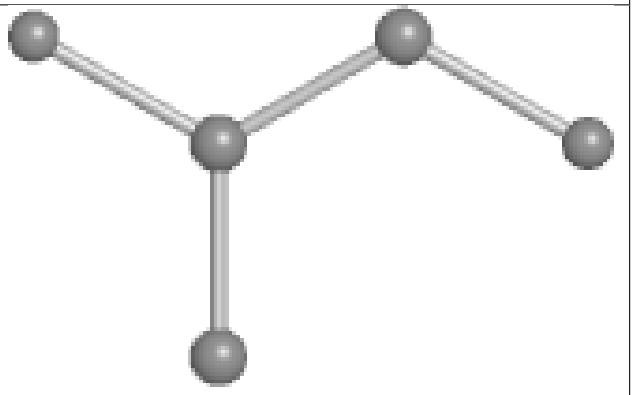
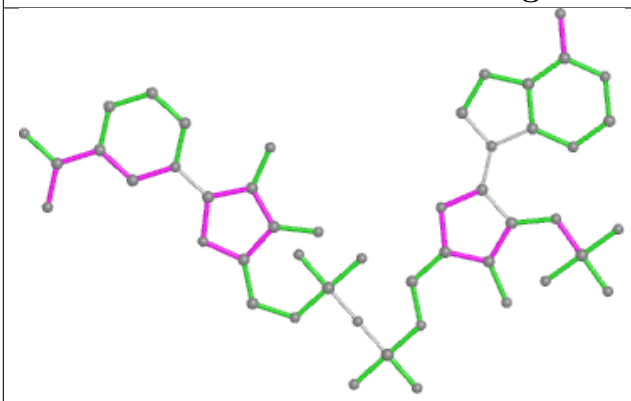
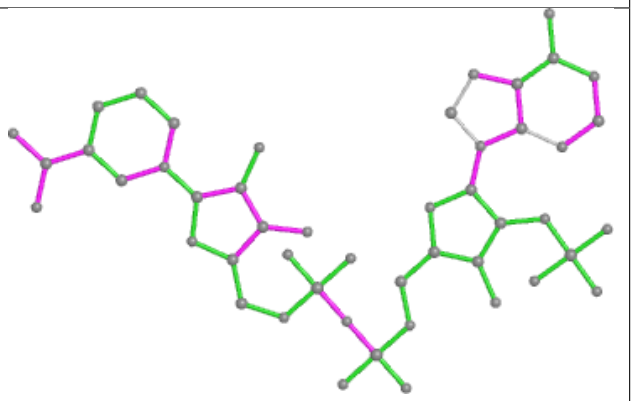


Rings

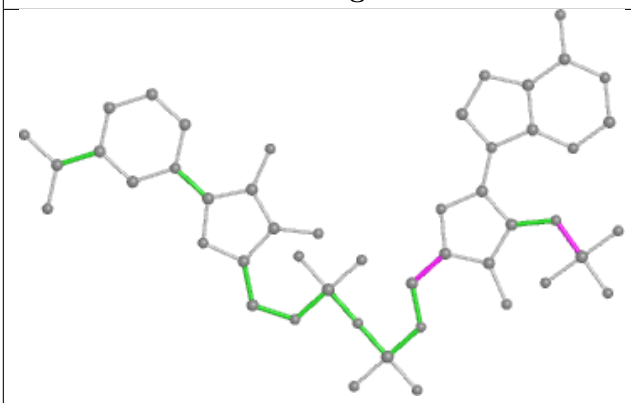
Ligand NAP B 301



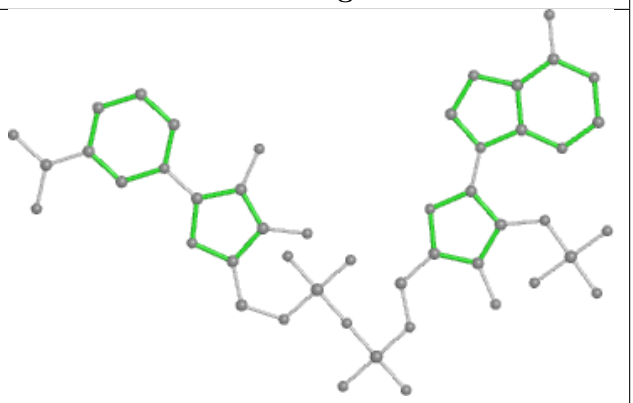
Bond lengths



Bond angles

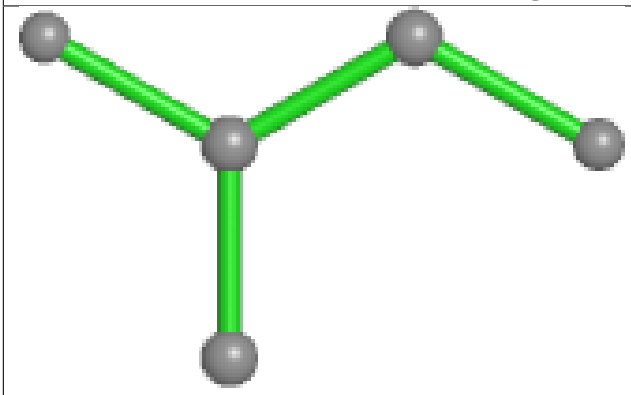


Torsions

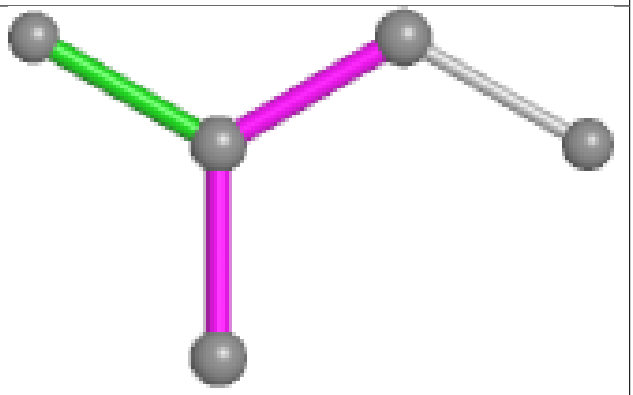


Rings

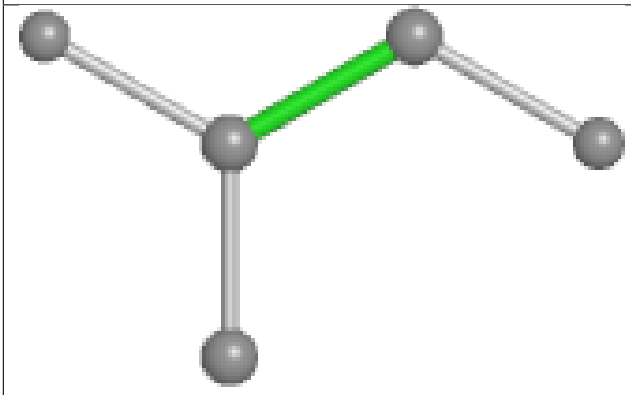
Ligand F3V G 302



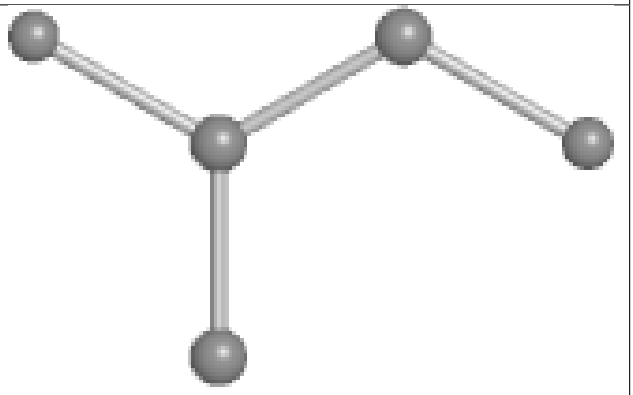
Bond lengths



Bond angles

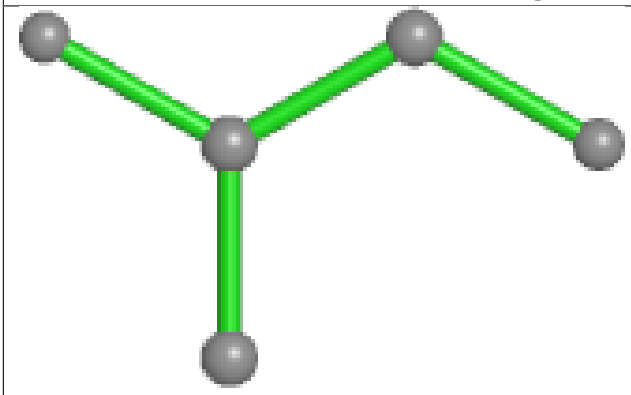


Torsions



Rings

Ligand F3V E 302



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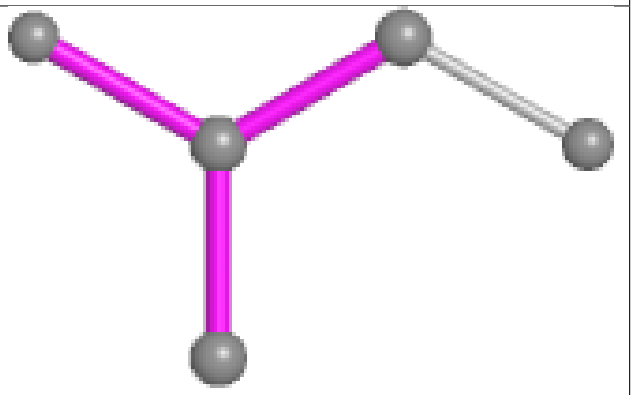
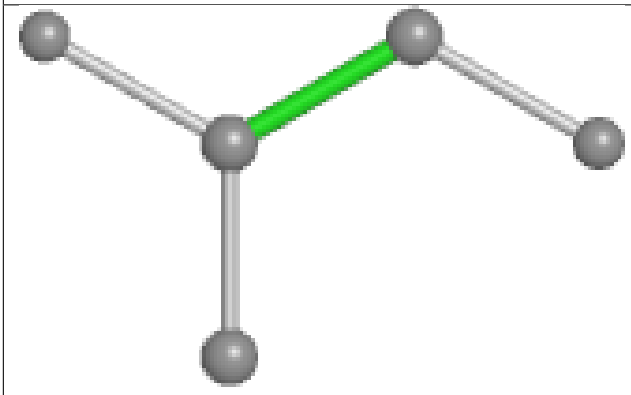
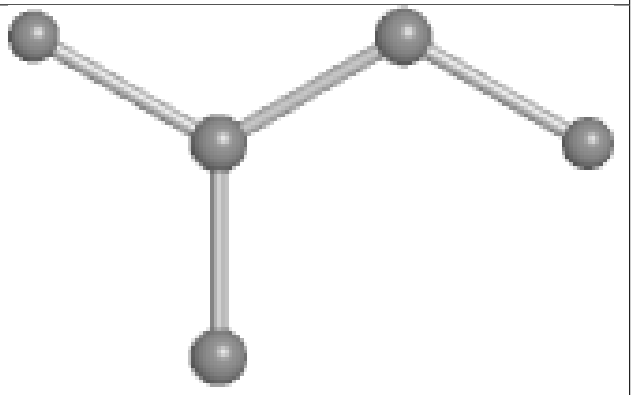


Bond angles

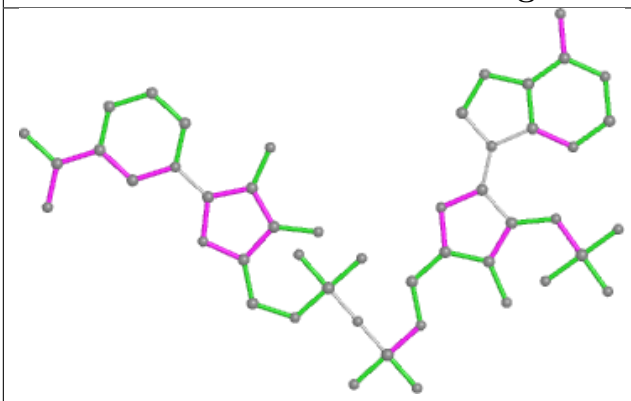


Torsions

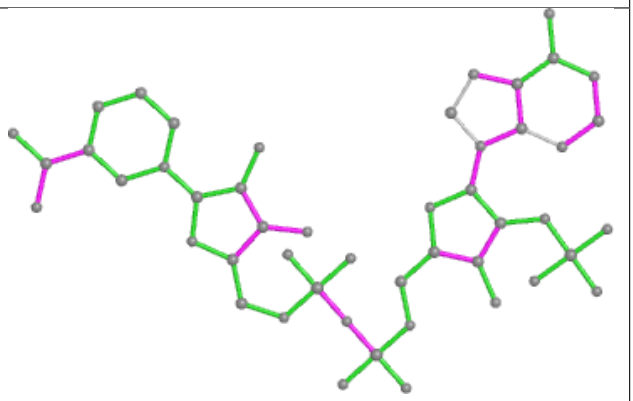


Rings

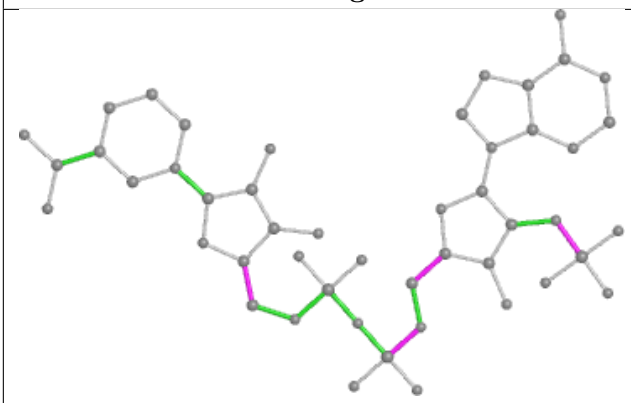
Ligand NAP M 301



Bond lengths



Bond angles



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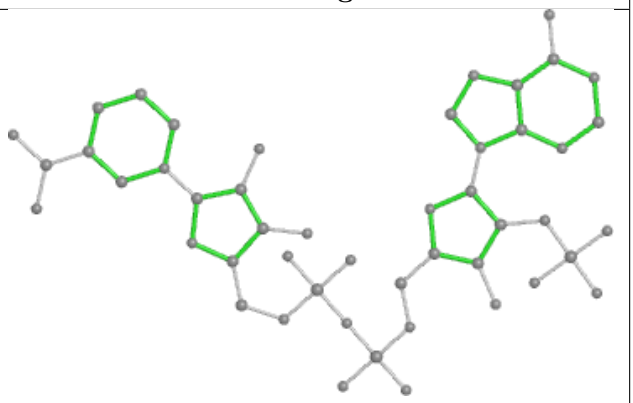
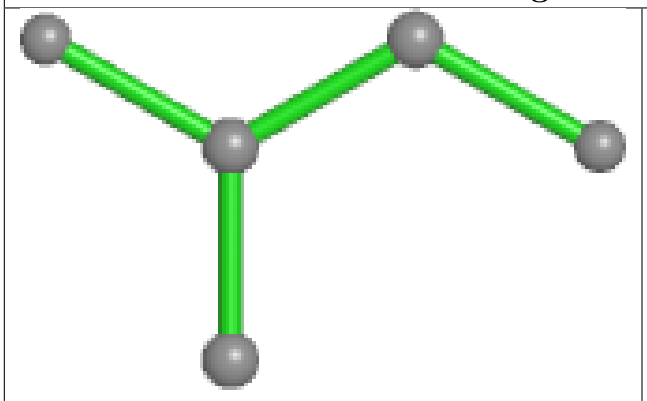
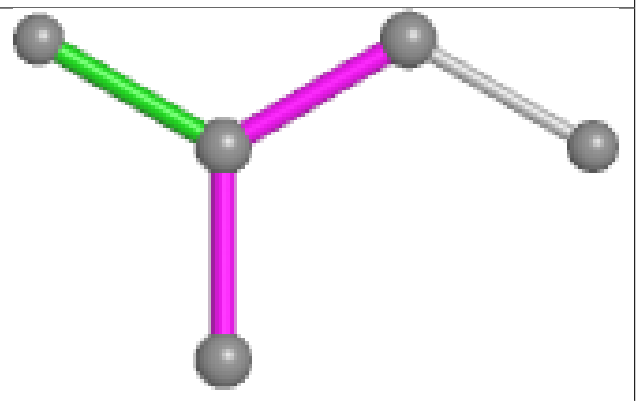


Rings

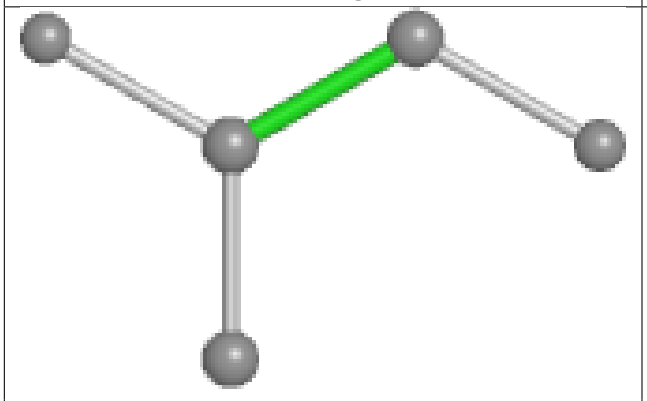
Ligand F3V L 302



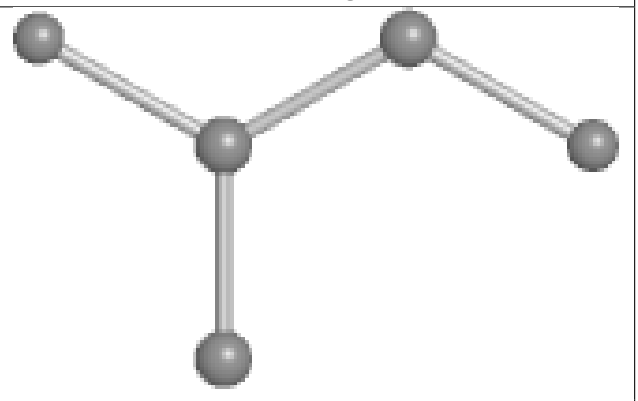
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	256/259 (98%)	-0.02	14 (5%)	25	28	13, 26, 67, 97	0
1	B	255/259 (98%)	0.12	15 (5%)	22	25	18, 33, 67, 102	0
1	C	258/259 (99%)	0.22	13 (5%)	28	32	19, 32, 51, 81	0
1	D	259/259 (100%)	0.27	8 (3%)	49	51	18, 34, 50, 84	0
1	E	255/259 (98%)	-0.00	4 (1%)	72	74	17, 31, 54, 67	0
1	F	254/259 (98%)	0.14	11 (4%)	35	38	16, 28, 56, 79	0
1	G	256/259 (98%)	0.34	19 (7%)	14	16	20, 35, 61, 71	0
1	H	253/259 (97%)	0.01	3 (1%)	79	81	18, 30, 49, 63	0
1	I	258/259 (99%)	0.32	13 (5%)	28	32	27, 43, 67, 81	0
1	J	257/259 (99%)	0.59	20 (7%)	13	14	29, 44, 72, 105	0
1	K	255/259 (98%)	0.48	28 (10%)	5	6	27, 47, 79, 106	0
1	L	253/259 (97%)	0.22	12 (4%)	31	34	28, 41, 66, 82	0
1	M	256/259 (98%)	0.54	29 (11%)	5	5	27, 45, 81, 110	0
1	N	254/259 (98%)	0.19	10 (3%)	39	42	29, 47, 67, 79	0
1	O	253/259 (97%)	0.31	11 (4%)	35	38	30, 45, 64, 76	0
1	P	255/259 (98%)	0.51	22 (8%)	10	12	29, 42, 67, 93	0
All	All	4087/4144 (98%)	0.26	232 (5%)	23	26	13, 38, 66, 110	0

The worst 5 of 232 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	254	LEU	12.3
1	D	254	LEU	11.4
1	B	203	LEU	11.3
1	J	253	HIS	8.5
1	K	205	GLN	8.5

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
5	MG	F	304	1/1	0.59	0.11	52,52,52,52	0
5	MG	O	304	1/1	0.70	0.18	45,45,45,45	0
3	F3V	M	302	5/5	0.76	0.15	66,68,68,68	0
5	MG	J	304	1/1	0.79	0.09	42,42,42,42	0
5	MG	H	304	1/1	0.79	0.11	28,28,28,28	0
3	F3V	B	302	5/5	0.83	0.14	38,42,44,46	0
3	F3V	N	302	5/5	0.83	0.11	42,43,44,45	0
3	F3V	E	302	5/5	0.83	0.11	25,27,31,33	0
2	NAP	M	301	48/48	0.84	0.13	42,53,62,63	48
3	F3V	G	302	5/5	0.84	0.11	39,39,40,41	0
4	CL	A	304	1/1	0.86	0.10	82,82,82,82	0
2	NAP	G	301	48/48	0.87	0.12	19,27,32,32	48
3	F3V	I	302	5/5	0.87	0.15	44,44,47,48	0
5	MG	M	304	1/1	0.87	0.13	71,71,71,71	0
2	NAP	B	301	48/48	0.87	0.13	24,32,41,42	48
3	F3V	P	302	5/5	0.88	0.19	45,47,49,50	0
2	NAP	K	301	48/48	0.88	0.12	35,38,42,44	48
5	MG	C	304	1/1	0.88	0.08	24,24,24,24	0
2	NAP	I	301	48/48	0.88	0.12	31,37,43,46	48
2	NAP	N	301	48/48	0.89	0.11	31,41,51,52	48
2	NAP	P	301	48/48	0.89	0.11	32,35,41,45	48
3	F3V	F	302	5/5	0.89	0.12	35,39,41,42	0
2	NAP	E	301	48/48	0.90	0.11	20,27,32,34	48
2	NAP	L	301	48/48	0.90	0.10	32,45,49,51	0
4	CL	J	303	1/1	0.90	0.18	56,56,56,56	0
4	CL	P	303	1/1	0.90	0.14	49,49,49,49	0
3	F3V	C	302	5/5	0.90	0.17	24,24,26,26	0

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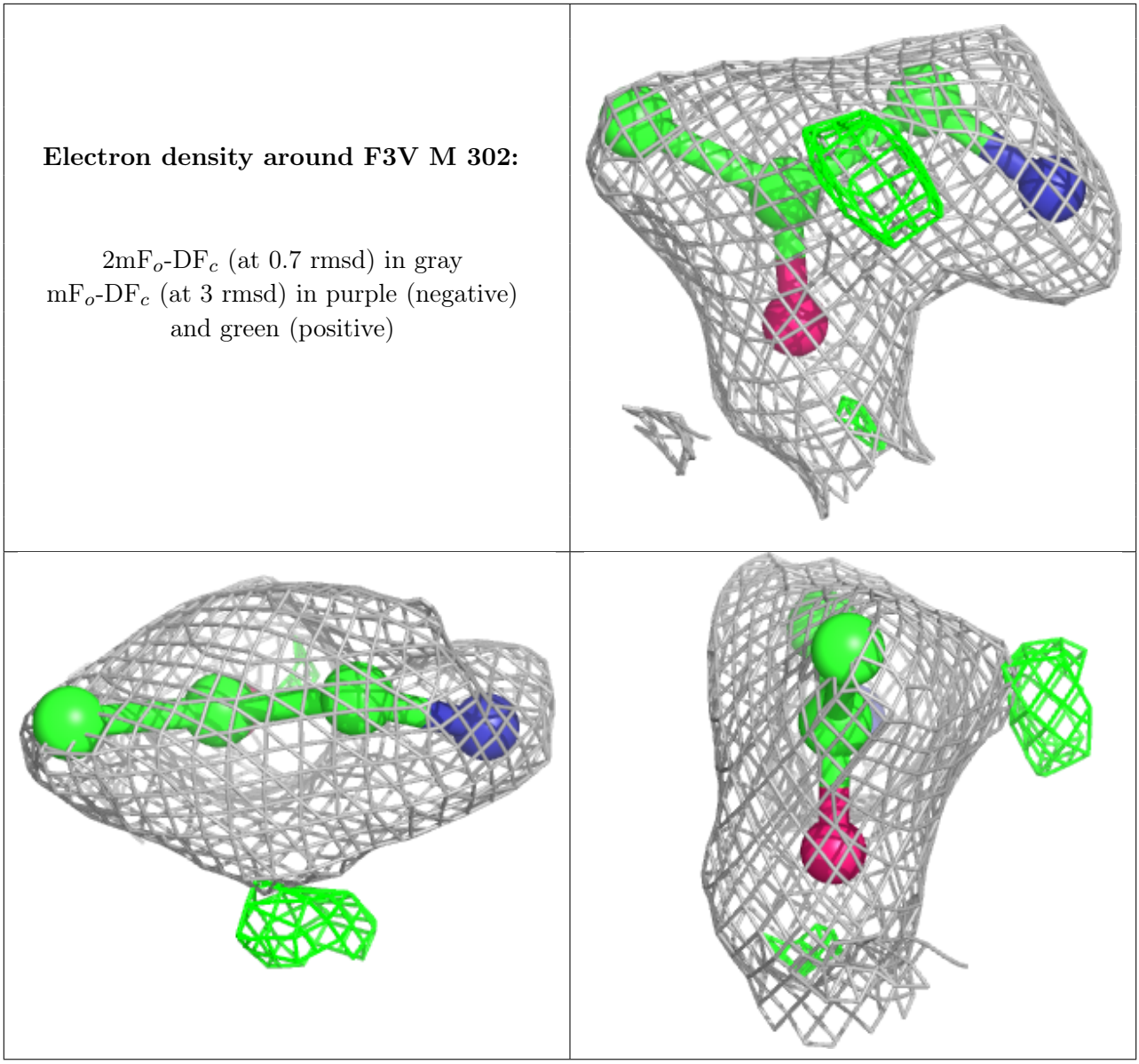
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	O	303	1/1	0.91	0.08	47,47,47,47	0
2	NAP	D	301	48/48	0.91	0.10	17,22,27,30	0
2	NAP	A	301	48/48	0.91	0.10	16,29,34,36	48
2	NAP	F	301	48/48	0.91	0.10	17,32,38,41	48
3	F3V	D	302	5/5	0.91	0.11	22,23,23,26	0
4	CL	E	303	1/1	0.91	0.07	36,36,36,36	0
3	F3V	K	302	5/5	0.91	0.12	45,46,48,50	0
4	CL	M	303	1/1	0.91	0.15	53,53,53,53	0
4	CL	L	303	1/1	0.92	0.15	52,52,52,52	0
2	NAP	J	301	48/48	0.92	0.11	28,34,36,38	0
5	MG	A	305	1/1	0.92	0.04	43,43,43,43	0
2	NAP	H	301	48/48	0.93	0.10	12,18,24,25	0
2	NAP	O	301	48/48	0.93	0.09	31,35,42,45	0
3	F3V	H	302	5/5	0.93	0.14	23,24,24,26	0
2	NAP	C	301	48/48	0.93	0.10	12,19,25,32	0
3	F3V	J	302	5/5	0.93	0.13	43,45,45,46	0
4	CL	F	303	1/1	0.93	0.07	33,33,33,33	0
4	CL	I	303	1/1	0.93	0.39	65,65,65,65	0
3	F3V	A	302	5/5	0.93	0.12	35,36,37,37	0
5	MG	L	304	1/1	0.93	0.06	66,66,66,66	0
4	CL	K	303	1/1	0.93	0.08	57,57,57,57	0
3	F3V	L	302	5/5	0.93	0.09	47,50,52,53	0
4	CL	C	303	1/1	0.94	0.06	31,31,31,31	0
4	CL	A	303	1/1	0.94	0.07	31,31,31,31	0
4	CL	B	303	1/1	0.95	0.09	37,37,37,37	0
4	CL	N	303	1/1	0.95	0.09	47,47,47,47	0
3	F3V	O	302	5/5	0.95	0.14	35,35,39,40	0
4	CL	D	303	1/1	0.96	0.06	33,33,33,33	0
4	CL	H	303	1/1	0.96	0.07	34,34,34,34	0
4	CL	G	303	1/1	0.97	0.07	33,33,33,33	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.

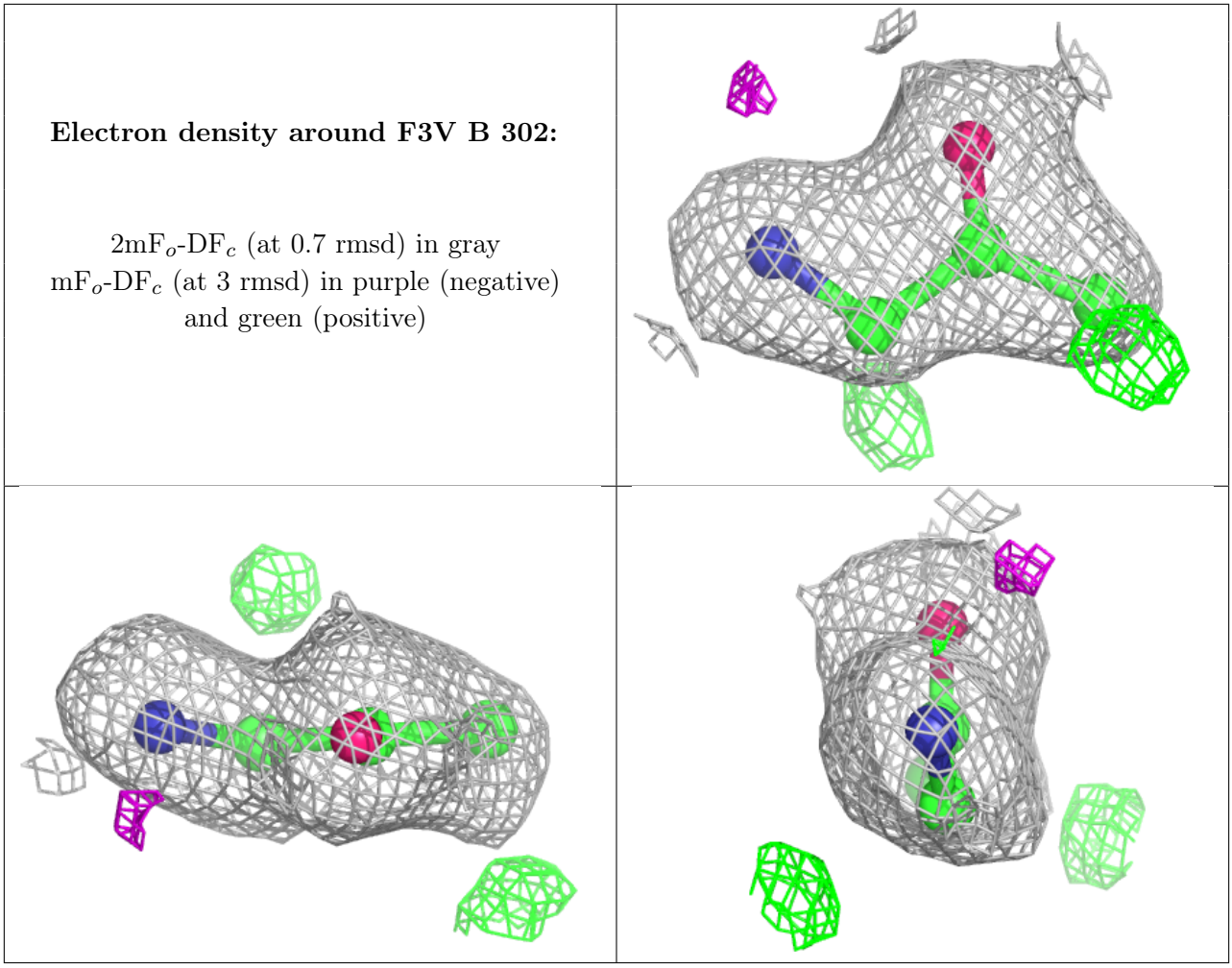
Electron density around F3V M 302:

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



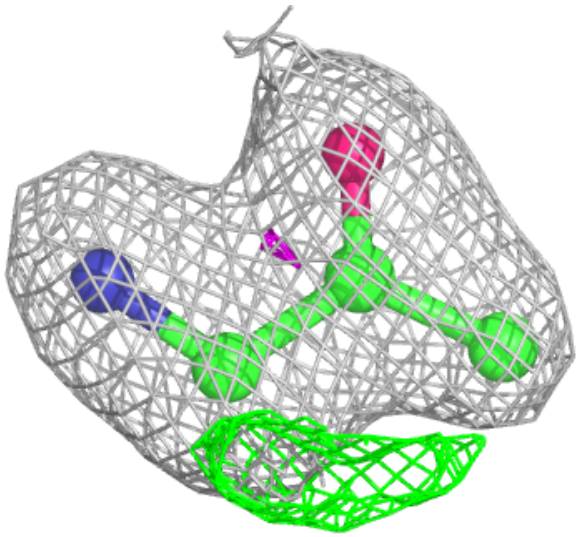
Electron density around F3V B 302:

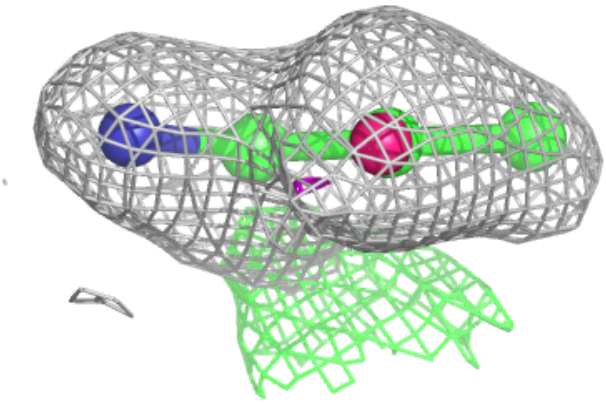
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

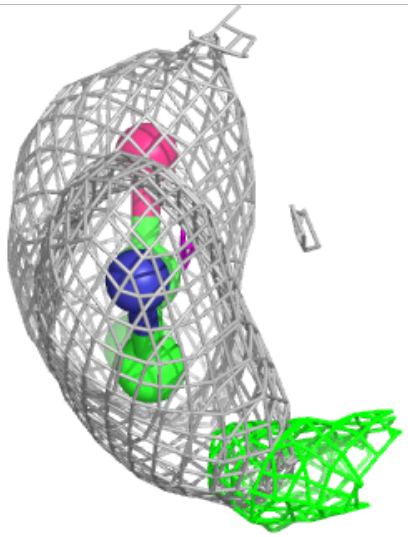


Electron density around F3V N 302:

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

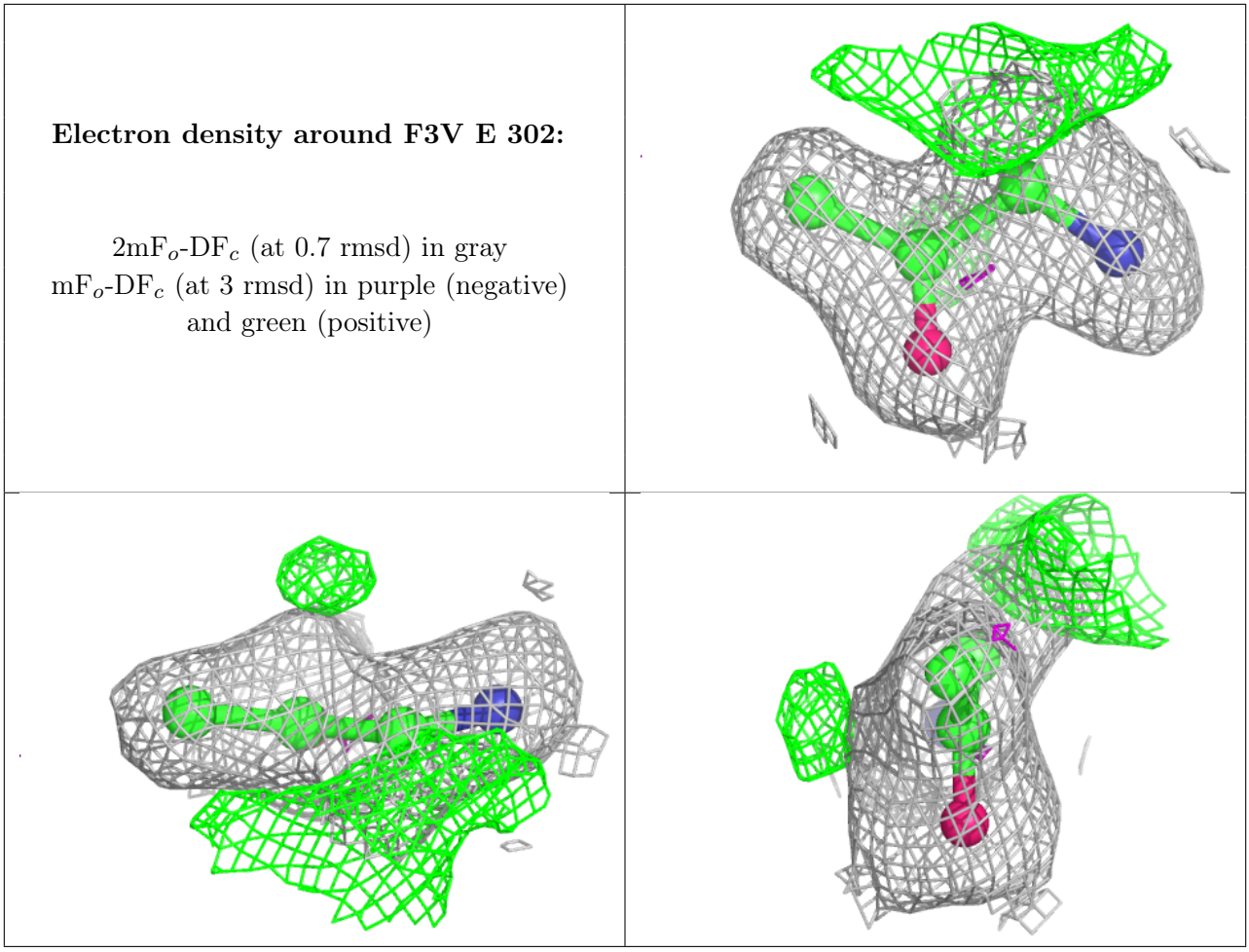






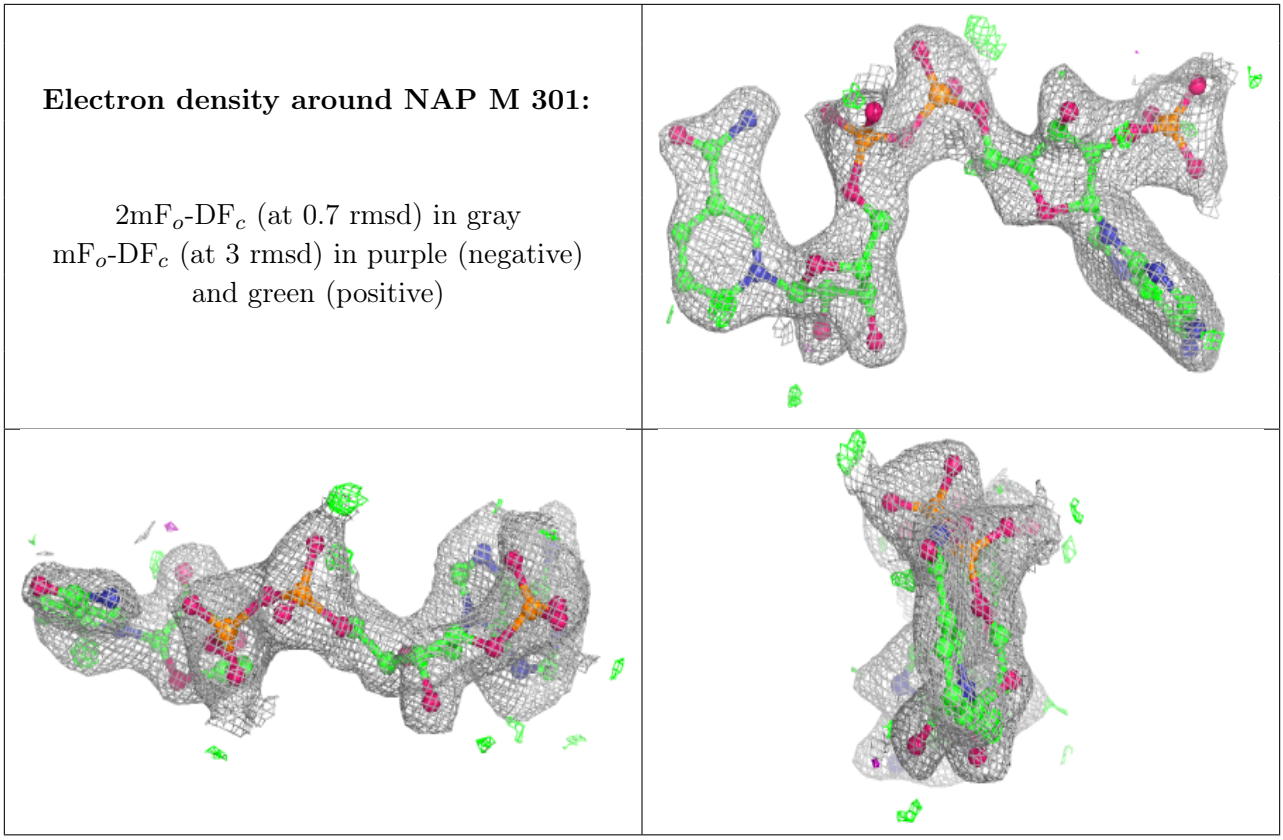
Electron density around F3V E 302:

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



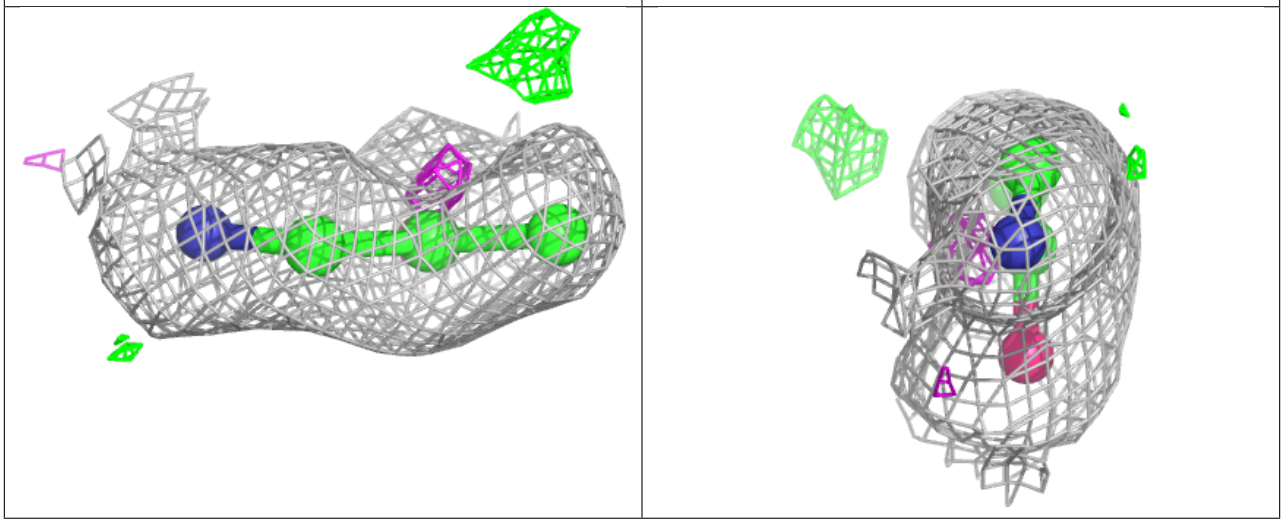
Electron density around NAP M 301:

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



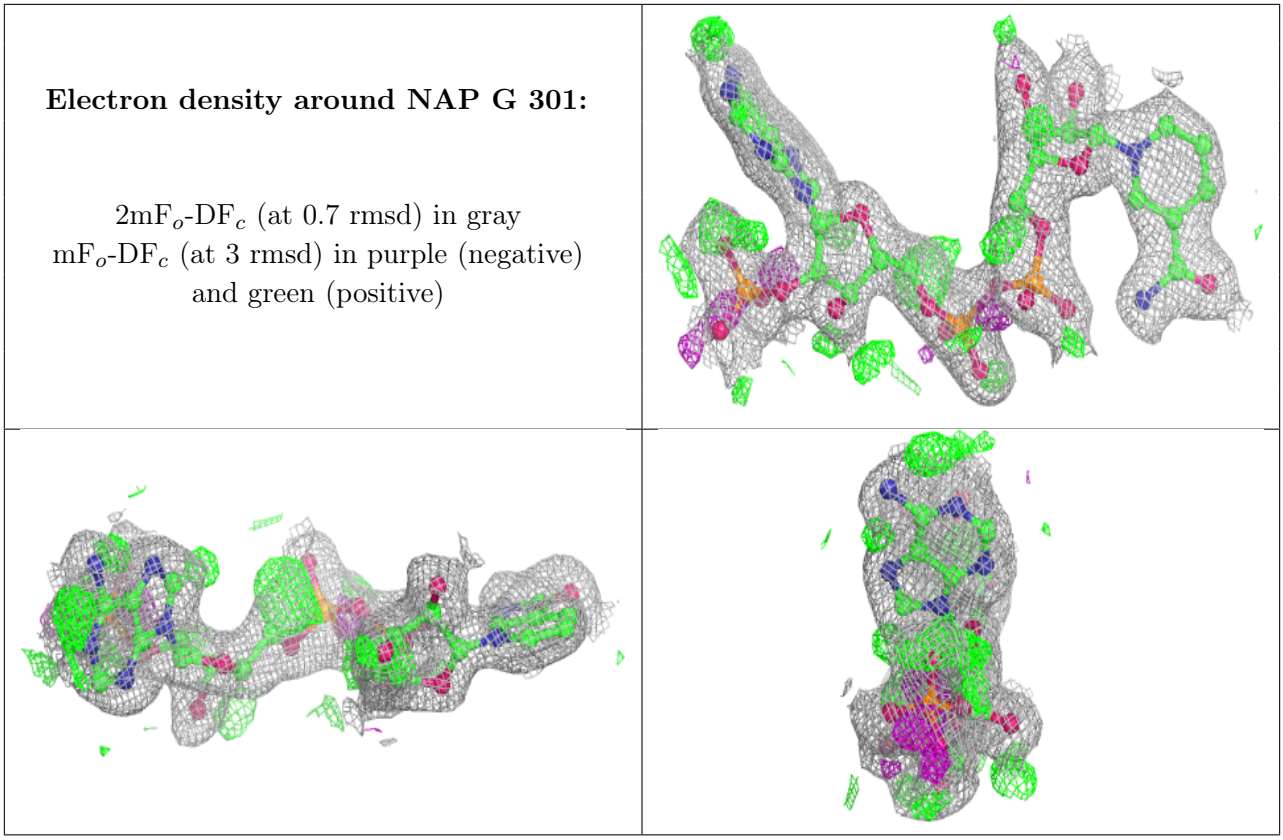
Electron density around F3V G 302:

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



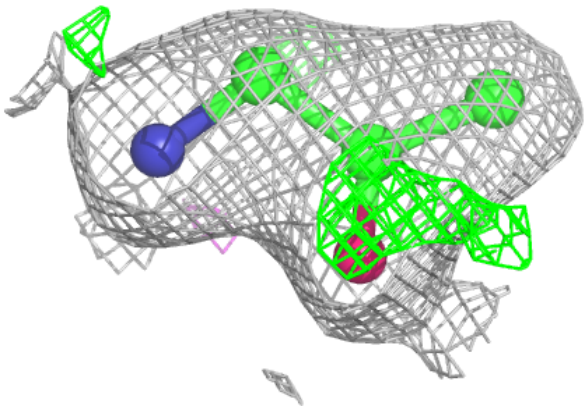
Electron density around NAP G 301:

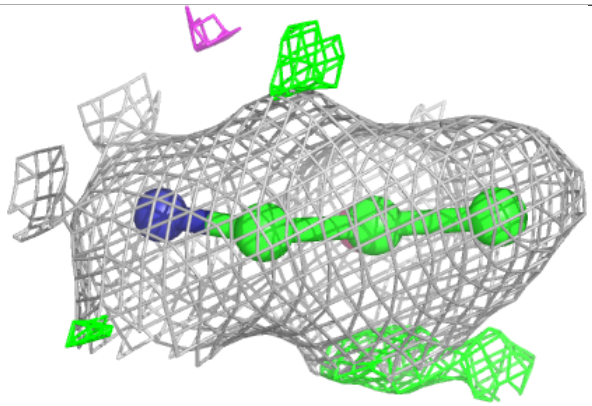
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

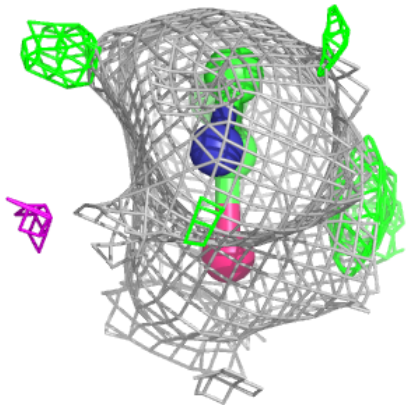


Electron density around F3V I 302:

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

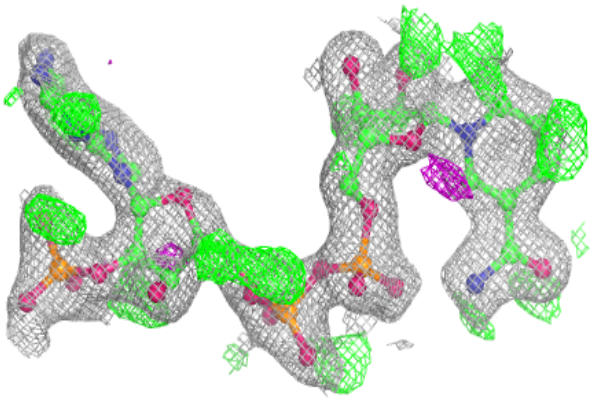


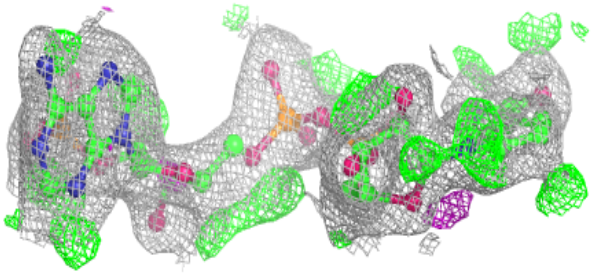


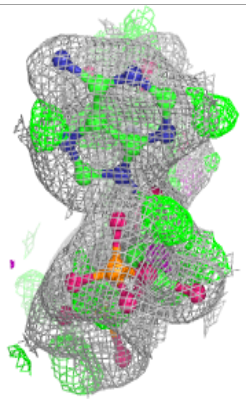


Electron density around NAP B 301:

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

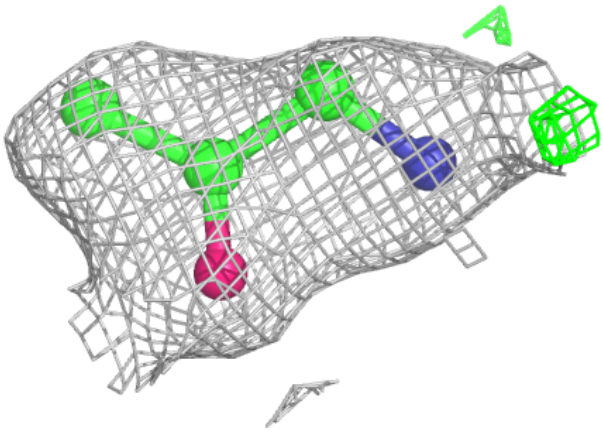


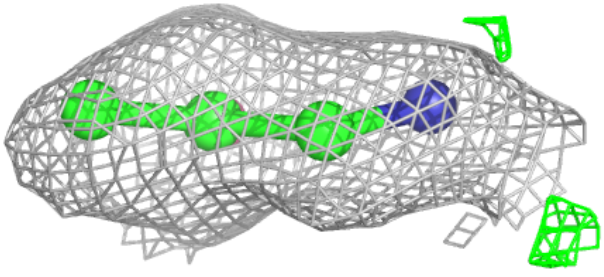


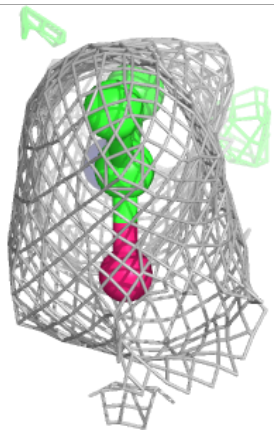


Electron density around F3V P 302:

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

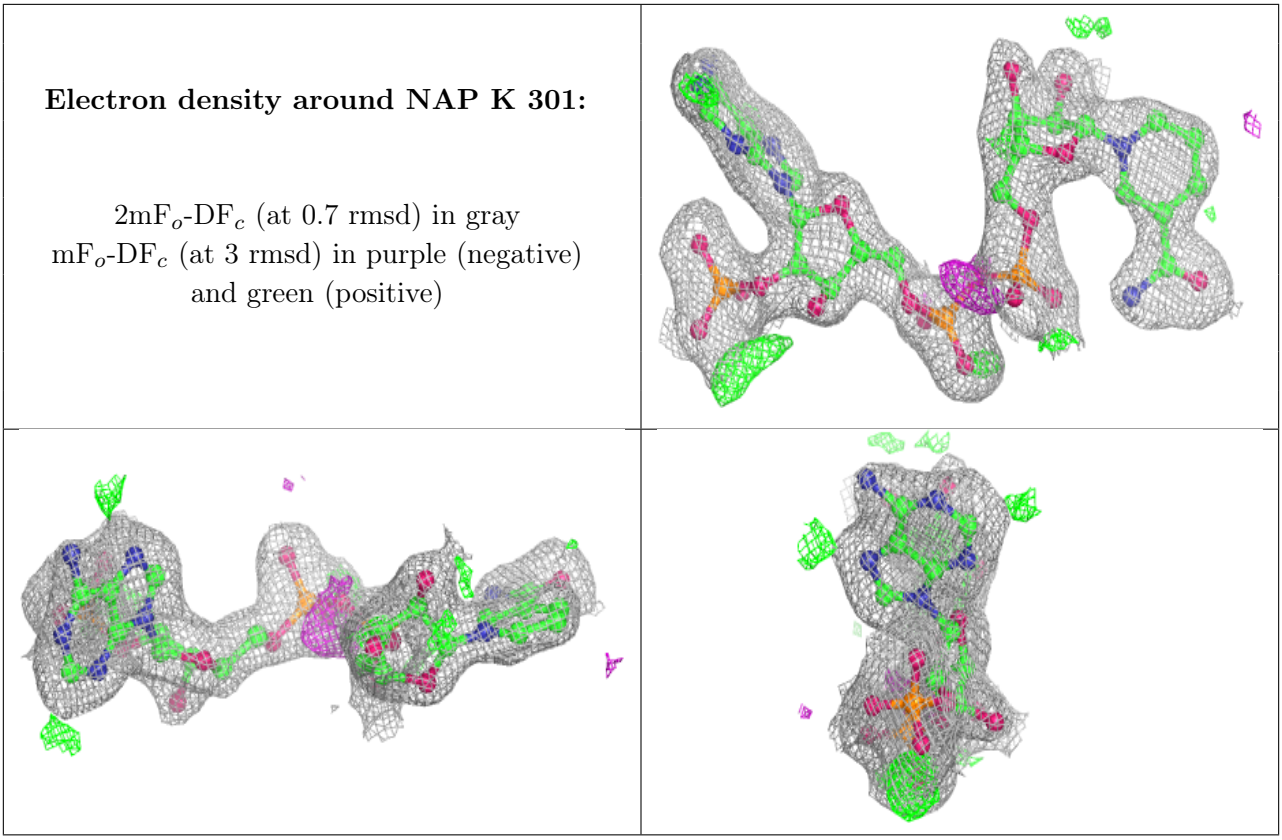






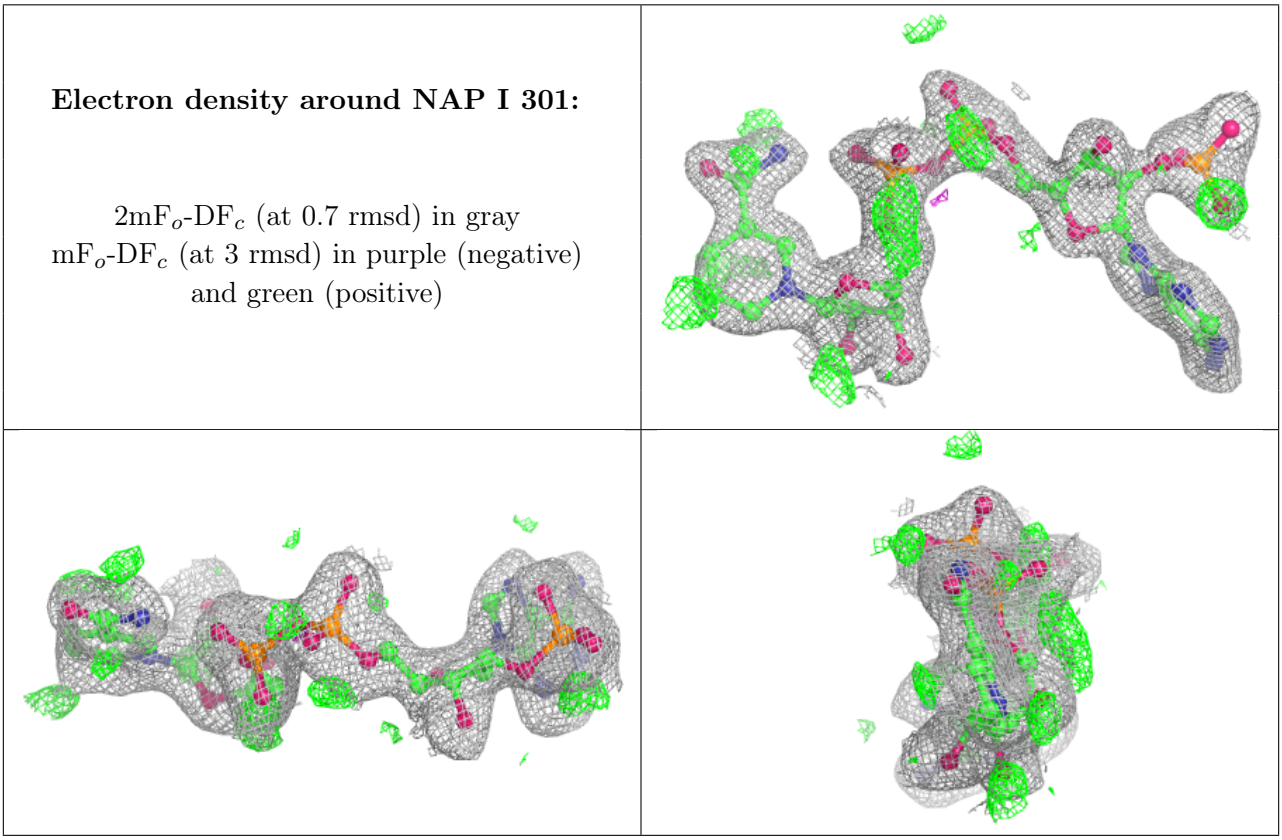
Electron density around NAP K 301:

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



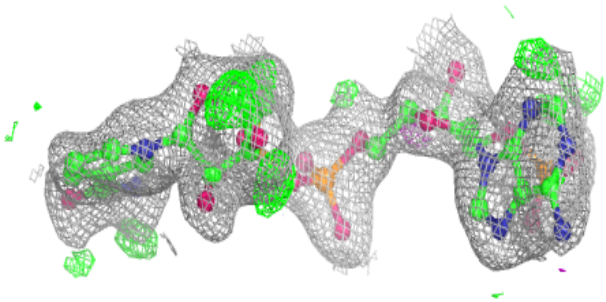
Electron density around NAP I 301:

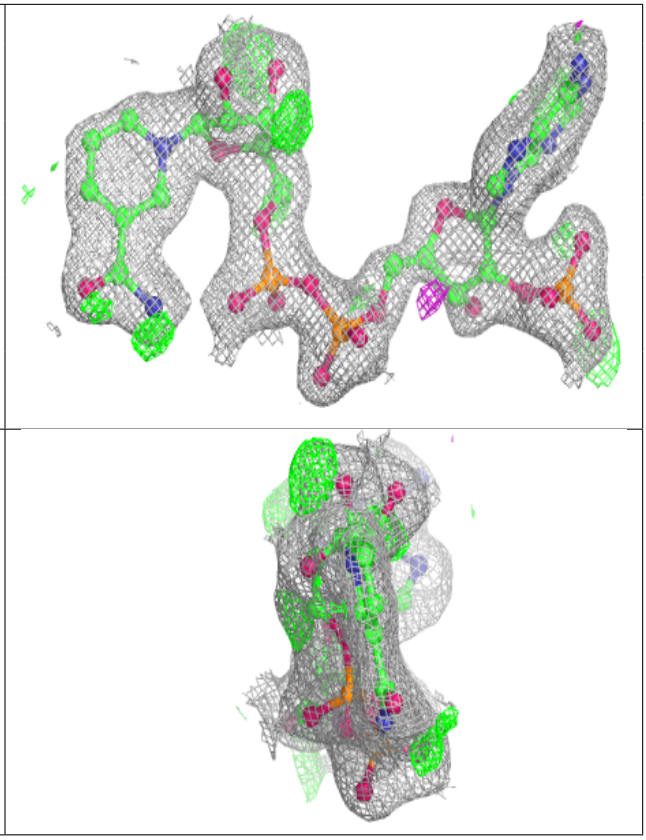
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAP N 301:

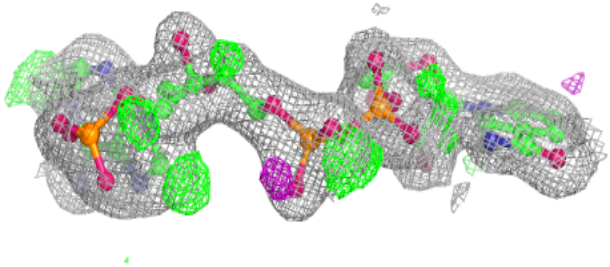
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

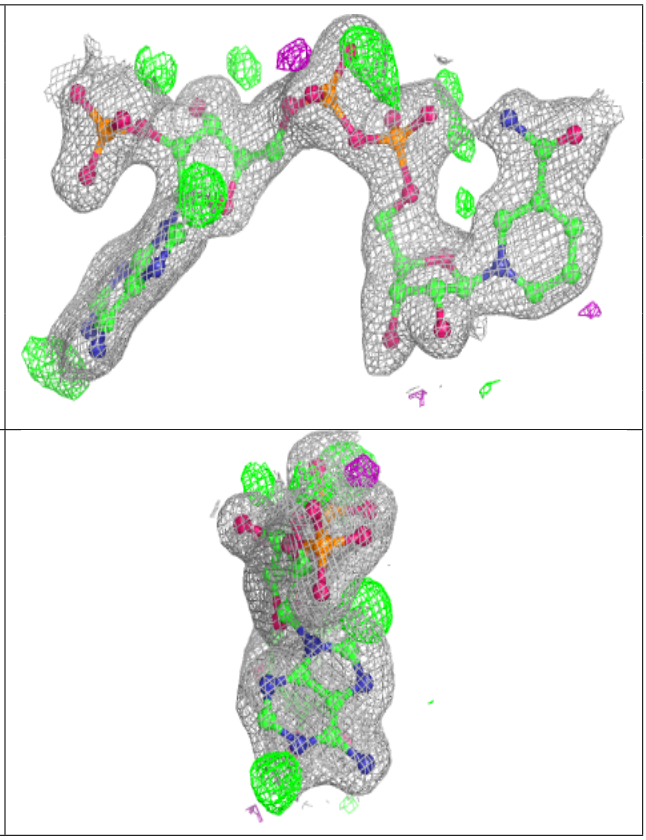




Electron density around NAP P 301:

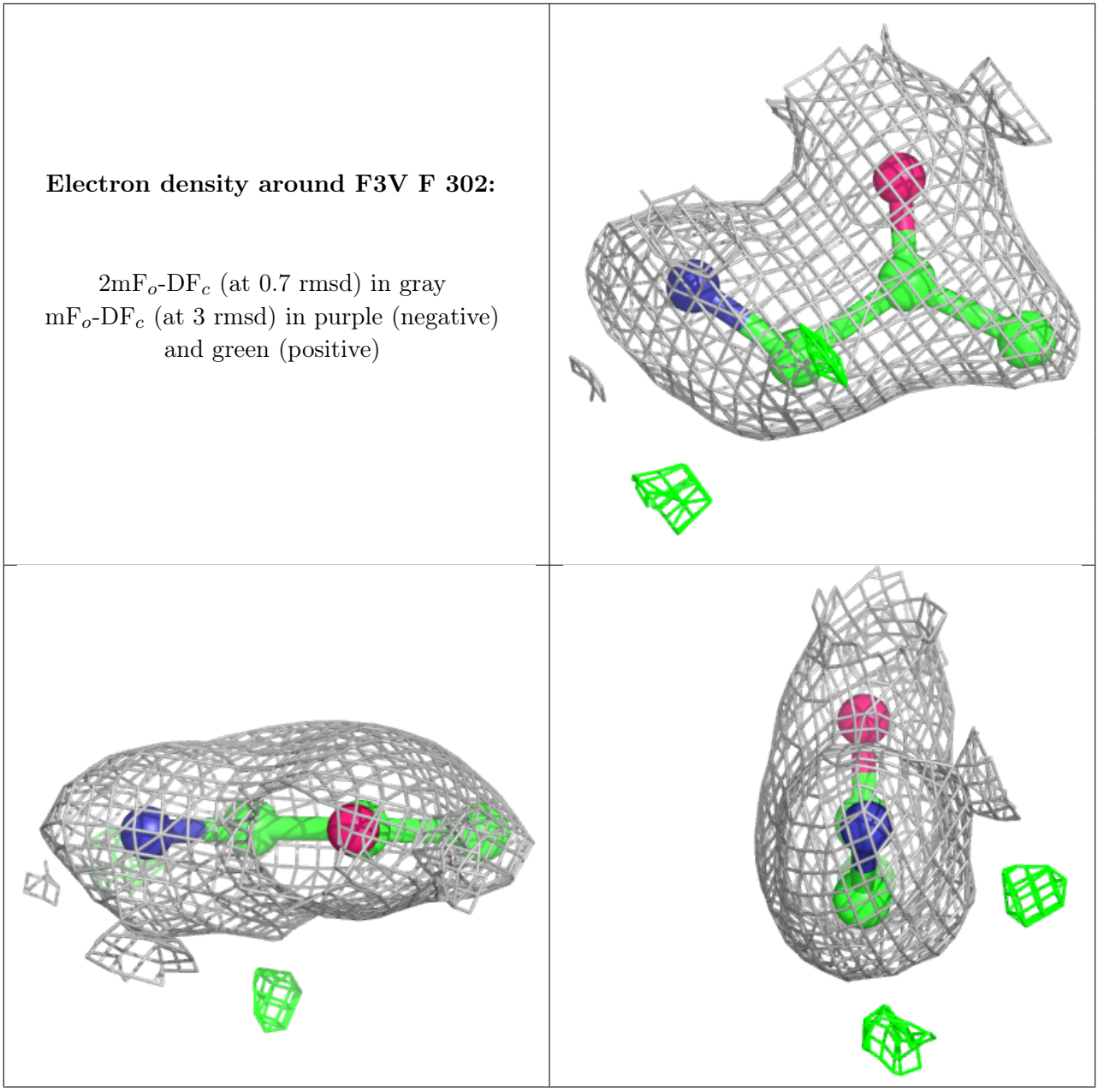
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





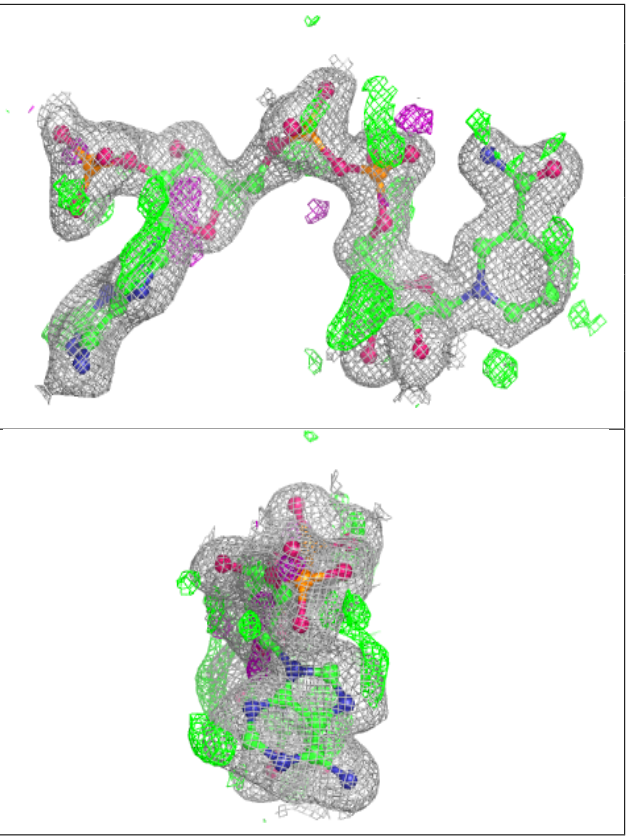
Electron density around F3V F 302:

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



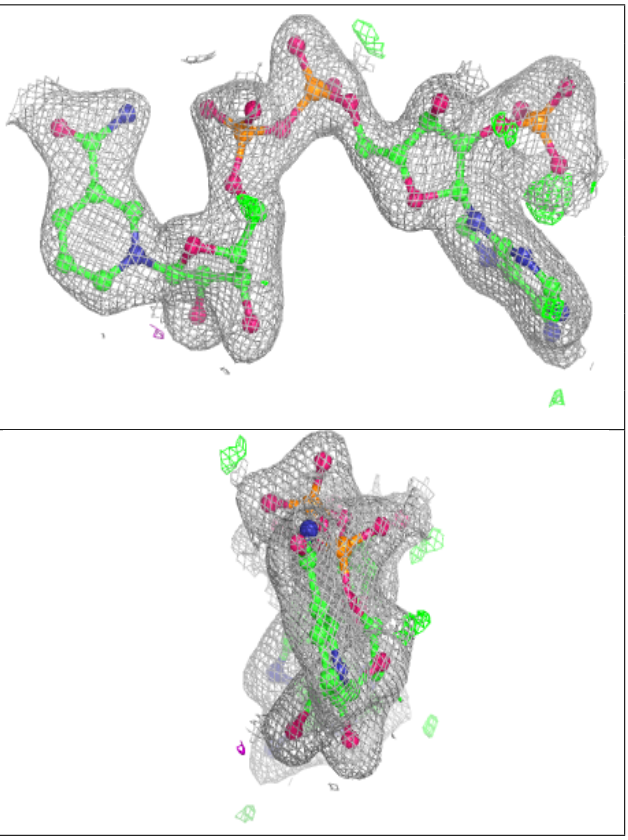
Electron density around NAP E 301:

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



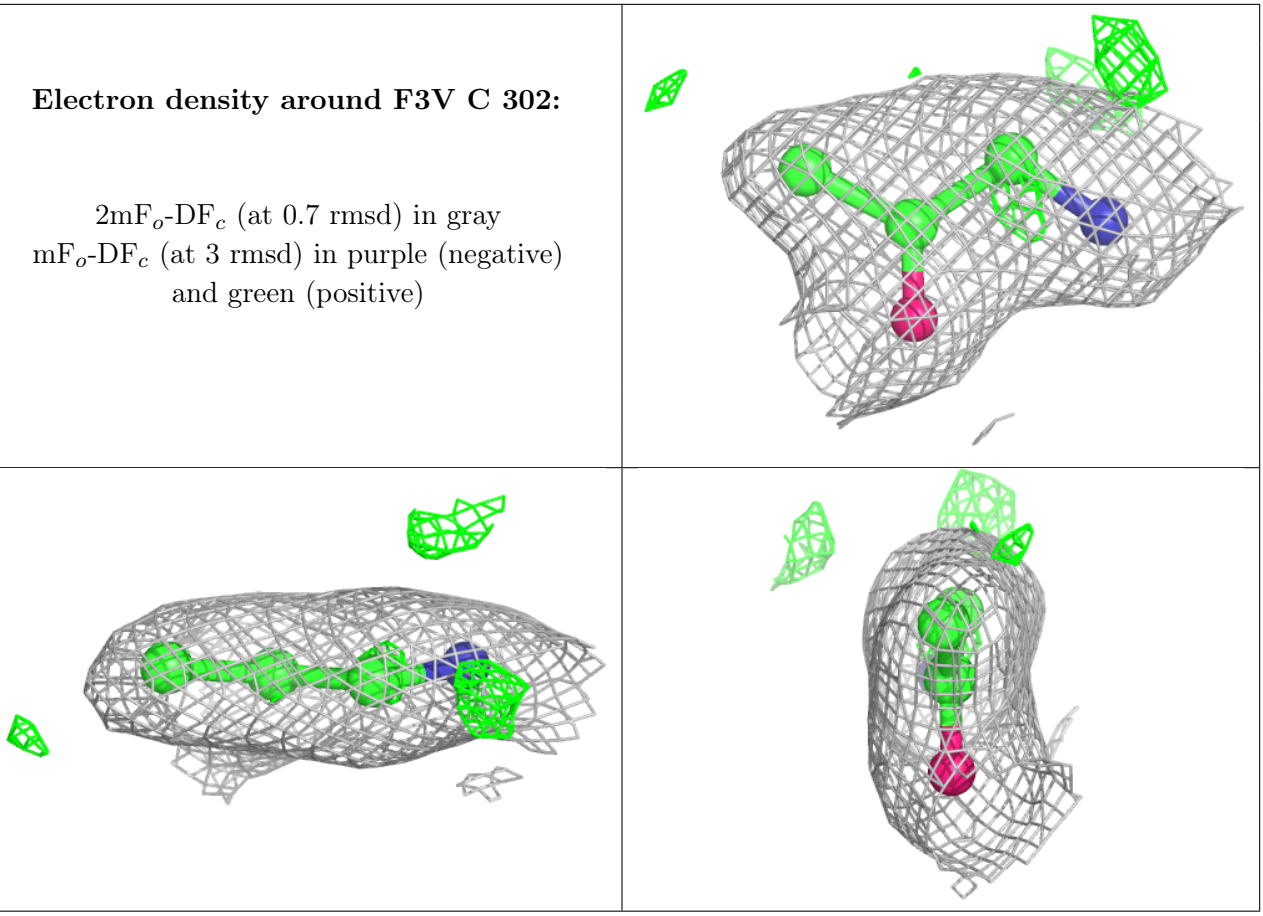
Electron density around NAP L 301:

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



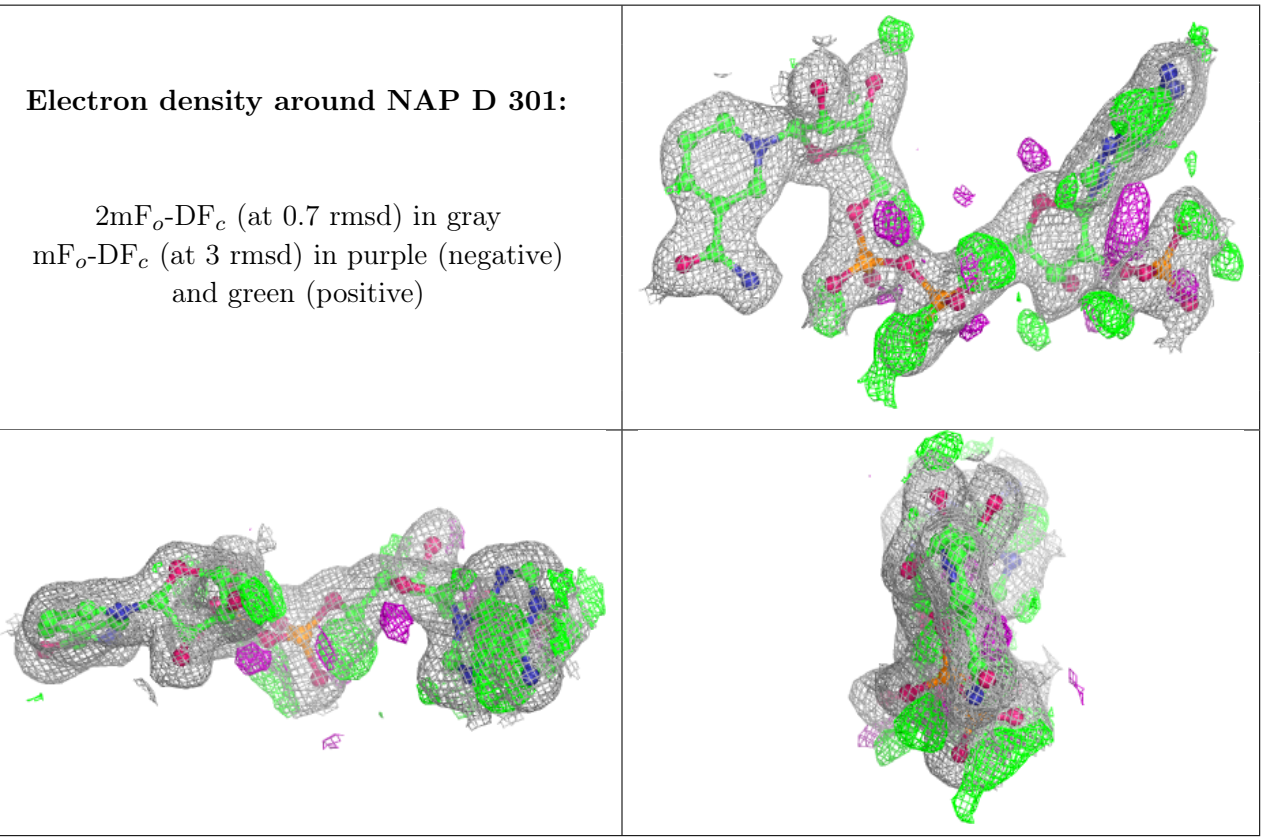
Electron density around F3V C 302:

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



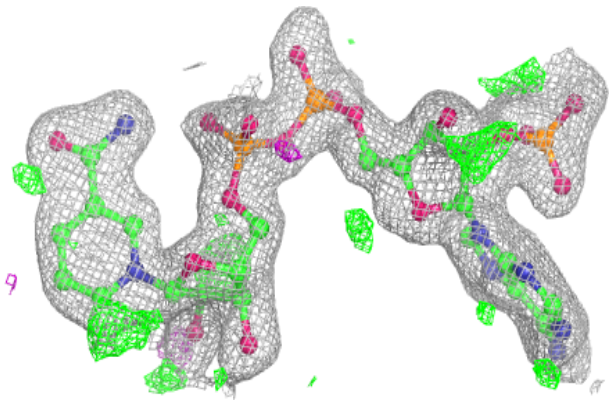
Electron density around NAP D 301:

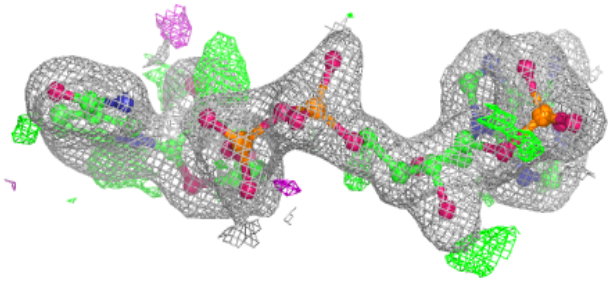
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

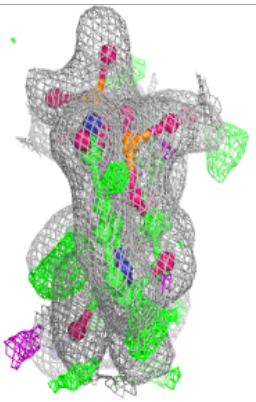


Electron density around NAP A 301:

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

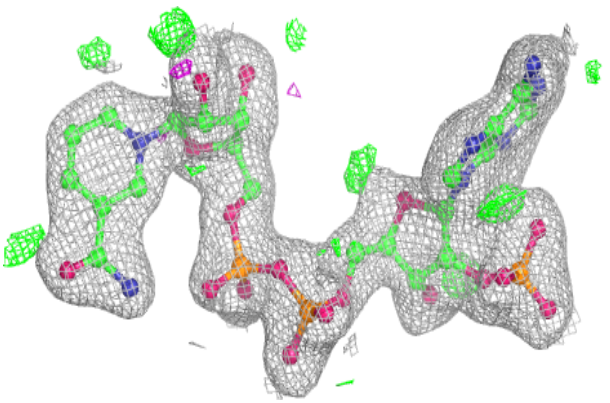


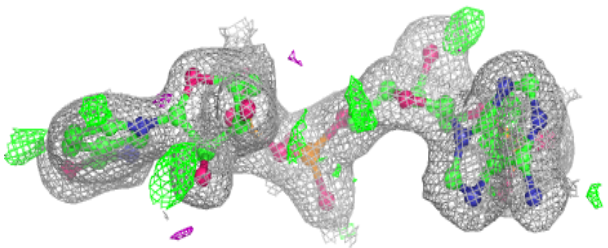


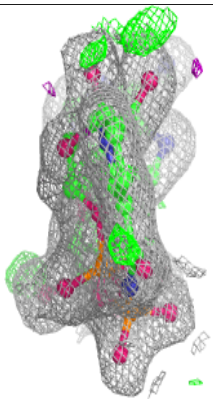


Electron density around NAP F 301:

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

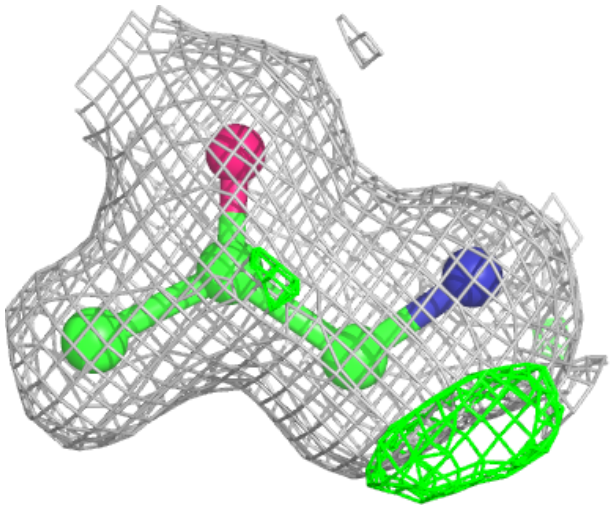


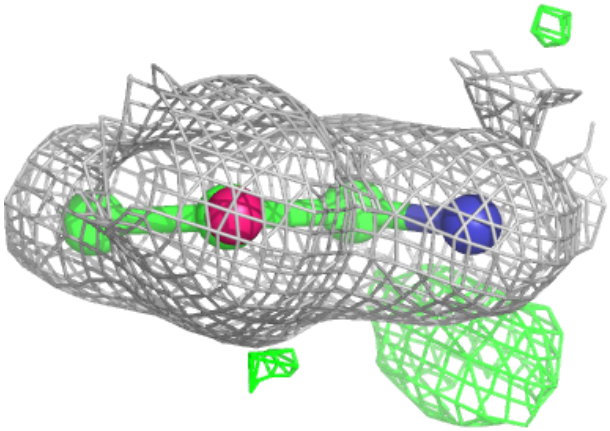


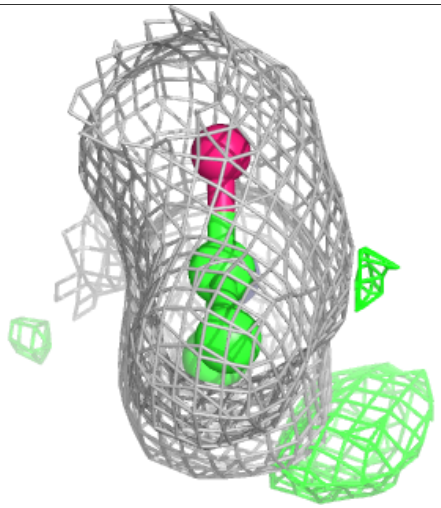


Electron density around F3V D 302:

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

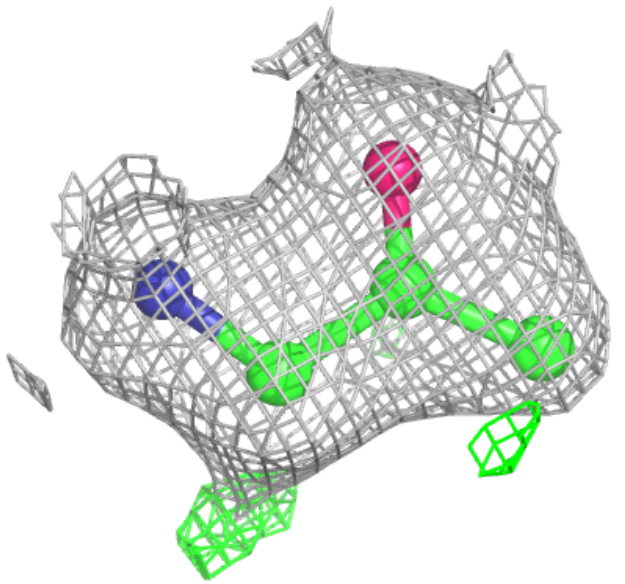


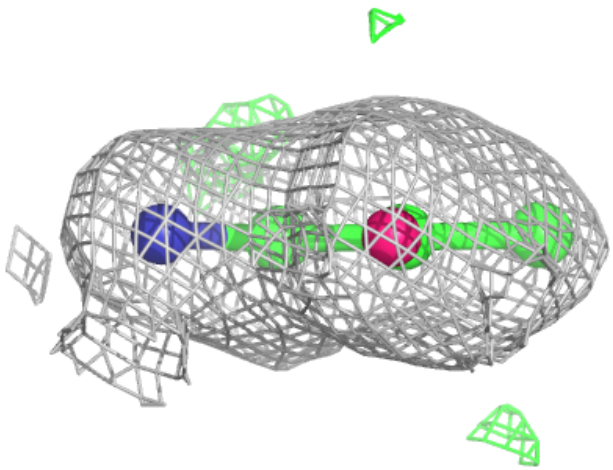


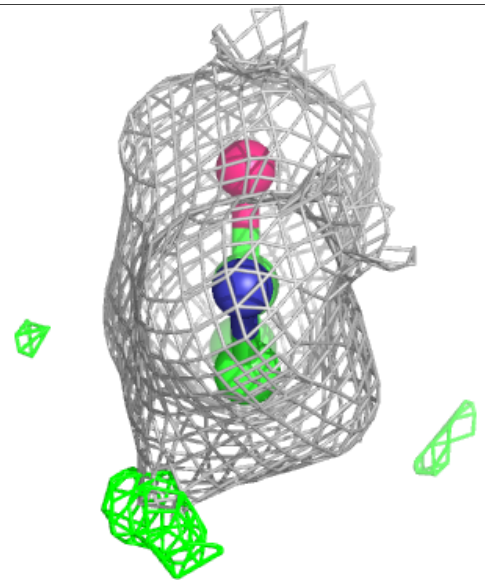


Electron density around F3V K 302:

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

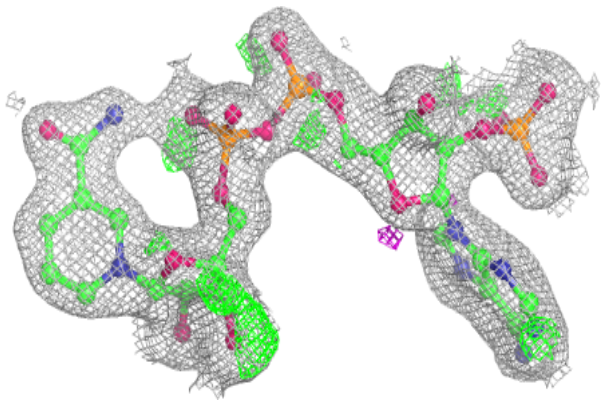


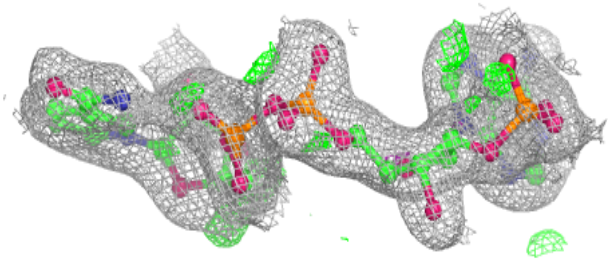


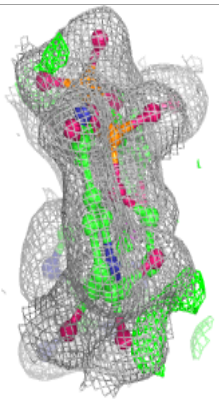


Electron density around NAP J 301:

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

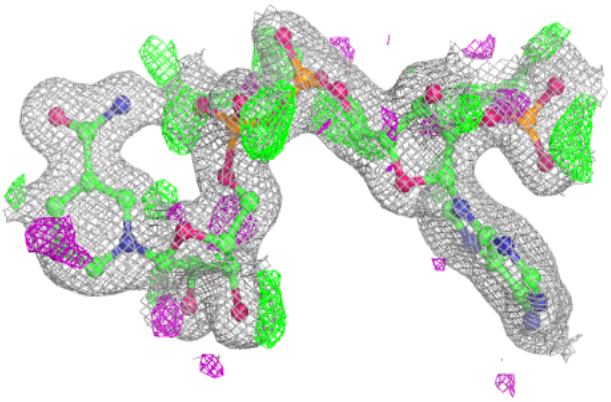


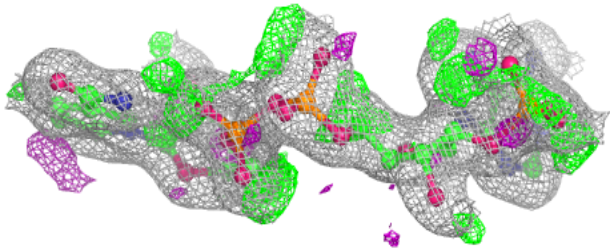


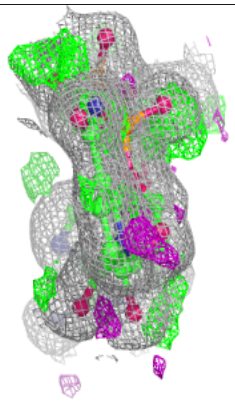


Electron density around NAP H 301:

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

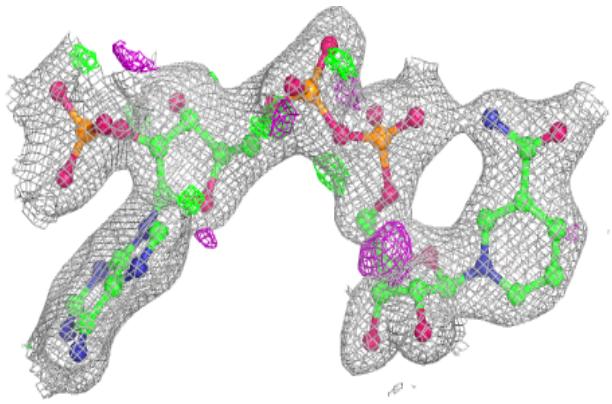


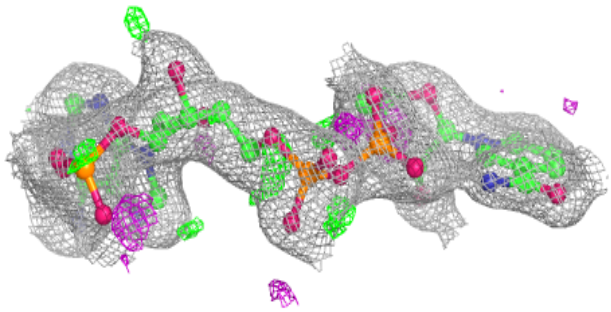


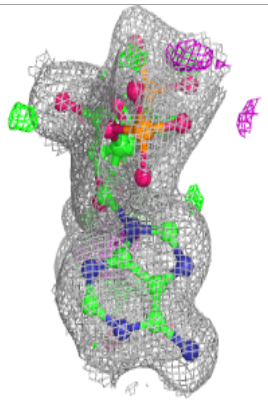


Electron density around NAP O 301:

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

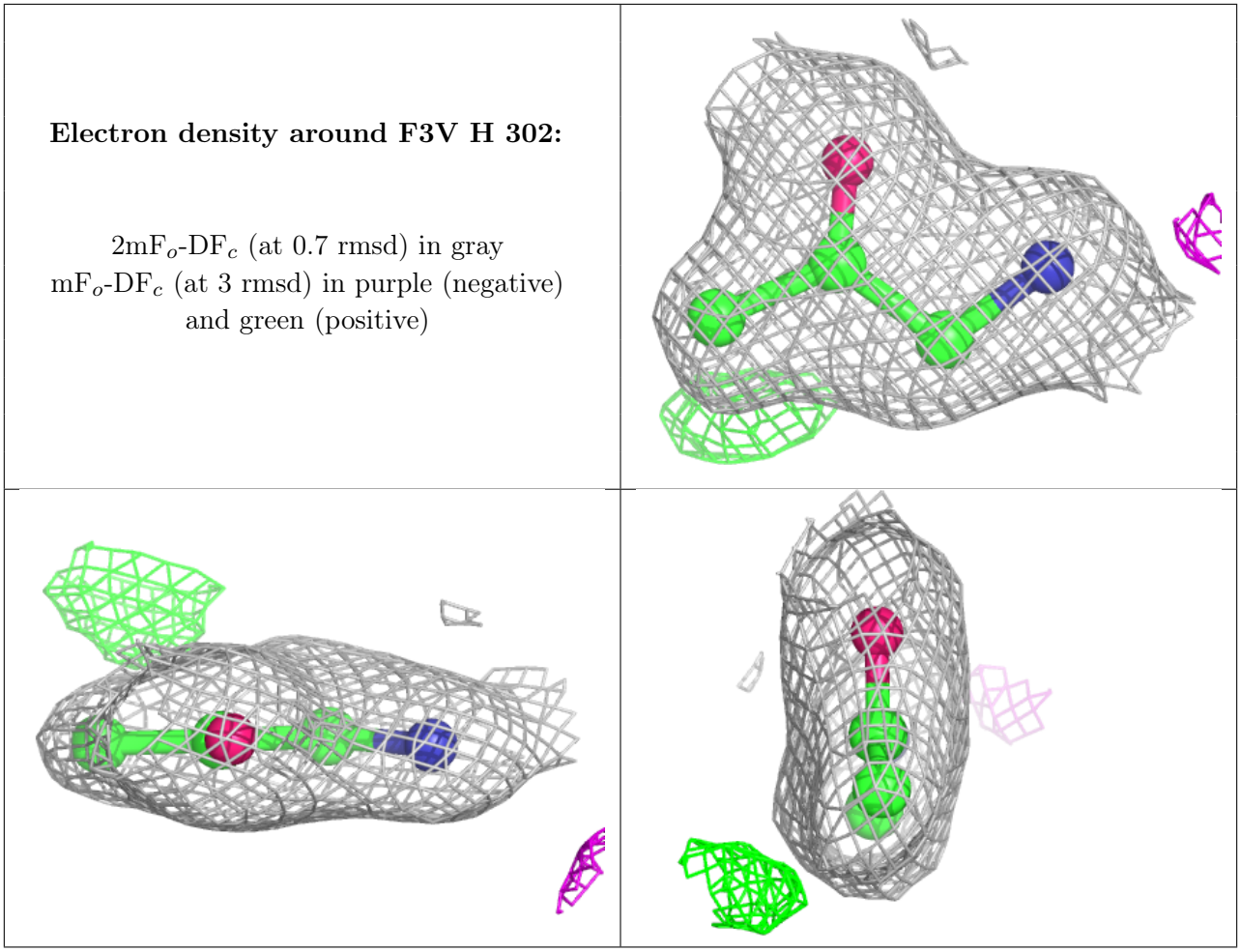






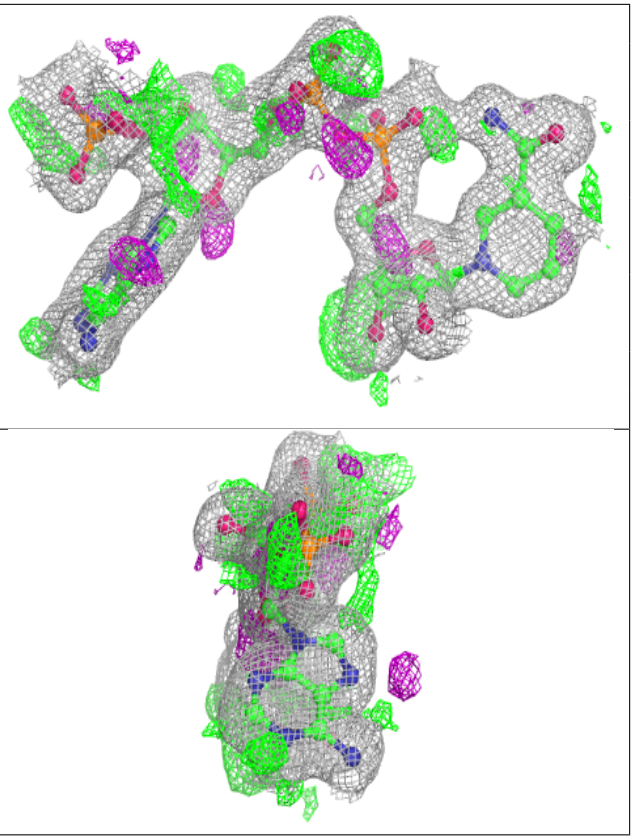
Electron density around F3V H 302:

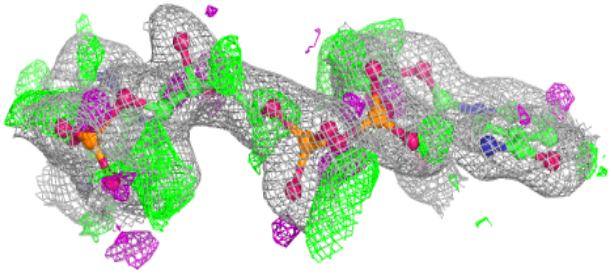
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAP C 301:

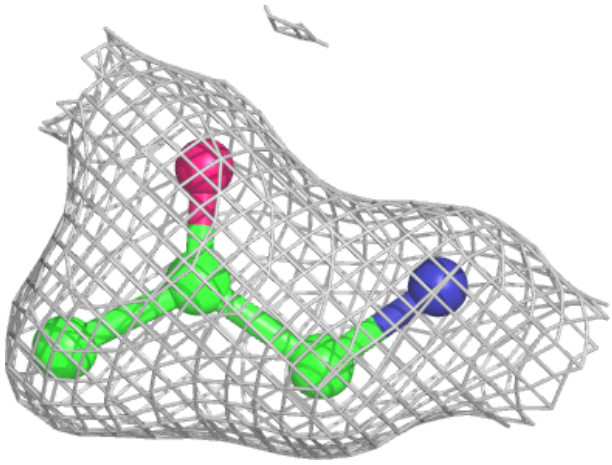
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

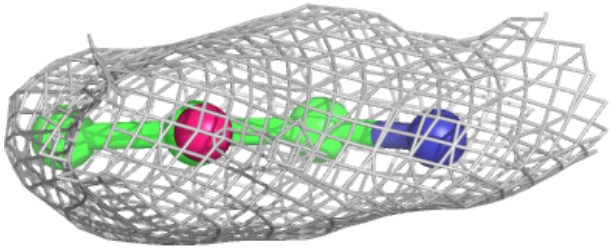


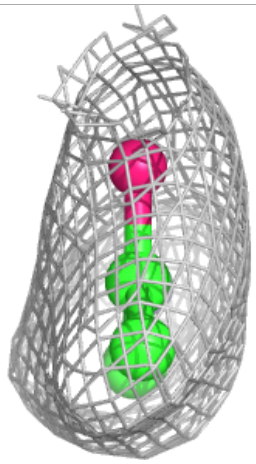


Electron density around F3V J 302:

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

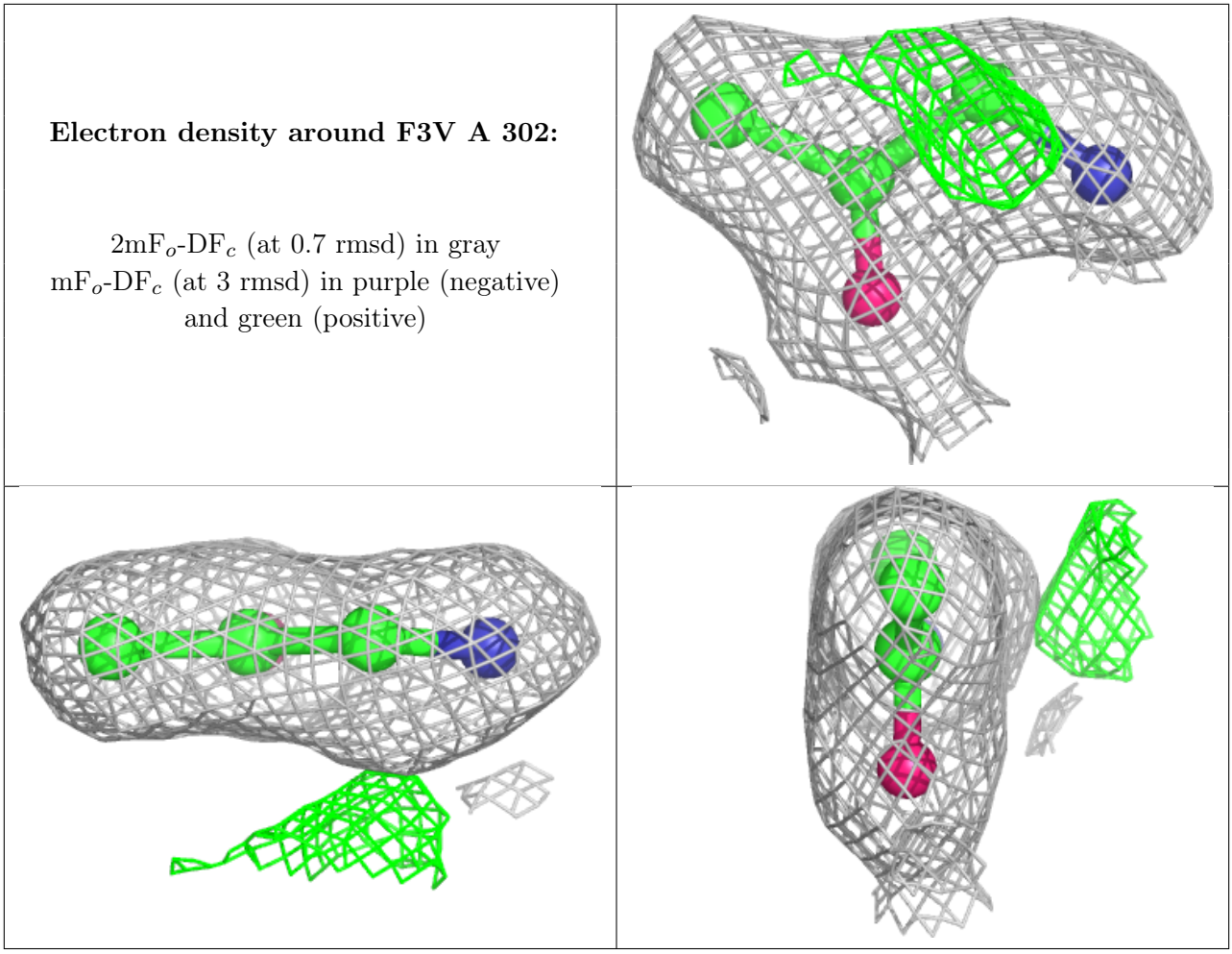






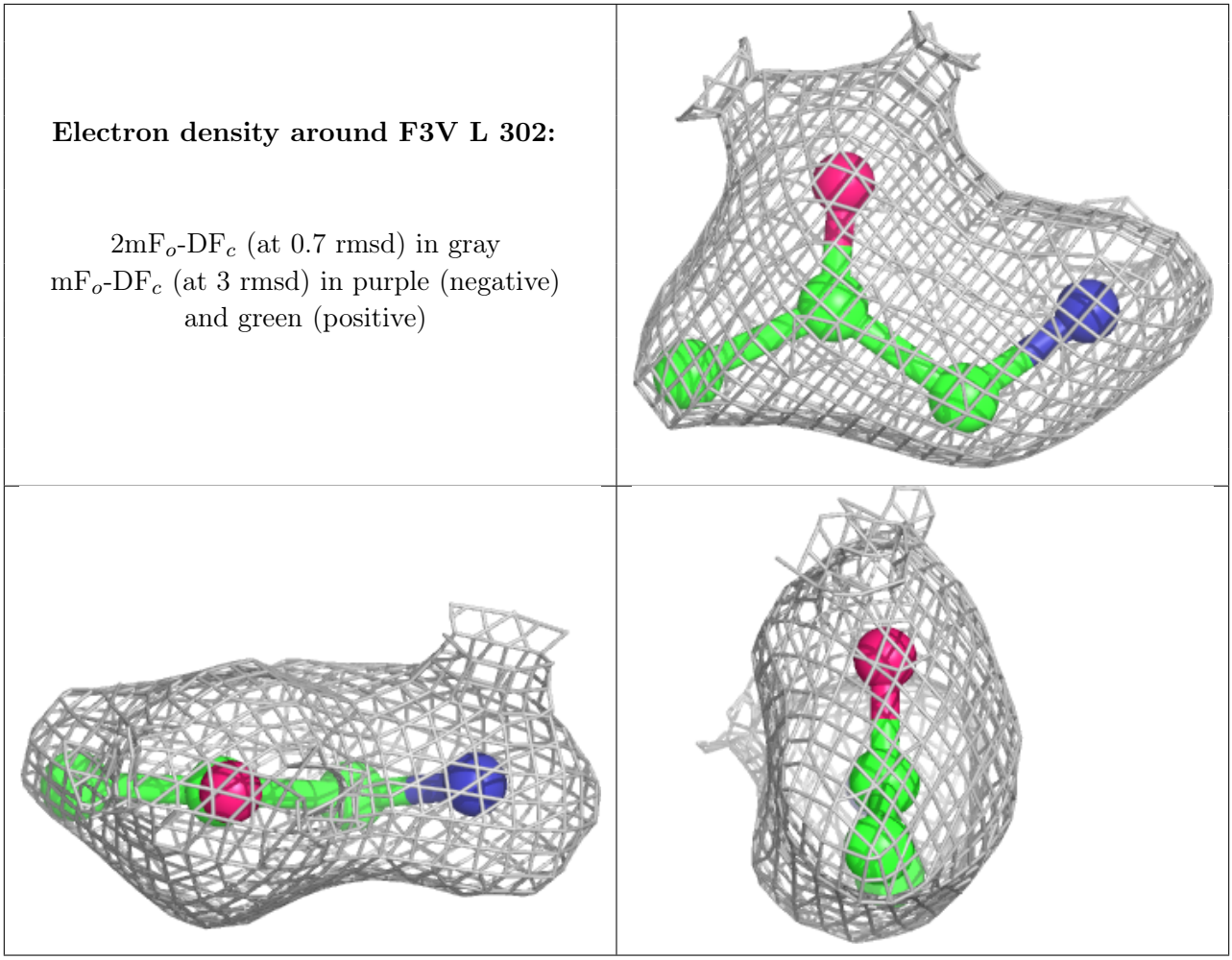
Electron density around F3V A 302:

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



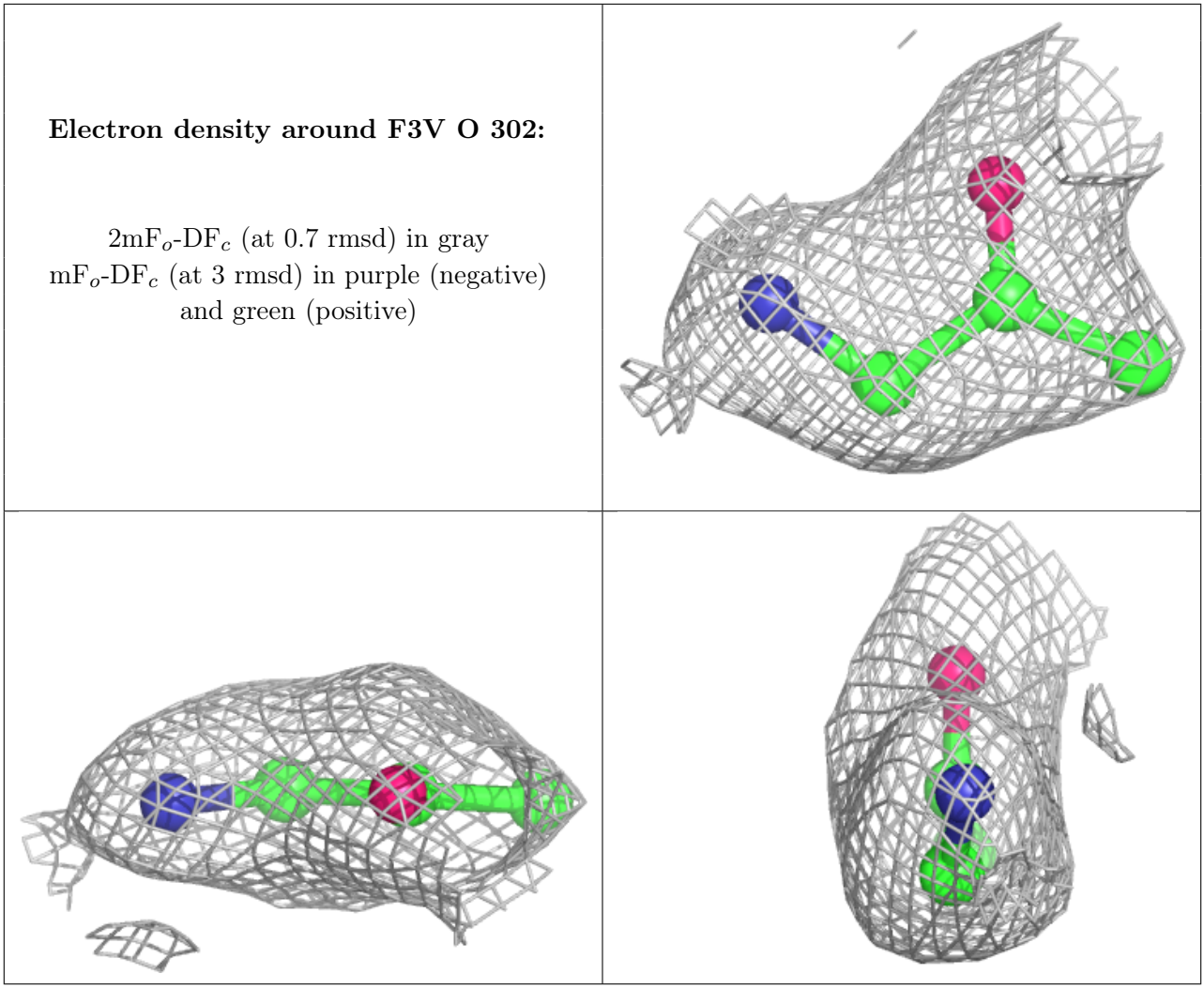
Electron density around F3V L 302:

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



Electron density around F3V O 302:

$2mF_o$-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

There are no such residues in this entry.