wwPDB X-ray Structure Validation Summary Report (i)

Apr 15, 2024 – 04:40 PM EDT

PDB ID	:	8UPP
Title	:	Campylobacter jejuni ketol-acid reductoisomerase in complex with NADPH and Hoe704
Authors	:	Lin, X.; Lv, Y.; Lonhienne, T.; Guddat, L.W.
Deposited on	:	2023-10-23
Resolution	:	1.78 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:

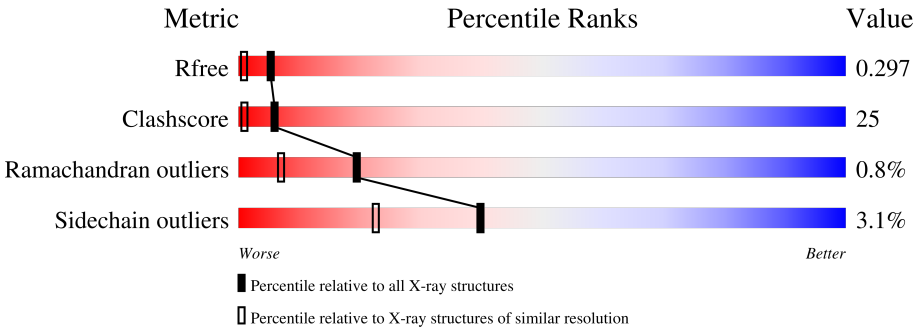
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)

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%

Mol	Chain	Length	Quality of chain
1	A	330	66% 31%
1	B	330	64% 32%
1	C	330	61% 35%
1	D	330	70% 27%
1	E	330	67% 31%
1	F	330	68% 29%
1	G	330	64% 34%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	330	
1	I	330	
1	J	330	
1	K	330	
1	L	330	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32370 atoms, of which 96 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 Ketol-acid reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	H	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	K	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	I	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	D	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	G	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	J	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	E	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	L	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	C	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	F	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0
1	A	327	Total 2495	C 1582	N 424	O 473	S 16	0	1	0

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

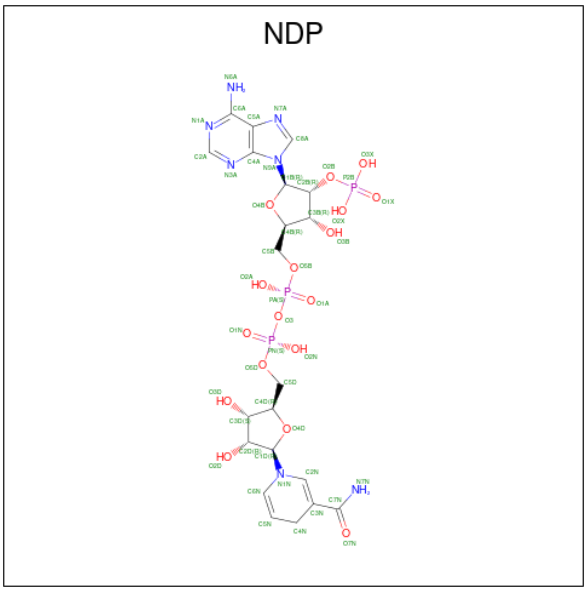
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mg 2	0	0
2	H	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

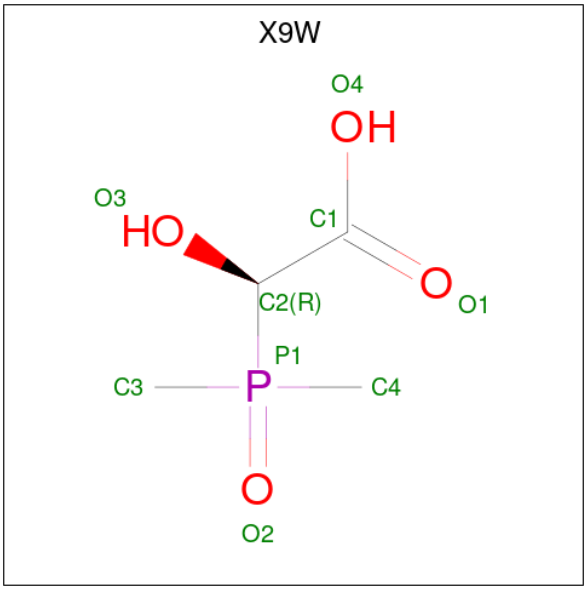
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	2	Total Mg 2 2	0	0
2	I	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	G	2	Total Mg 2 2	0	0
2	J	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	L	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is (2R)-(dimethylphosphoryl)(hydroxy)acetic acid (three-letter code: X9W) (formula: $C_4H_9O_4P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	H	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	H	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	I	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	D	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	G	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	J	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	E	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	L	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	C	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	F	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	A	1	Total	C	H	O	P	0	0
			17	4	8	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	142	Total	O	0	0
			142	142		
5	H	141	Total	O	0	0
			141	141		
5	K	114	Total	O	0	0
			114	114		
5	I	135	Total	O	0	0
			135	135		
5	D	127	Total	O	0	0
			127	127		
5	G	136	Total	O	0	0
			136	136		
5	J	145	Total	O	0	0
			145	145		
5	E	142	Total	O	0	0
			142	142		

Continued on next page...

Continued from previous page...

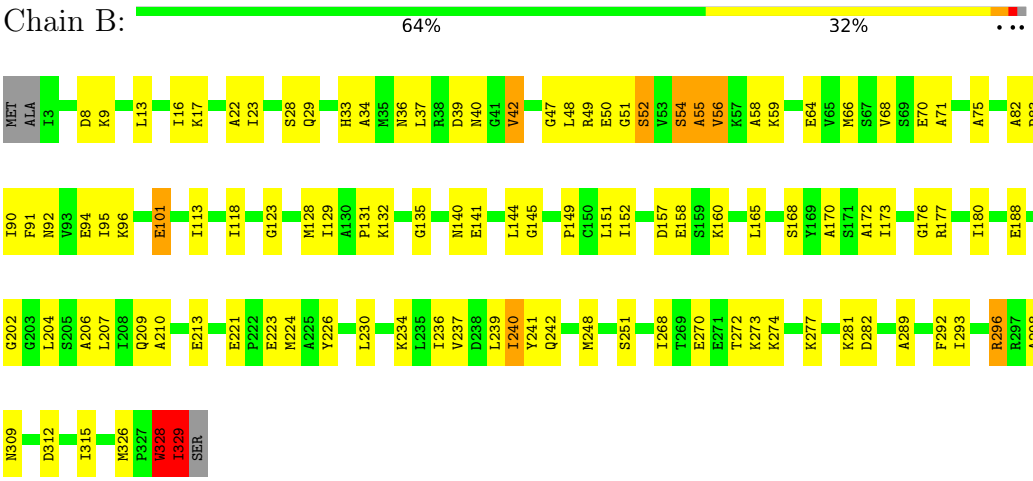
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	123	Total O 123 123	0	0
5	C	124	Total O 124 124	0	0
5	F	146	Total O 146 146	0	0
5	A	151	Total O 151 151	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

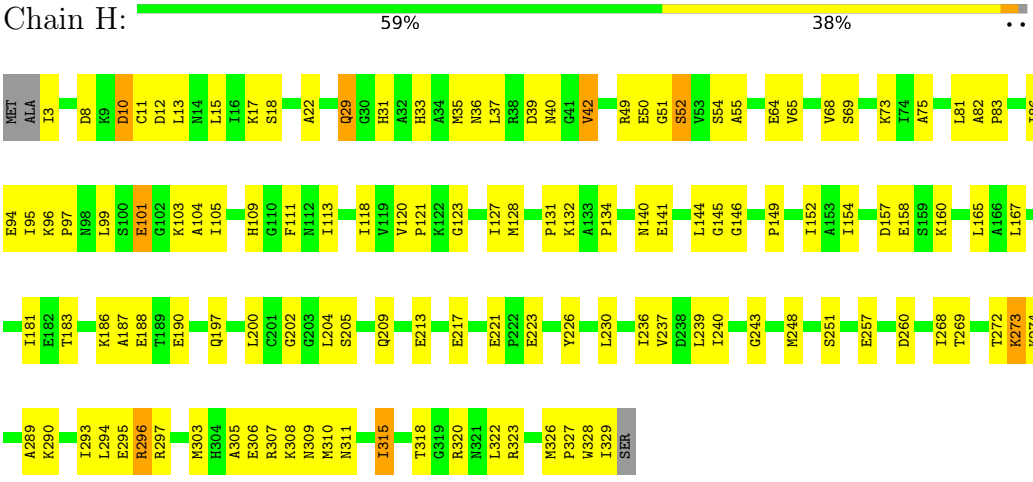
• Molecule 1: Ketol-acid reductoisomerase

Chain B:



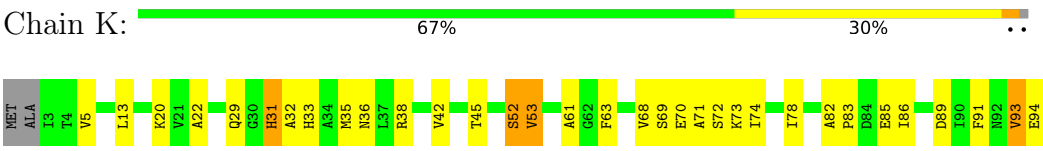
• Molecule 1: Ketol-acid reductoisomerase

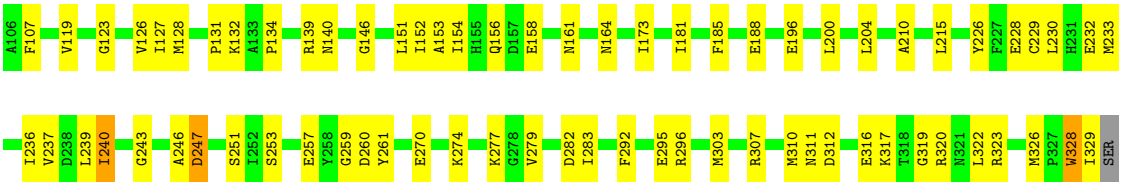
Chain H:



• Molecule 1: Ketol-acid reductoisomerase

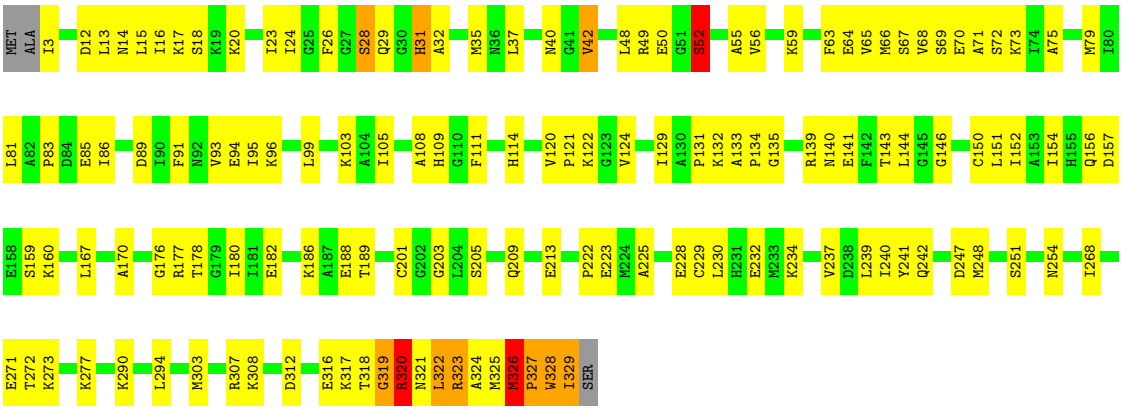
Chain K:





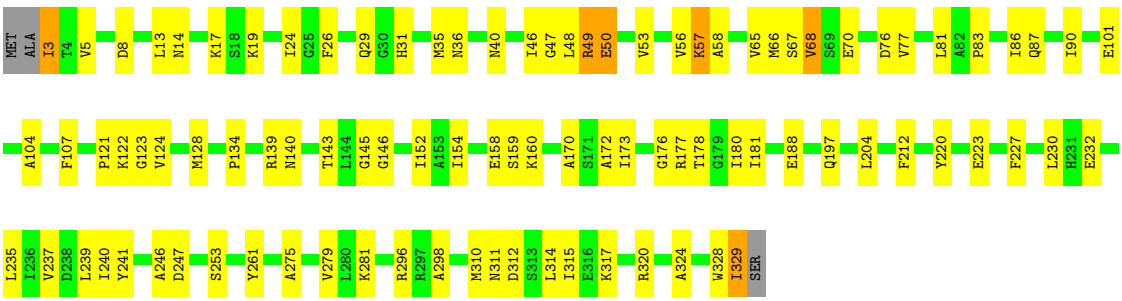
• Molecule 1: Ketol-acid reductoisomerase

Chain I:



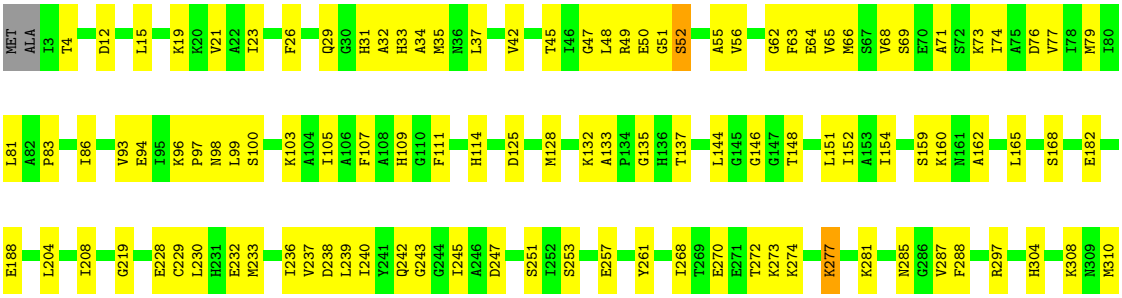
• Molecule 1: Ketol-acid reductoisomerase

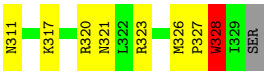
Chain D:



• Molecule 1: Ketol-acid reductoisomerase

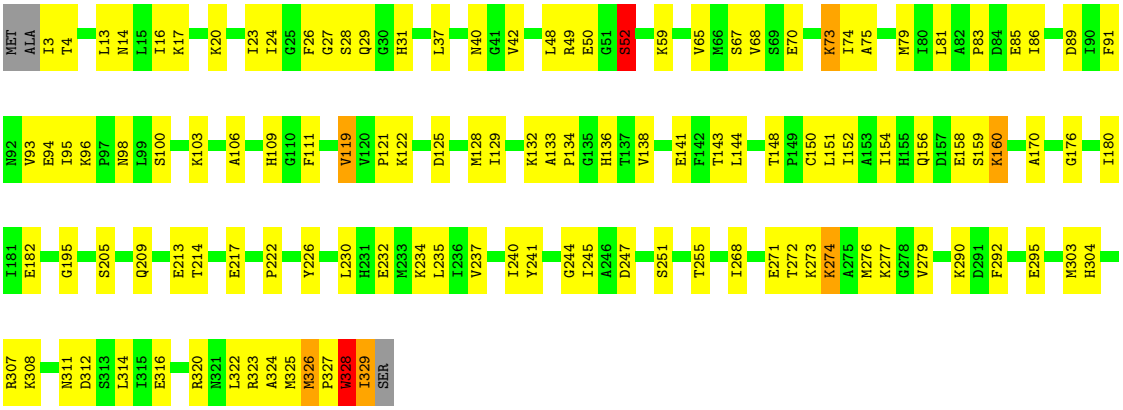
Chain G:





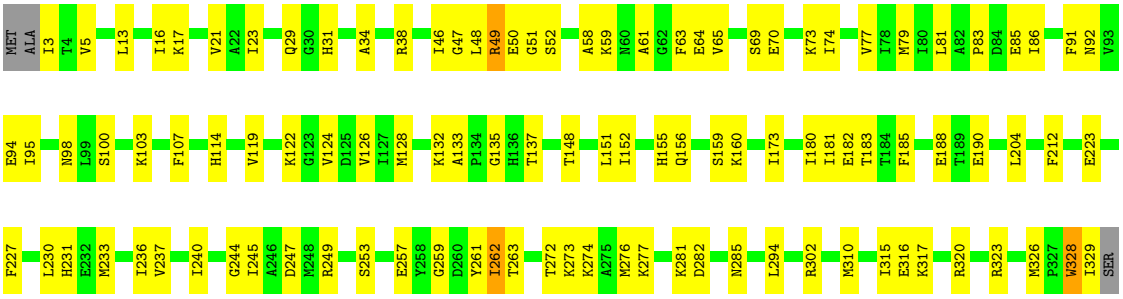
• Molecule 1: Ketol-acid reductoisomerase

Chain J:



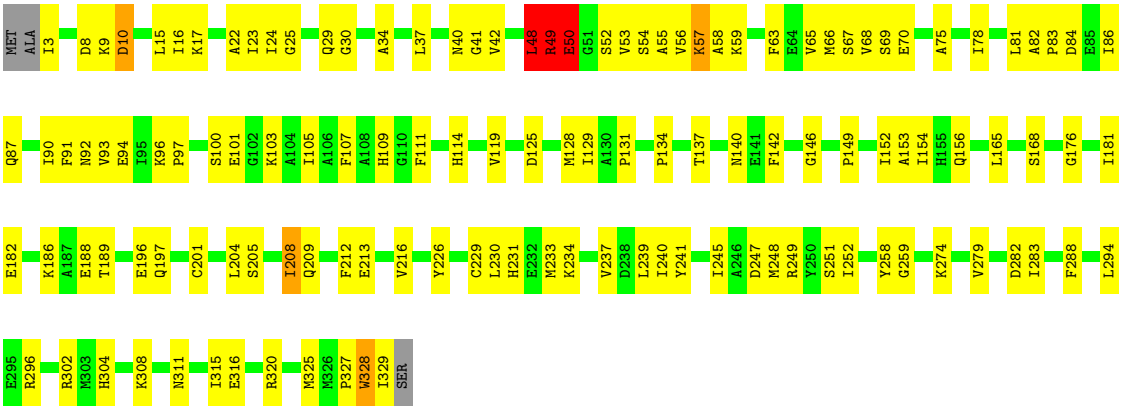
• Molecule 1: Ketol-acid reductoisomerase

Chain E:



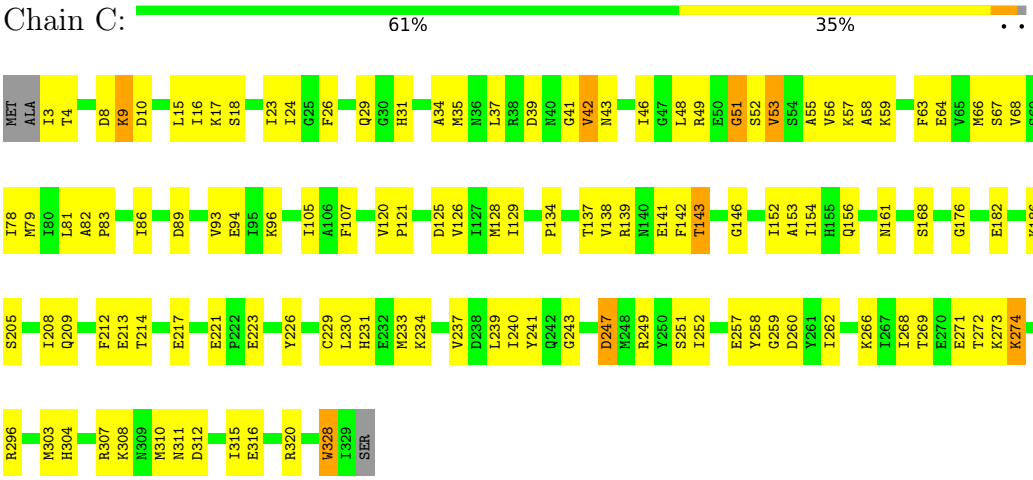
• Molecule 1: Ketol-acid reductoisomerase

Chain L:



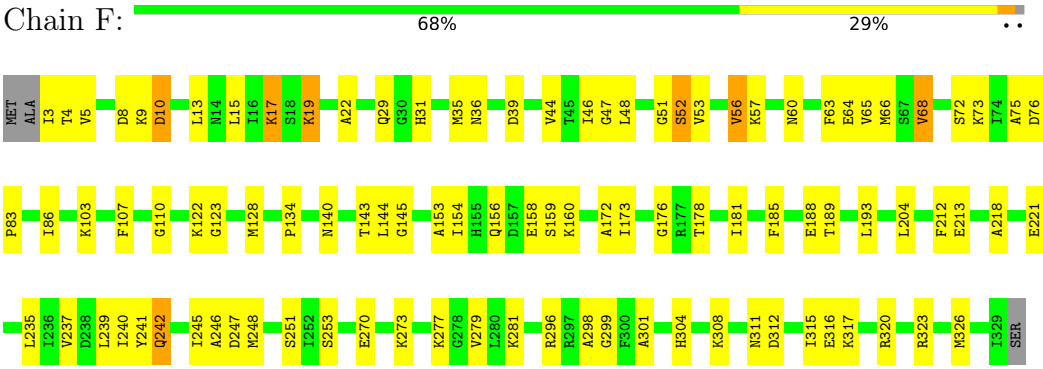
• Molecule 1: Ketol-acid reductoisomerase

Chain C:



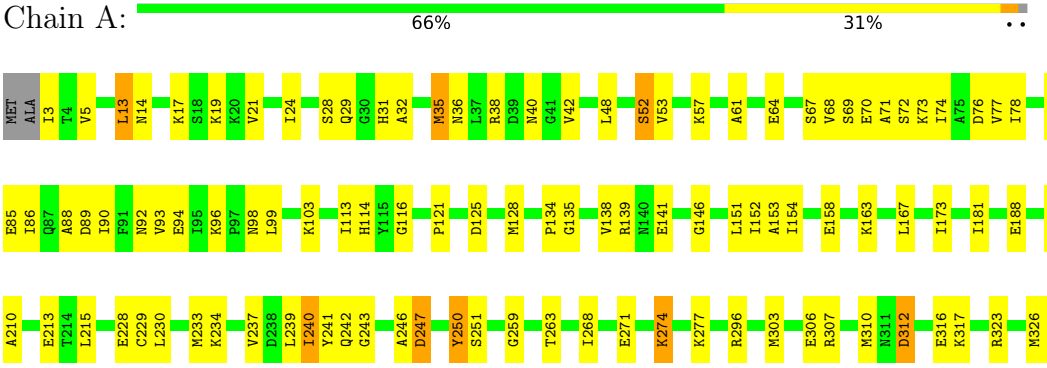
• Molecule 1: Ketol-acid reductoisomerase

Chain F:



• Molecule 1: Ketol-acid reductoisomerase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	111.95Å 111.95Å 111.94Å 110.91° 107.73° 109.76°	Depositor
Resolution (Å)	34.35 – 1.78 34.35 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.3 (34.35-1.78) 93.2 (34.35-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.264 , 0.298 0.264 , 0.297	Depositor DCC
R_{free} test set	1907 reflections (0.51%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 27.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage

Continued on next page...

[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.

Continued from previous page...

Property	Value	Source
Estimated twinning fraction	0.096 for -k,h+k+l,-h 0.096 for -l,-h,h+k+l 0.097 for -k,-l,h+k+l 0.097 for h+k+l,-h,-k 0.089 for h+k+l,-l,-h 0.089 for -l,h+k+l,-k 0.109 for -h-k-l,h,l 0.109 for k,-h-k-l,l 0.108 for l,k,-h-k-l 0.108 for -h-k-l,k,h 0.108 for h,-h-k-l,k 0.108 for h,l,-h-k-l 0.108 for l,h,k 0.108 for k,l,h 0.457 for -h-k-l,l,k 0.096 for -h,-l,-k 0.468 for l,-h-k-l,h 0.097 for -l,-k,-h 0.457 for k,h,-h-k-l 0.089 for -k,-h,-l 0.096 for h+k+l,-k,-l 0.098 for -h,h+k+l,-l 0.090 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32370	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, X9W, NDP

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	0/2539	0.61	0/3422
1	B	0.44	0/2539	0.63	1/3422 (0.0%)
1	C	0.43	0/2539	0.58	0/3422
1	D	0.46	0/2539	0.60	0/3422
1	E	0.45	0/2539	0.61	0/3422
1	F	0.48	0/2539	0.62	0/3422
1	G	0.44	0/2539	0.60	0/3422
1	H	0.43	0/2539	0.62	0/3422
1	I	0.43	0/2539	0.60	0/3422
1	J	0.45	0/2539	0.61	0/3422
1	K	0.43	0/2539	0.61	0/3422
1	L	0.43	0/2539	0.61	1/3422 (0.0%)
All	All	0.44	0/30468	0.61	2/41064 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	I	0	1
1	J	0	1
1	L	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	329	ILE	N-CA-C	-6.30	93.98	111.00
1	L	48	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	328	TRP	Peptide
1	I	326	MET	Peptide
1	J	50	GLU	Peptide
1	L	49	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2495	0	2516	125	0
1	B	2495	0	2516	139	0
1	C	2495	0	2516	120	0
1	D	2495	0	2516	137	0
1	E	2495	0	2516	125	0
1	F	2495	0	2516	123	0
1	G	2495	0	2516	138	0
1	H	2495	0	2516	139	1
1	I	2495	0	2516	190	0
1	J	2495	0	2516	155	1
1	K	2495	0	2516	117	0
1	L	2495	0	2516	137	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	48	0	26	9	0
3	B	48	0	26	7	0
3	C	48	0	26	7	0
3	D	48	0	26	10	0
3	E	48	0	26	7	0
3	F	48	0	26	4	0
3	G	48	0	26	5	0
3	H	48	0	26	12	0
3	I	48	0	26	9	0
3	J	48	0	26	7	0
3	K	48	0	26	7	0
3	L	48	0	26	7	0
4	A	9	8	0	0	0
4	B	9	8	0	0	0
4	C	9	8	0	0	0
4	D	9	8	0	1	0
4	E	9	8	0	0	0
4	F	9	8	0	1	0
4	G	9	8	0	1	0
4	H	18	16	0	1	0
4	I	9	8	0	1	0
4	J	9	8	0	1	0
4	L	9	8	0	0	0
5	A	151	0	0	21	0
5	B	142	0	0	30	0
5	C	124	0	0	18	0
5	D	127	0	0	24	0
5	E	142	0	0	19	0
5	F	146	0	0	26	1
5	G	136	0	0	16	0
5	H	141	0	0	24	0
5	I	135	0	0	28	0
5	J	145	0	0	25	1
5	K	114	0	0	23	0
5	L	123	0	0	30	0
All	All	32274	96	30504	1527	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 1527 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:H:157:ASP:O	1:H:160:LYS:NZ	1.72	1.22
1:C:73:LYS:NZ	5:C:501:HOH:O	1.80	1.15
1:J:17:LYS:NZ	1:J:40:ASN:O	1.80	1.14
1:I:59:LYS:HA	1:I:59:LYS:HE2	1.25	1.12
1:D:5:VAL:HG22	1:D:181:ILE:HD11	1.20	1.11

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:GLU:OE1	1:J:160:LYS:NZ[1_565]	1.75	0.45
5:J:642:HOH:O	5:F:629:HOH:O[1_655]	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	326/330 (99%)	306 (94%)	18 (6%)	2 (1%)	25 11
1	B	326/330 (99%)	308 (94%)	14 (4%)	4 (1%)	13 3
1	C	326/330 (99%)	312 (96%)	11 (3%)	3 (1%)	17 5
1	D	326/330 (99%)	308 (94%)	17 (5%)	1 (0%)	41 25
1	E	326/330 (99%)	313 (96%)	11 (3%)	2 (1%)	25 11
1	F	326/330 (99%)	313 (96%)	11 (3%)	2 (1%)	25 11
1	G	326/330 (99%)	311 (95%)	13 (4%)	2 (1%)	25 11
1	H	326/330 (99%)	310 (95%)	15 (5%)	1 (0%)	41 25
1	I	326/330 (99%)	305 (94%)	16 (5%)	5 (2%)	10 2
1	J	326/330 (99%)	313 (96%)	11 (3%)	2 (1%)	25 11
1	K	326/330 (99%)	312 (96%)	12 (4%)	2 (1%)	25 11
1	L	326/330 (99%)	306 (94%)	15 (5%)	5 (2%)	10 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3912/3960 (99%)	3717 (95%)	164 (4%)	31 (1%)	19 7

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	SER
1	B	55	ALA
1	B	56	VAL
1	K	52	SER
1	K	328	TRP

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	262/263 (100%)	252 (96%)	10 (4%)	33 16
1	B	262/263 (100%)	254 (97%)	8 (3%)	40 22
1	C	262/263 (100%)	252 (96%)	10 (4%)	33 16
1	D	262/263 (100%)	256 (98%)	6 (2%)	50 34
1	E	262/263 (100%)	256 (98%)	6 (2%)	50 34
1	F	262/263 (100%)	254 (97%)	8 (3%)	40 22
1	G	262/263 (100%)	259 (99%)	3 (1%)	73 65
1	H	262/263 (100%)	255 (97%)	7 (3%)	44 28
1	I	262/263 (100%)	249 (95%)	13 (5%)	24 9
1	J	262/263 (100%)	251 (96%)	11 (4%)	30 13
1	K	262/263 (100%)	255 (97%)	7 (3%)	44 28
1	L	262/263 (100%)	254 (97%)	8 (3%)	40 22
All	All	3144/3156 (100%)	3047 (97%)	97 (3%)	40 22

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	119	VAL
1	C	49	ARG
1	E	262	ILE
1	L	119	VAL
1	C	143	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	29	GLN
1	A	31	HIS
1	A	156	GLN
1	A	98	ASN
1	G	29	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 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	$\#\|Z\|>2$
4	X9W	L	404	2	3,8,8	1.07	0	7,12,12	1.47	1 (14%)
3	NDP	E	404	-	45,52,52	2.44	7 (15%)	53,80,80	1.71	10 (18%)
4	X9W	E	401	2	3,8,8	2.07	1 (33%)	7,12,12	1.40	2 (28%)
3	NDP	B	403	-	45,52,52	2.22	6 (13%)	53,80,80	1.72	8 (15%)
3	NDP	A	404	-	45,52,52	2.28	5 (11%)	53,80,80	1.71	9 (16%)
4	X9W	D	404	2	3,8,8	1.62	1 (33%)	7,12,12	1.59	1 (14%)
4	X9W	B	404	2	3,8,8	2.00	1 (33%)	7,12,12	1.44	0
3	NDP	K	403	-	45,52,52	2.49	6 (13%)	53,80,80	1.67	10 (18%)
4	X9W	J	403	2	3,8,8	1.63	1 (33%)	7,12,12	2.14	3 (42%)
4	X9W	I	403	2	3,8,8	1.80	1 (33%)	7,12,12	2.21	4 (57%)
3	NDP	L	403	-	45,52,52	2.32	6 (13%)	53,80,80	1.51	5 (9%)
4	X9W	C	401	2	3,8,8	1.50	0	7,12,12	1.71	2 (28%)
3	NDP	I	404	-	45,52,52	2.44	5 (11%)	53,80,80	1.65	10 (18%)
4	X9W	H	403	2	3,8,8	1.44	0	7,12,12	2.47	3 (42%)
3	NDP	D	403	-	45,52,52	2.24	6 (13%)	53,80,80	1.62	8 (15%)
4	X9W	F	401	2	3,8,8	1.36	0	7,12,12	2.18	2 (28%)
3	NDP	G	403	-	45,52,52	2.63	8 (17%)	53,80,80	1.72	9 (16%)
3	NDP	H	404	-	45,52,52	2.49	5 (11%)	53,80,80	1.65	7 (13%)
3	NDP	J	404	-	45,52,52	2.37	5 (11%)	53,80,80	1.57	9 (16%)
4	X9W	G	404	2	3,8,8	2.32	1 (33%)	7,12,12	1.81	2 (28%)
4	X9W	A	401	2	3,8,8	1.44	0	7,12,12	1.43	2 (28%)
3	NDP	F	404	-	45,52,52	2.34	5 (11%)	53,80,80	1.58	9 (16%)
4	X9W	H	405	2	3,8,8	1.65	0	7,12,12	1.88	2 (28%)
3	NDP	C	404	-	45,52,52	2.48	8 (17%)	53,80,80	1.54	9 (16%)

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
4	X9W	L	404	2	-	2/4/10/10	-
3	NDP	E	404	-	-	6/30/77/77	0/5/5/5
4	X9W	E	401	2	-	2/4/10/10	-
3	NDP	B	403	-	-	14/30/77/77	0/5/5/5
3	NDP	A	404	-	-	8/30/77/77	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	X9W	D	404	2	-	1/4/10/10	-
4	X9W	B	404	2	-	1/4/10/10	-
3	NDP	K	403	-	-	13/30/77/77	0/5/5/5
4	X9W	J	403	2	-	0/4/10/10	-
4	X9W	I	403	2	-	2/4/10/10	-
3	NDP	L	403	-	-	10/30/77/77	0/5/5/5
4	X9W	C	401	2	-	0/4/10/10	-
3	NDP	I	404	-	-	10/30/77/77	0/5/5/5
4	X9W	H	403	2	-	2/4/10/10	-
3	NDP	D	403	-	-	7/30/77/77	0/5/5/5
4	X9W	F	401	2	-	3/4/10/10	-
3	NDP	G	403	-	-	8/30/77/77	0/5/5/5
3	NDP	H	404	-	-	11/30/77/77	0/5/5/5
3	NDP	J	404	-	-	10/30/77/77	0/5/5/5
4	X9W	G	404	2	-	3/4/10/10	-
4	X9W	A	401	2	-	2/4/10/10	-
3	NDP	F	404	-	-	5/30/77/77	0/5/5/5
4	X9W	H	405	2	-	3/4/10/10	-
3	NDP	C	404	-	-	6/30/77/77	0/5/5/5

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	403	NDP	P2B-O2B	14.87	1.87	1.59
3	I	404	NDP	P2B-O2B	14.31	1.86	1.59
3	H	404	NDP	P2B-O2B	14.30	1.86	1.59
3	K	403	NDP	P2B-O2B	14.23	1.86	1.59
3	J	404	NDP	P2B-O2B	13.73	1.85	1.59

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	403	NDP	PN-O3-PA	-7.05	108.64	132.83
3	G	403	NDP	PN-O3-PA	-6.69	109.87	132.83
3	K	403	NDP	PN-O3-PA	-6.58	110.25	132.83
3	H	404	NDP	PN-O3-PA	-6.53	110.41	132.83
3	A	404	NDP	PN-O3-PA	-6.37	110.97	132.83

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	NDP	C2B-O2B-P2B-O1X
3	B	403	NDP	C5D-O5D-PN-O3
3	B	403	NDP	C5D-O5D-PN-O1N
3	B	403	NDP	O4D-C4D-C5D-O5D
3	H	404	NDP	C5B-O5B-PA-O1A

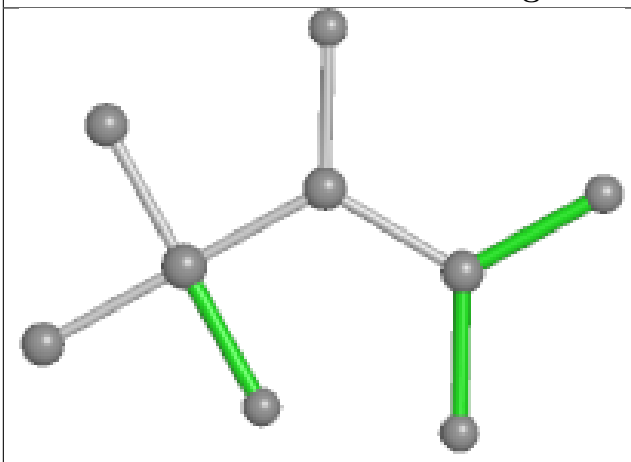
There are no ring outliers.

18 monomers are involved in 95 short contacts:

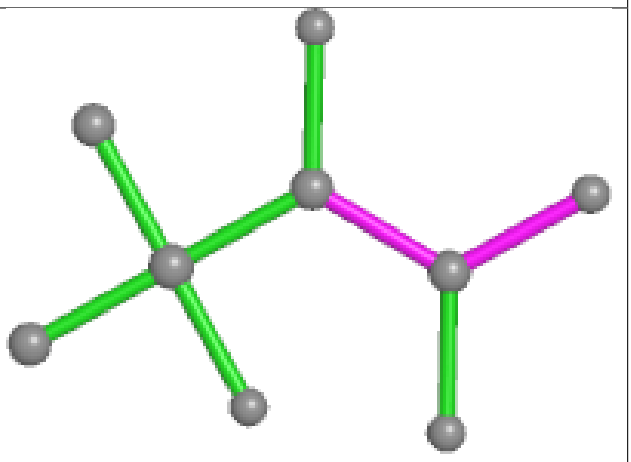
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	404	NDP	7	0
3	B	403	NDP	7	0
3	A	404	NDP	9	0
4	D	404	X9W	1	0
3	K	403	NDP	7	0
4	J	403	X9W	1	0
4	I	403	X9W	1	0
3	L	403	NDP	7	0
3	I	404	NDP	9	0
4	H	403	X9W	1	0
3	D	403	NDP	10	0
4	F	401	X9W	1	0
3	G	403	NDP	5	0
3	H	404	NDP	12	0
3	J	404	NDP	7	0
4	G	404	X9W	1	0
3	F	404	NDP	4	0
3	C	404	NDP	7	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.

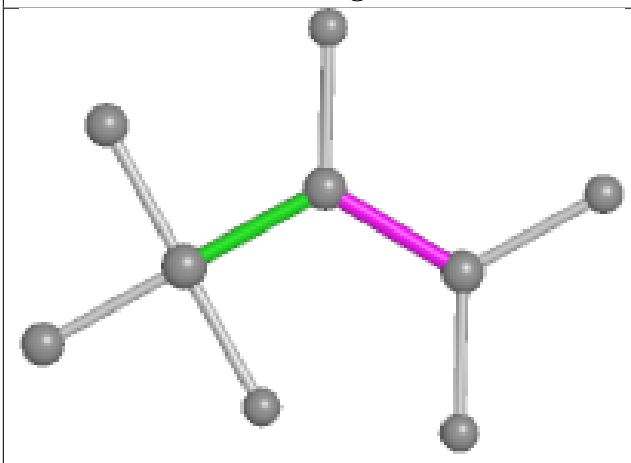
Ligand X9W L 404



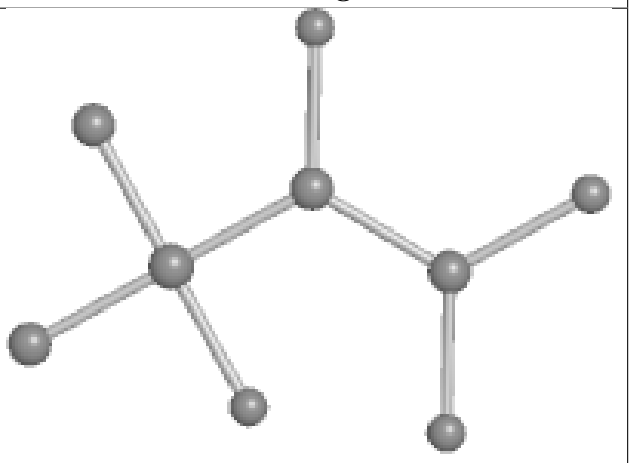
Bond lengths



Bond angles

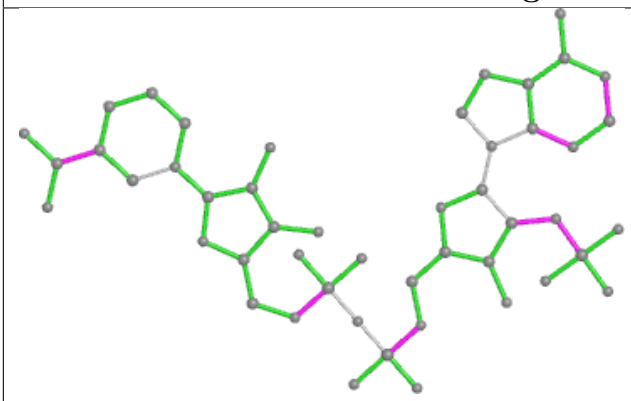


Torsions

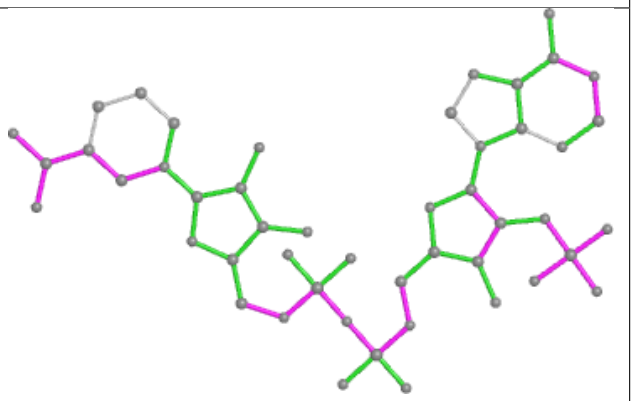


Rings

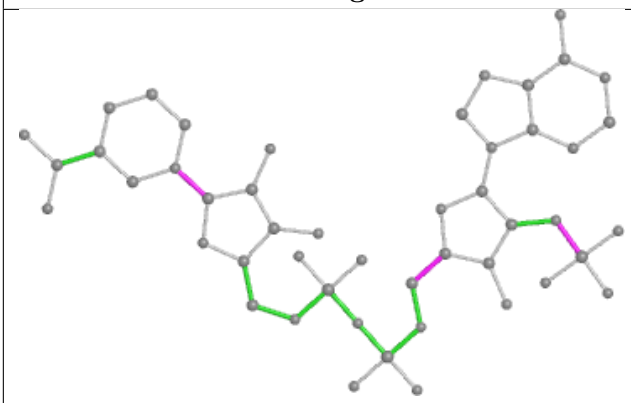
Ligand NDP E 404



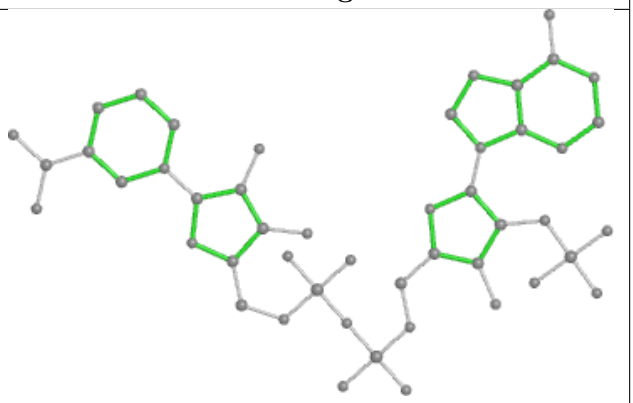
Bond lengths



Bond angles

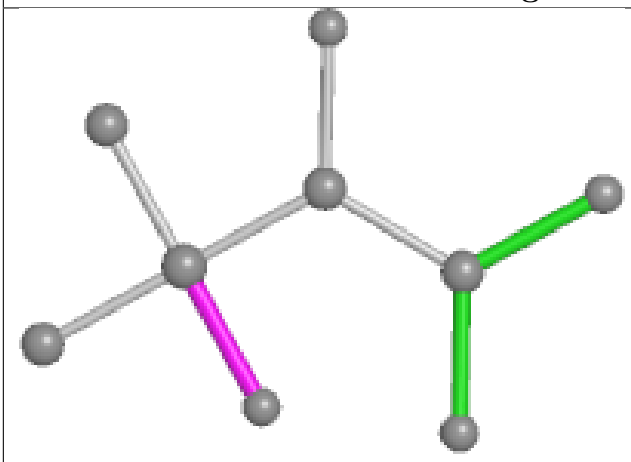


Torsions

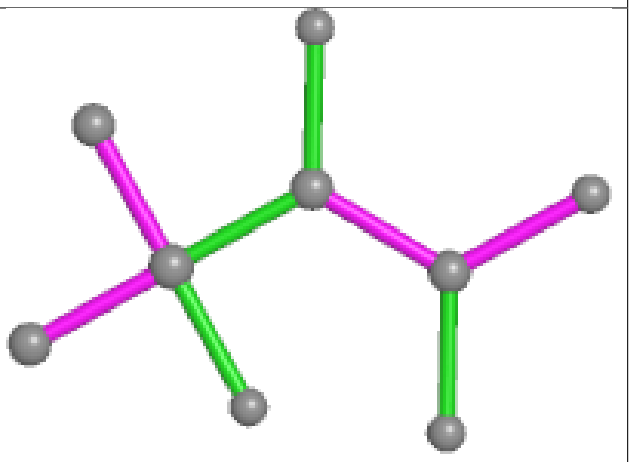


Rings

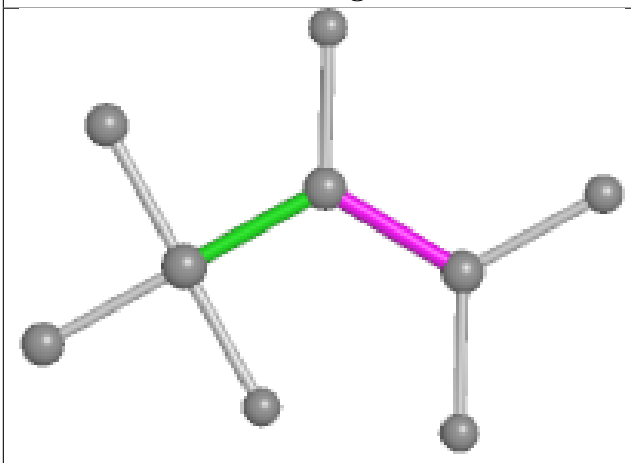
Ligand X9W E 401



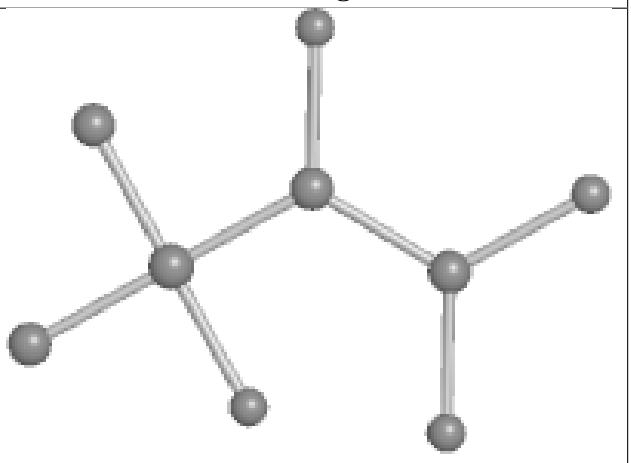
Bond lengths



Bond angles

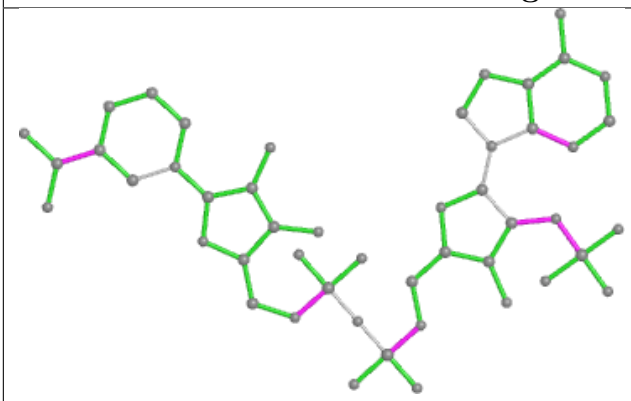


Torsions

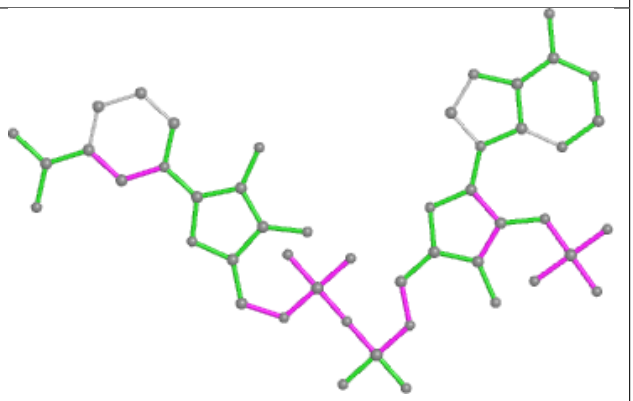


Rings

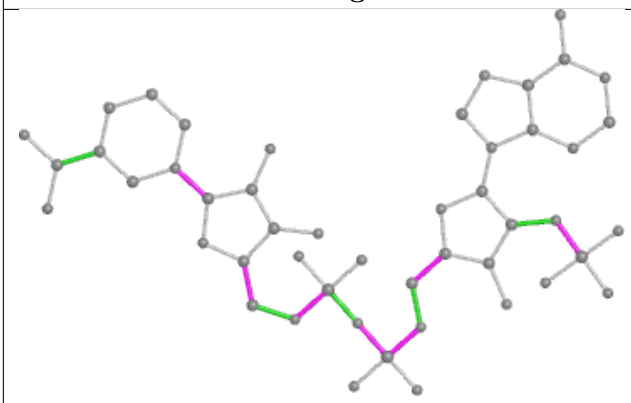
Ligand NDP B 403



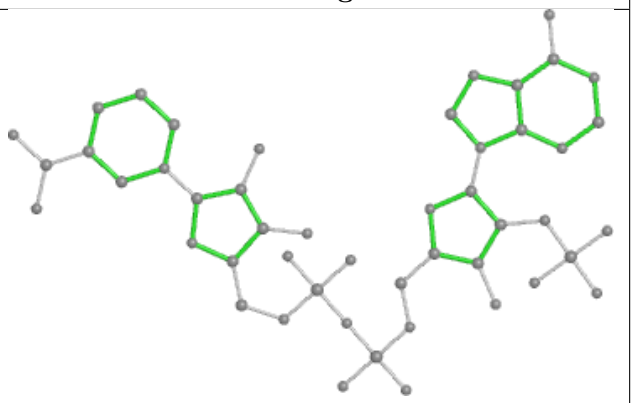
Bond lengths



Bond angles

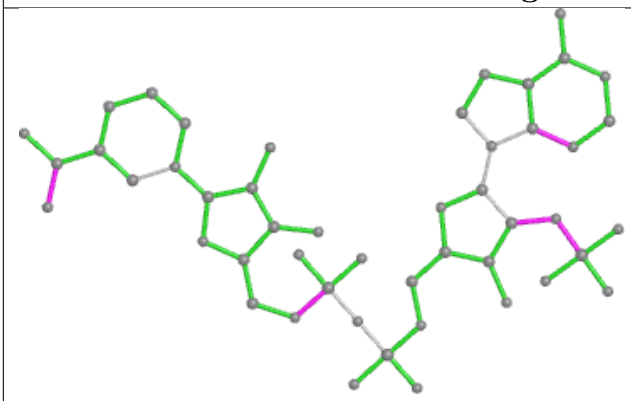


Torsions

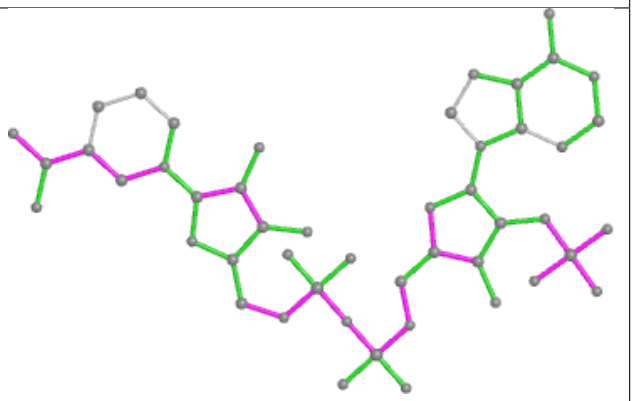


Rings

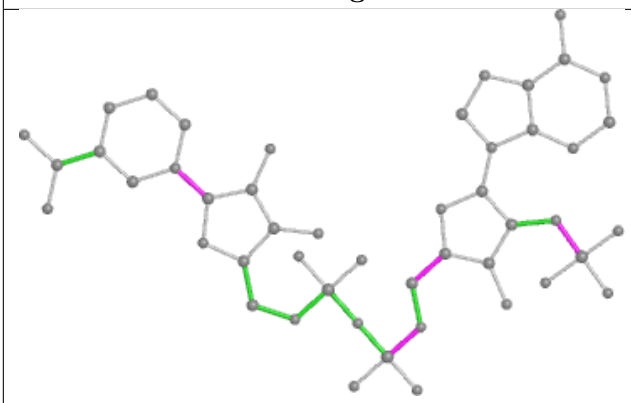
Ligand NDP A 404



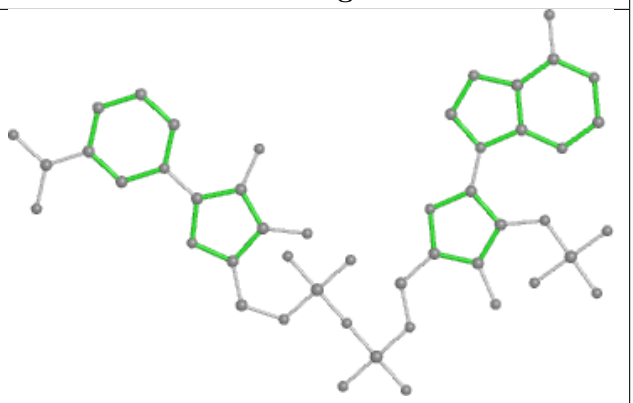
Bond lengths



Bond angles

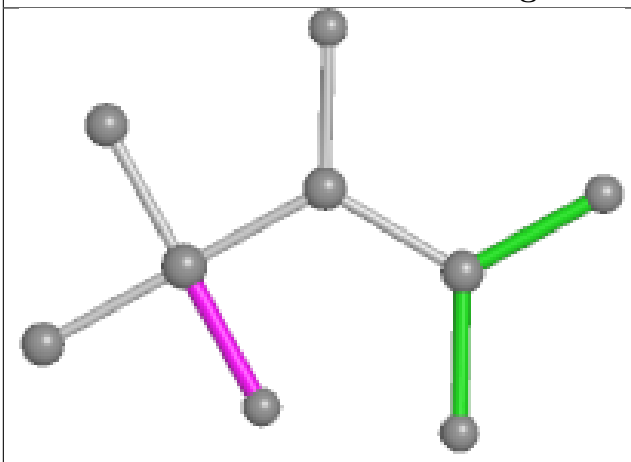


Torsions

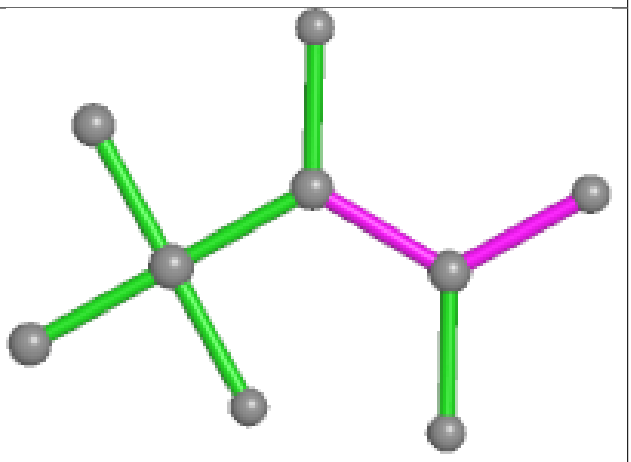


Rings

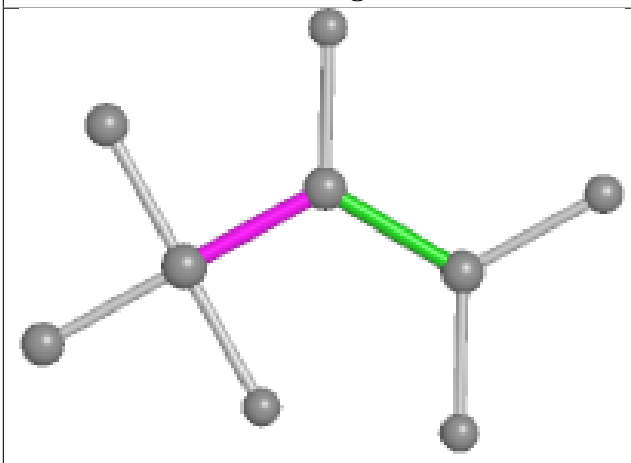
Ligand X9W D 404



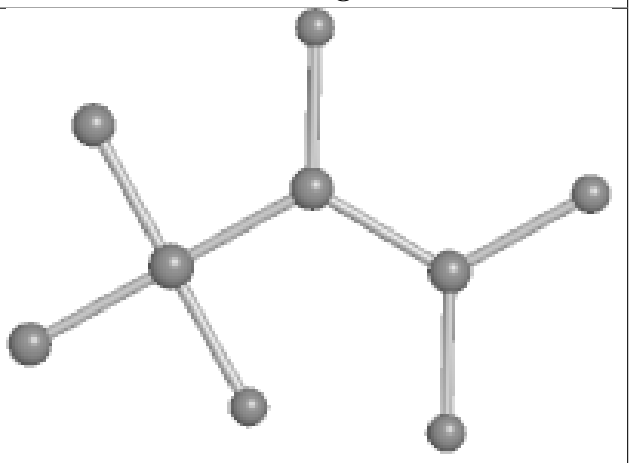
Bond lengths



Bond angles

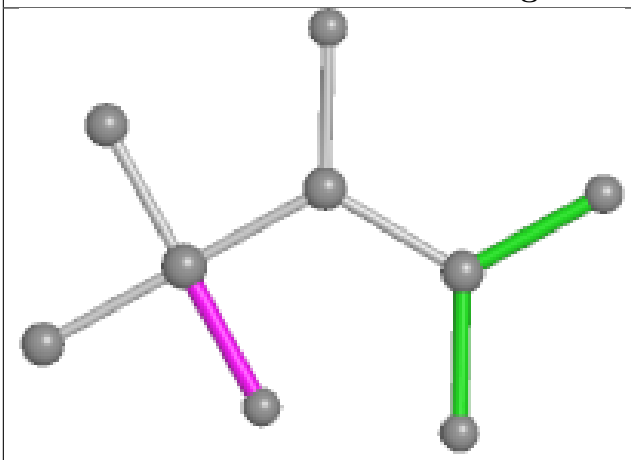


Torsions

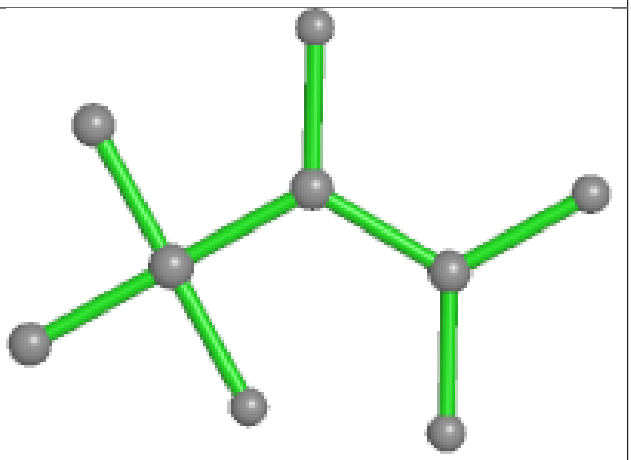


Rings

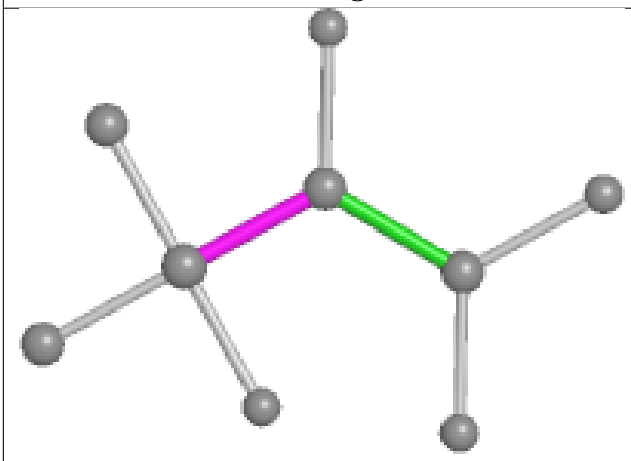
Ligand X9W B 404



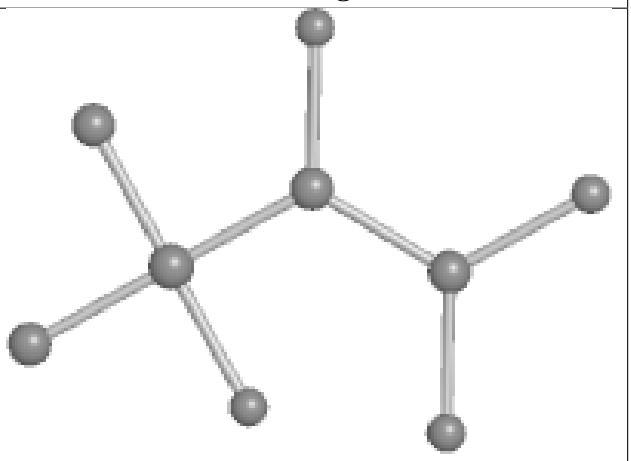
Bond lengths



Bond angles

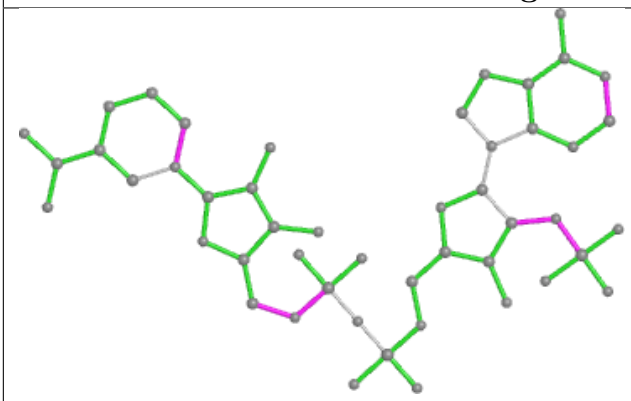


Torsions

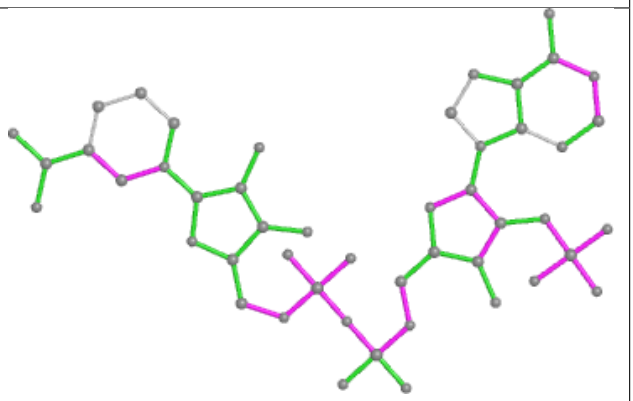


Rings

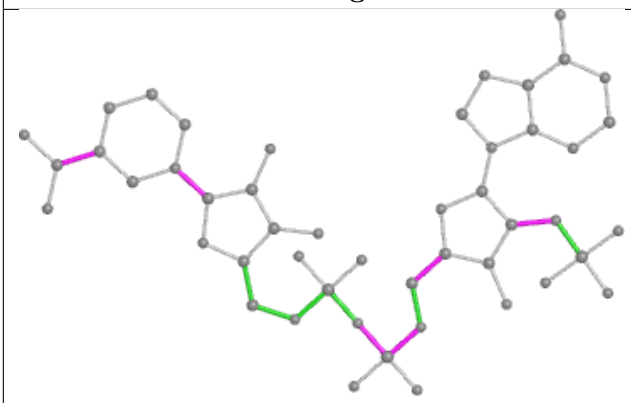
Ligand NDP K 403



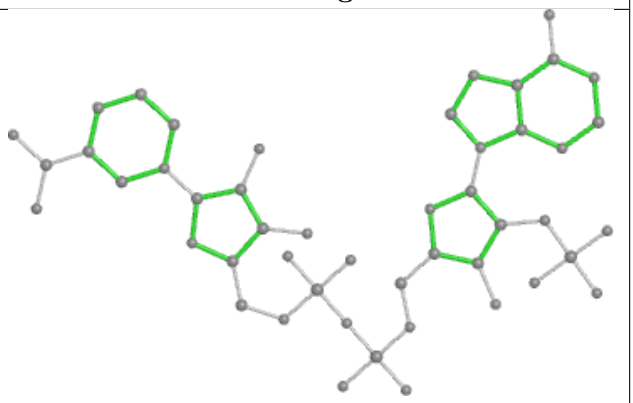
Bond lengths



Bond angles

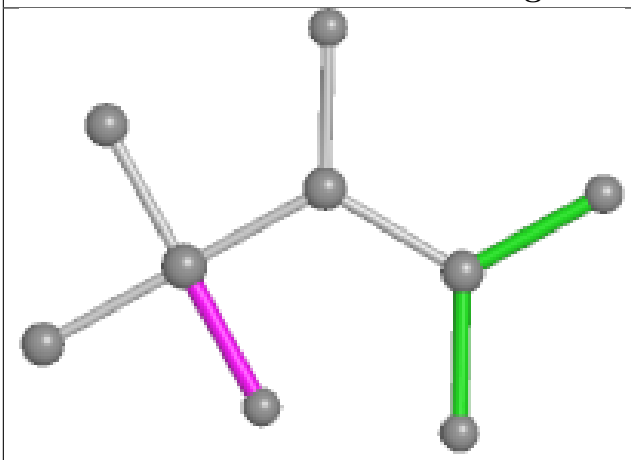


Torsions

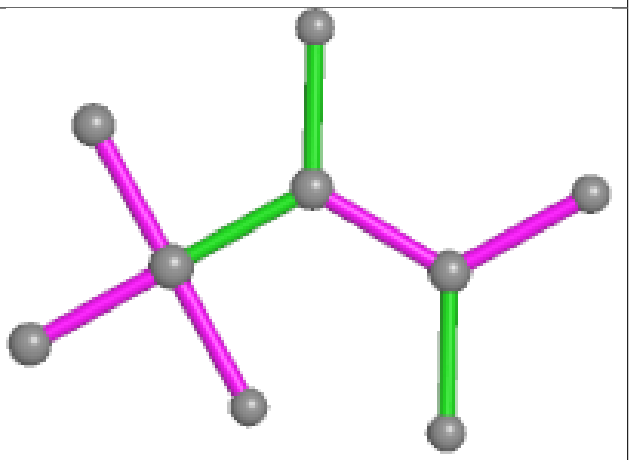


Rings

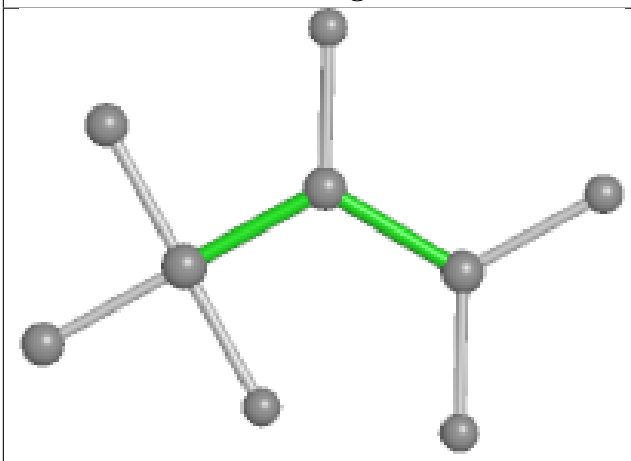
Ligand X9W J 403



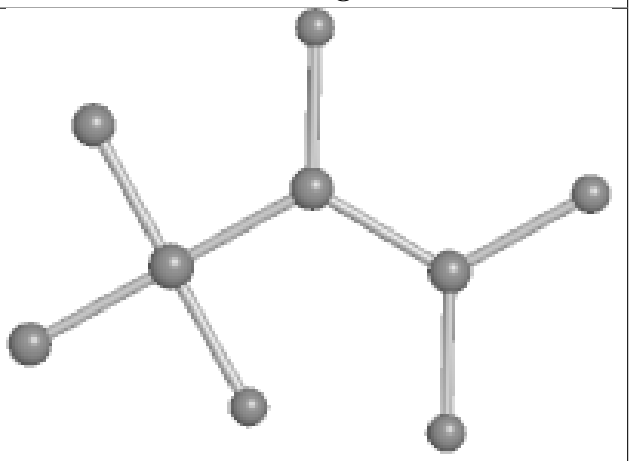
Bond lengths



Bond angles

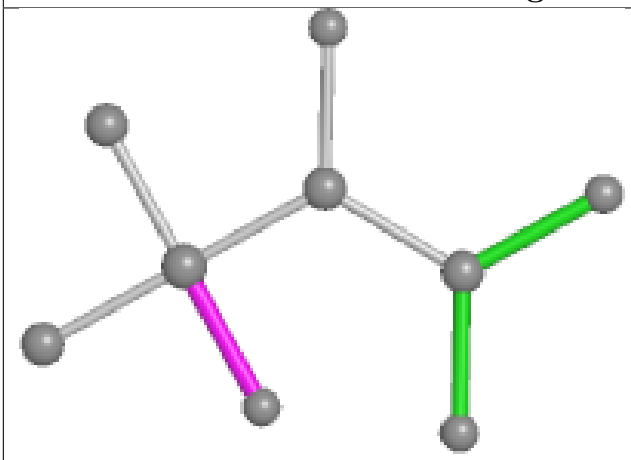


Torsions

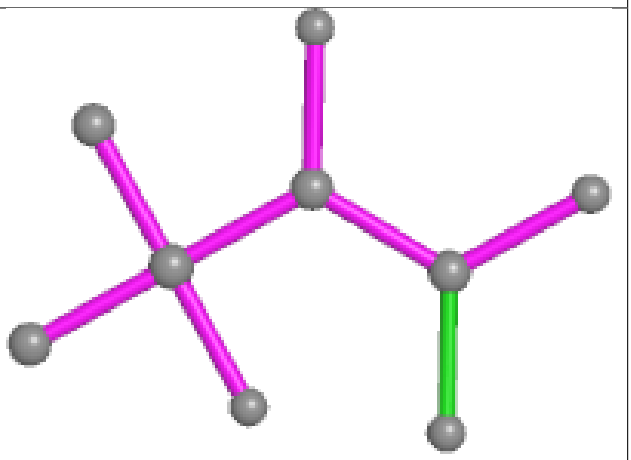


Rings

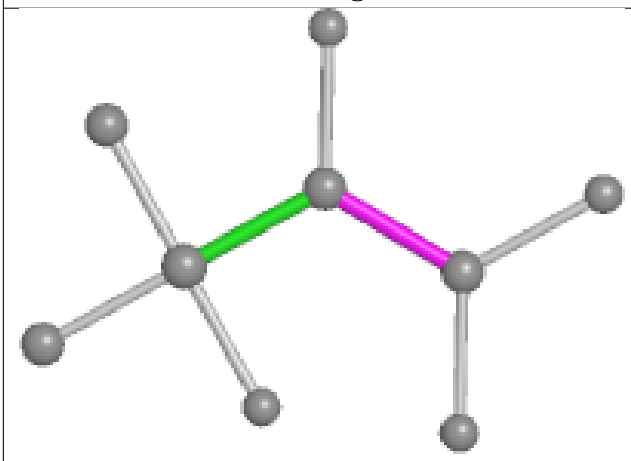
Ligand X9W I 403



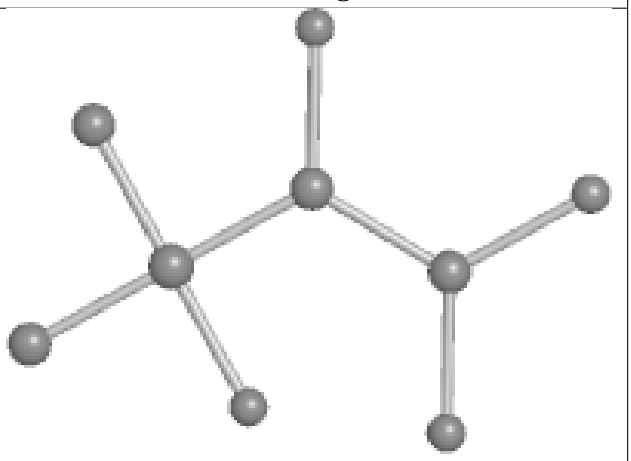
Bond lengths



Bond angles

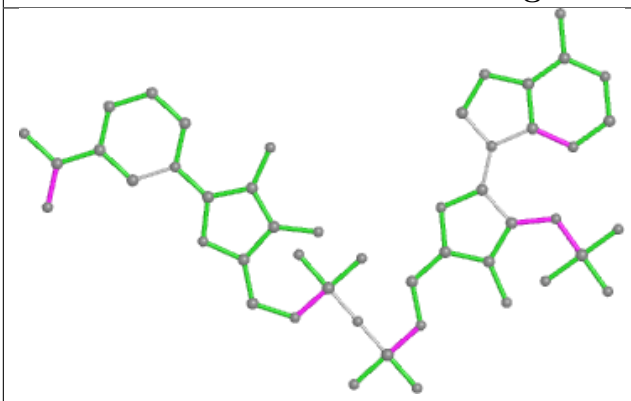


Torsions

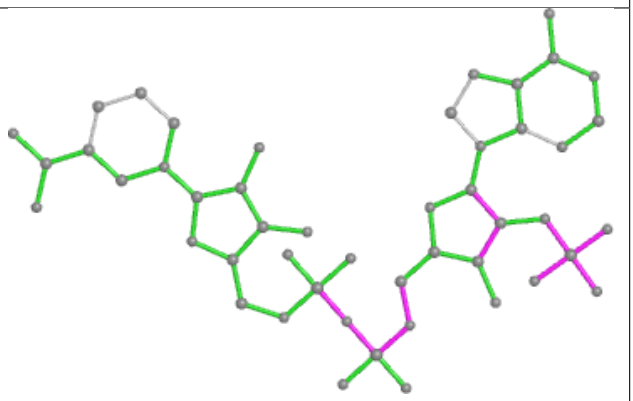


Rings

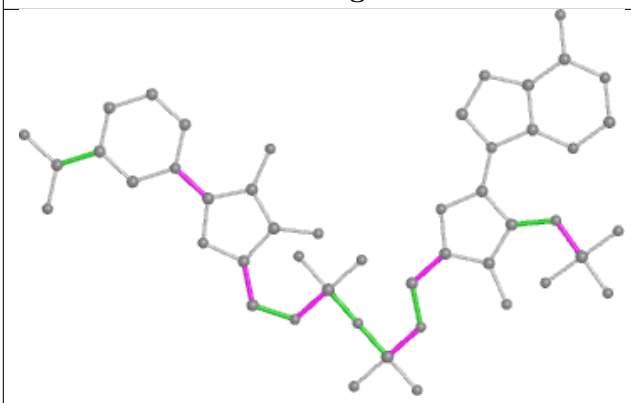
Ligand NDP L 403



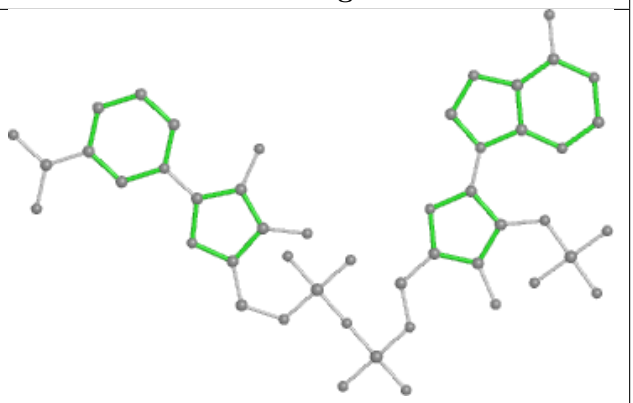
Bond lengths



Bond angles

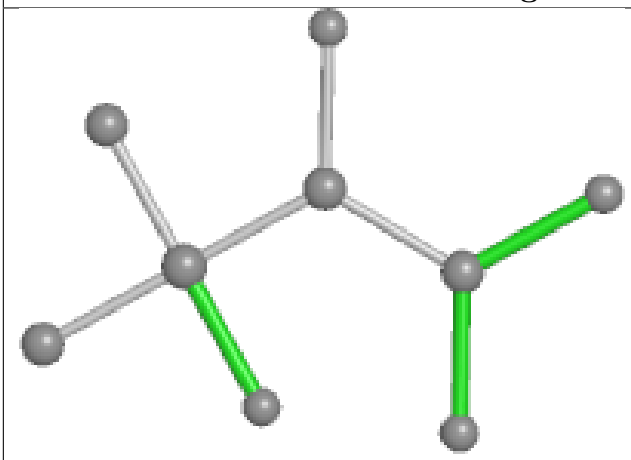


Torsions

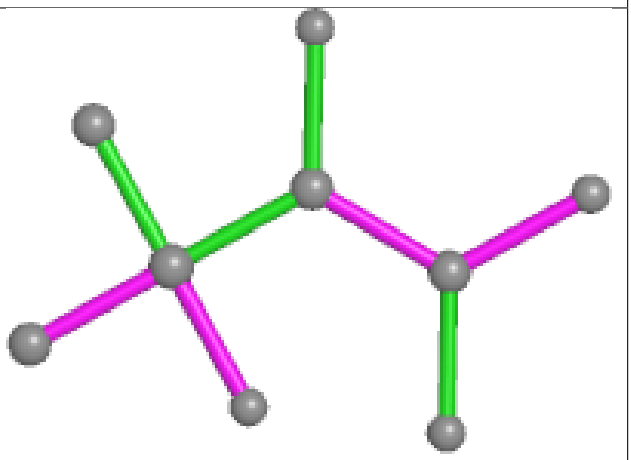


Rings

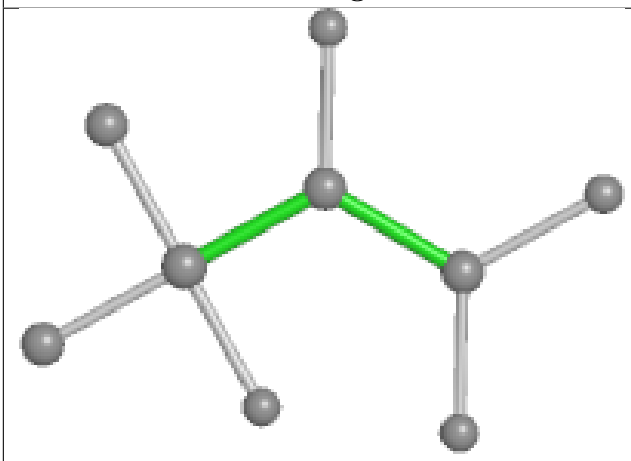
Ligand X9W C 401



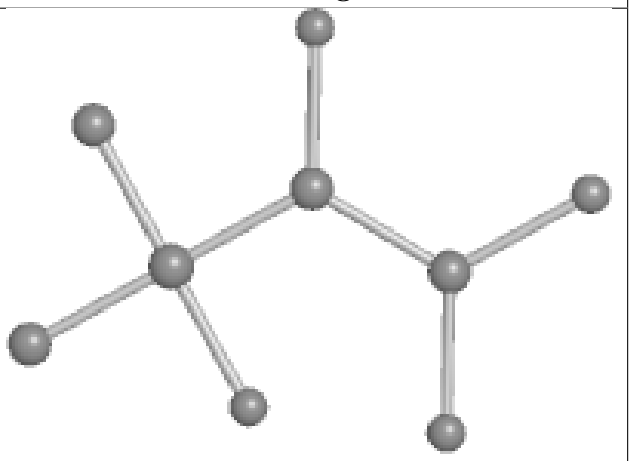
Bond lengths



Bond angles

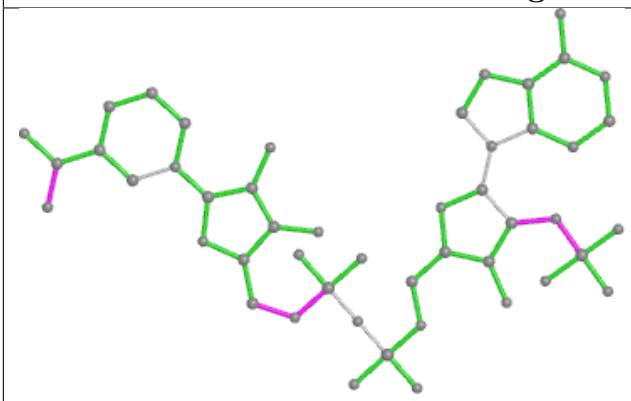


Torsions

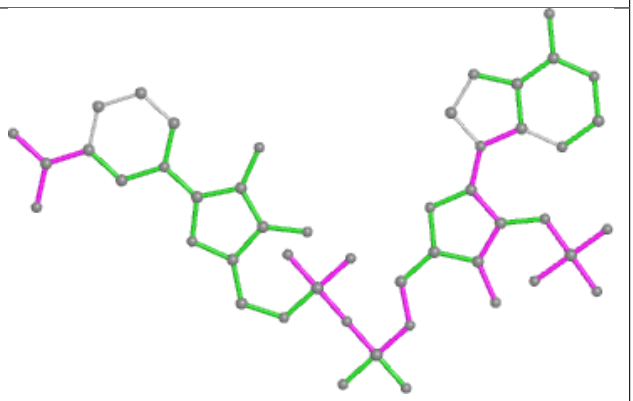


Rings

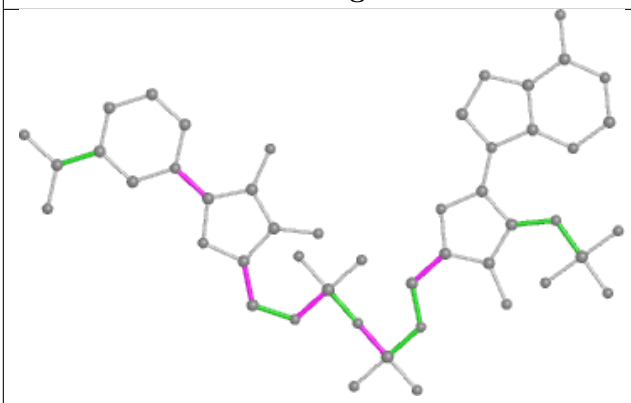
Ligand NDP I 404



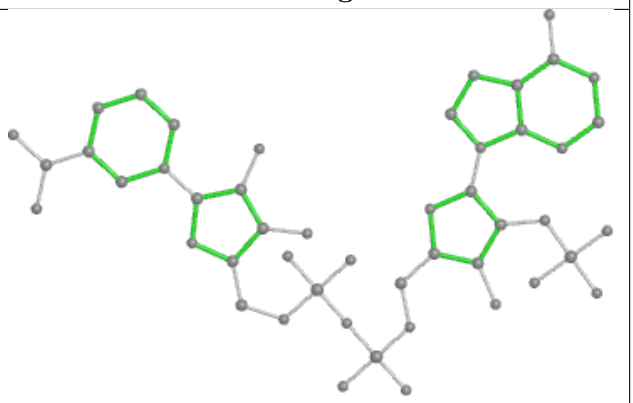
Bond lengths



Bond angles

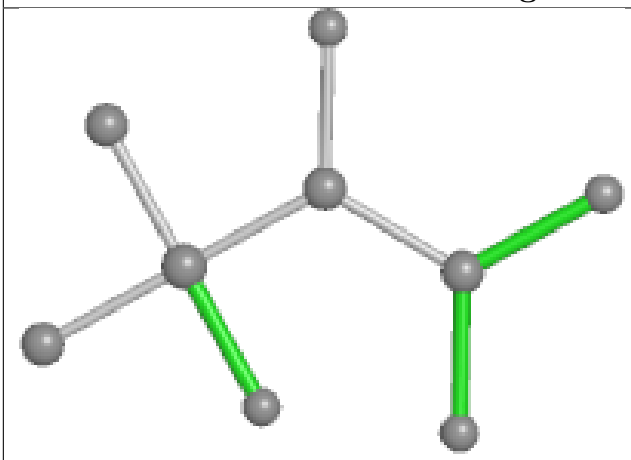


Torsions

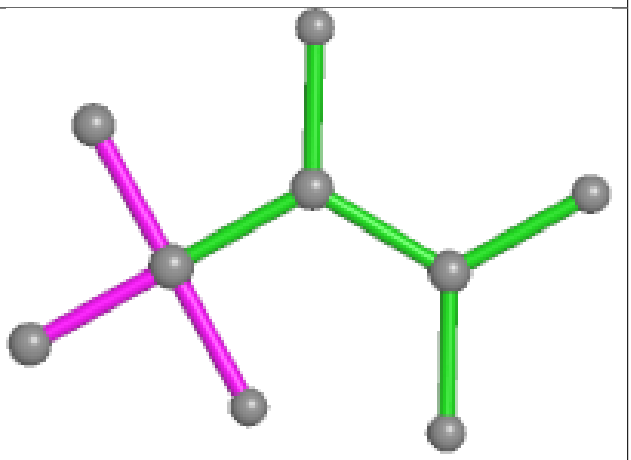


Rings

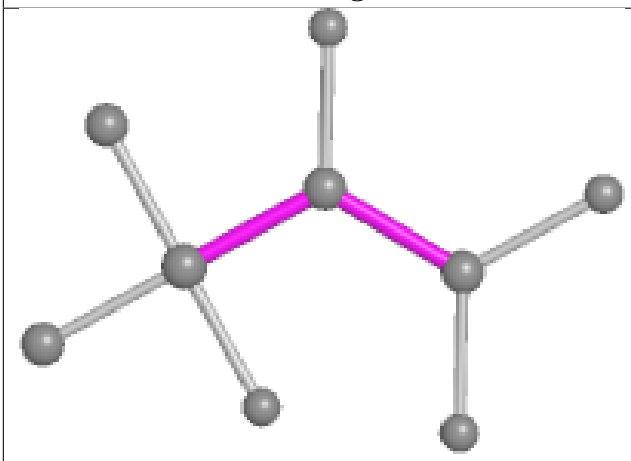
Ligand X9W H 403



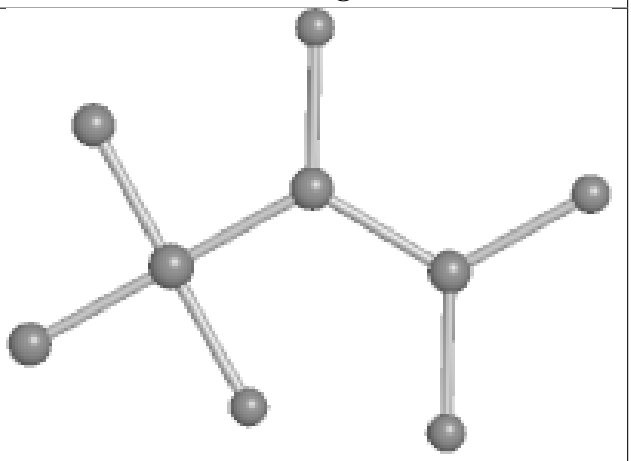
Bond lengths



Bond angles

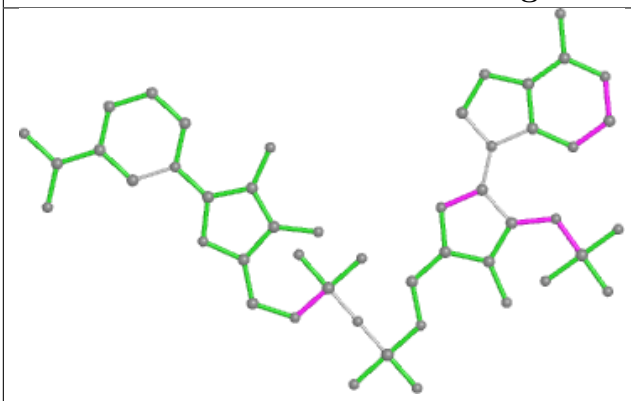


Torsions

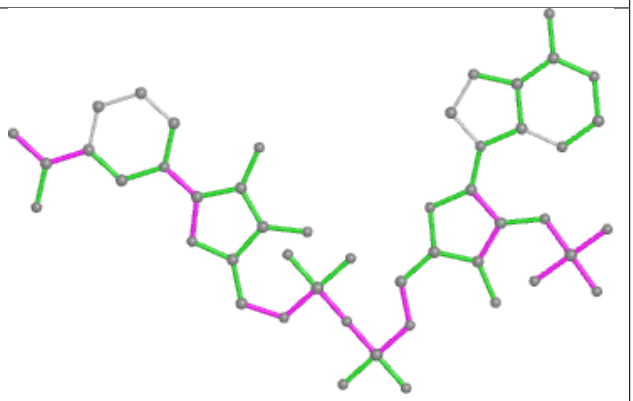


Rings

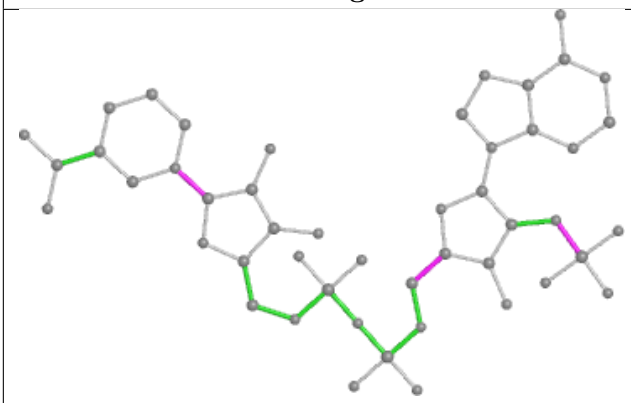
Ligand NDP D 403



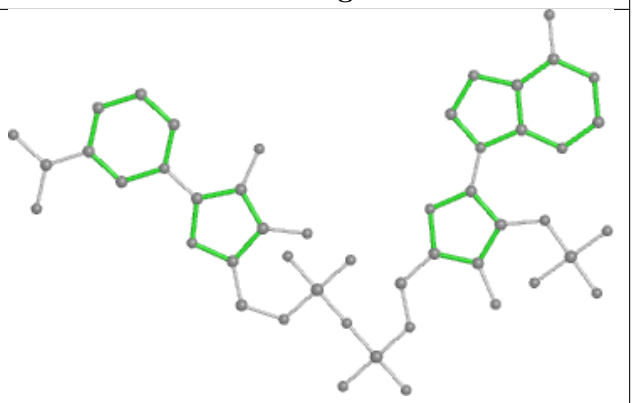
Bond lengths



Bond angles

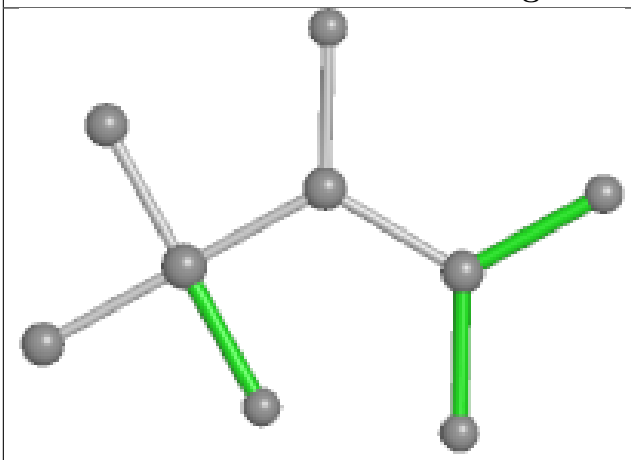


Torsions

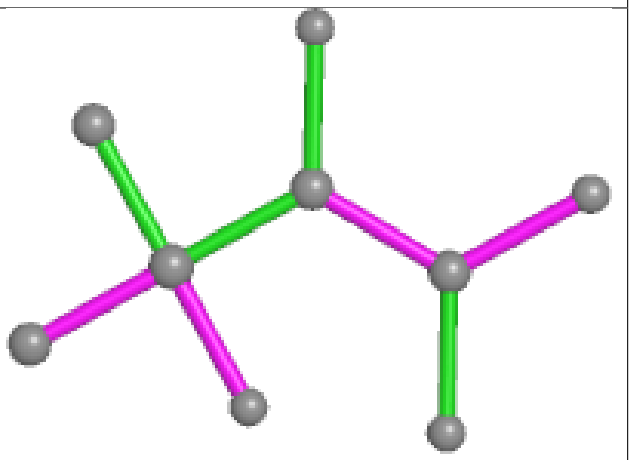


Rings

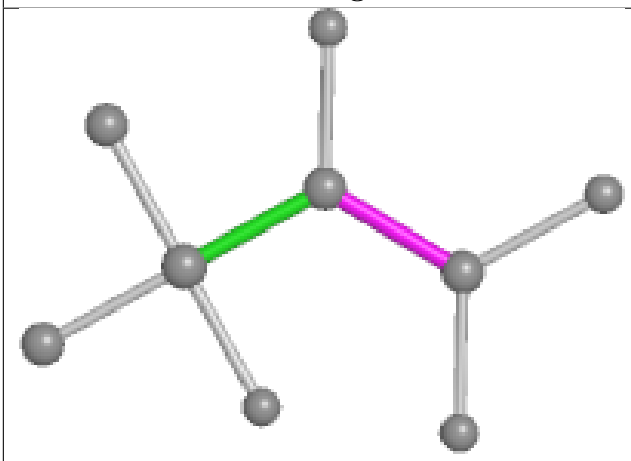
Ligand X9W F 401



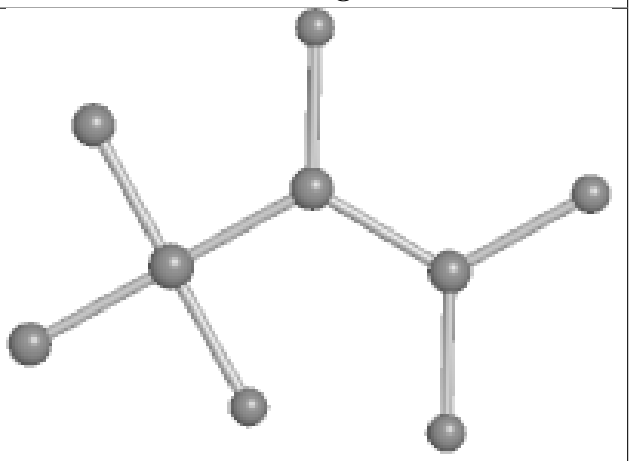
Bond lengths



Bond angles

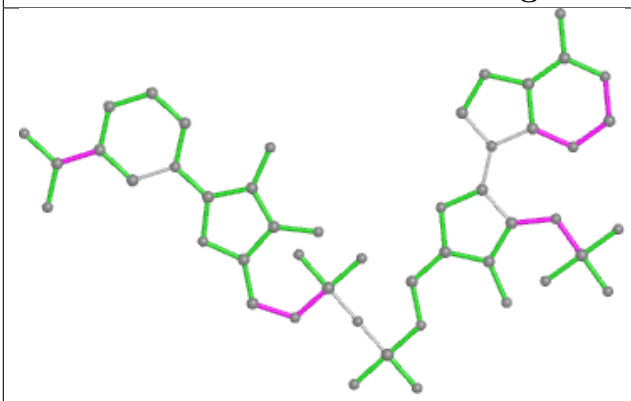


Torsions

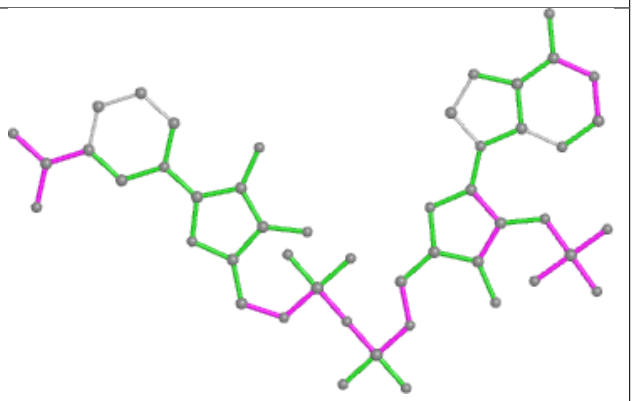


Rings

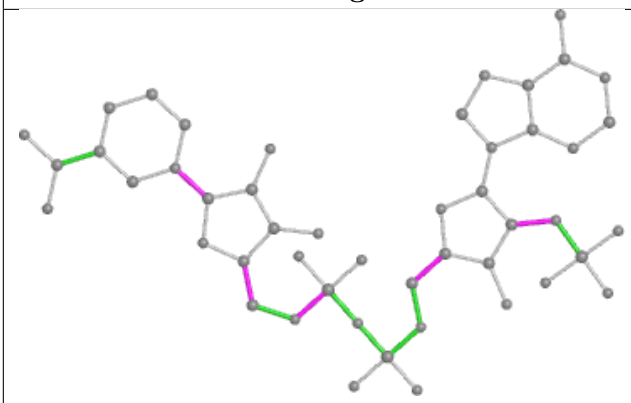
Ligand NDP G 403



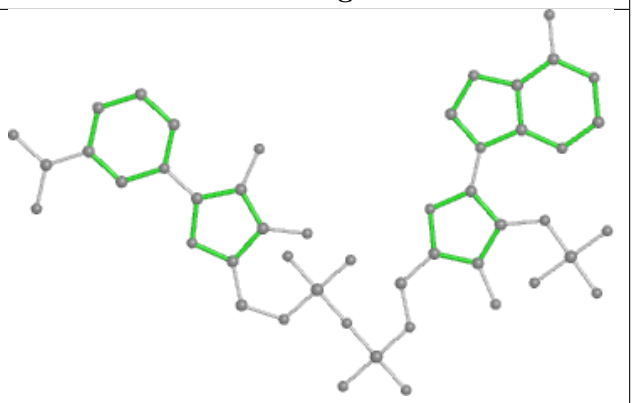
Bond lengths



Bond angles

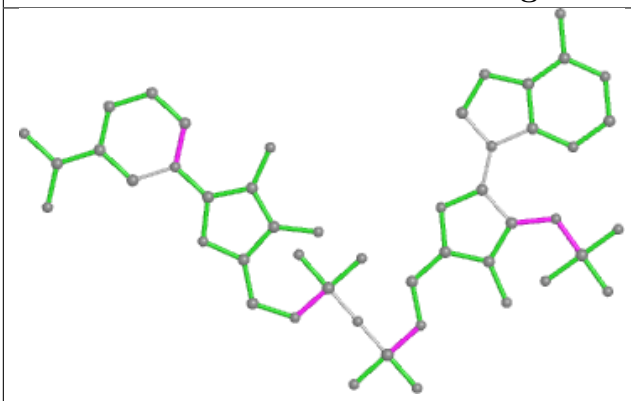


Torsions

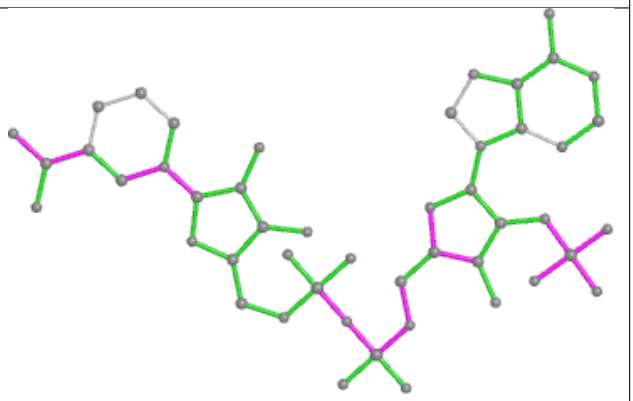


Rings

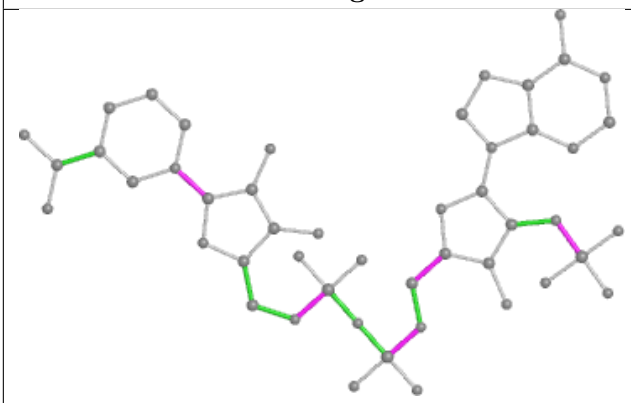
Ligand NDP H 404



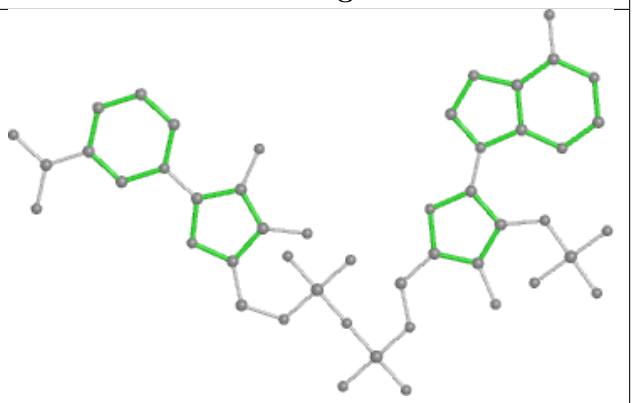
Bond lengths



Bond angles

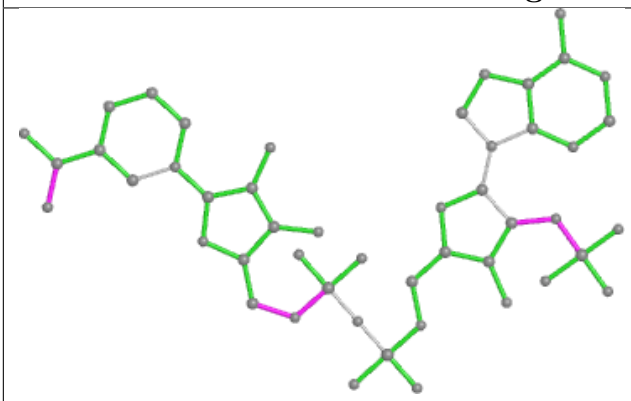


Torsions

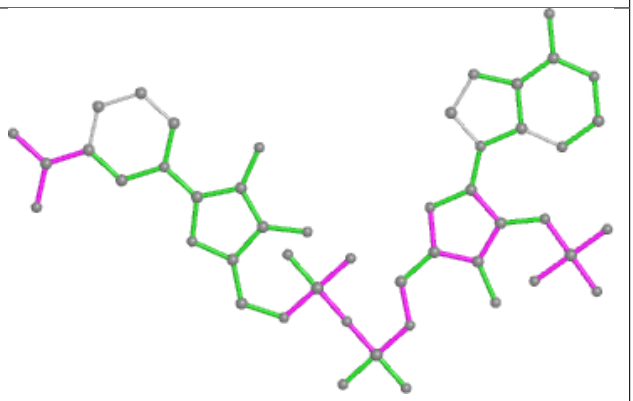


Rings

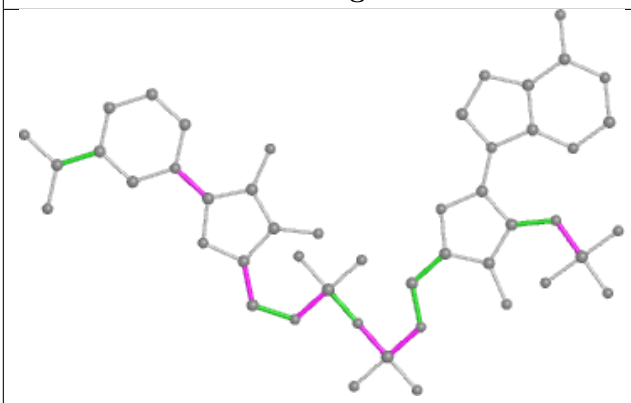
Ligand NDP J 404



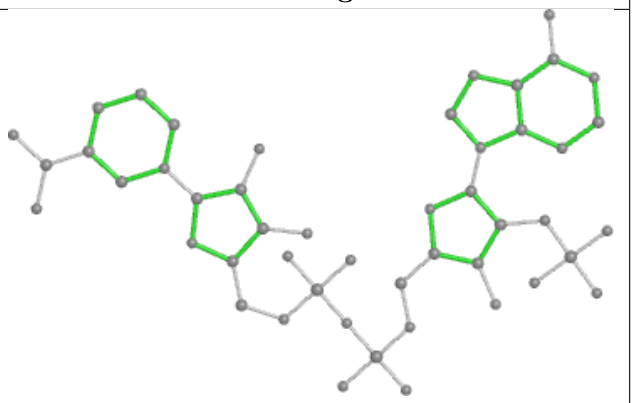
Bond lengths



Bond angles

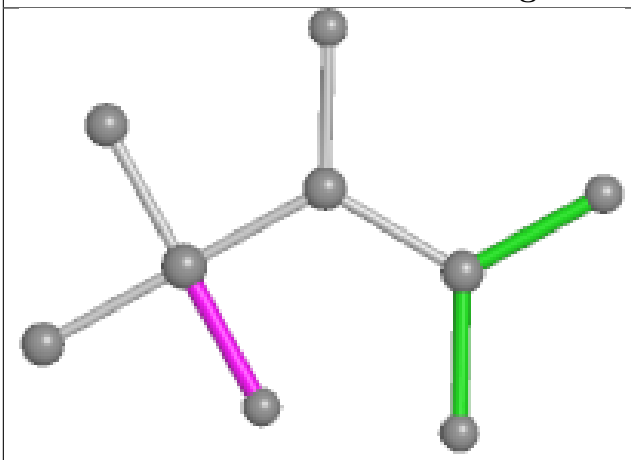


Torsions

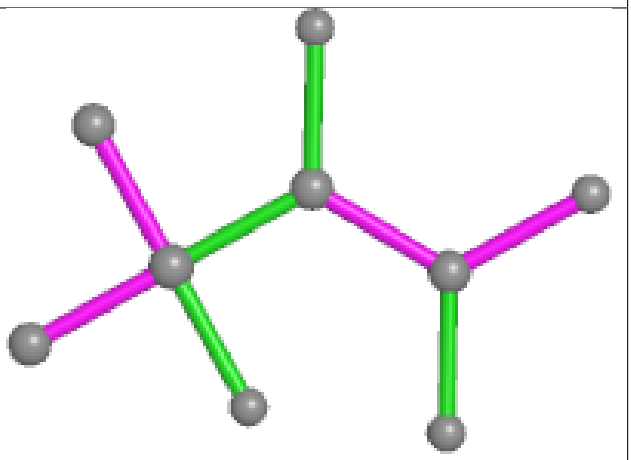


Rings

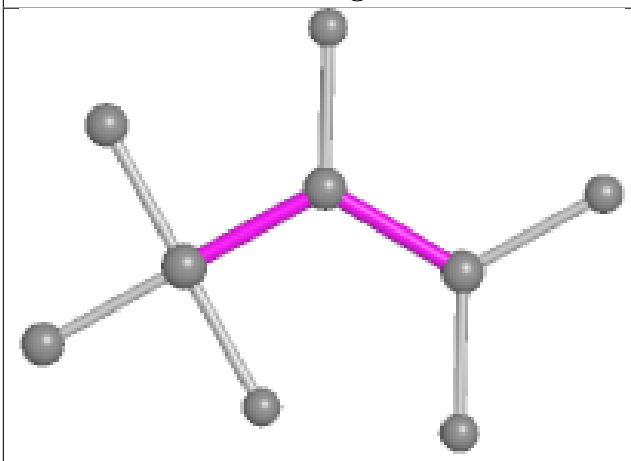
Ligand X9W G 404



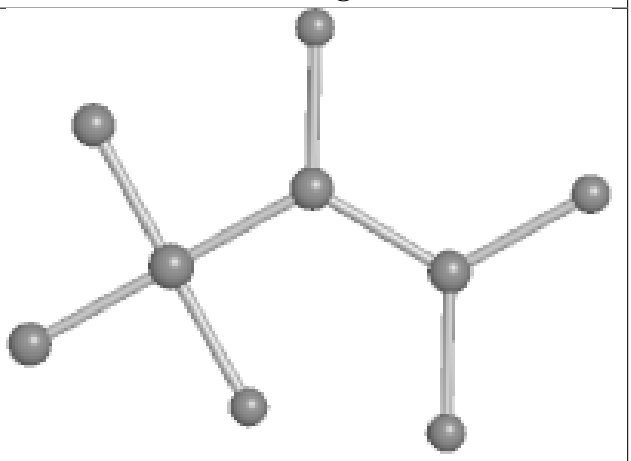
Bond lengths



Bond angles

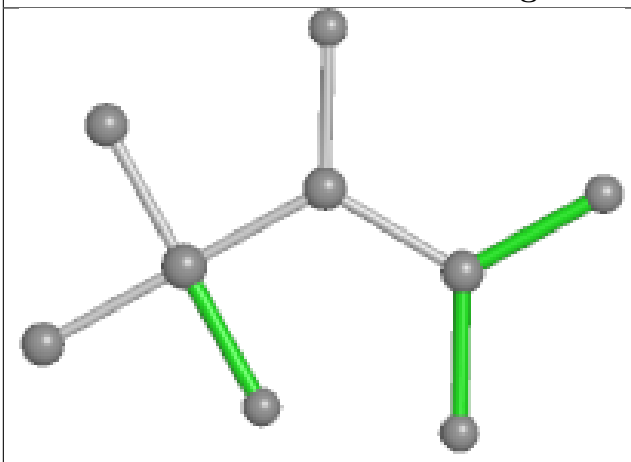


Torsions

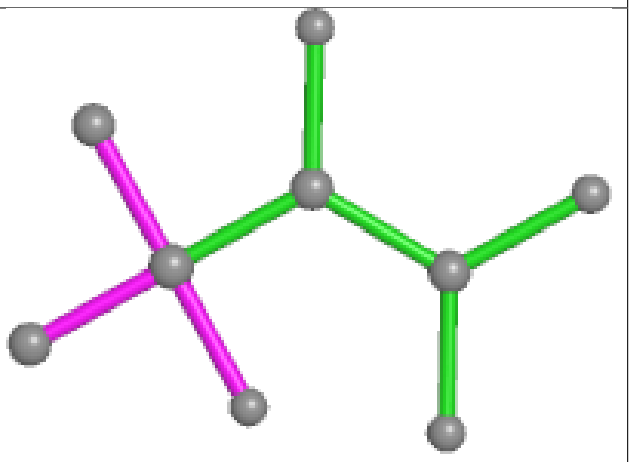


Rings

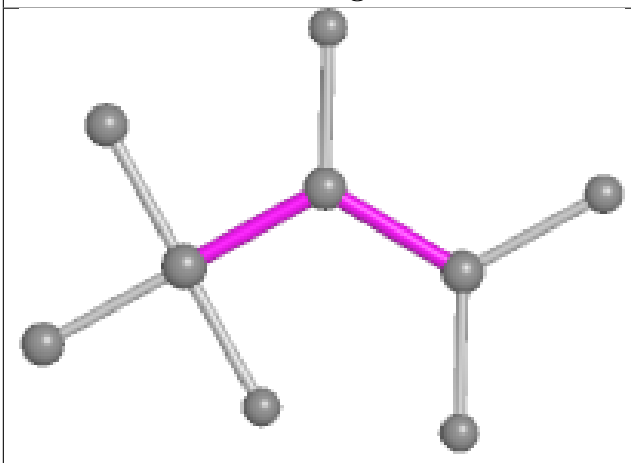
Ligand X9W A 401



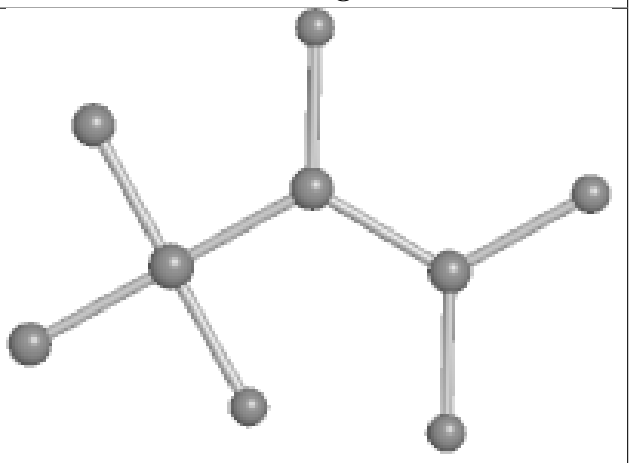
Bond lengths



Bond angles

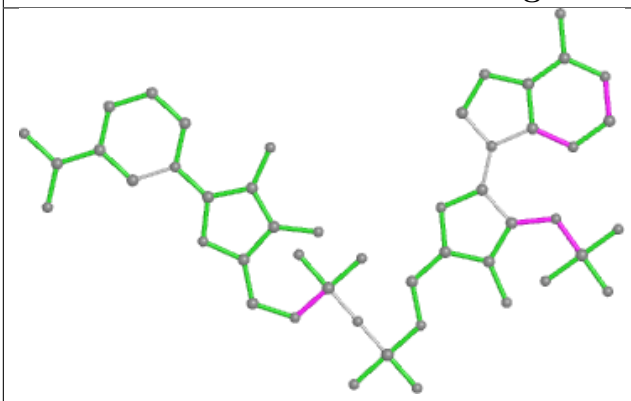


Torsions

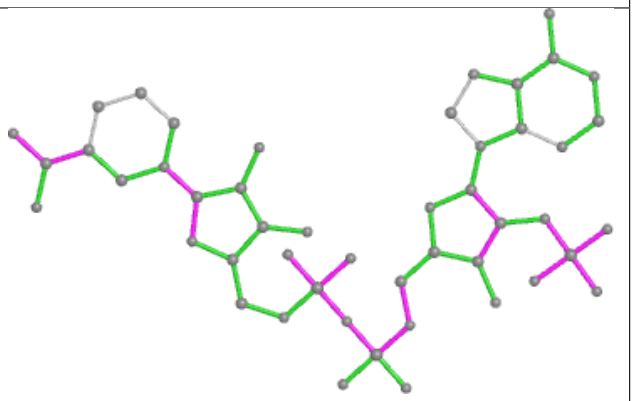


Rings

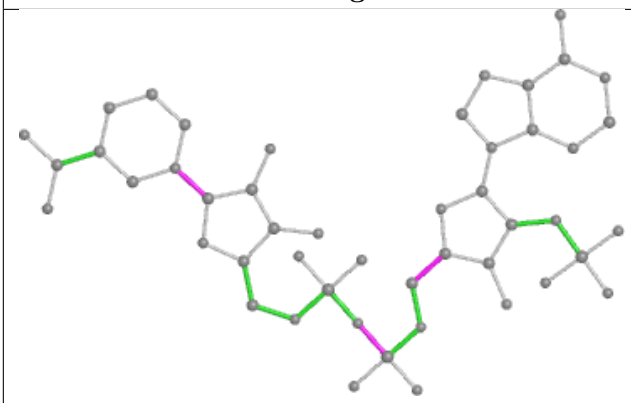
Ligand NDP F 404



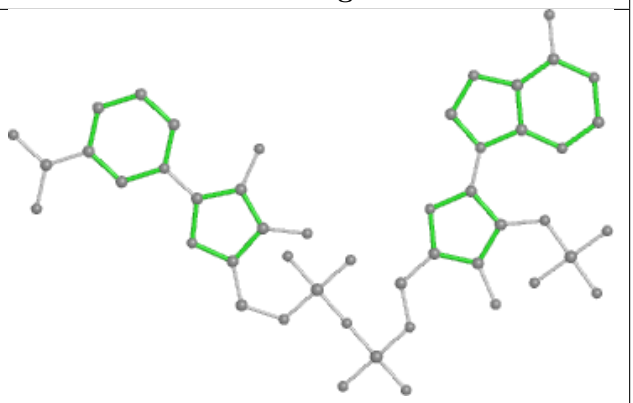
Bond lengths



Bond angles

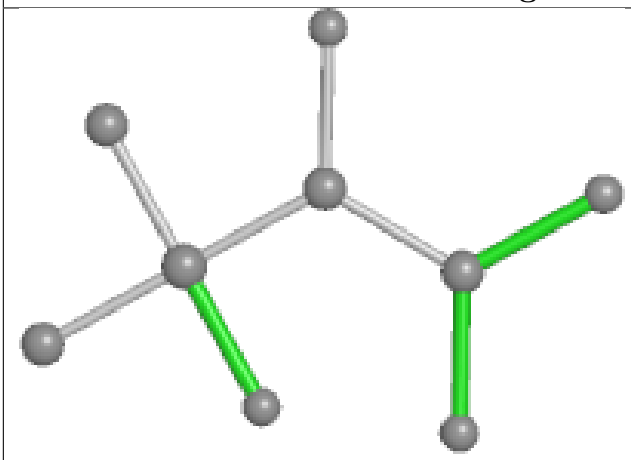


Torsions

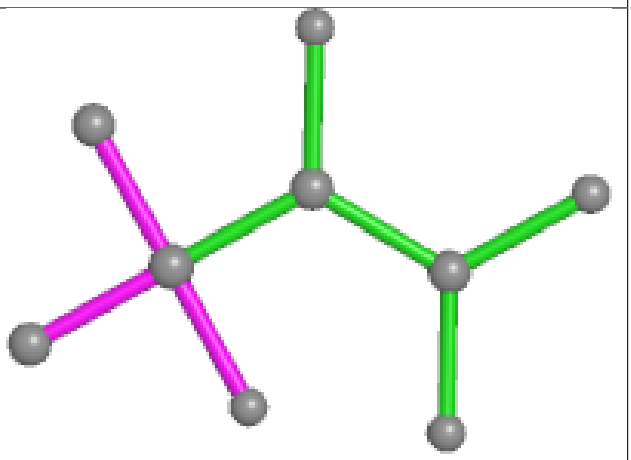


Rings

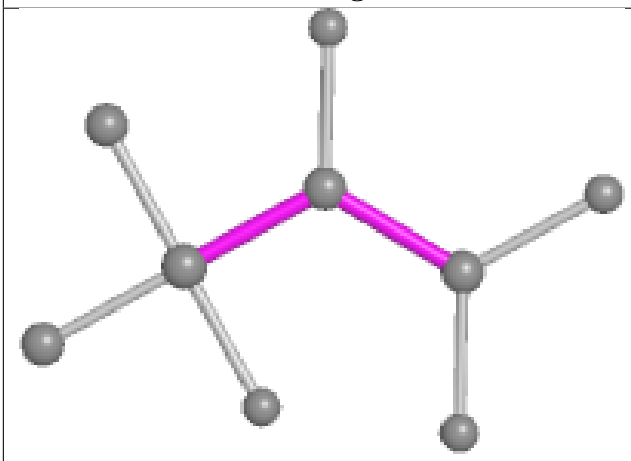
Ligand X9W H 405



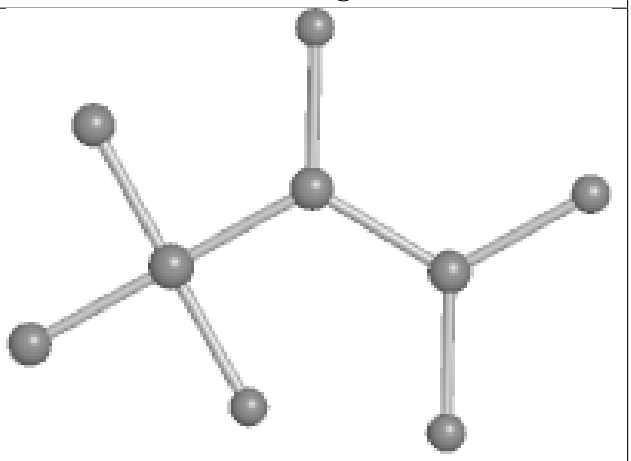
Bond lengths



Bond angles

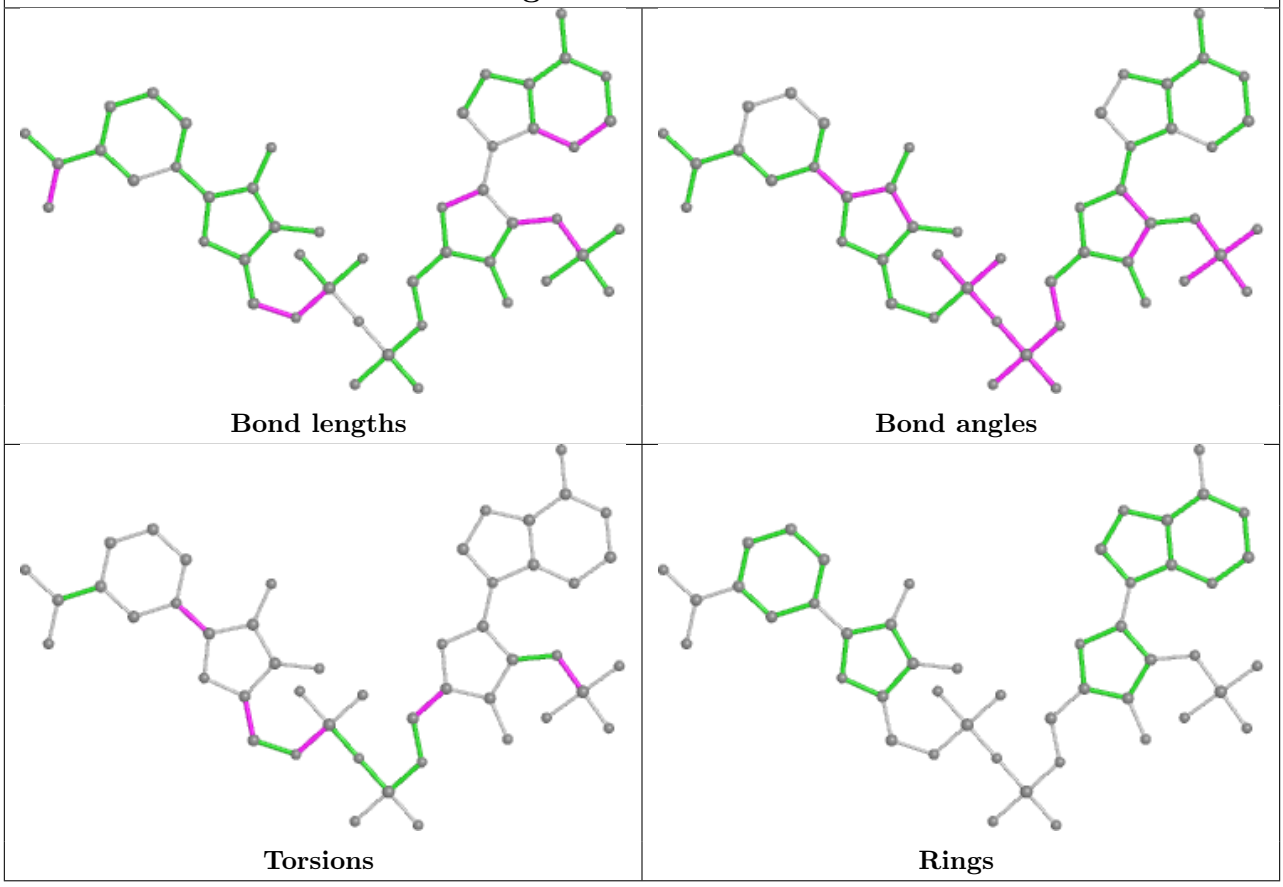


Torsions



Rings

Ligand NDP C 404



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

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

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

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

6.3 Carbohydrates

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

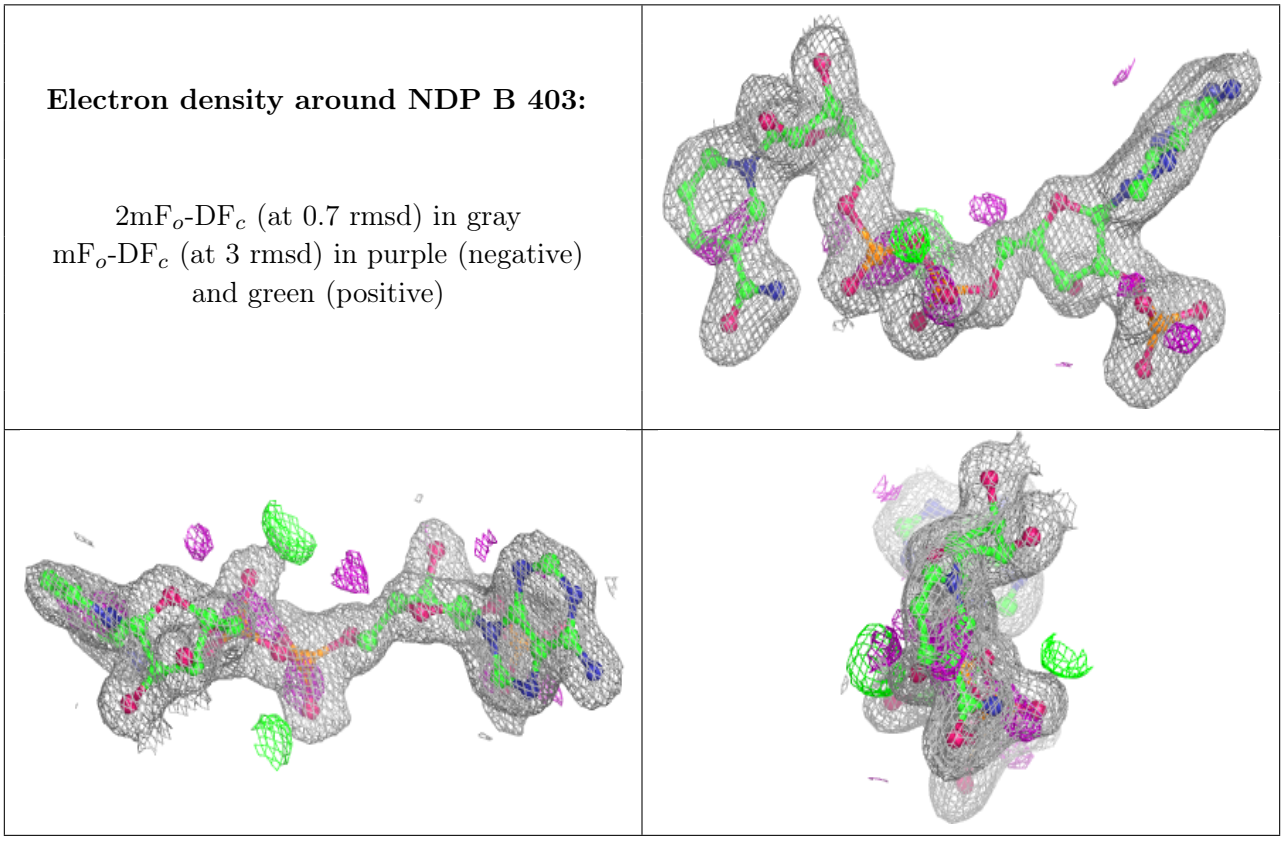
6.4 Ligands

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

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

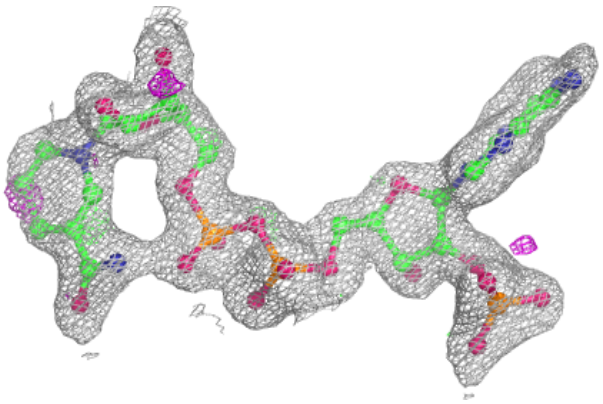
Electron density around NDP B 403:

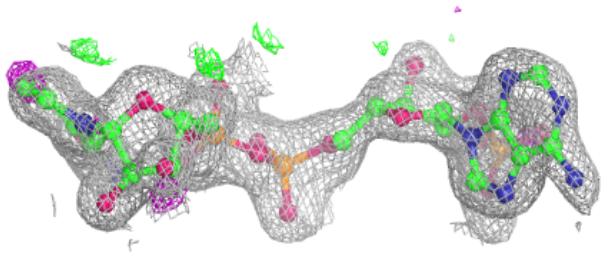
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

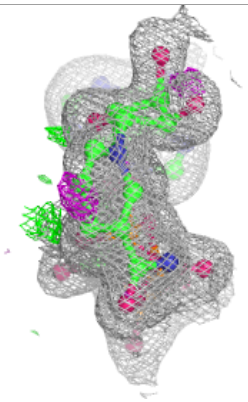


Electron density around NDP H 404:

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

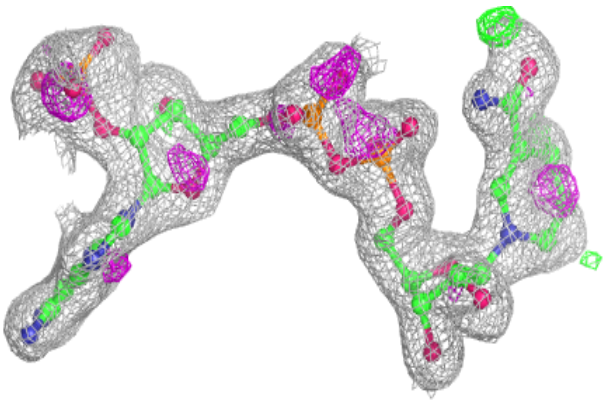


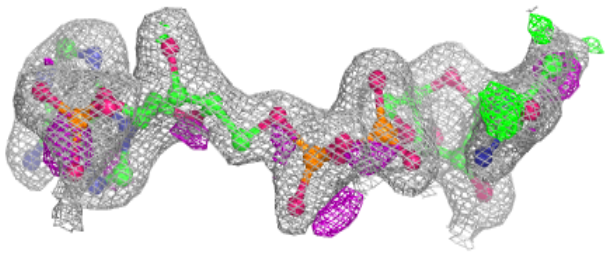


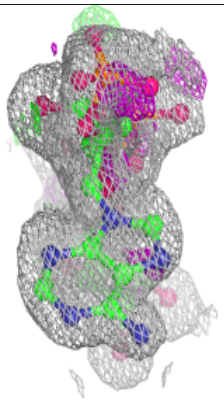


Electron density around NDP K 403:

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

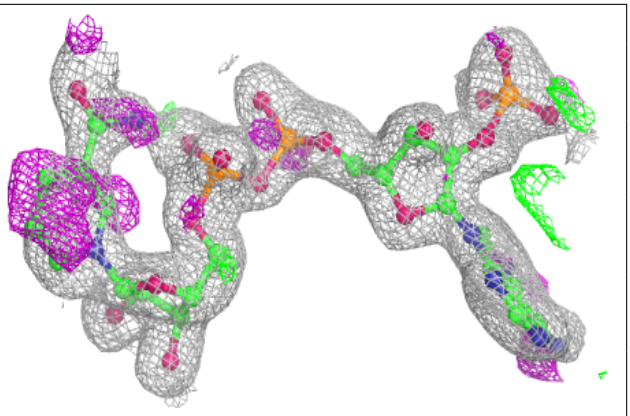


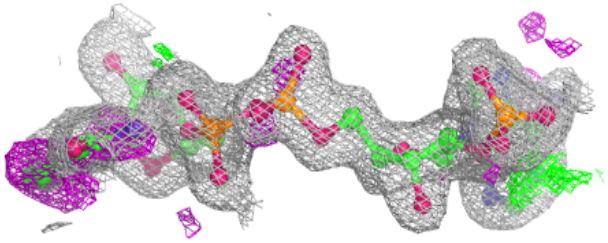


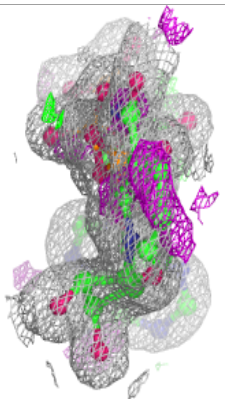


Electron density around NDP I 404:

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

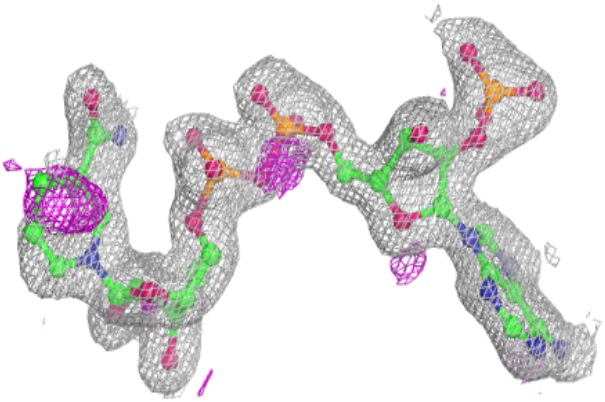


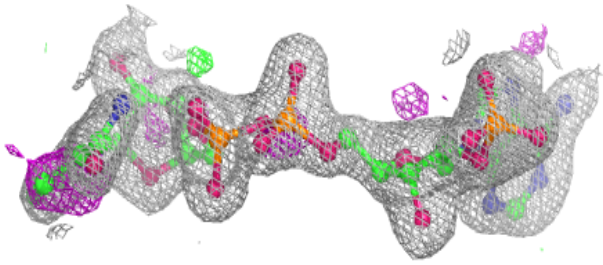


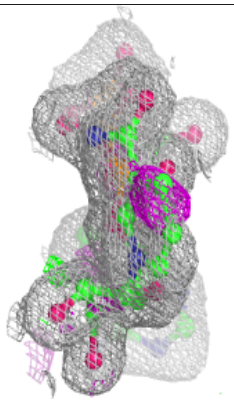


Electron density around NDP D 403:

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

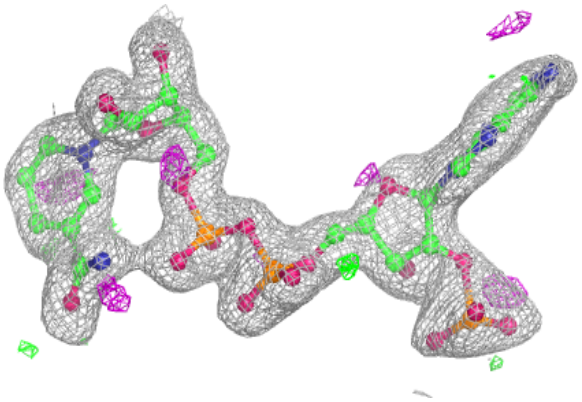


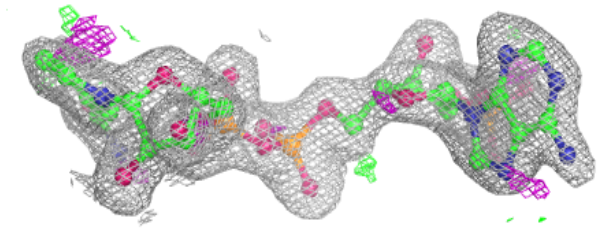


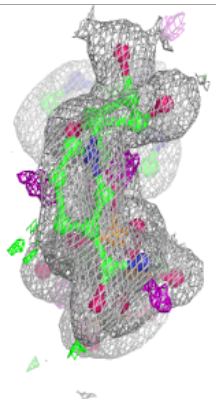


Electron density around NDP G 403:

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

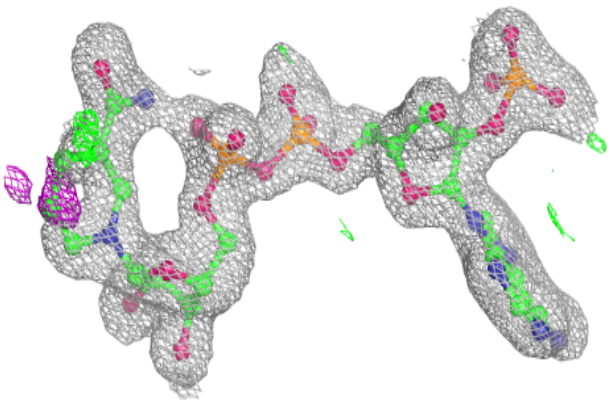


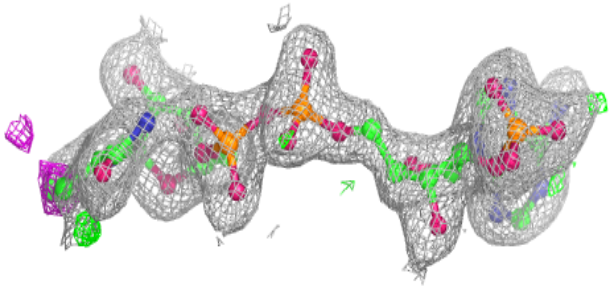


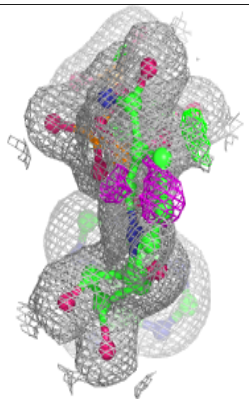


Electron density around NDP J 404:

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

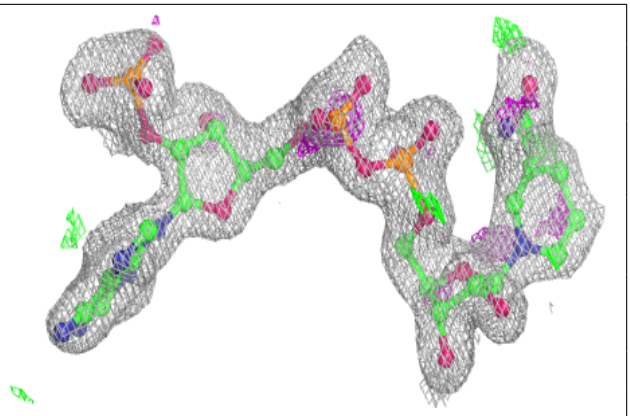


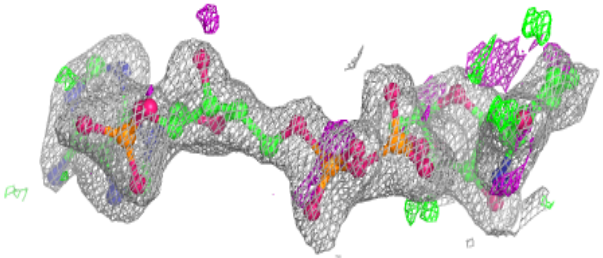


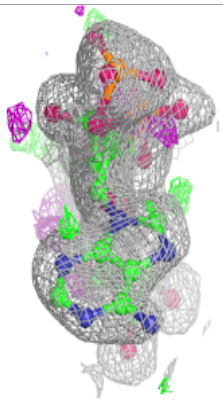


Electron density around NDP E 404:

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

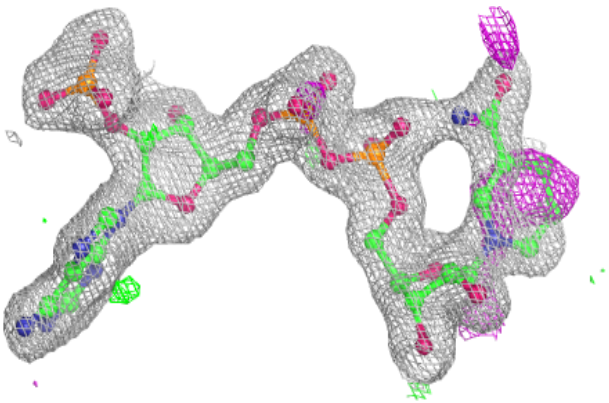


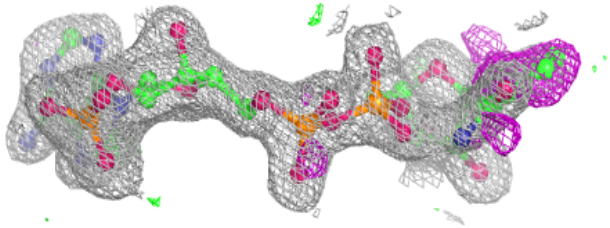


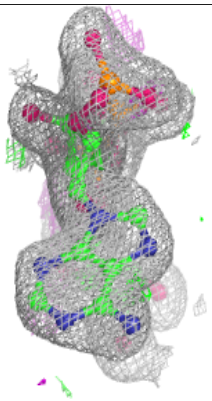


Electron density around NDP L 403:

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

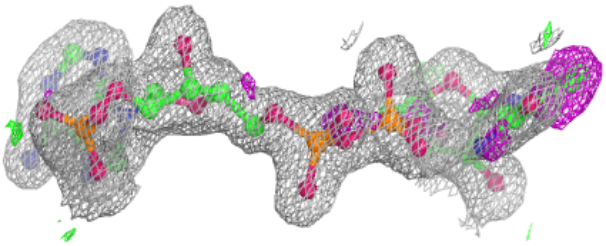


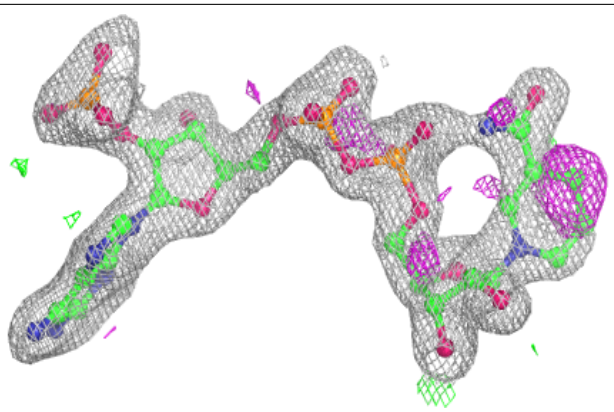


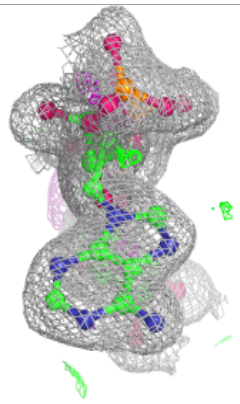


Electron density around NDP C 404:

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

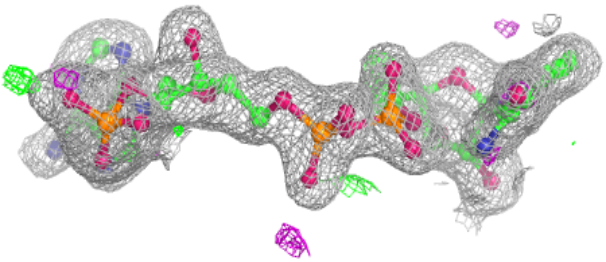


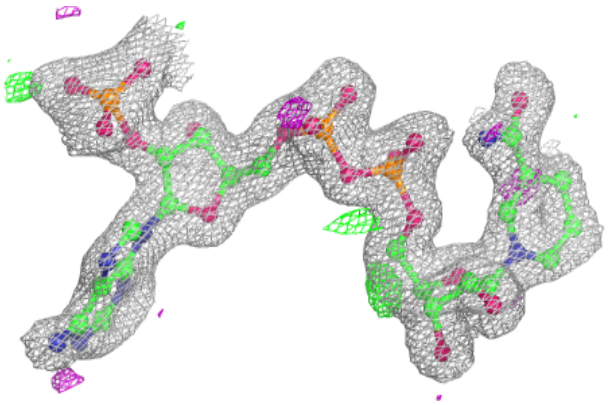


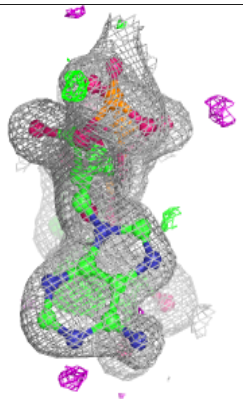


Electron density around NDP F 404:

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

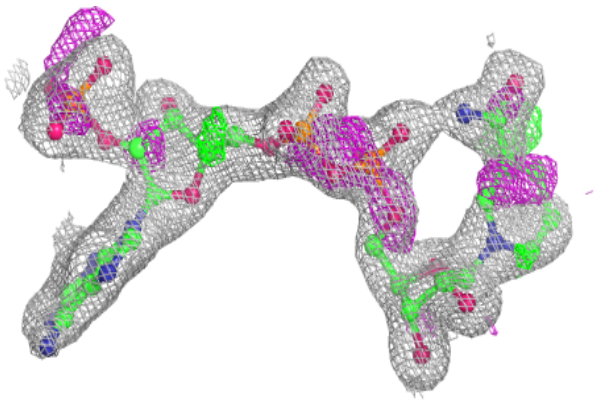


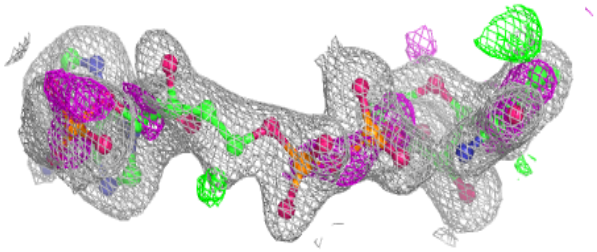


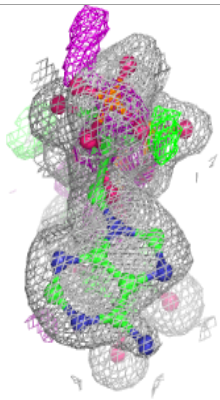


Electron density around NDP A 404:

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

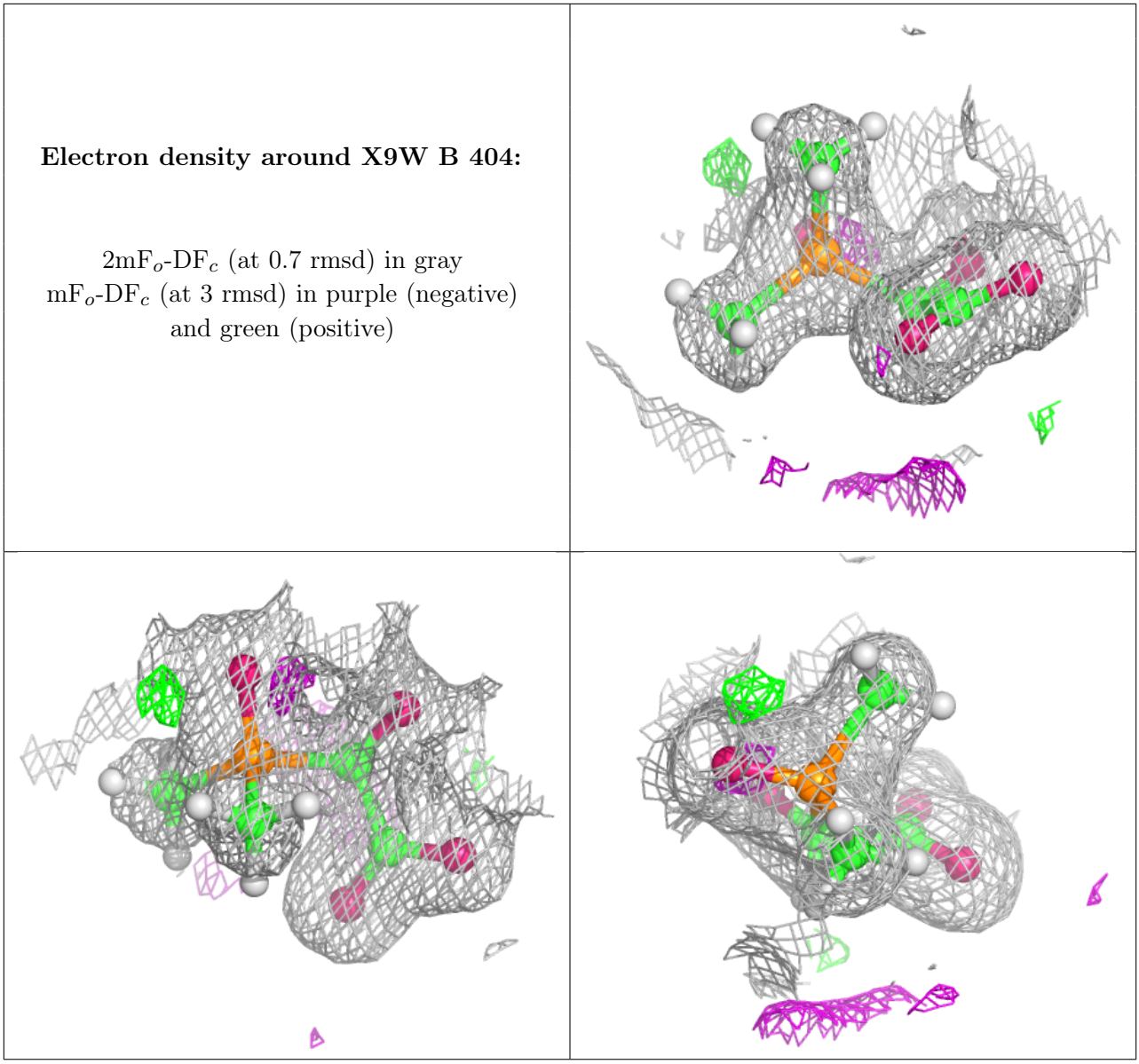






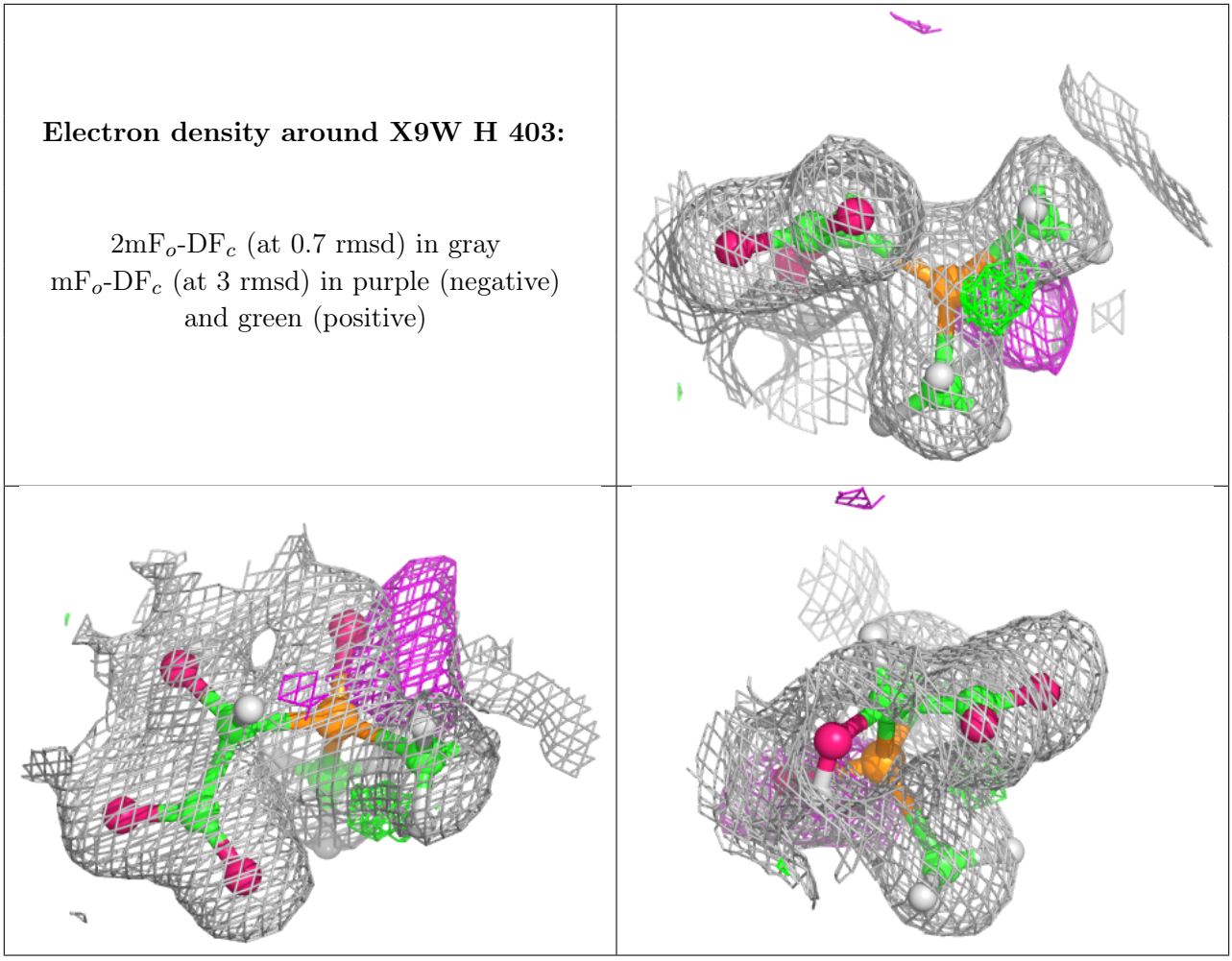
Electron density around X9W B 404:

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



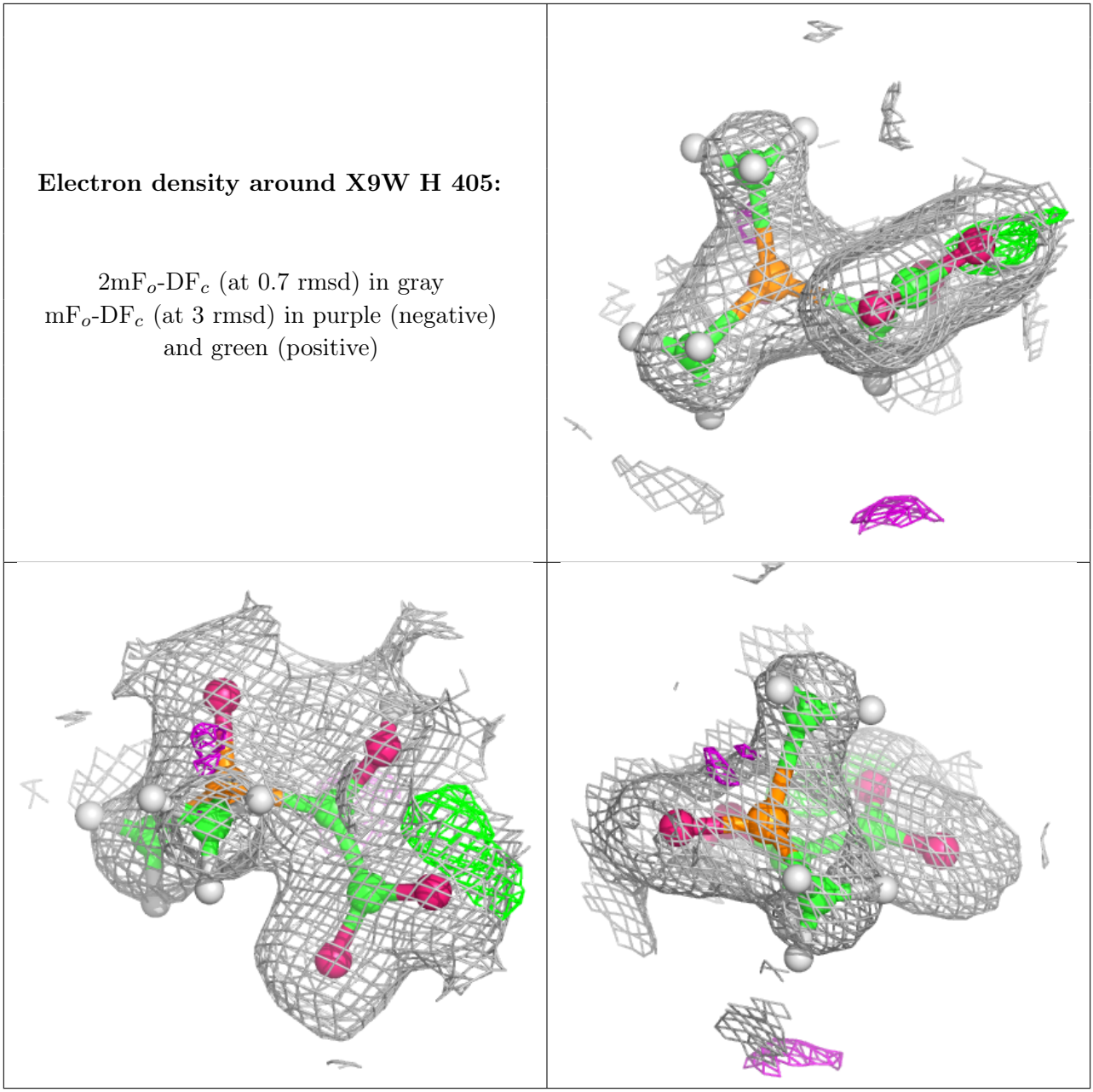
Electron density around X9W H 403:

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



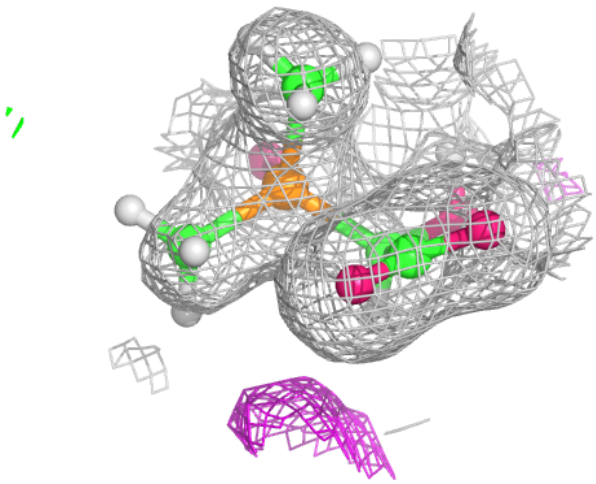
Electron density around X9W H 405:

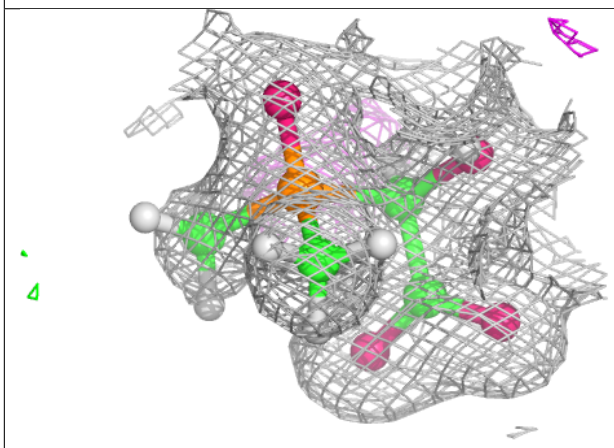
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

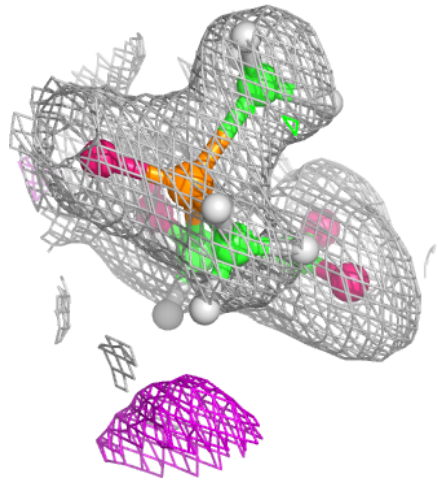


Electron density around X9W I 403:

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

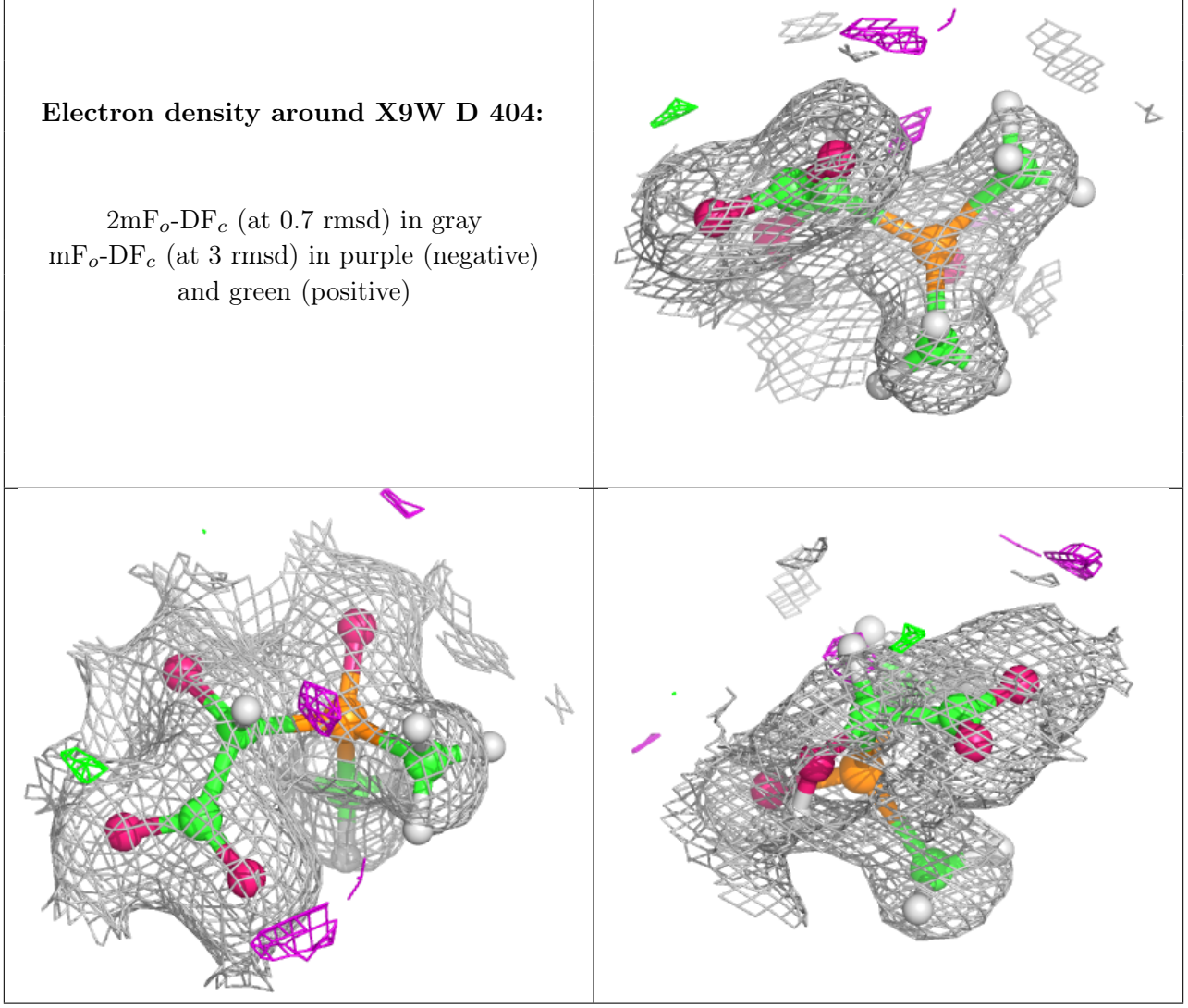






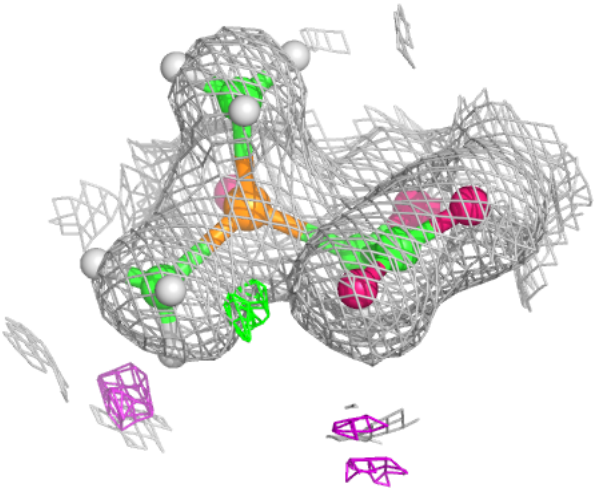
Electron density around X9W D 404:

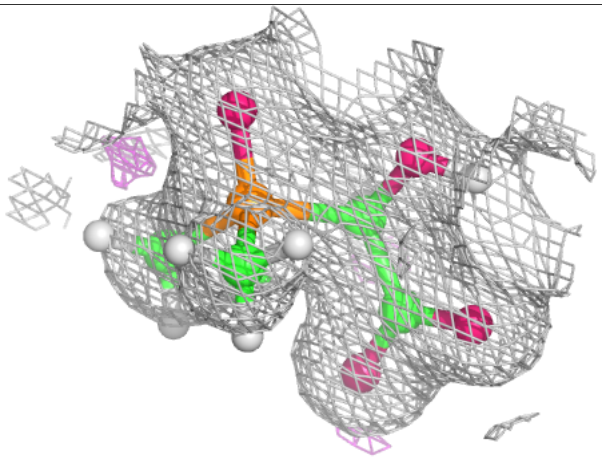
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

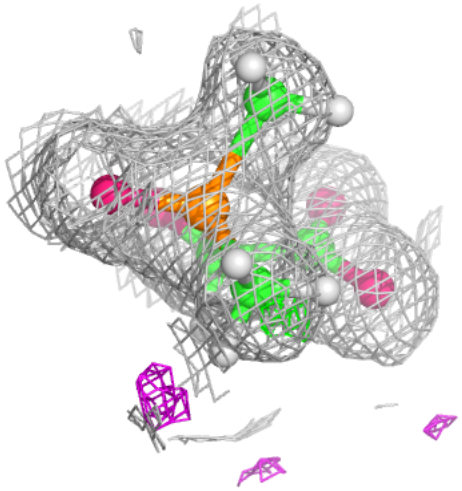


Electron density around X9W G 404:

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

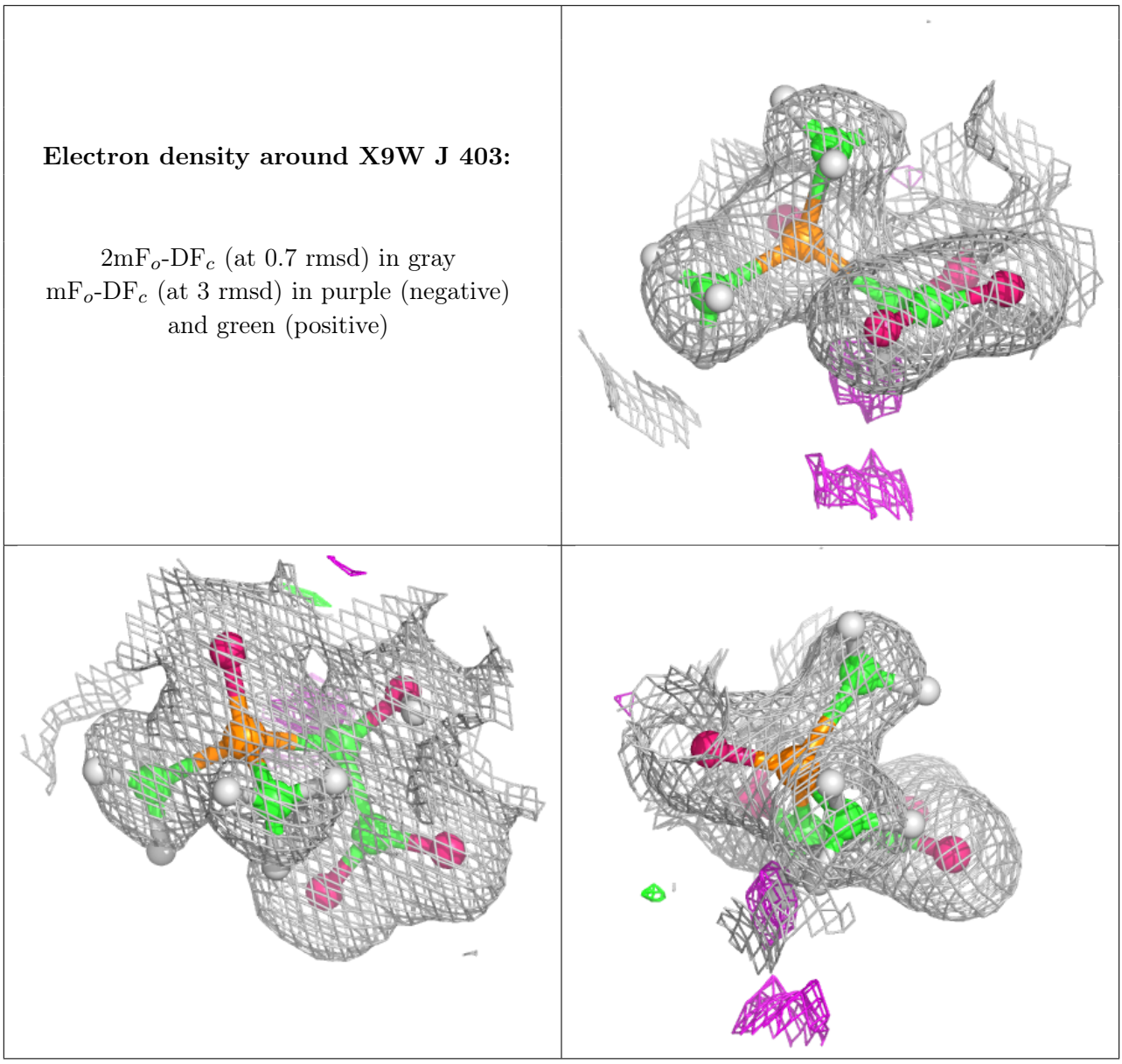






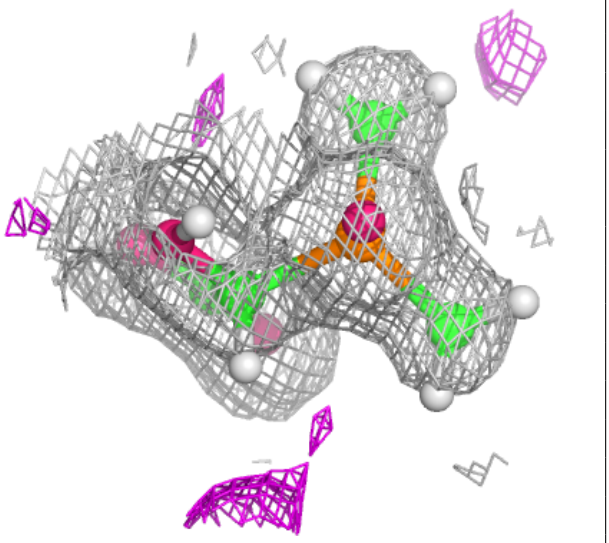
Electron density around X9W J 403:

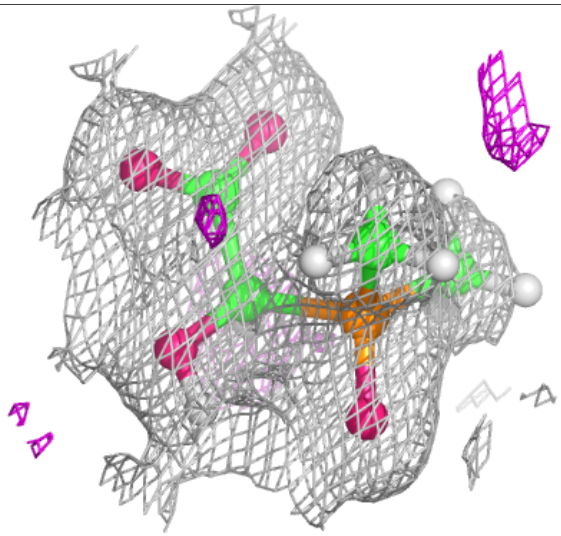
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

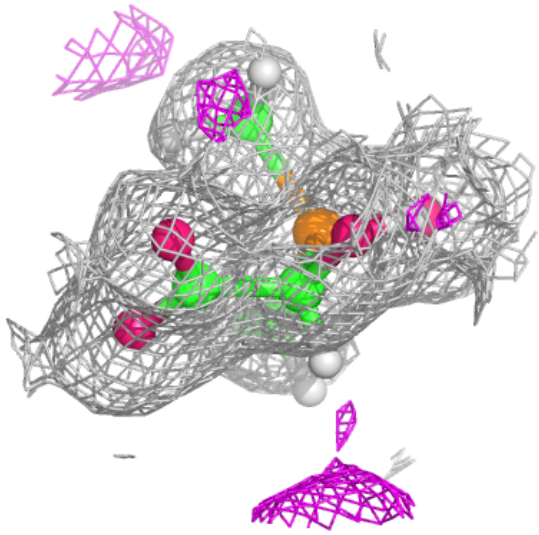


Electron density around X9W E 401:

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

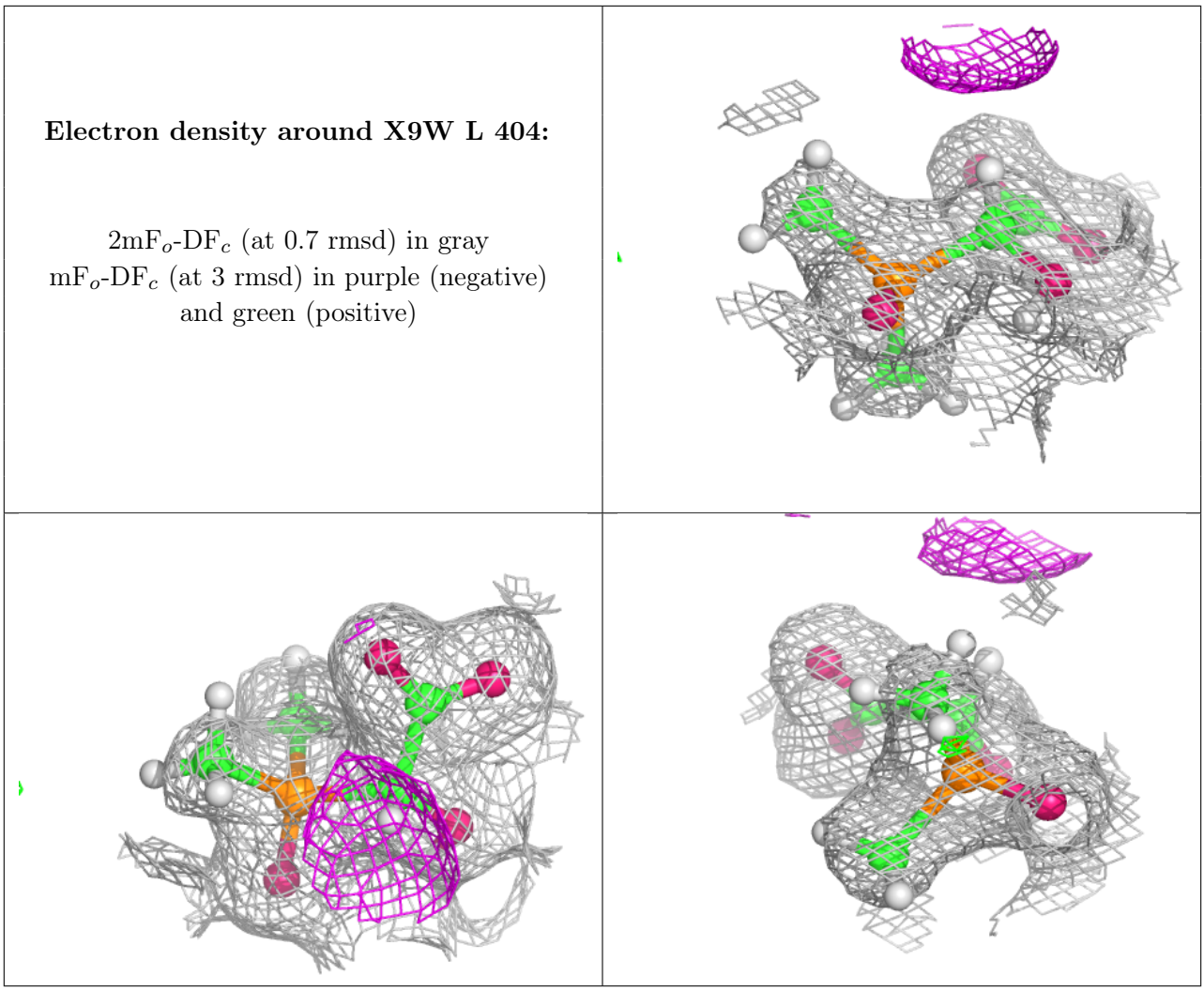






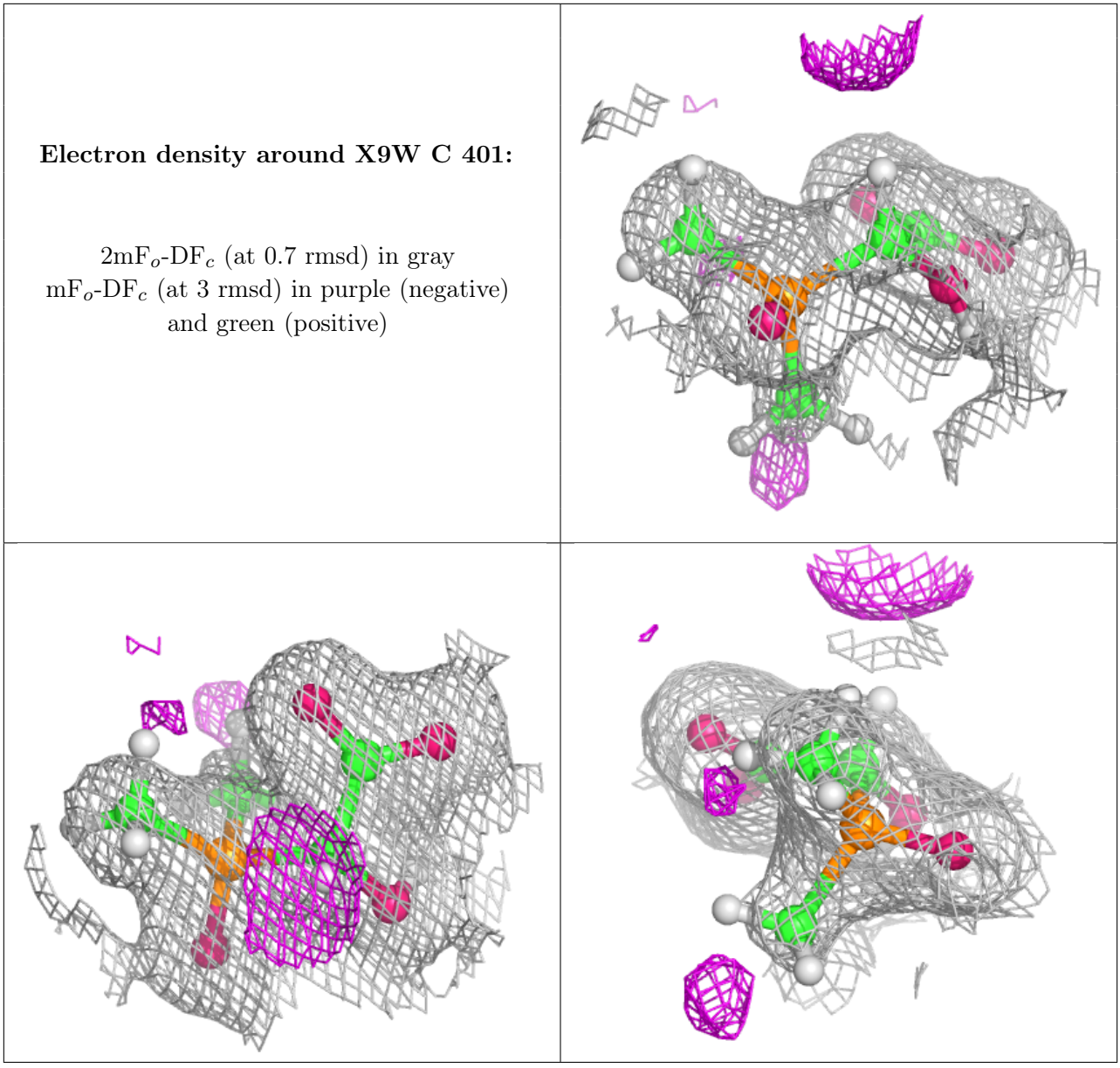
Electron density around X9W L 404:

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



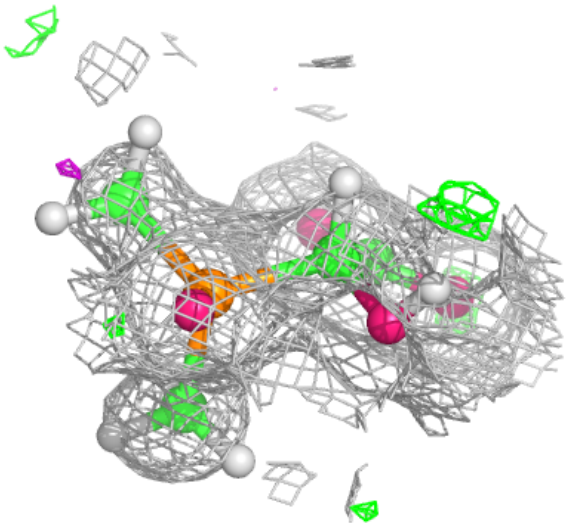
Electron density around X9W C 401:

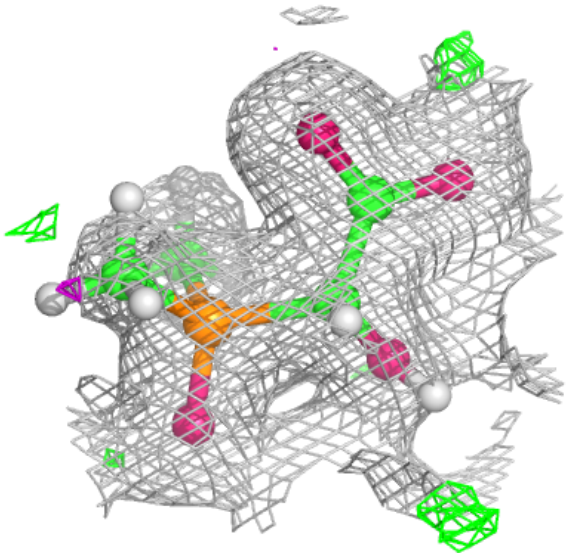
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

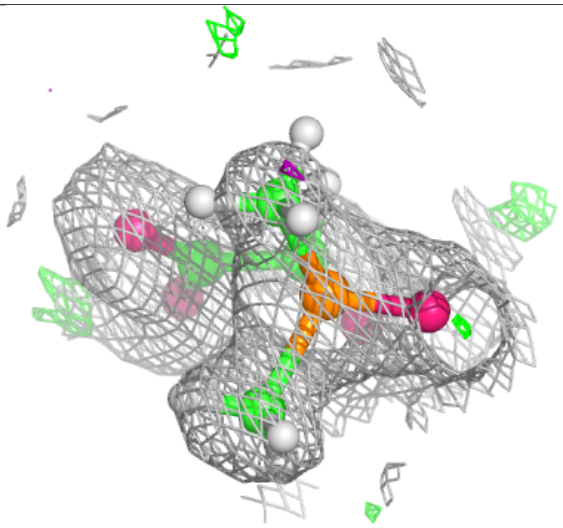


Electron density around X9W F 401:

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

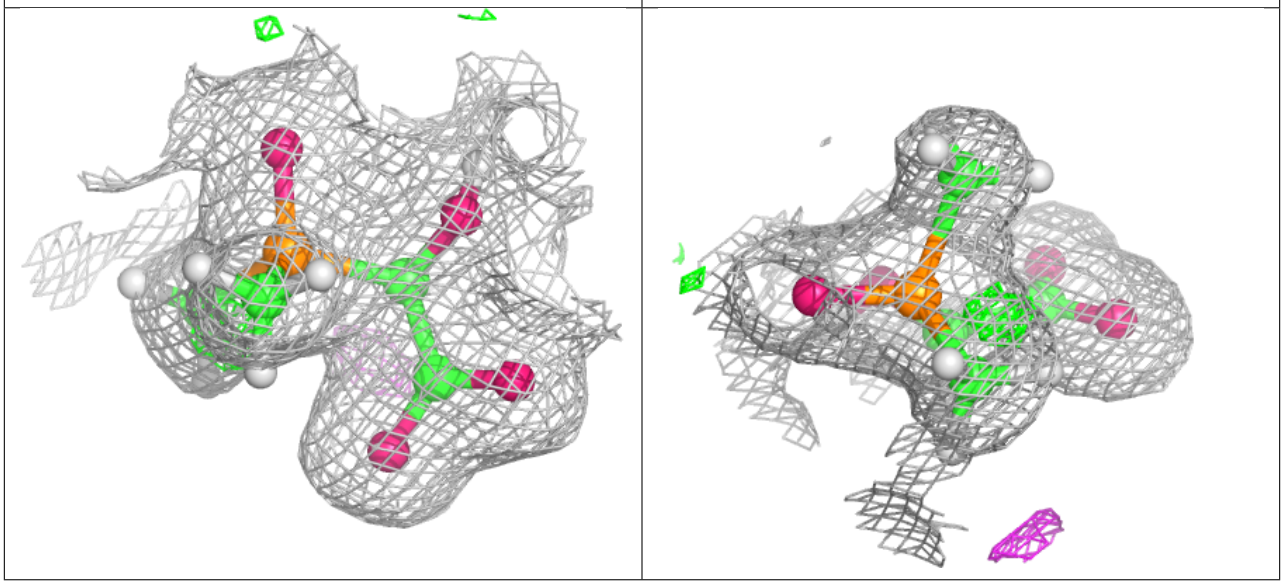






Electron density around X9W A 401:

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



6.5 Other polymers (i)

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