wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 06:36 PM EDT

PDB ID	:	6OM8
Title	:	Caenorhabditis Elegans UDP-Glucose Dehydrogenase in complex with UDP-Xylose
Authors	:	Beattie, N.R.; McDonald, W.E.; Hicks Sirmans, T.N.; Wood, Z.A.
Deposited on	:	2019-04-18
Resolution	:	2.45 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:

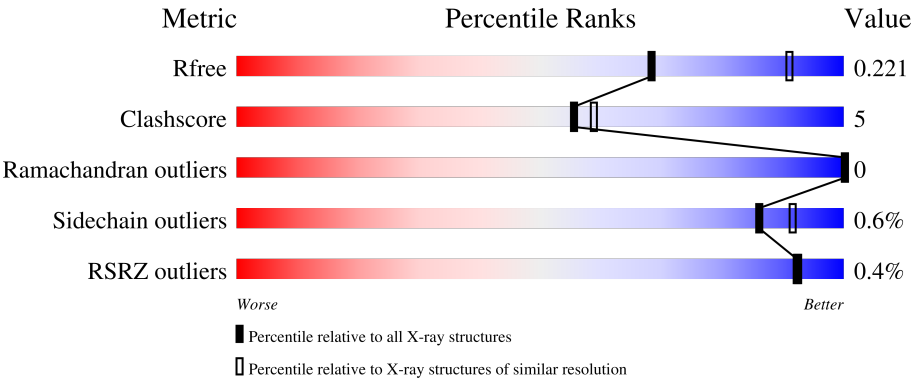
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.45 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	481	85% 11% ·
1	B	481	2% 85% 11% ·
1	C	481	87% 9% ·
1	D	481	84% 13% ·
1	E	481	86% 10% ·

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Mol	Chain	Length	Quality of chain
1	F	481	86% 11%
1	G	481	84% 12%
1	H	481	86% 10%
1	I	481	84% 12%
1	J	481	% 82% 12% 5%
1	K	481	88% 9%
1	L	481	% 85% 10%

2 Entry composition (i)

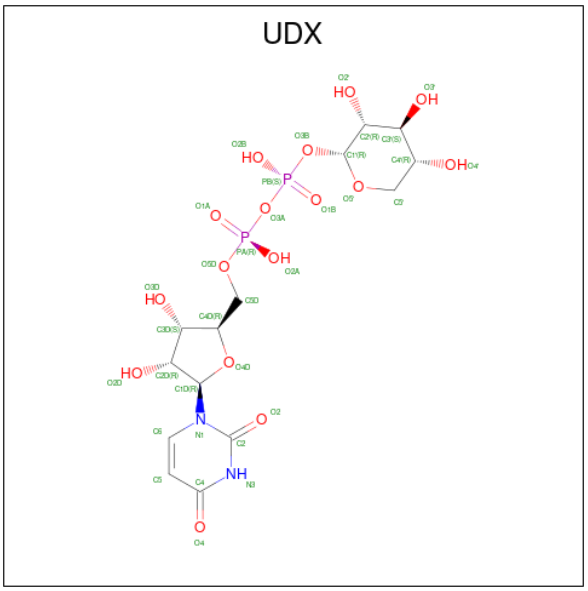
There are 3 unique types of molecules in this entry. The entry contains 44931 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3574	2268	614	677	15			
1	B	463	Total	C	N	O	S	0	1	0
			3577	2270	614	678	15			
1	C	463	Total	C	N	O	S	0	1	0
			3577	2270	614	678	15			
1	D	468	Total	C	N	O	S	0	1	0
			3615	2295	620	685	15			
1	E	461	Total	C	N	O	S	0	2	0
			3564	2261	612	676	15			
1	F	465	Total	C	N	O	S	0	3	0
			3598	2284	617	682	15			
1	G	462	Total	C	N	O	S	0	2	0
			3572	2268	613	676	15			
1	H	462	Total	C	N	O	S	0	3	0
			3580	2275	614	676	15			
1	I	462	Total	C	N	O	S	0	2	0
			3572	2268	613	676	15			
1	J	456	Total	C	N	O	S	0	1	0
			3525	2240	602	669	14			
1	K	464	Total	C	N	O	S	0	2	0
			3591	2280	616	680	15			
1	L	463	Total	C	N	O	S	0	2	0
			3576	2270	614	676	16			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-XYLOPYRANOSE (three-letter code: UDX) (formula: $C_{14}H_{22}N_2O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	A	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	B	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	B	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	C	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	C	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	D	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	D	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	E	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	E	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	F	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	F	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	G	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	G	1	Total	C	N	O	P	0	0
			34	14	2	16	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	H	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	I	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	I	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	J	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	J	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	K	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	K	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	L	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	L	1	Total	C	N	O	P	0	0
			34	14	2	16	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	90	Total	O	0	0
			90	90		
3	C	125	Total	O	0	0
			125	125		
3	D	135	Total	O	0	0
			135	135		
3	E	117	Total	O	0	0
			117	117		
3	F	123	Total	O	0	0
			123	123		
3	G	74	Total	O	0	0
			74	74		
3	H	107	Total	O	0	0
			107	107		
3	I	74	Total	O	0	0
			74	74		

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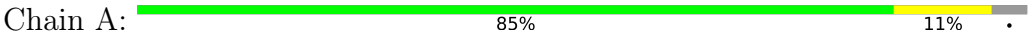
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	42	Total O 42 42	0	0
3	K	107	Total O 107 107	0	0
3	L	73	Total O 73 73	0	0

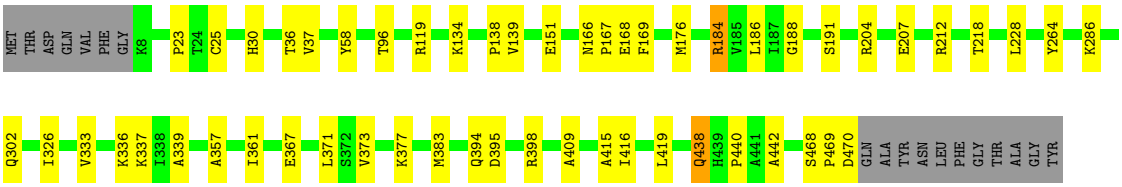
3 Residue-property plots (i)

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: UDP-glucose 6-dehydrogenase

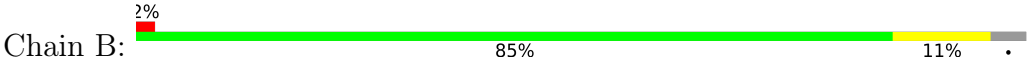
Chain A:

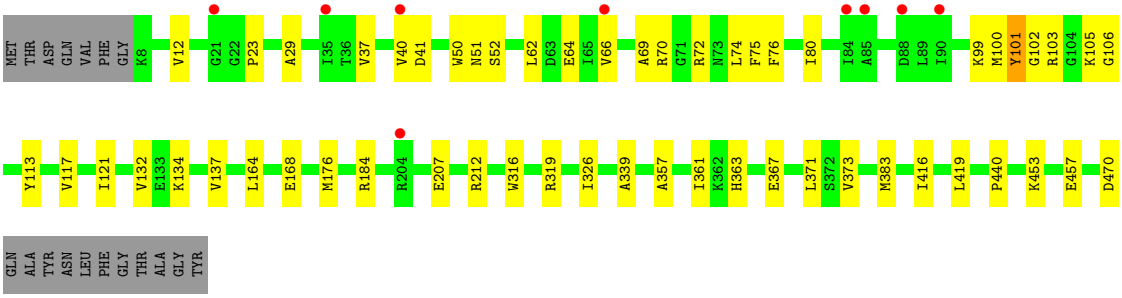




• Molecule 1: UDP-glucose 6-dehydrogenase

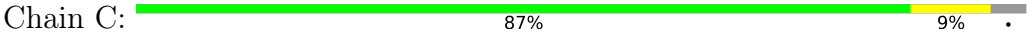
Chain B:

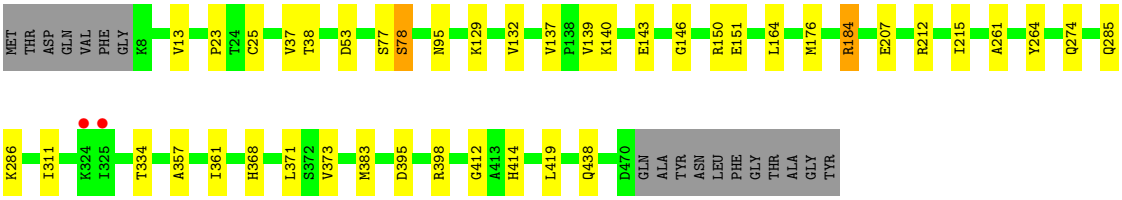




• Molecule 1: UDP-glucose 6-dehydrogenase

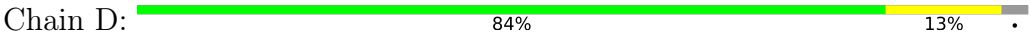
Chain C:

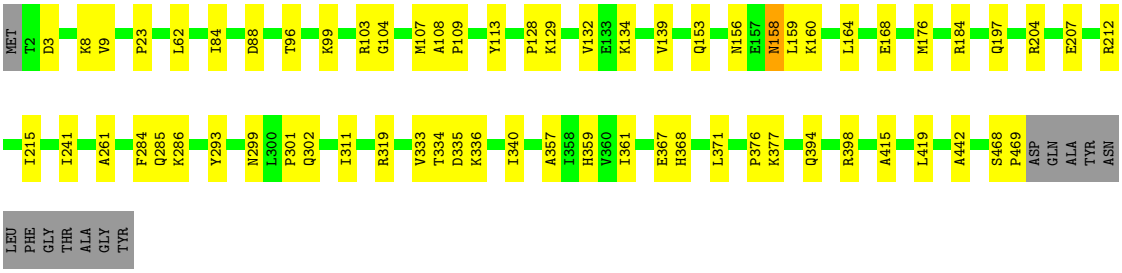




• Molecule 1: UDP-glucose 6-dehydrogenase

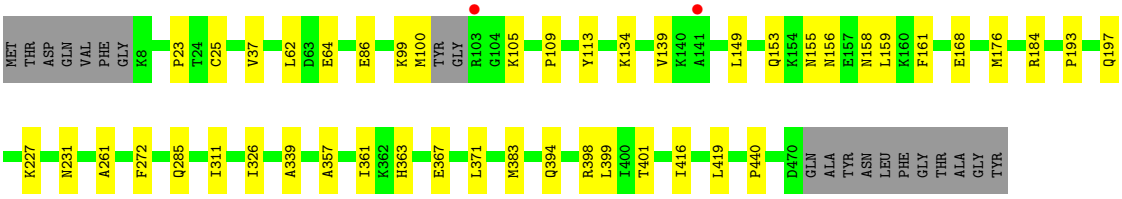
Chain D:





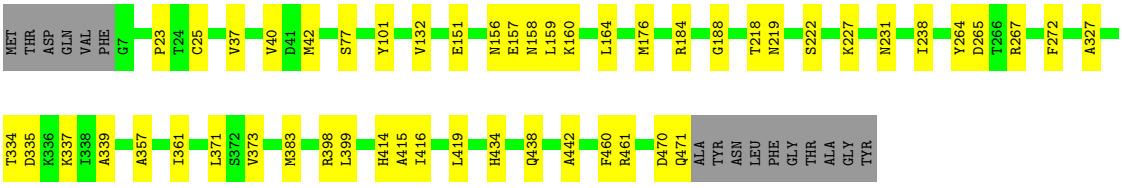
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain E:



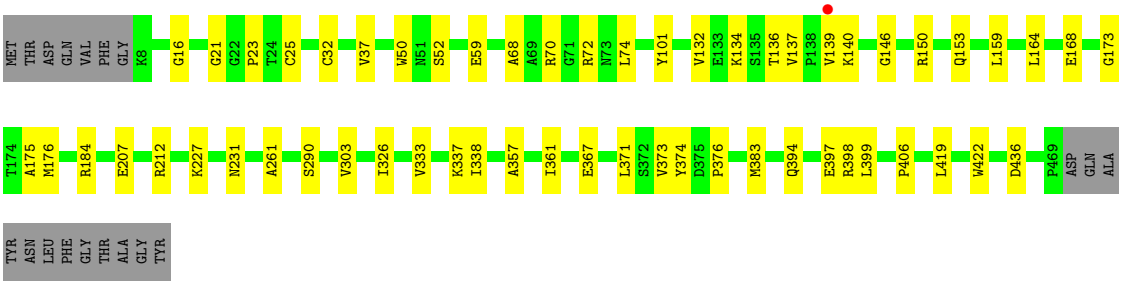
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain F:



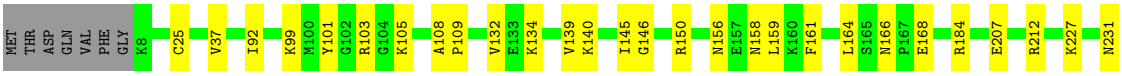
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain G:



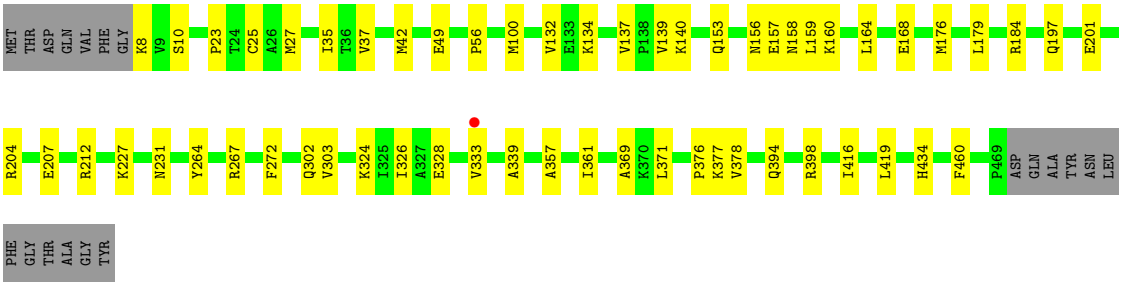
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain H:



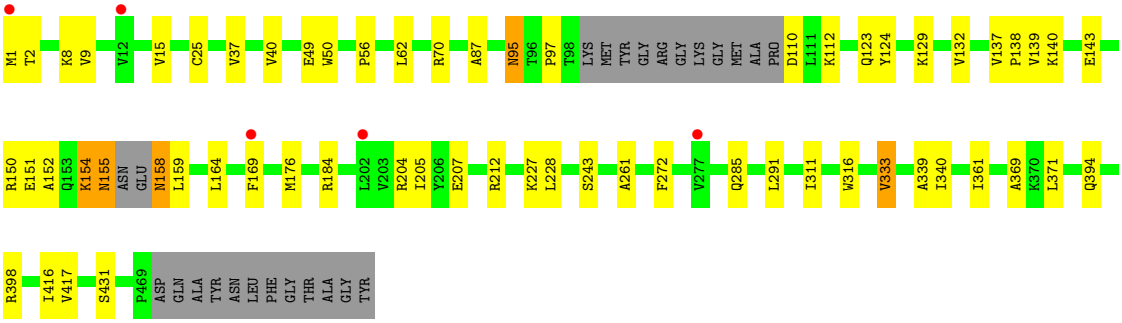
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain I:



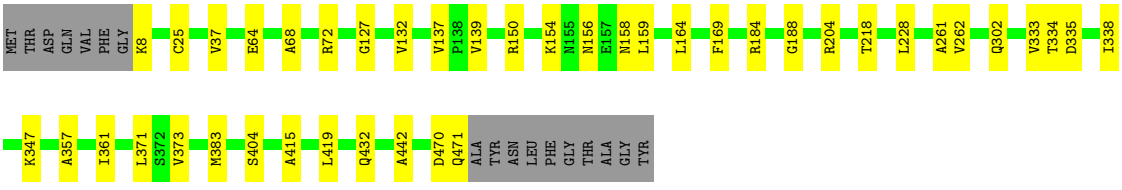
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain J:



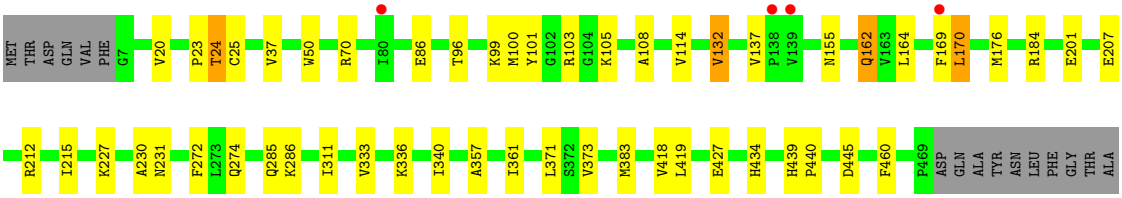
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain K:



• Molecule 1: UDP-glucose 6-dehydrogenase

Chain L:



GLY
TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	157.71Å 168.17Å 279.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.70 – 2.45 88.82 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.1 (52.70-2.45) 98.1 (88.82-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.194 , 0.220 0.194 , 0.221	Depositor DCC
R_{free} test set	1847 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	44931	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: UDX

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	0.49	0/3643	0.52	0/4941
1	B	0.43	0/3649	0.52	0/4949
1	C	0.43	0/3649	0.53	0/4949
1	D	0.44	0/3688	0.51	0/5002
1	E	0.41	0/3637	0.52	0/4931
1	F	0.47	0/3676	0.52	0/4985
1	G	0.37	0/3647	0.51	0/4946
1	H	0.43	0/3658	0.50	0/4961
1	I	0.38	0/3647	0.49	0/4946
1	J	0.47	0/3594	0.56	0/4875
1	K	0.44	0/3666	0.53	0/4972
1	L	0.42	0/3651	0.50	0/4951
All	All	0.43	0/43805	0.52	0/59408

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3574	0	3584	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3577	0	3589	49	0
1	C	3577	0	3589	31	0
1	D	3615	0	3625	44	0
1	E	3564	0	3581	37	0
1	F	3598	0	3616	38	0
1	G	3572	0	3590	42	0
1	H	3580	0	3604	30	0
1	I	3572	0	3590	40	0
1	J	3525	0	3536	62	0
1	K	3591	0	3608	29	0
1	L	3576	0	3593	40	0
2	A	68	0	40	0	0
2	B	68	0	40	0	0
2	C	68	0	40	1	0
2	D	68	0	40	2	0
2	E	68	0	40	1	0
2	F	68	0	40	1	0
2	G	68	0	40	1	0
2	H	68	0	40	0	0
2	I	68	0	40	1	0
2	J	68	0	40	1	0
2	K	68	0	40	0	0
2	L	68	0	40	0	0
3	A	127	0	0	5	0
3	B	90	0	0	3	0
3	C	125	0	0	3	0
3	D	135	0	0	3	0
3	E	117	0	0	7	0
3	F	123	0	0	2	0
3	G	74	0	0	5	0
3	H	107	0	0	0	0
3	I	74	0	0	2	0
3	J	42	0	0	1	0
3	K	107	0	0	4	0
3	L	73	0	0	4	0
All	All	44931	0	43585	444	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 444 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:E:184:ARG:NH1	1:F:265:ASP:HB2	1.49	1.27
1:B:40:VAL:HG11	1:B:80:ILE:HG12	1.31	1.12
1:A:204:ARG:HD3	3:A:663:HOH:O	1.53	1.07
1:I:333:VAL:HG12	1:I:369:ALA:HB2	1.36	1.07
1:E:184:ARG:HH12	1:F:265:ASP:HB2	0.97	1.06

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/481 (96%)	444 (96%)	17 (4%)	0	100	100
1	B	462/481 (96%)	444 (96%)	18 (4%)	0	100	100
1	C	462/481 (96%)	446 (96%)	16 (4%)	0	100	100
1	D	467/481 (97%)	448 (96%)	19 (4%)	0	100	100
1	E	459/481 (95%)	444 (97%)	15 (3%)	0	100	100
1	F	466/481 (97%)	448 (96%)	18 (4%)	0	100	100
1	G	462/481 (96%)	448 (97%)	14 (3%)	0	100	100
1	H	463/481 (96%)	446 (96%)	17 (4%)	0	100	100
1	I	462/481 (96%)	449 (97%)	13 (3%)	0	100	100
1	J	451/481 (94%)	437 (97%)	14 (3%)	0	100	100
1	K	464/481 (96%)	451 (97%)	13 (3%)	0	100	100
1	L	463/481 (96%)	449 (97%)	14 (3%)	0	100	100
All	All	5542/5772 (96%)	5354 (97%)	188 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	386/399 (97%)	384 (100%)	2 (0%)	88 93
1	B	387/399 (97%)	384 (99%)	3 (1%)	81 88
1	C	387/399 (97%)	385 (100%)	2 (0%)	88 93
1	D	391/399 (98%)	390 (100%)	1 (0%)	92 95
1	E	387/399 (97%)	387 (100%)	0	100 100
1	F	390/399 (98%)	388 (100%)	2 (0%)	88 93
1	G	387/399 (97%)	384 (99%)	3 (1%)	81 88
1	H	388/399 (97%)	387 (100%)	1 (0%)	92 95
1	I	387/399 (97%)	386 (100%)	1 (0%)	92 95
1	J	383/399 (96%)	377 (98%)	6 (2%)	62 74
1	K	389/399 (98%)	388 (100%)	1 (0%)	92 95
1	L	387/399 (97%)	379 (98%)	8 (2%)	53 66
All	All	4649/4788 (97%)	4619 (99%)	30 (1%)	86 91

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	272	PHE
1	L	162	GLN
1	J	155	ASN
1	L	272	PHE
1	L	114	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	219	ASN
1	F	452	GLN
1	K	158	ASN
1	J	158	ASN

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Mol	Chain	Res	Type
1	B	414	HIS

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)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	UDX	K	500	-	33,36,36	0.95	2 (6%)	50,55,55	1.44	6 (12%)
2	UDX	K	501	-	33,36,36	0.95	2 (6%)	50,55,55	1.38	7 (14%)
2	UDX	F	500	-	33,36,36	0.99	4 (12%)	50,55,55	1.40	5 (10%)
2	UDX	E	501	-	33,36,36	0.97	2 (6%)	50,55,55	1.42	5 (10%)
2	UDX	D	500	-	33,36,36	0.96	2 (6%)	50,55,55	1.40	7 (14%)
2	UDX	C	500	-	33,36,36	0.98	2 (6%)	50,55,55	1.43	5 (10%)
2	UDX	G	500	-	33,36,36	0.98	2 (6%)	50,55,55	1.36	6 (12%)
2	UDX	I	501	-	33,36,36	0.93	3 (9%)	50,55,55	1.44	6 (12%)
2	UDX	B	500	-	33,36,36	0.96	2 (6%)	50,55,55	1.46	7 (14%)
2	UDX	G	501	-	33,36,36	0.94	2 (6%)	50,55,55	1.46	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	UDX	L	500	-	33,36,36	0.95	3 (9%)	50,55,55	1.49	6 (12%)
2	UDX	L	501	-	33,36,36	0.98	3 (9%)	50,55,55	1.36	5 (10%)
2	UDX	C	501	-	33,36,36	0.97	2 (6%)	50,55,55	1.37	6 (12%)
2	UDX	D	501	-	33,36,36	1.00	3 (9%)	50,55,55	1.48	6 (12%)
2	UDX	H	501	-	33,36,36	0.95	2 (6%)	50,55,55	1.36	5 (10%)
2	UDX	J	501	-	33,36,36	0.97	3 (9%)	50,55,55	1.42	6 (12%)
2	UDX	A	500	-	33,36,36	0.94	1 (3%)	50,55,55	1.43	6 (12%)
2	UDX	E	500	-	33,36,36	0.95	2 (6%)	50,55,55	1.45	7 (14%)
2	UDX	A	501	-	33,36,36	0.94	2 (6%)	50,55,55	1.45	7 (14%)
2	UDX	F	501	-	33,36,36	0.96	2 (6%)	50,55,55	1.52	7 (14%)
2	UDX	I	500	-	33,36,36	0.99	2 (6%)	50,55,55	1.43	6 (12%)
2	UDX	B	501	-	33,36,36	0.98	2 (6%)	50,55,55	1.41	5 (10%)
2	UDX	J	500	-	33,36,36	0.99	3 (9%)	50,55,55	1.33	5 (10%)
2	UDX	H	500	-	33,36,36	0.98	2 (6%)	50,55,55	1.40	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDX	K	500	-	-	6/21/54/54	0/3/3/3
2	UDX	K	501	-	-	4/21/54/54	0/3/3/3
2	UDX	F	500	-	-	4/21/54/54	0/3/3/3
2	UDX	E	501	-	-	1/21/54/54	0/3/3/3
2	UDX	D	500	-	-	5/21/54/54	0/3/3/3
2	UDX	C	500	-	-	6/21/54/54	0/3/3/3
2	UDX	G	500	-	-	5/21/54/54	0/3/3/3
2	UDX	I	501	-	-	4/21/54/54	0/3/3/3
2	UDX	B	500	-	-	8/21/54/54	0/3/3/3
2	UDX	G	501	-	-	6/21/54/54	0/3/3/3
2	UDX	L	500	-	-	5/21/54/54	0/3/3/3
2	UDX	L	501	-	-	4/21/54/54	0/3/3/3
2	UDX	C	501	-	-	4/21/54/54	0/3/3/3
2	UDX	D	501	-	-	4/21/54/54	0/3/3/3
2	UDX	H	501	-	-	4/21/54/54	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDX	J	501	-	-	5/21/54/54	0/3/3/3
2	UDX	A	500	-	-	6/21/54/54	0/3/3/3
2	UDX	E	500	-	-	4/21/54/54	0/3/3/3
2	UDX	A	501	-	-	4/21/54/54	0/3/3/3
2	UDX	F	501	-	-	9/21/54/54	0/3/3/3
2	UDX	I	500	-	-	6/21/54/54	0/3/3/3
2	UDX	B	501	-	-	8/21/54/54	0/3/3/3
2	UDX	J	500	-	-	4/21/54/54	0/3/3/3
2	UDX	H	500	-	-	6/21/54/54	0/3/3/3

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	UDX	C4-N3	-2.73	1.33	1.38
2	L	501	UDX	C4-N3	-2.69	1.33	1.38
2	D	501	UDX	C4-N3	-2.65	1.33	1.38
2	C	500	UDX	C4-N3	-2.63	1.33	1.38
2	B	501	UDX	C4-N3	-2.62	1.33	1.38

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	UDX	C4-N3-C2	-5.32	119.56	126.58
2	D	501	UDX	C4-N3-C2	-5.02	119.95	126.58
2	B	501	UDX	C4-N3-C2	-4.87	120.16	126.58
2	G	501	UDX	C4-N3-C2	-4.83	120.21	126.58
2	J	501	UDX	C4-N3-C2	-4.82	120.23	126.58

There are no chirality outliers.

5 of 122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	UDX	C1'-O3B-PB-O2B
2	A	501	UDX	PA-O3A-PB-O3B
2	B	500	UDX	C1'-O3B-PB-O2B
2	B	501	UDX	C5D-O5D-PA-O2A
2	C	500	UDX	C1'-O3B-PB-O2B

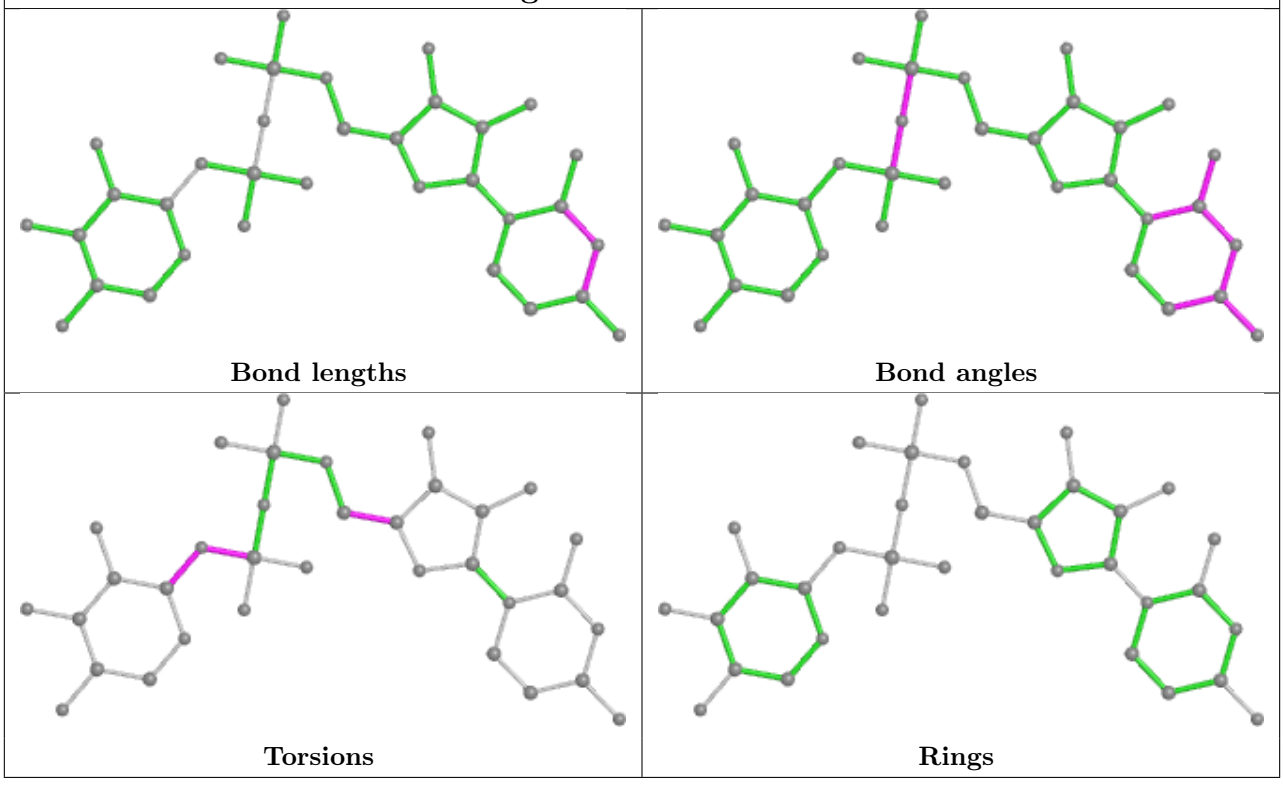
There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	500	UDX	1	0
2	D	500	UDX	1	0
2	C	500	UDX	1	0
2	G	500	UDX	1	0
2	D	501	UDX	1	0
2	E	500	UDX	1	0
2	I	500	UDX	1	0
2	J	500	UDX	1	0

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

Ligand UDX K 500



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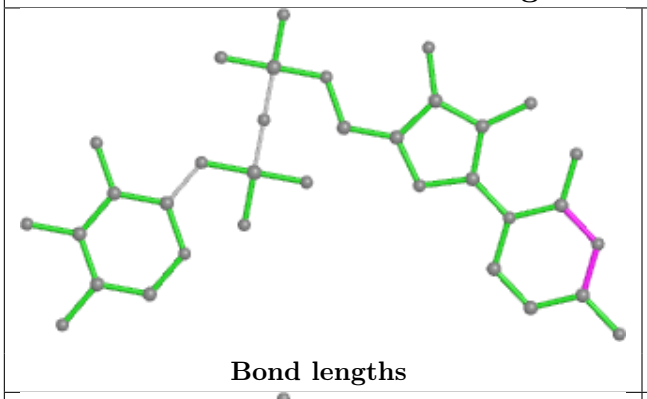
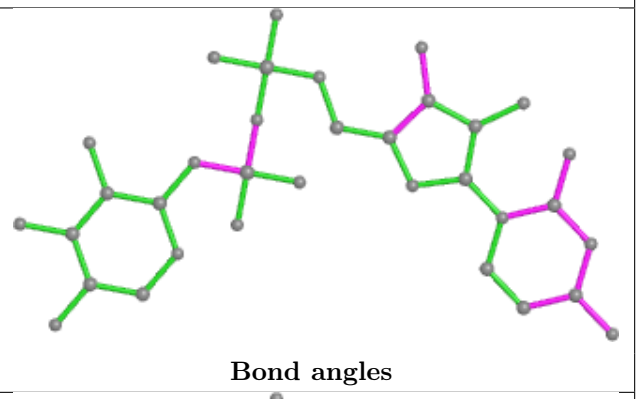
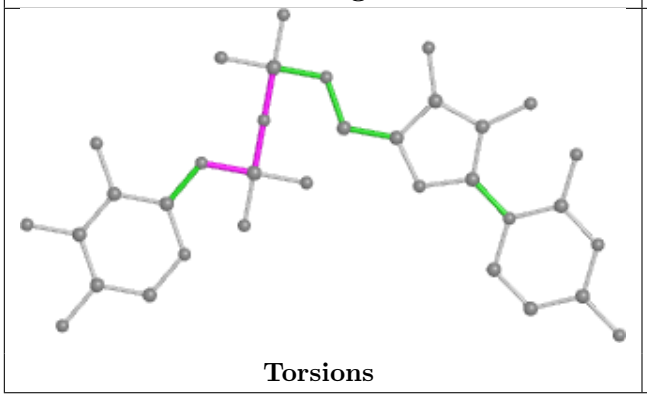


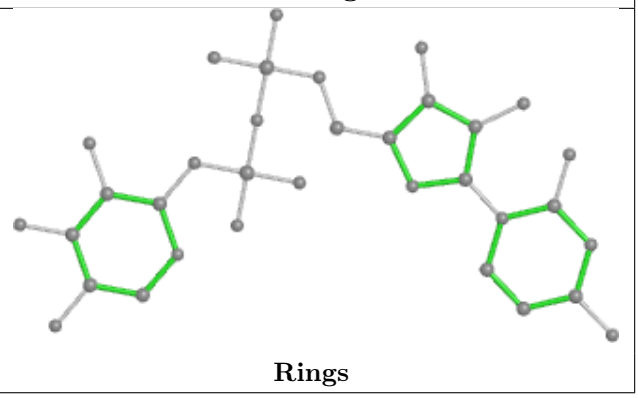
Bond lengths



Bond angles

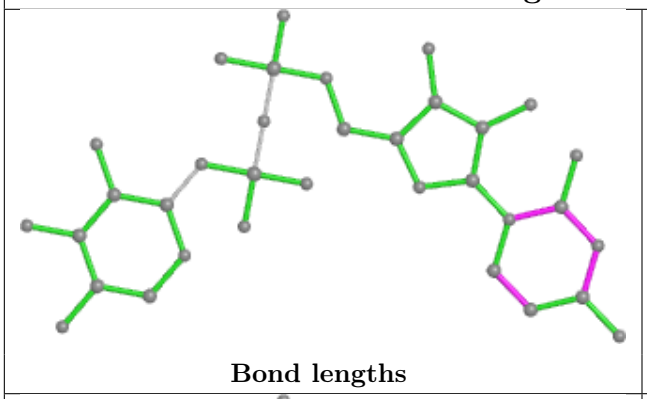


Torsions



Rings

Ligand UDX F 500



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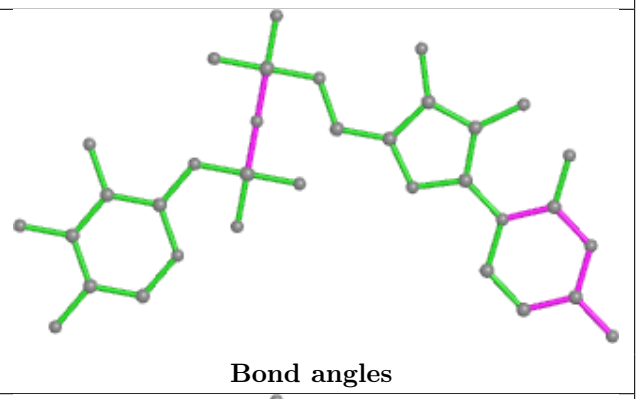

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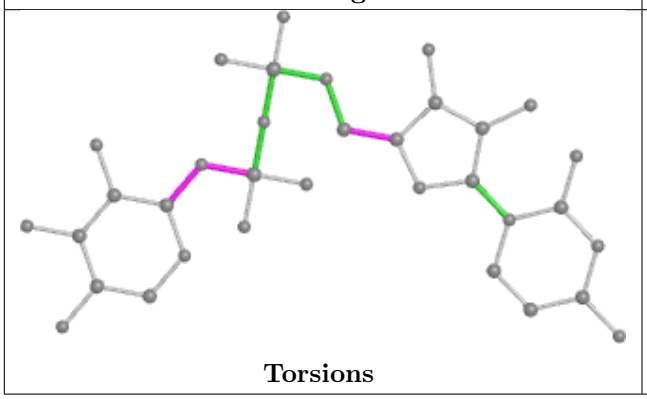

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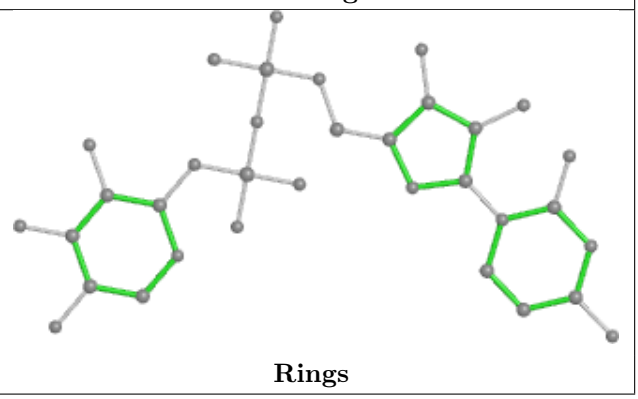

Rings

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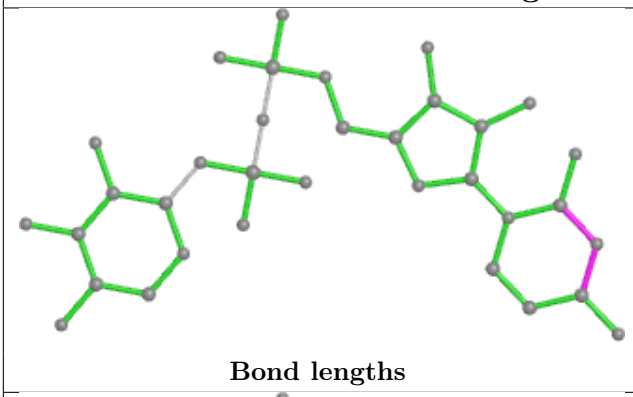

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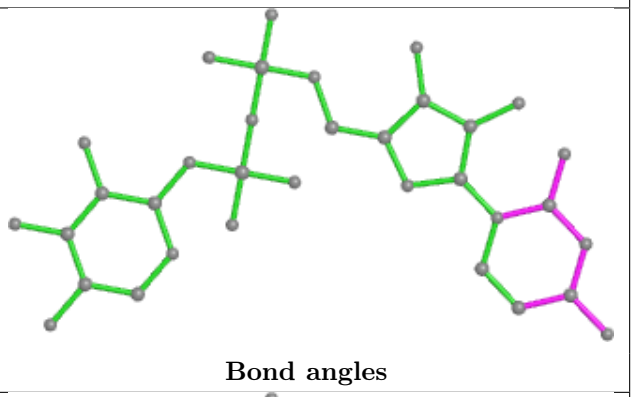
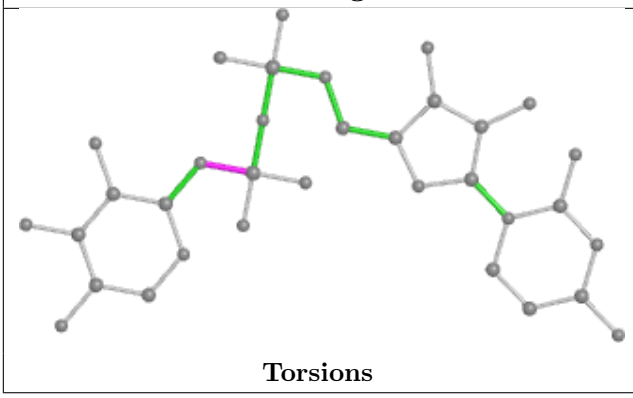


Bond angles



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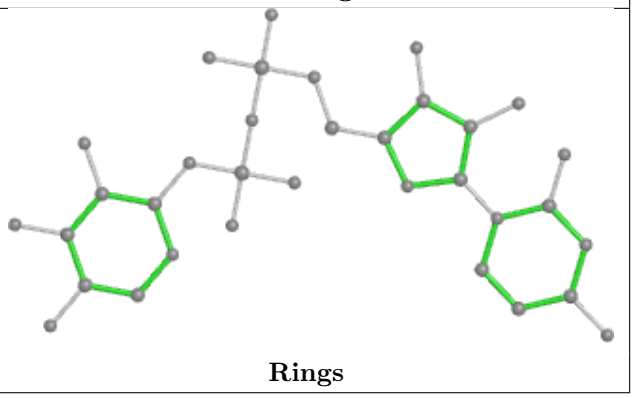

Rings

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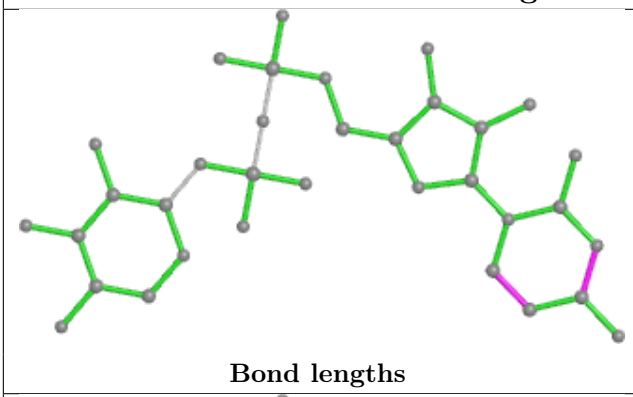

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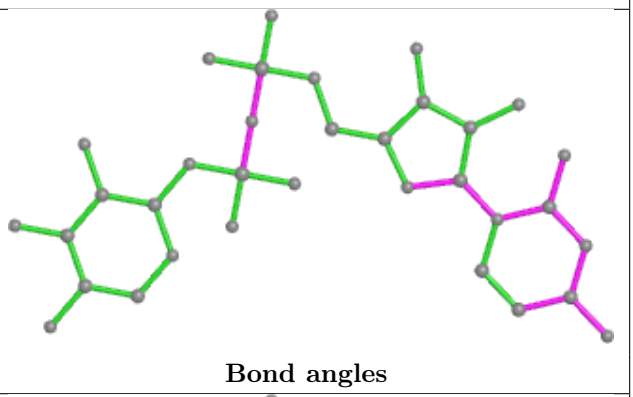

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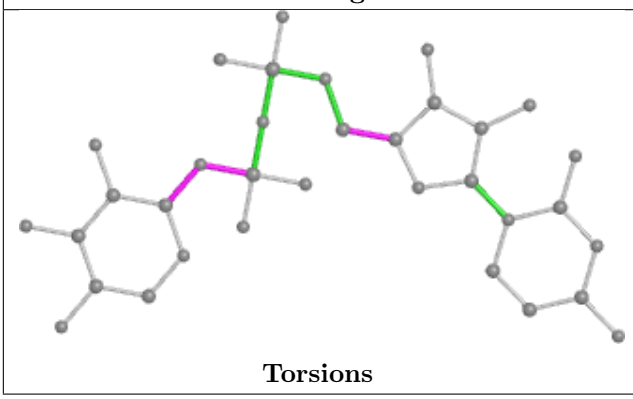

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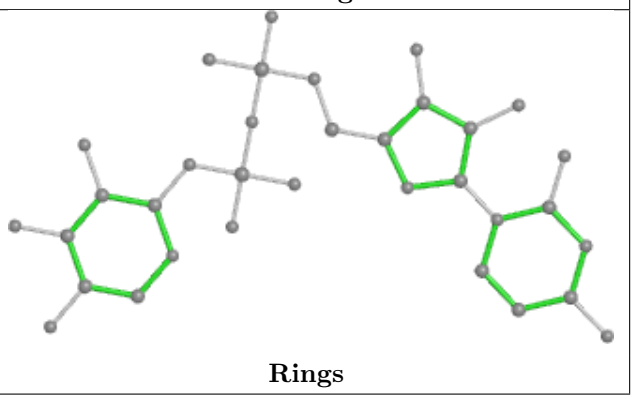

Rings

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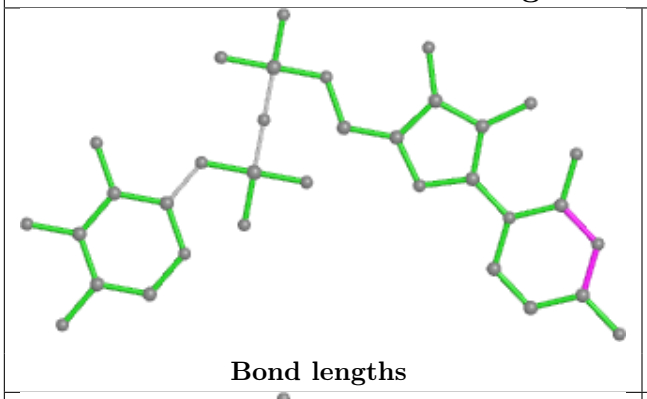

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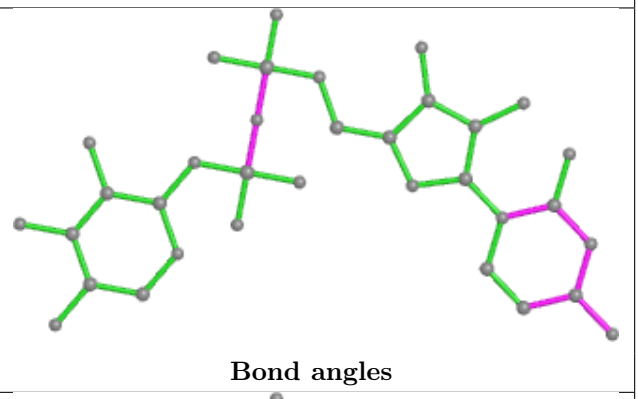
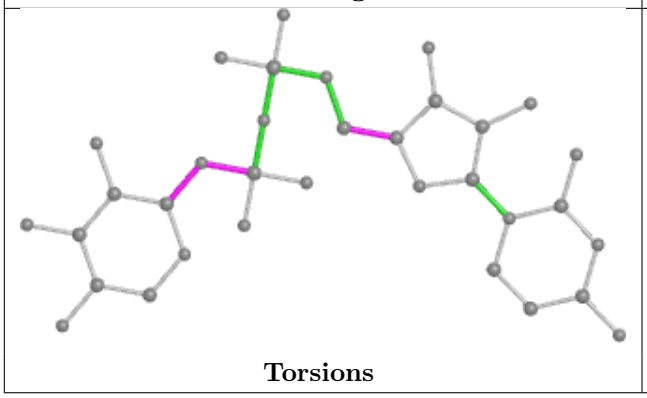


Bond angles



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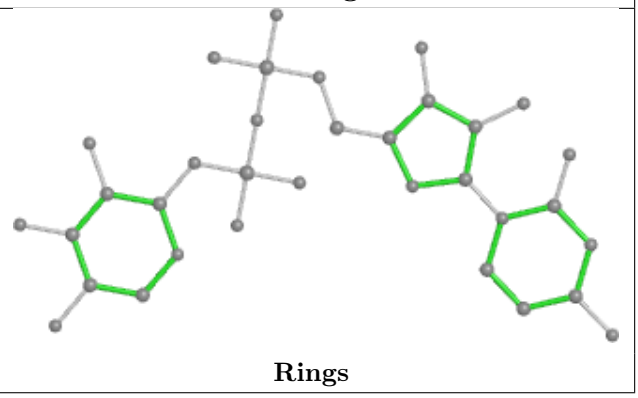
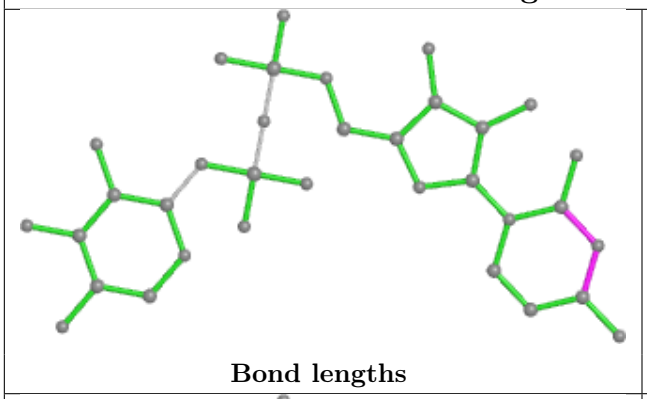
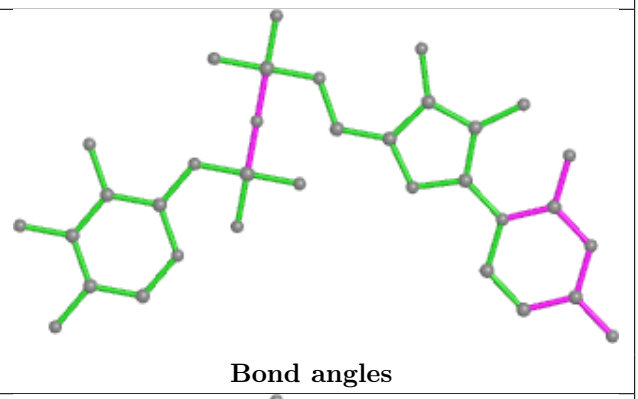


Rings

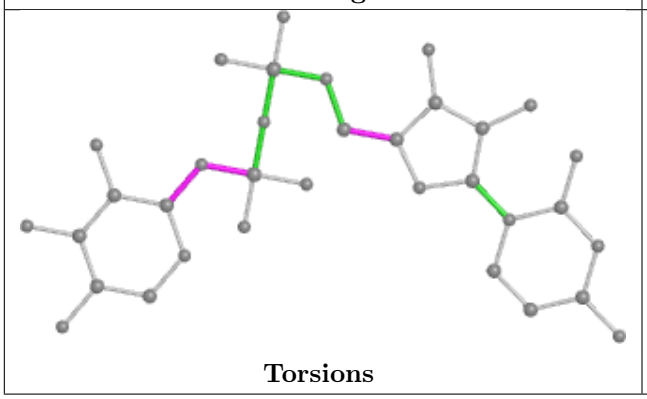
Ligand UDX G 500



Bond lengths



Bond angles



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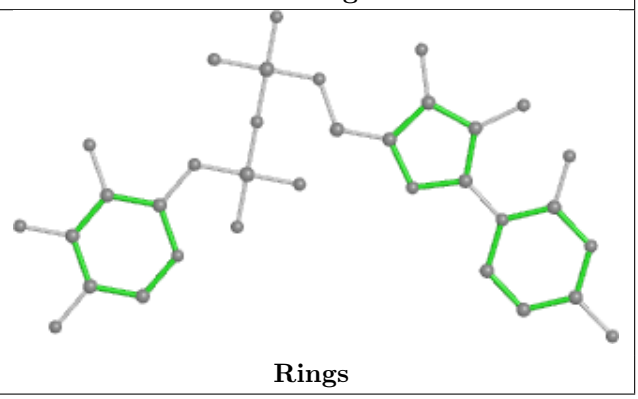
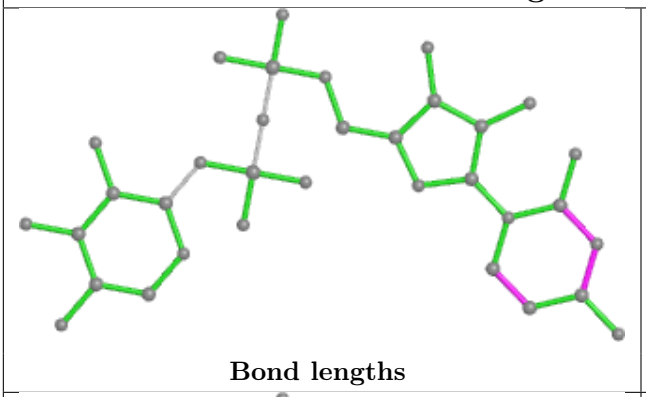


Rings

Ligand UDX I 501



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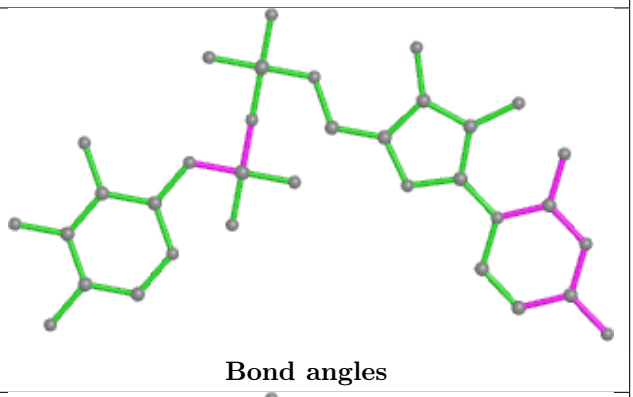
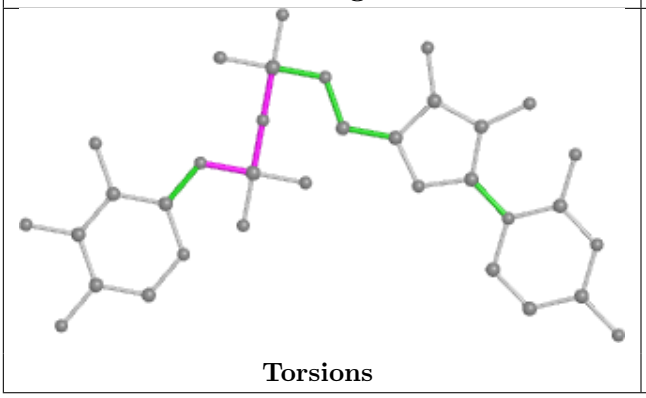
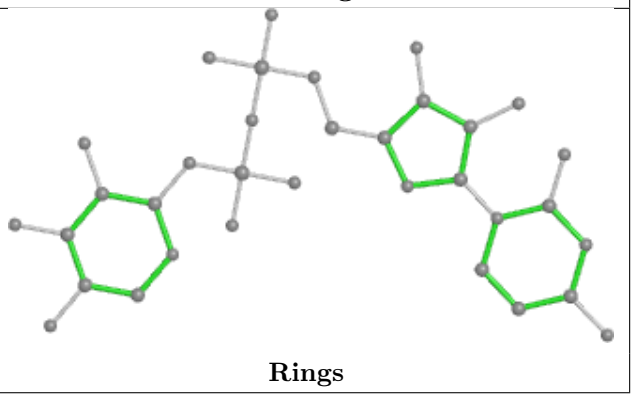


Bond angles

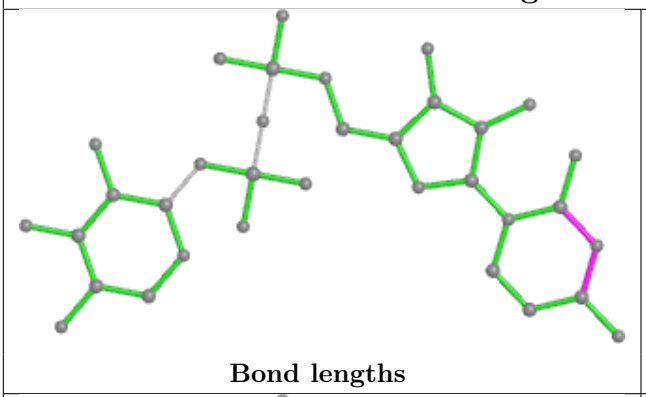


Torsions



Rings

Ligand UDX B 500



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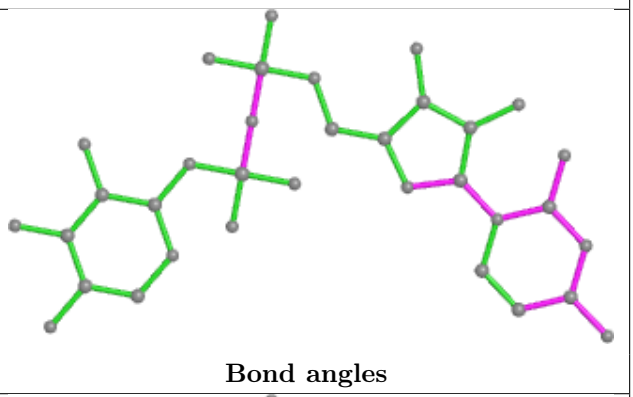
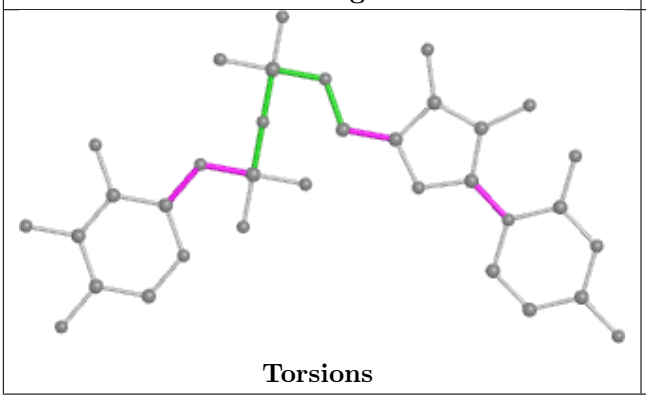


Bond angles



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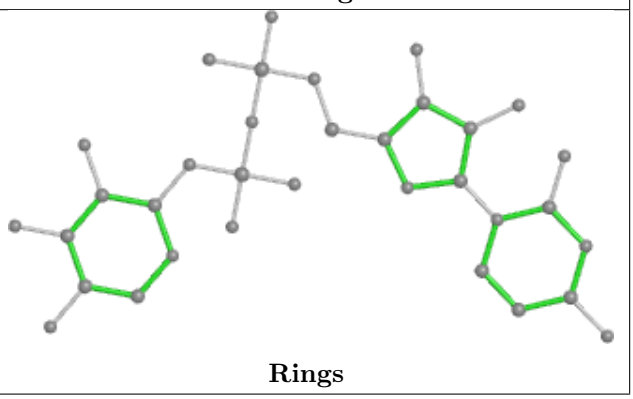

Rings

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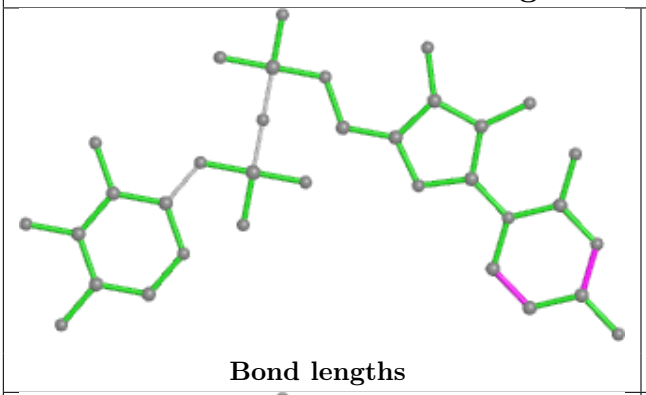

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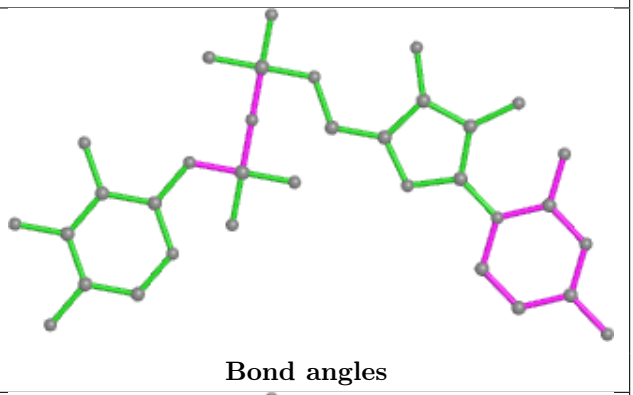

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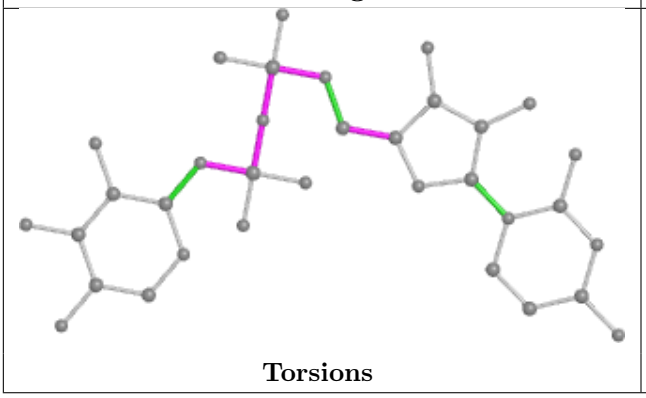

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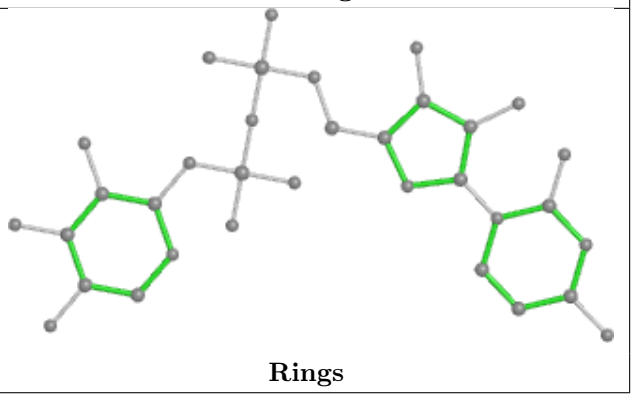

Rings

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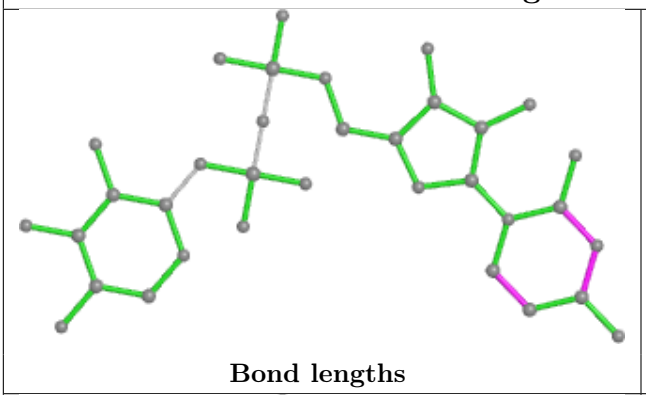

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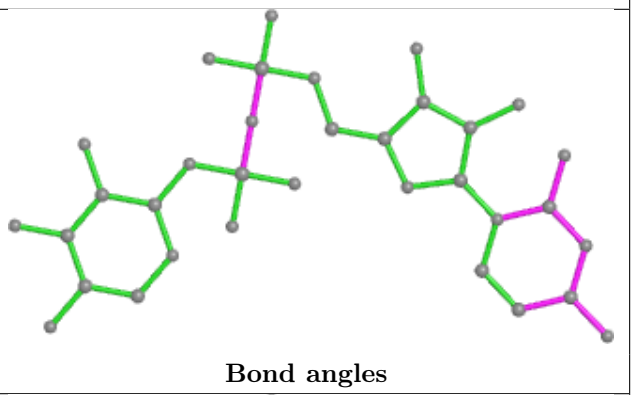
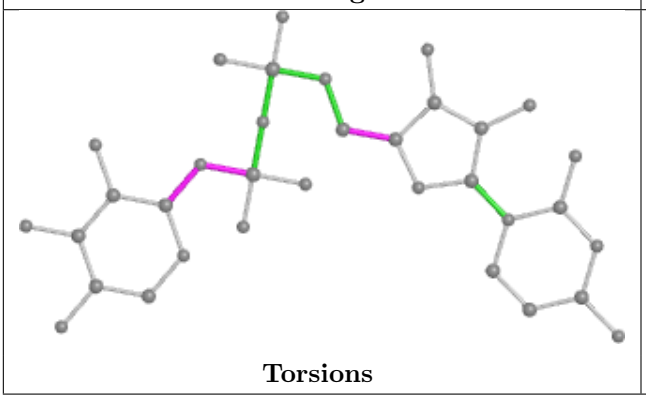


Bond angles



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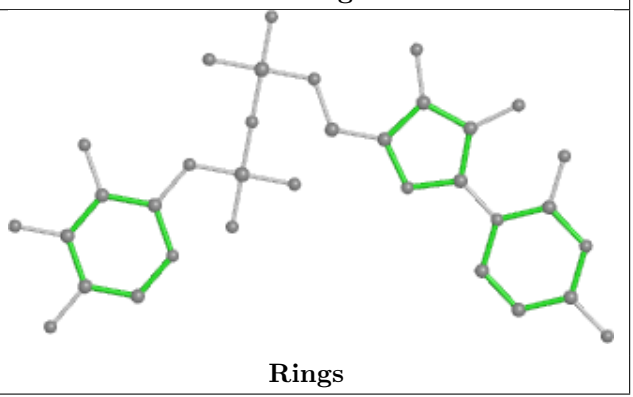
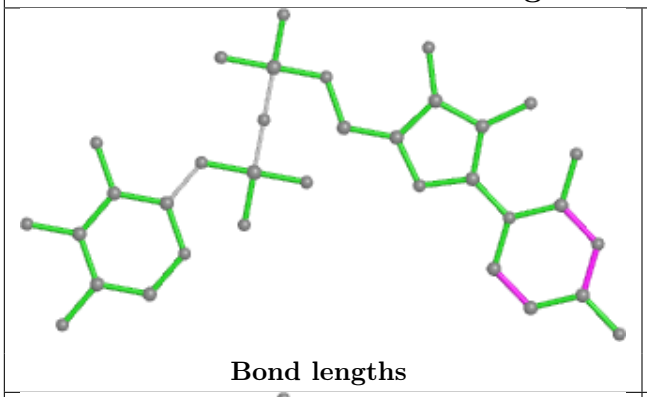


Rings

Ligand UDX L 501



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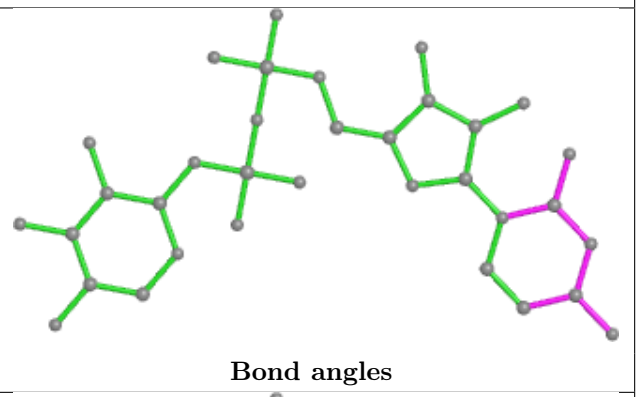
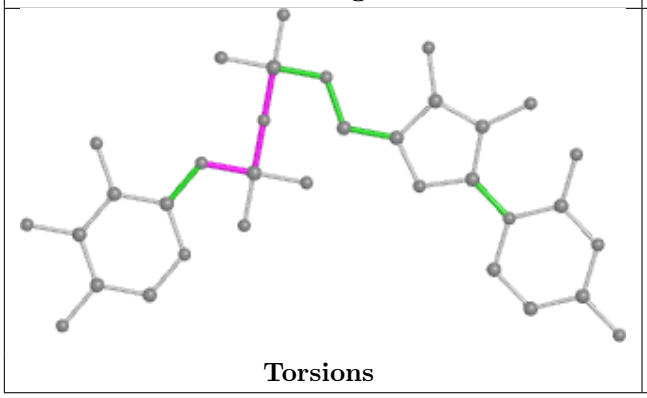


Bond angles



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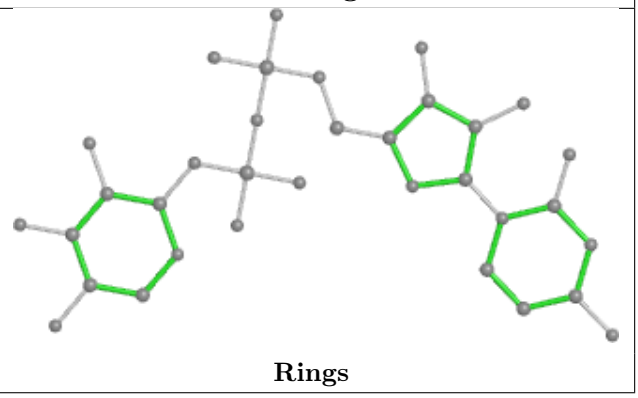

Rings

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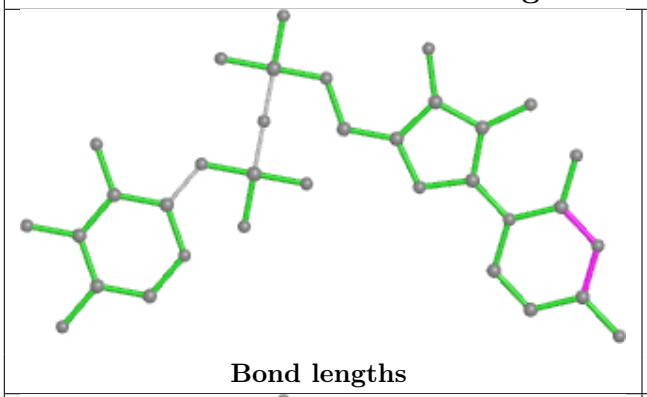

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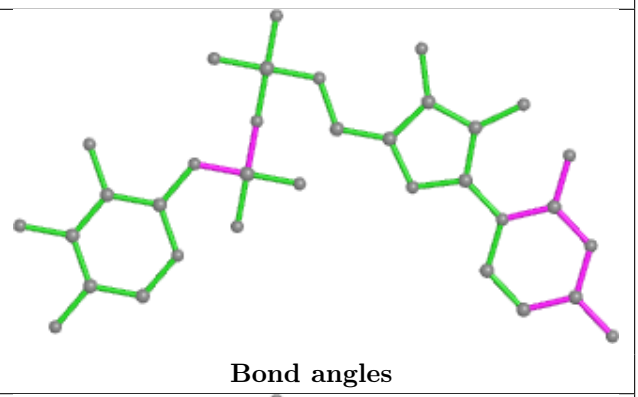

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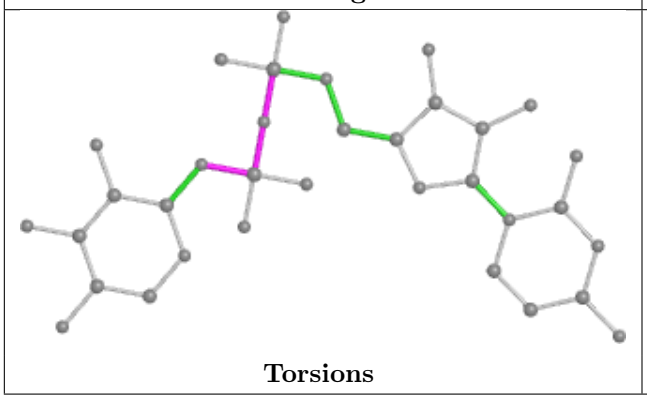

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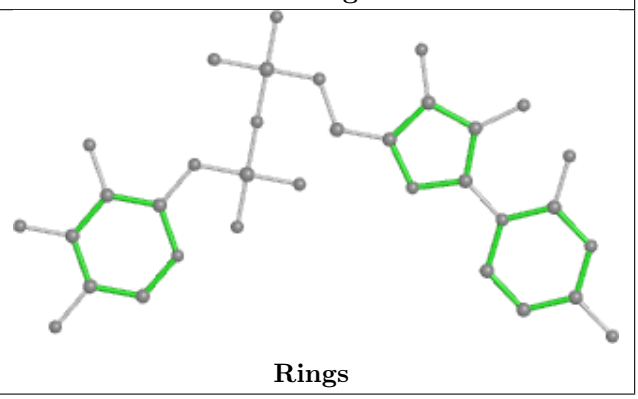

Rings

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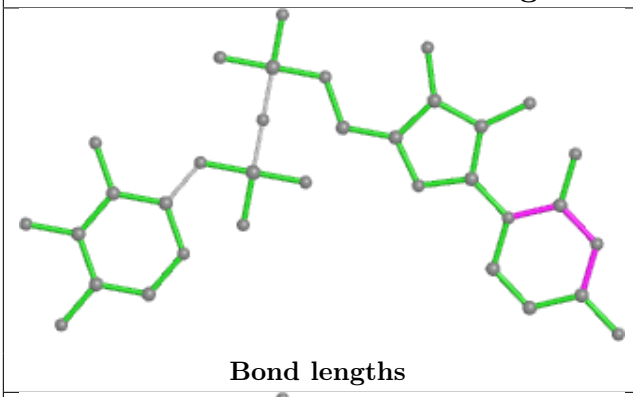

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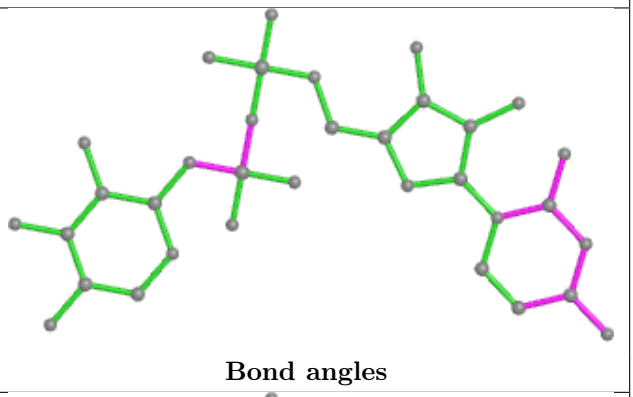

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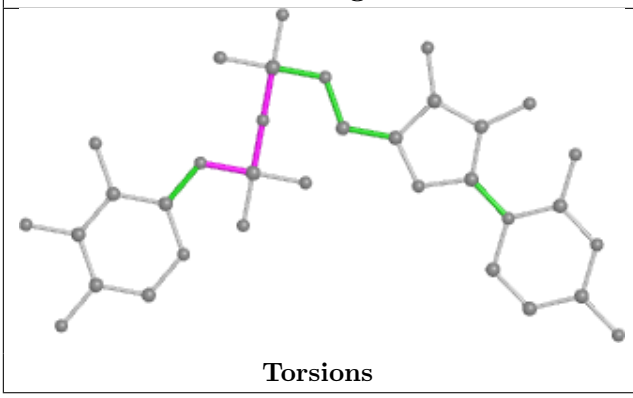

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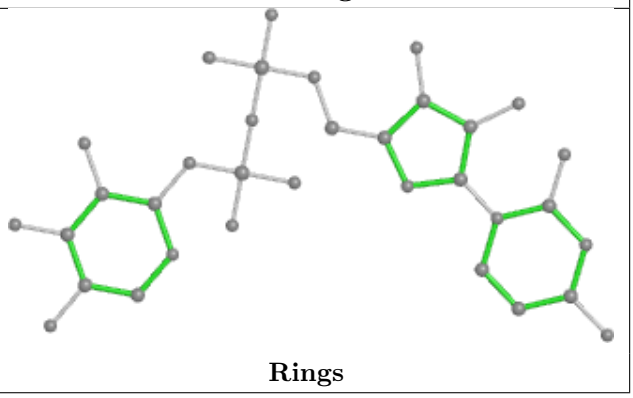

Rings

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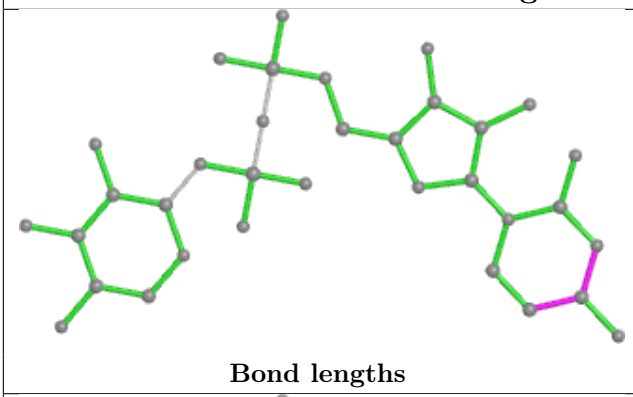

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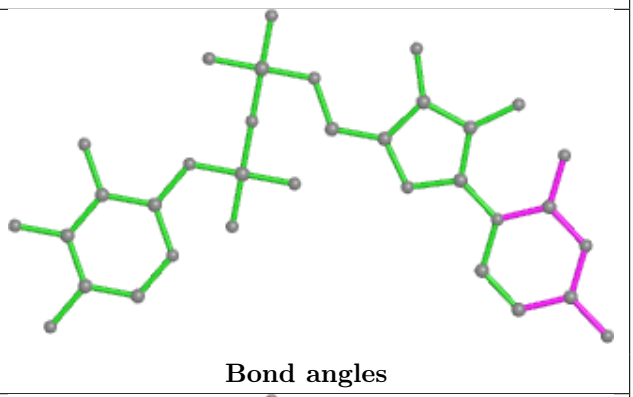

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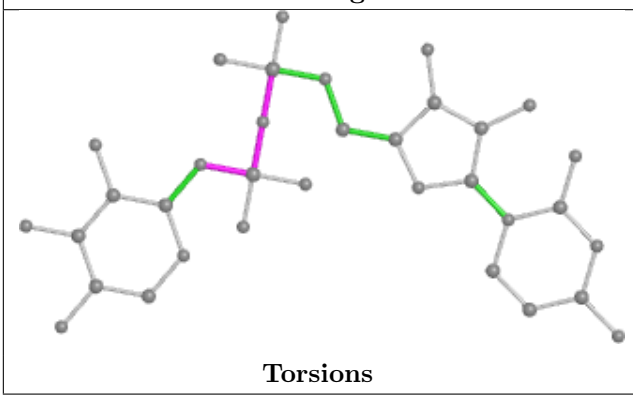

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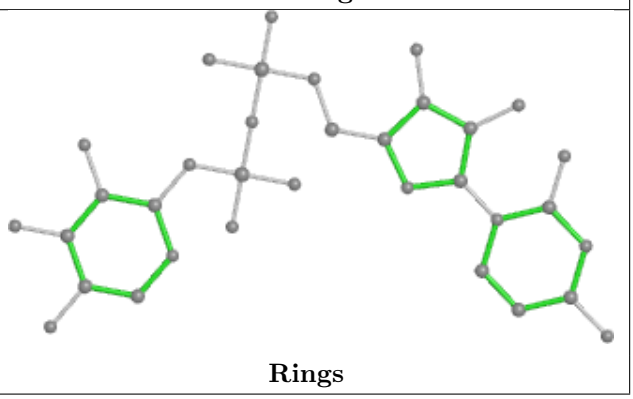

Rings

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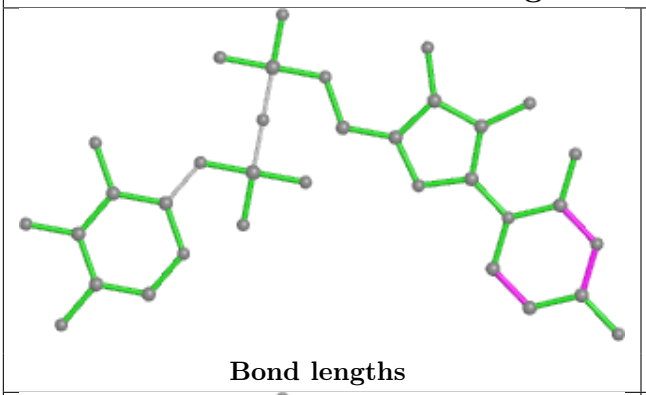

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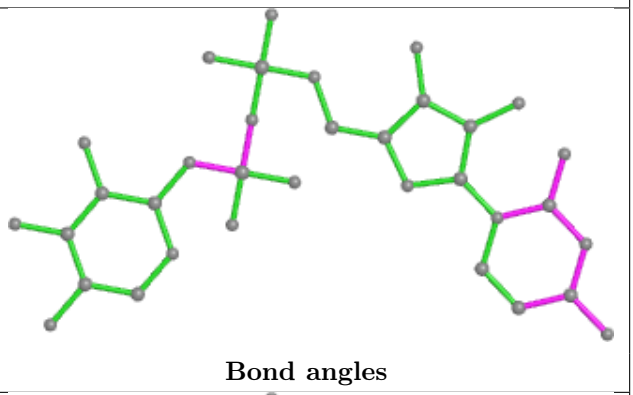

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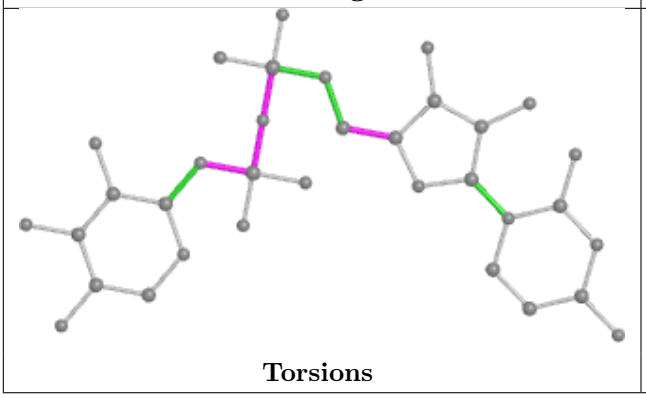

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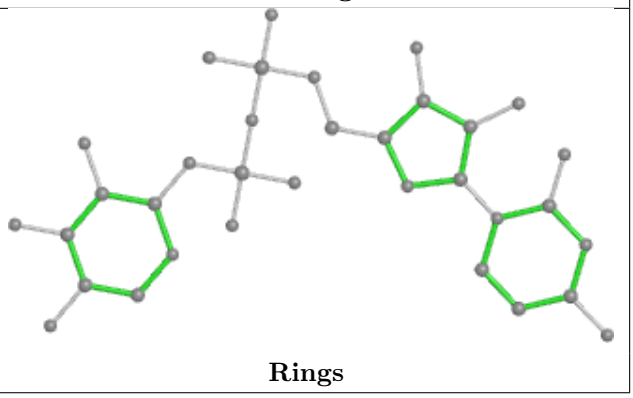

Rings

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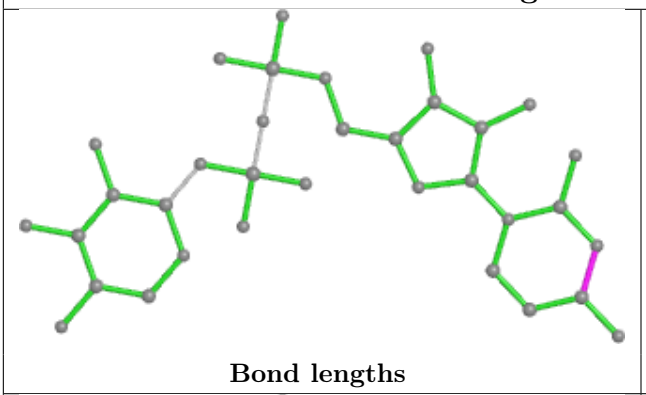

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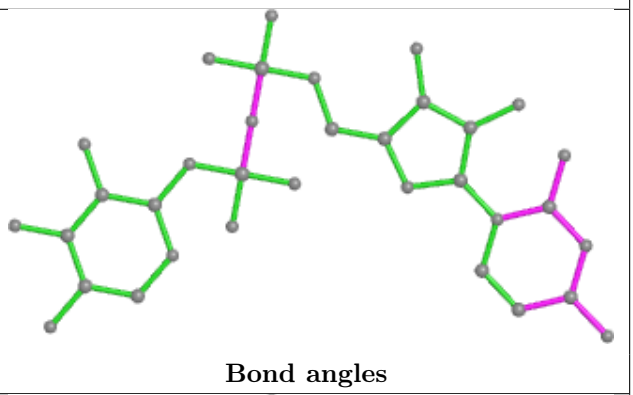

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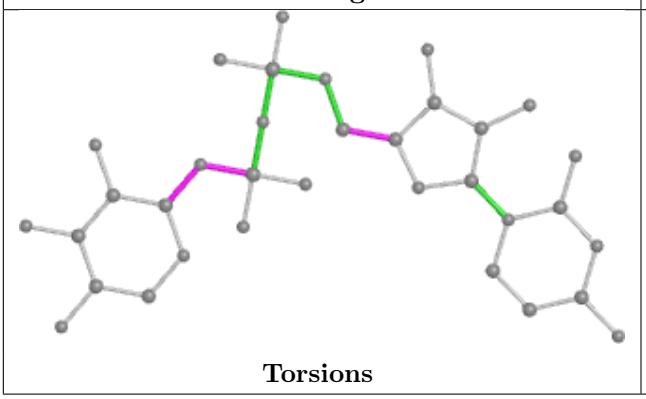

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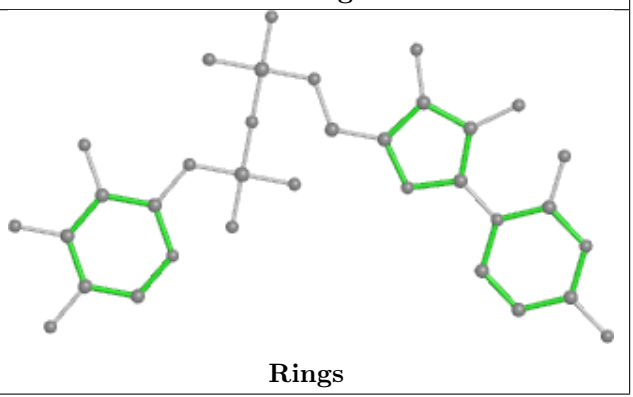

Rings

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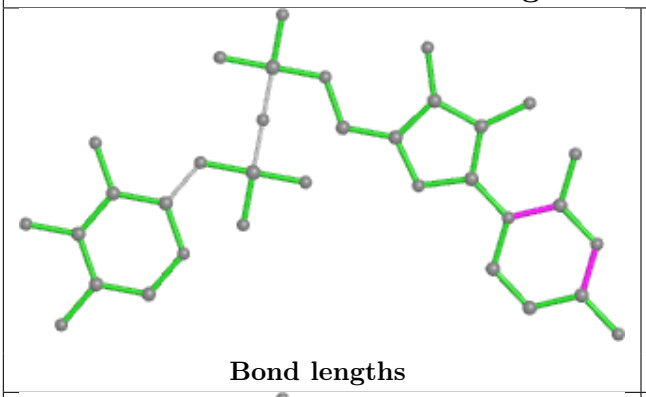

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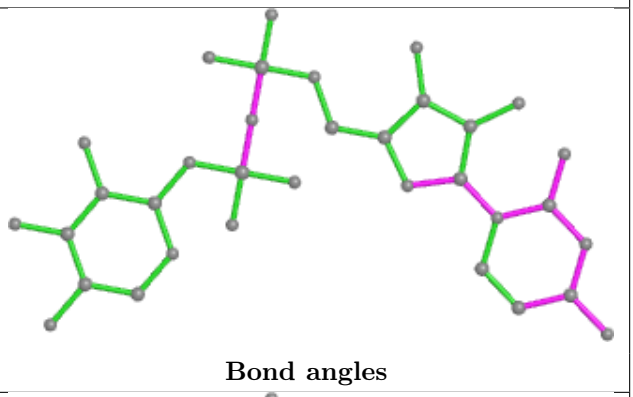

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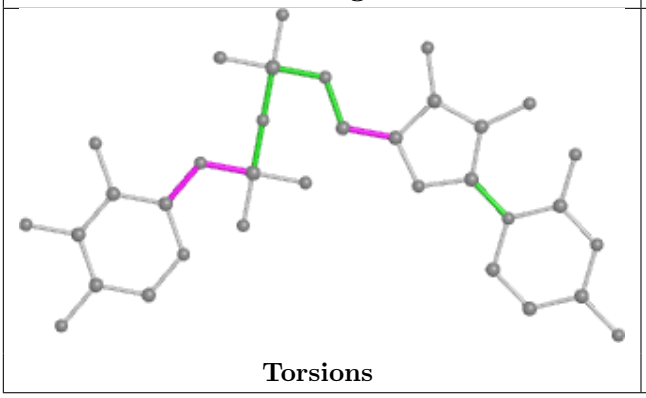

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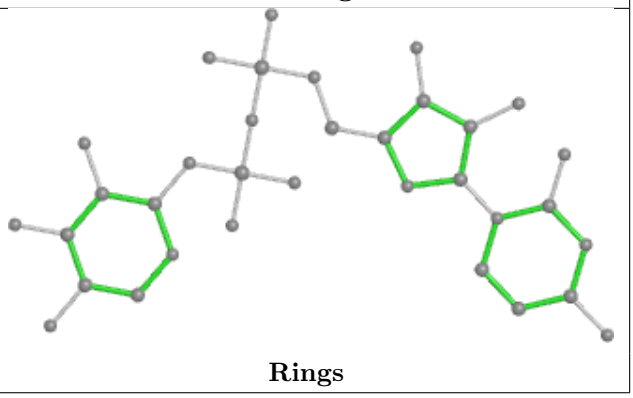

Rings

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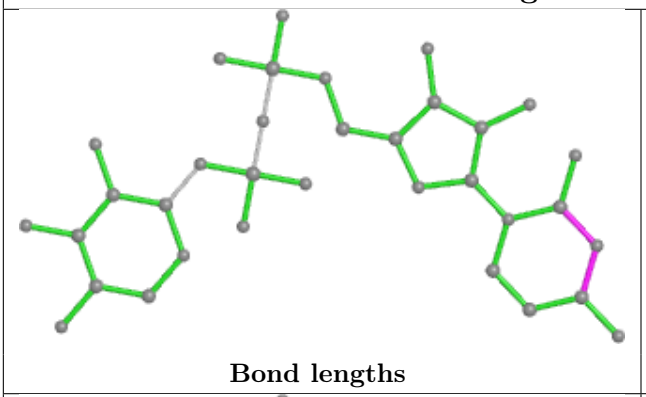

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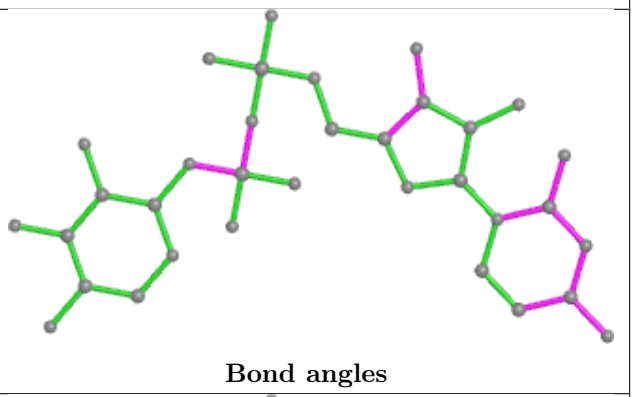

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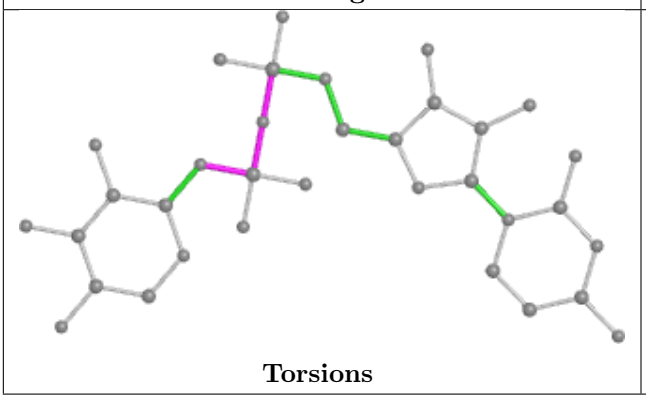

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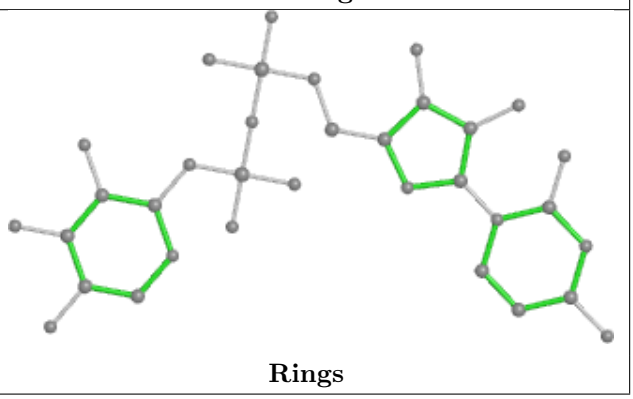
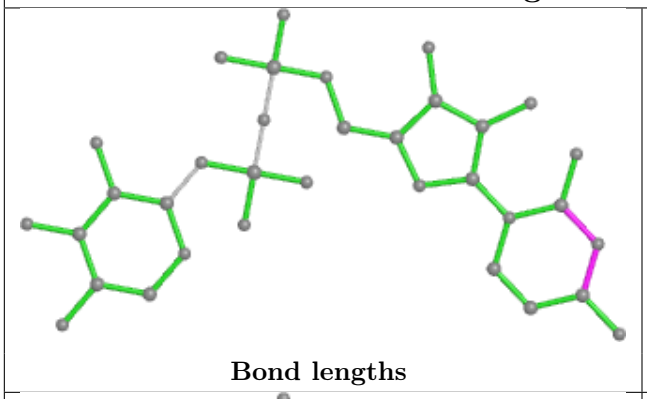


Rings

Ligand UDX F 501



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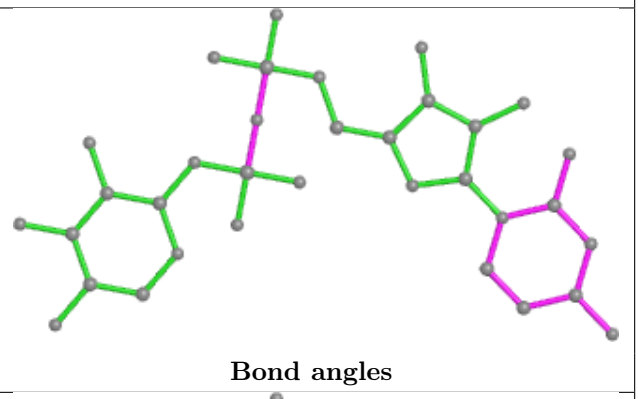

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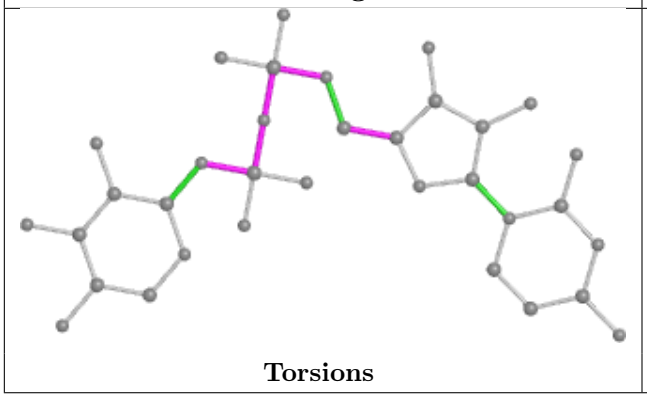

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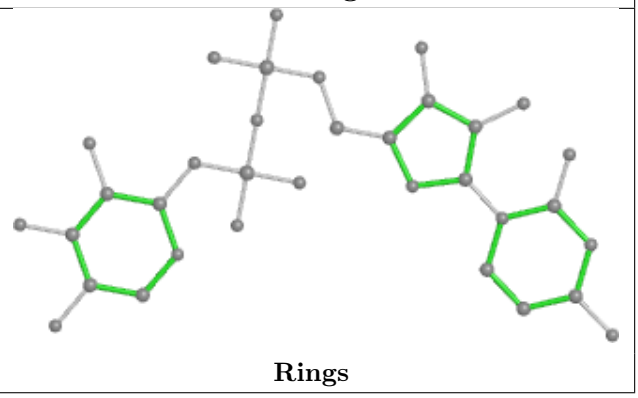
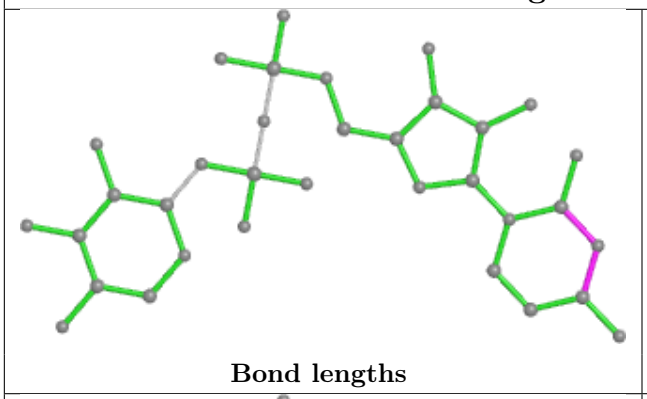


Rings

Ligand UDX I 500



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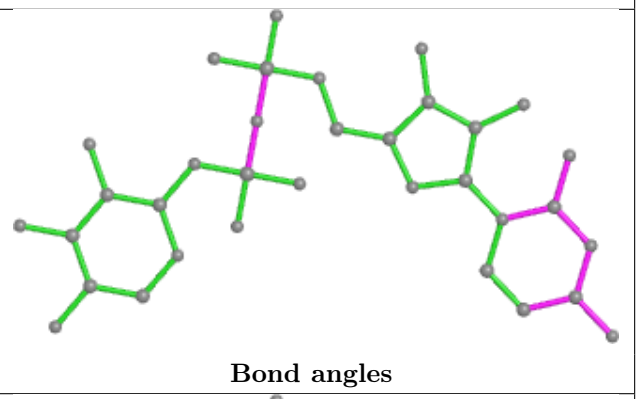
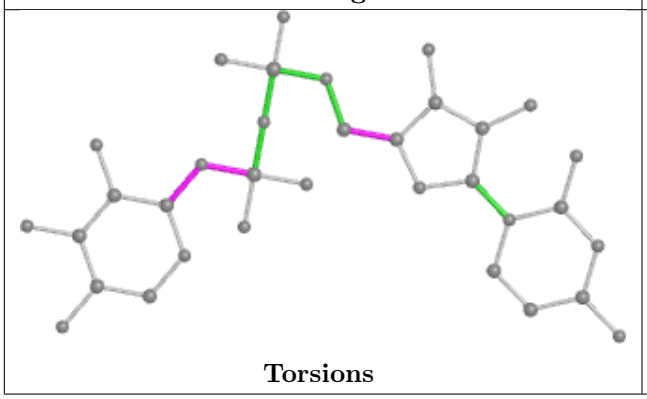
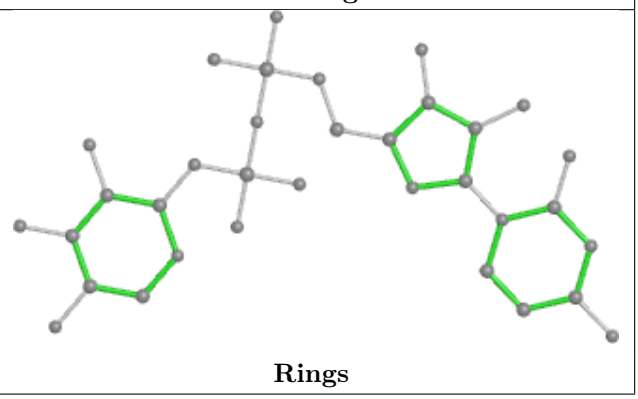


Bond angles

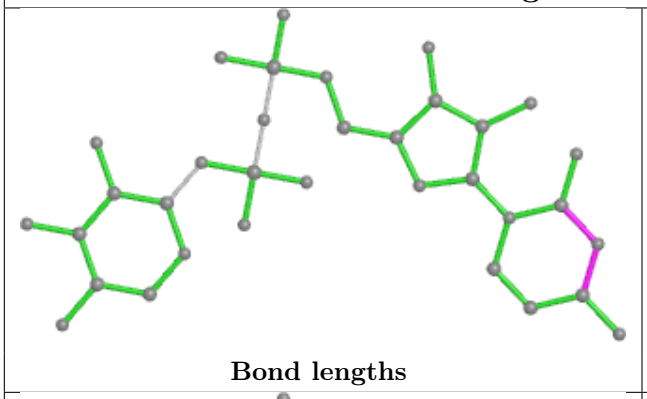


Torsions

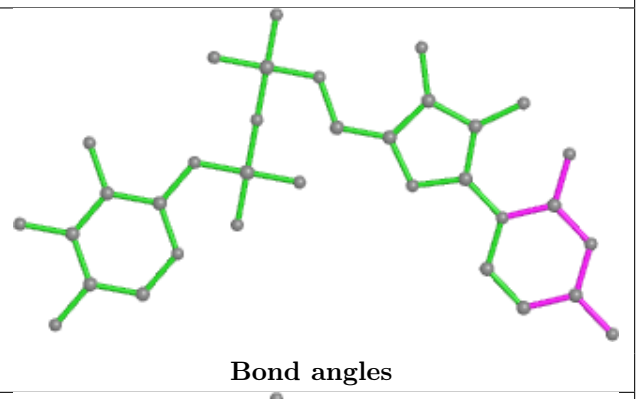


Rings

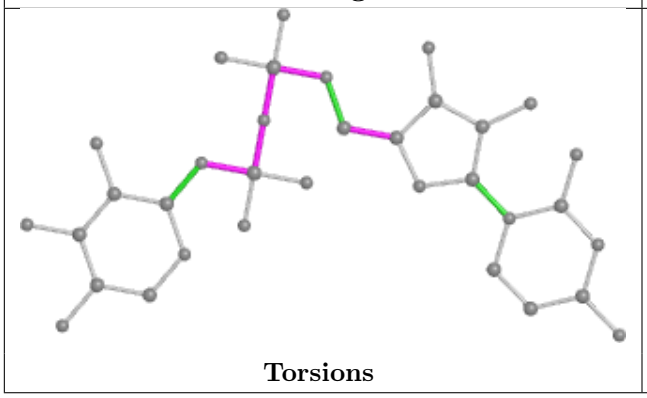
Ligand UDX B 501



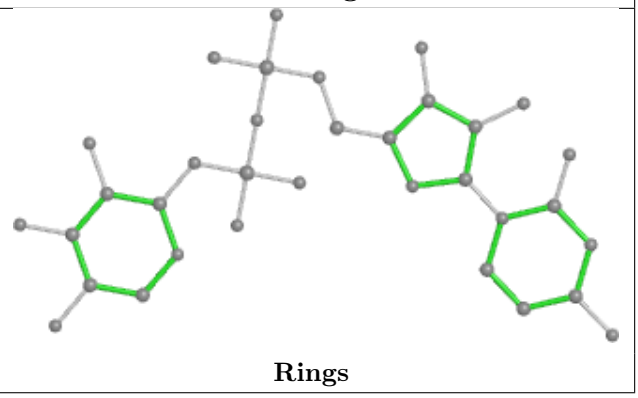
Bond lengths



Bond angles

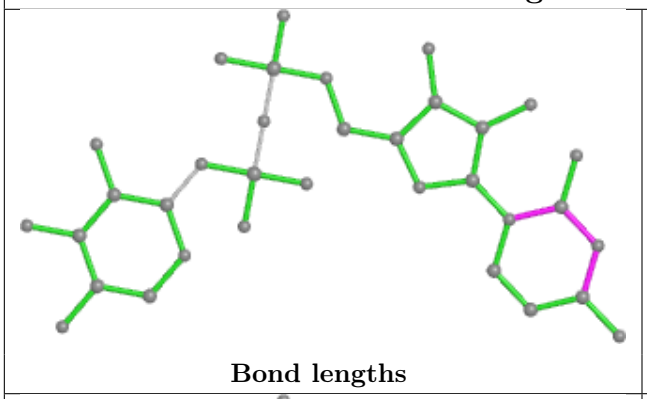


Torsions

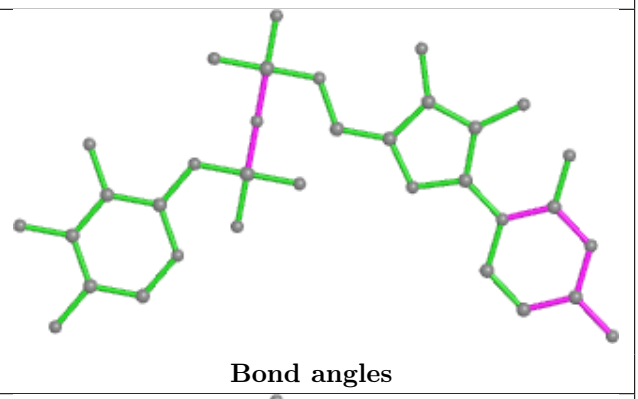


Rings

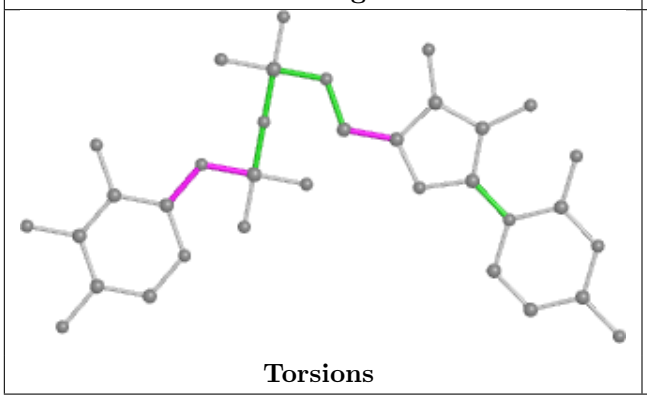
Ligand UDX J 500



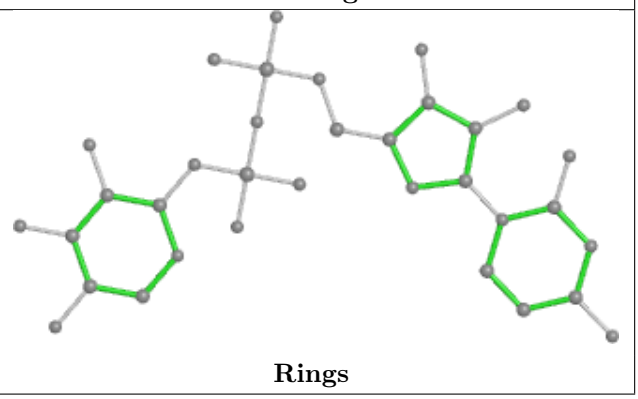
Bond lengths



Bond angles

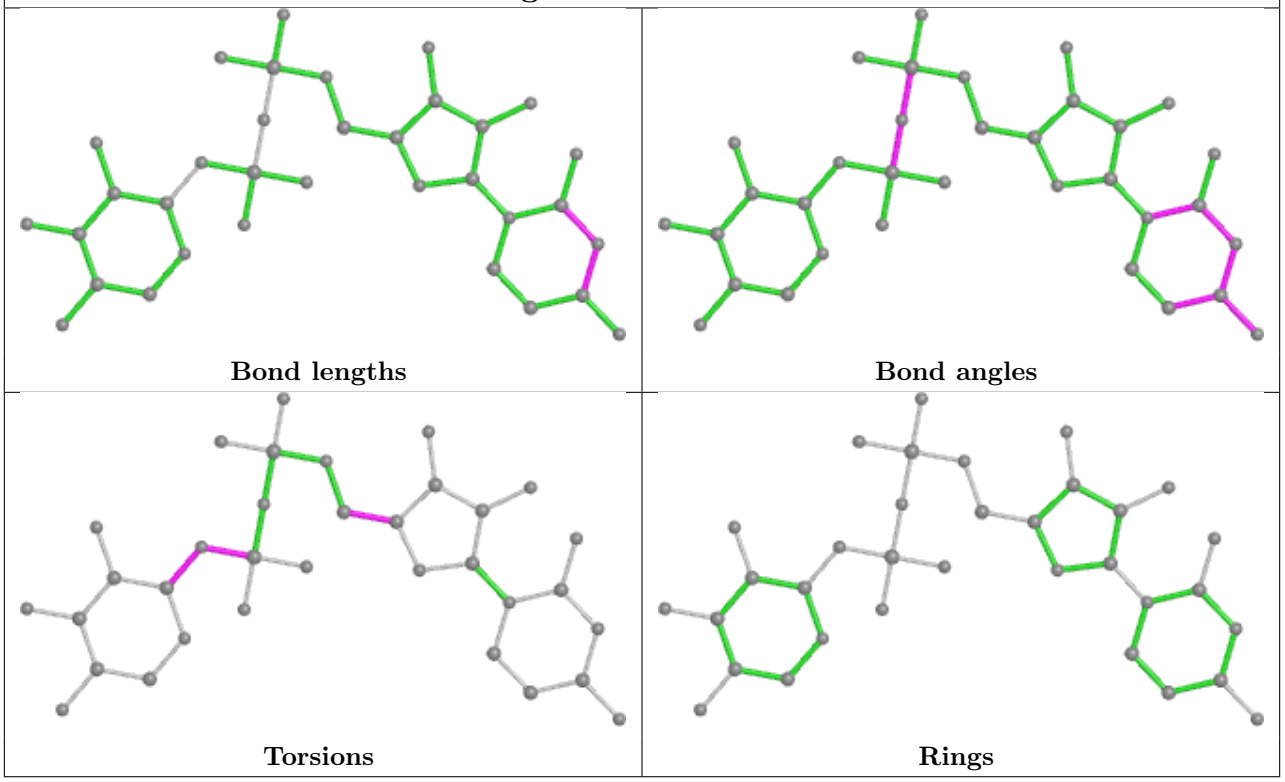


Torsions



Rings

Ligand UDX H 500



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	463/481 (96%)	0.05	0 100 100	30, 43, 63, 101	0
1	B	463/481 (96%)	0.23	9 (1%) 66 63	31, 54, 83, 109	0
1	C	463/481 (96%)	0.04	2 (0%) 92 92	31, 48, 70, 97	0
1	D	468/481 (97%)	-0.00	0 100 100	32, 45, 69, 124	0
1	E	461/481 (95%)	0.04	2 (0%) 92 92	33, 45, 69, 107	0
1	F	465/481 (96%)	0.07	0 100 100	31, 46, 67, 91	0
1	G	462/481 (96%)	0.03	1 (0%) 95 95	37, 56, 77, 97	0
1	H	462/481 (96%)	-0.00	0 100 100	38, 50, 72, 92	0
1	I	462/481 (96%)	0.12	1 (0%) 95 95	38, 56, 77, 109	0
1	J	456/481 (94%)	0.14	5 (1%) 80 79	42, 59, 86, 111	0
1	K	464/481 (96%)	0.08	0 100 100	34, 52, 78, 99	0
1	L	463/481 (96%)	0.11	4 (0%) 84 83	37, 54, 78, 116	0
All	All	5552/5772 (96%)	0.08	24 (0%) 92 92	30, 51, 76, 124	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	139	VAL	4.0
1	C	324	LYS	2.9
1	E	103	ARG	2.8
1	L	138	PRO	2.8
1	B	66	VAL	2.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

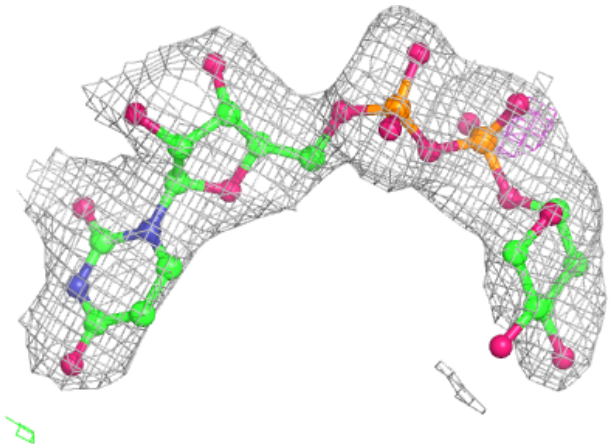
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

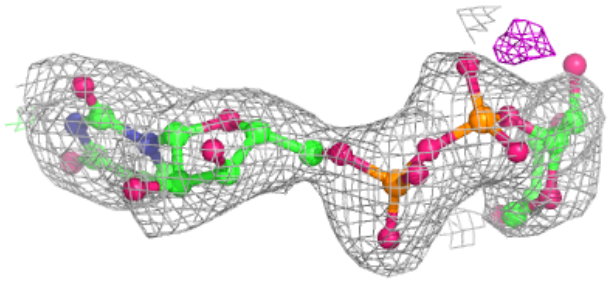
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UDX	J	500	34/34	0.91	0.21	77,91,99,102	0
2	UDX	E	500	34/34	0.97	0.19	42,58,68,69	0
2	UDX	G	500	34/34	0.97	0.16	50,58,66,67	0
2	UDX	I	500	34/34	0.97	0.14	41,49,61,61	0
2	UDX	B	500	34/34	0.97	0.17	51,58,63,65	0
2	UDX	K	500	34/34	0.97	0.16	43,54,66,66	0
2	UDX	L	500	34/34	0.97	0.20	49,59,76,77	0
2	UDX	E	501	34/34	0.98	0.15	30,37,42,44	0
2	UDX	F	500	34/34	0.98	0.15	33,49,54,61	0
2	UDX	F	501	34/34	0.98	0.16	29,36,39,47	0
2	UDX	A	500	34/34	0.98	0.16	35,41,50,53	0
2	UDX	G	501	34/34	0.98	0.14	33,41,49,51	0
2	UDX	H	500	34/34	0.98	0.17	46,54,62,67	0
2	UDX	H	501	34/34	0.98	0.15	35,41,48,55	0
2	UDX	B	501	34/34	0.98	0.18	34,45,51,56	0
2	UDX	I	501	34/34	0.98	0.17	38,45,51,52	0
2	UDX	C	500	34/34	0.98	0.15	38,50,54,55	0
2	UDX	J	501	34/34	0.98	0.13	40,50,58,60	0
2	UDX	D	500	34/34	0.98	0.16	35,47,67,71	0
2	UDX	K	501	34/34	0.98	0.16	30,40,45,47	0
2	UDX	A	501	34/34	0.98	0.16	28,37,42,45	0
2	UDX	L	501	34/34	0.98	0.15	35,43,45,48	0
2	UDX	C	501	34/34	0.99	0.16	29,36,42,43	0
2	UDX	D	501	34/34	0.99	0.15	29,37,45,50	0

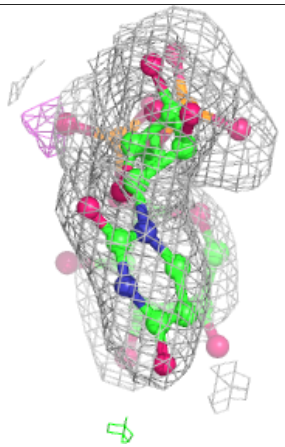
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDX J 500:

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

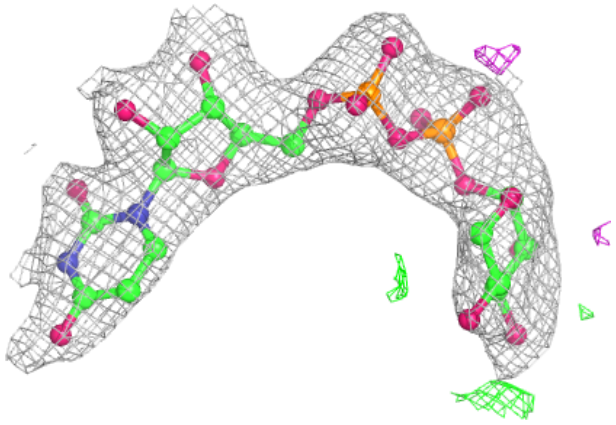


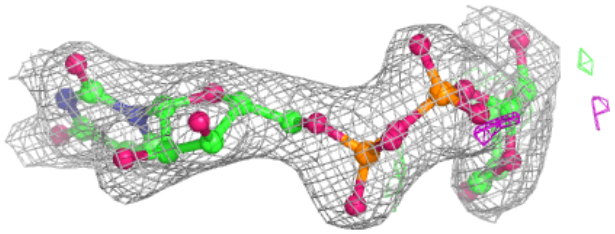


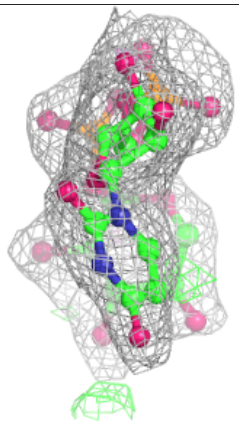


Electron density around UDX E 500:

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







Electron density around UDX G 500:

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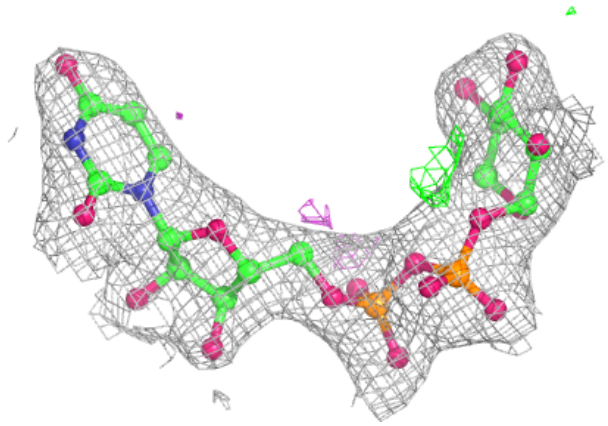
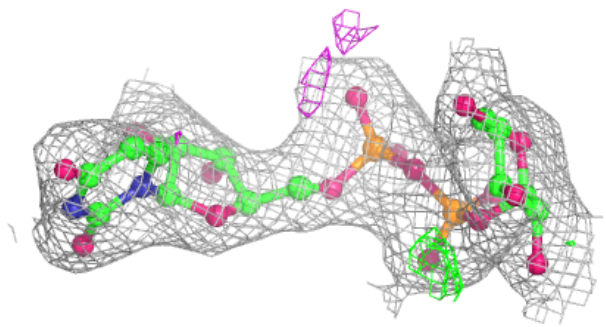
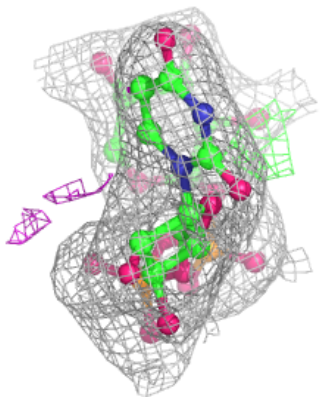
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around UDX I 500:

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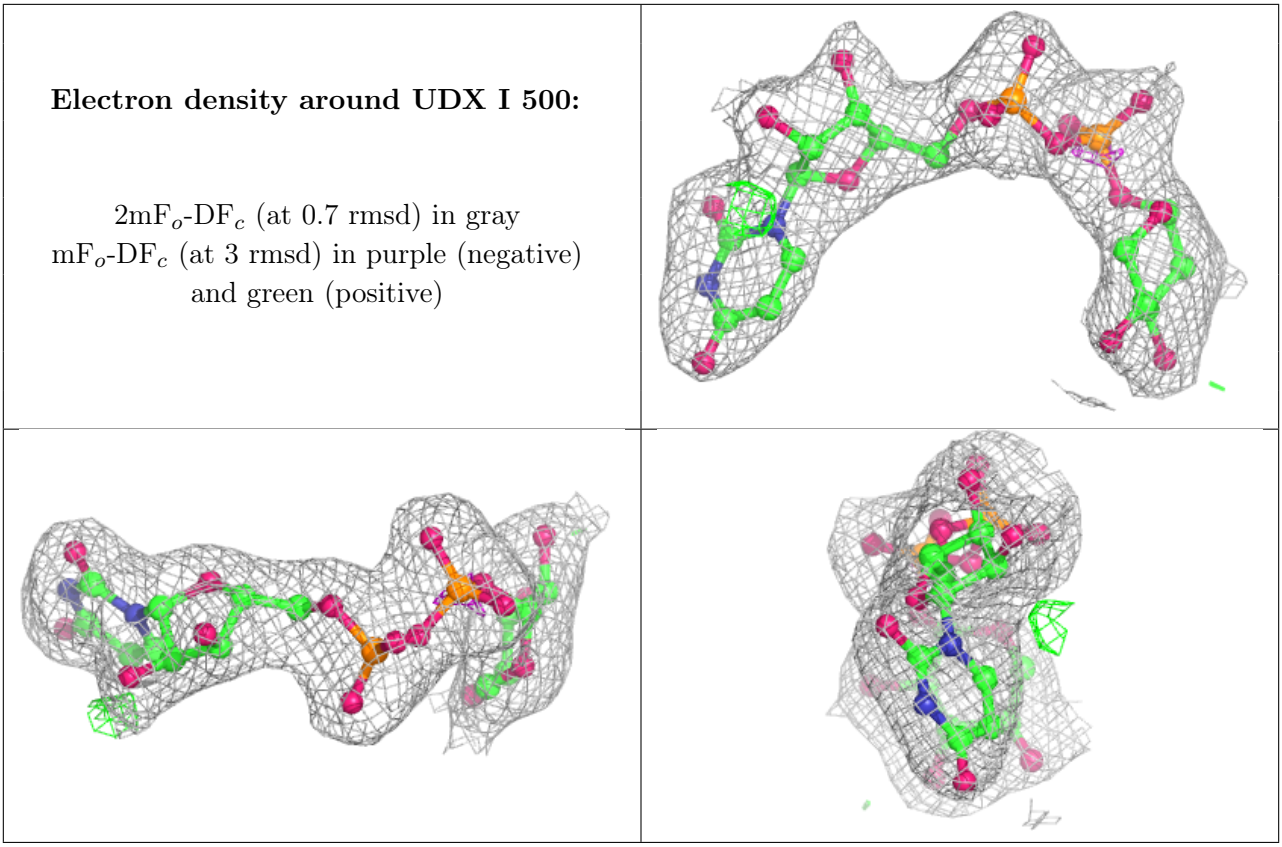
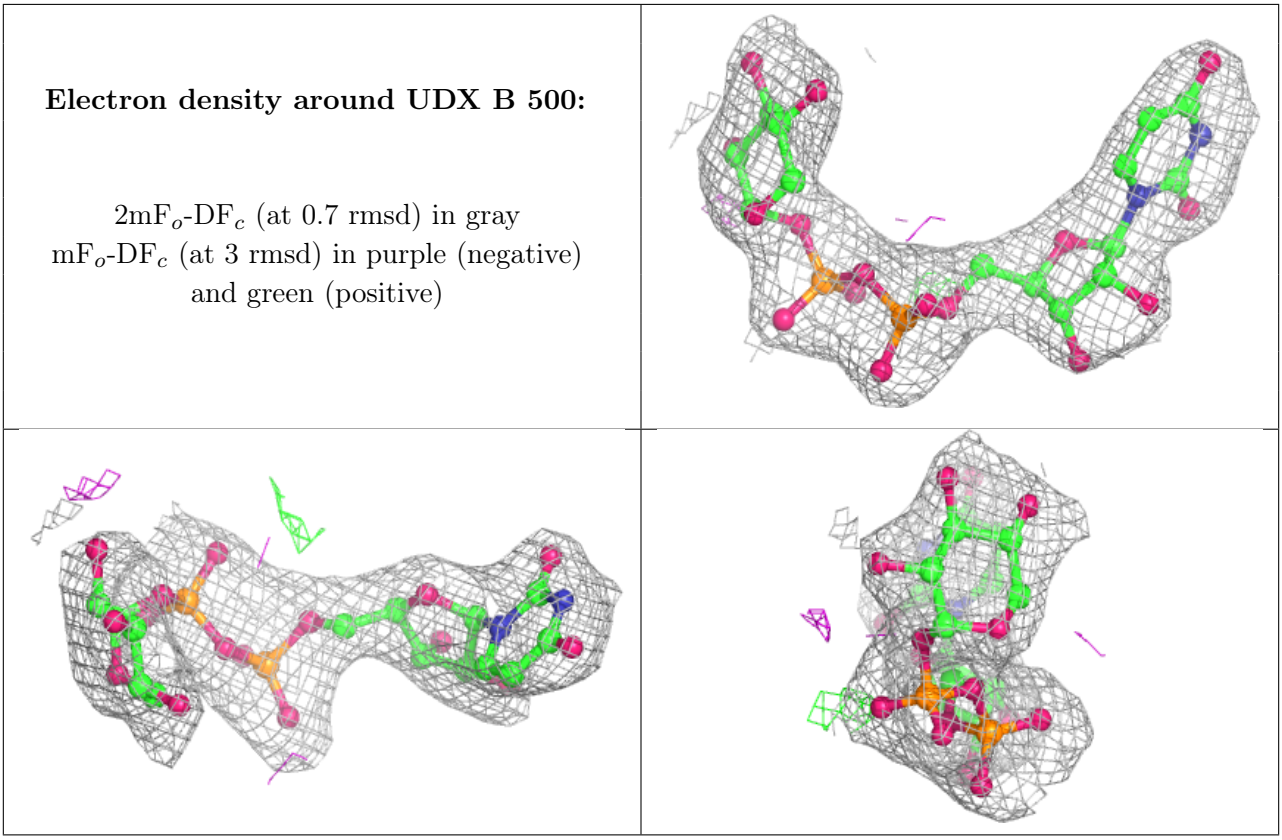
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



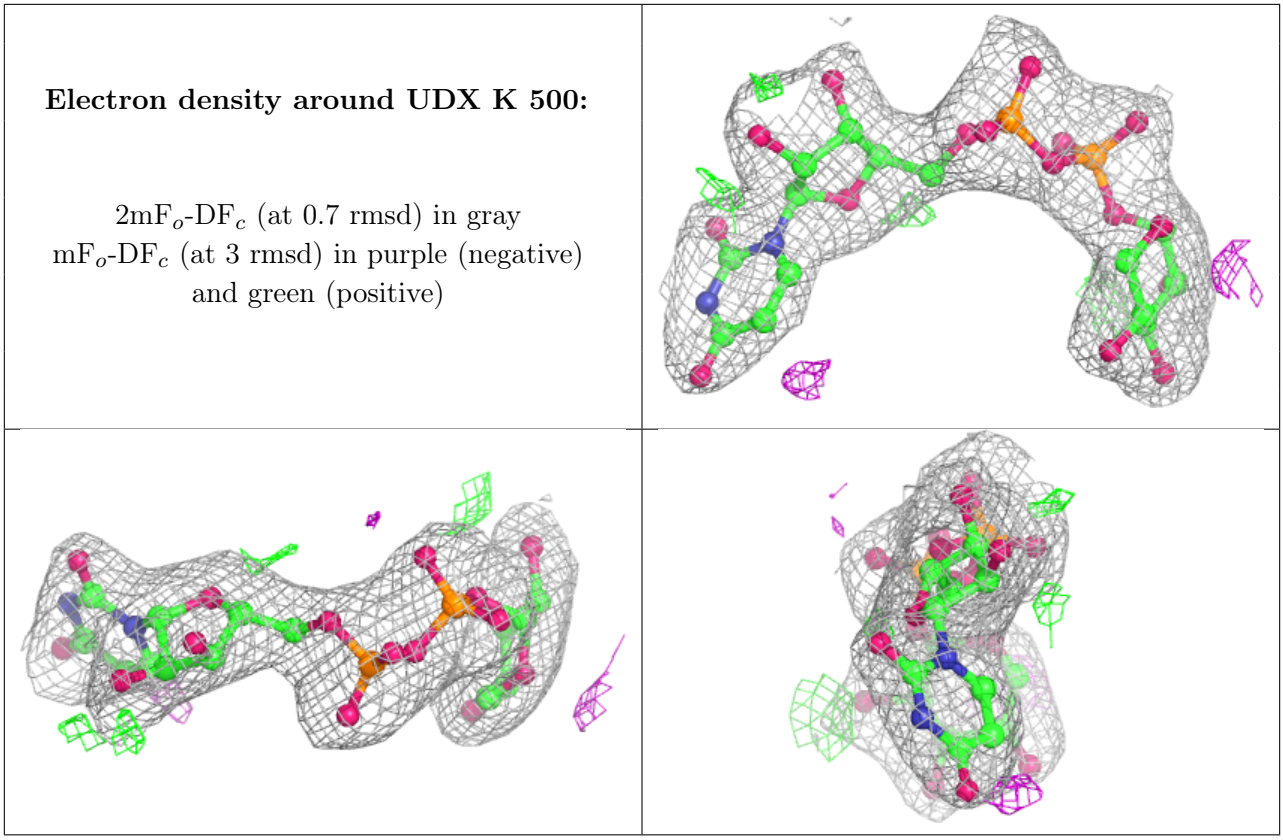
Electron density around UDX B 500:

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



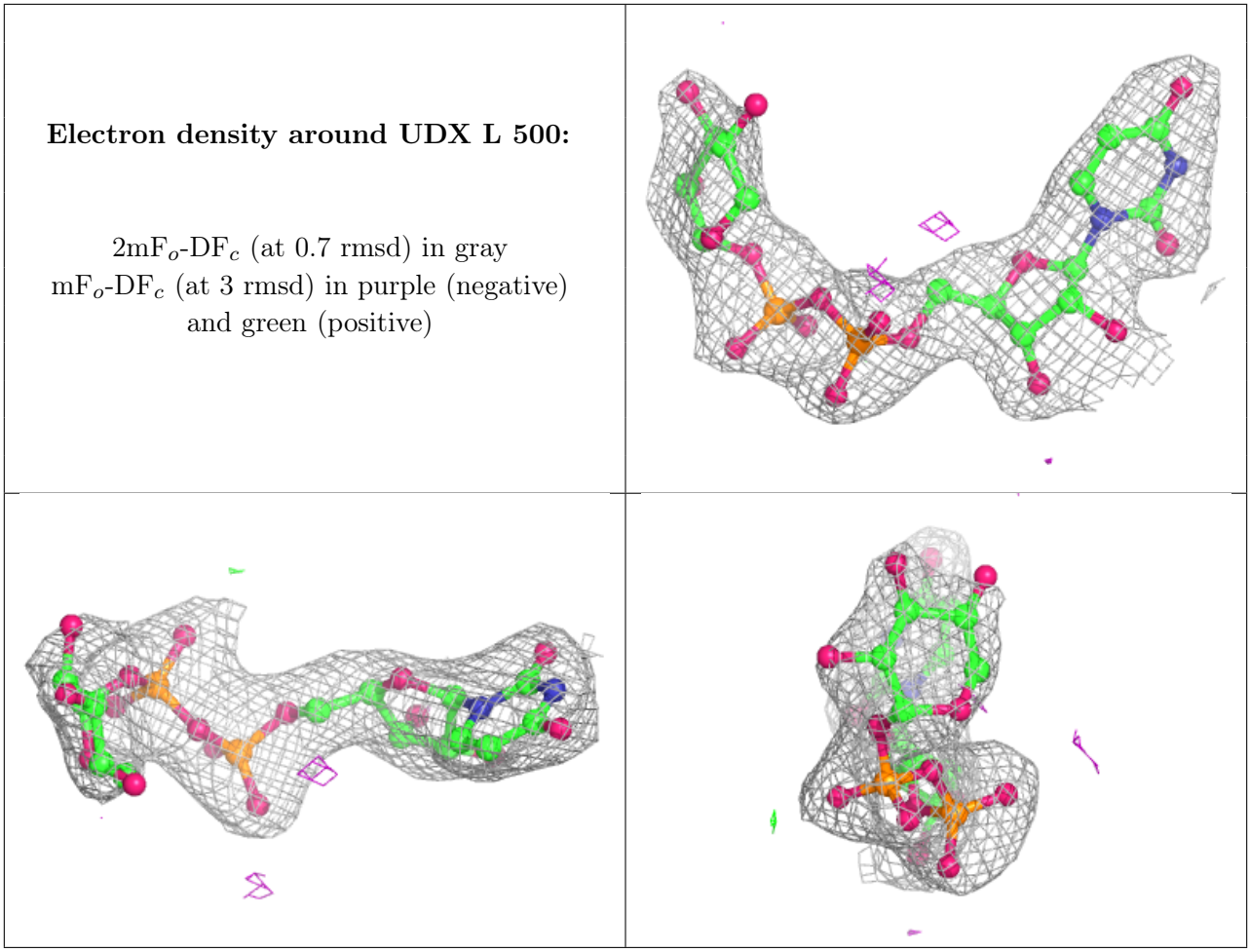
Electron density around UDX K 500:

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



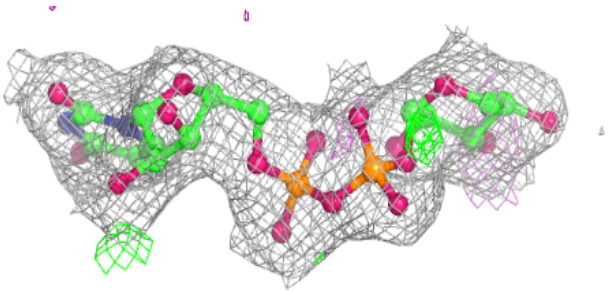
Electron density around UDX L 500:

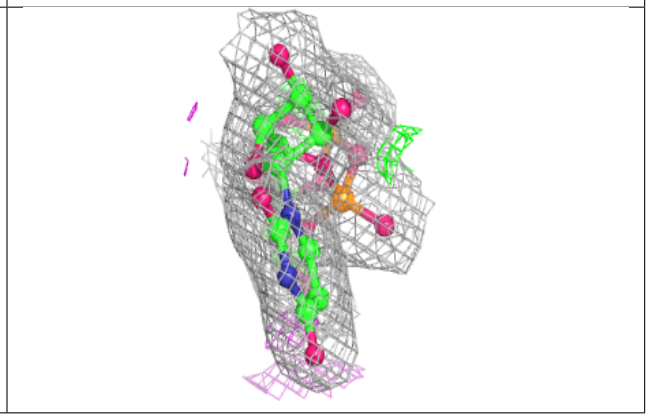
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around UDX E 501:

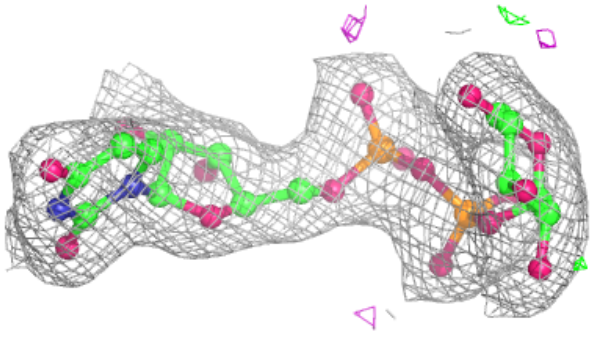
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

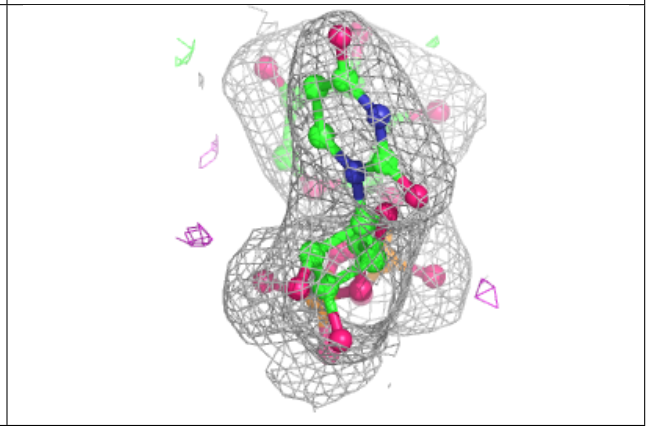




Electron density around UDX F 500:

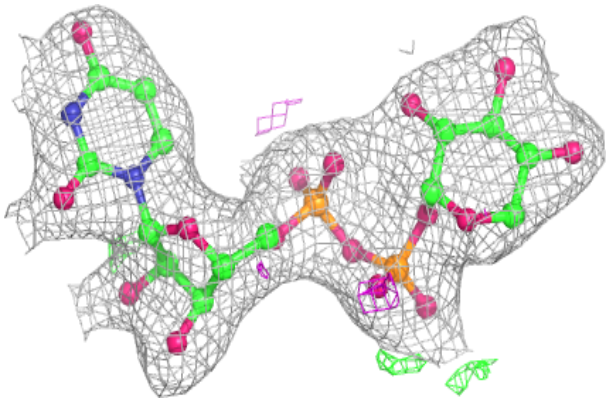
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

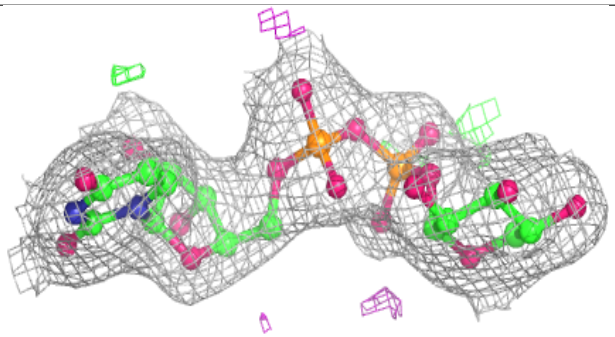


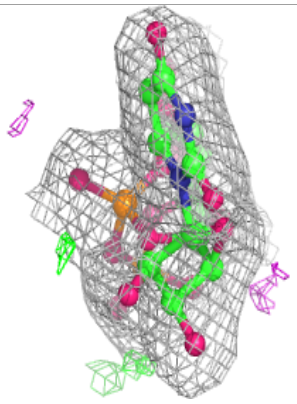


Electron density around UDX F 501:

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

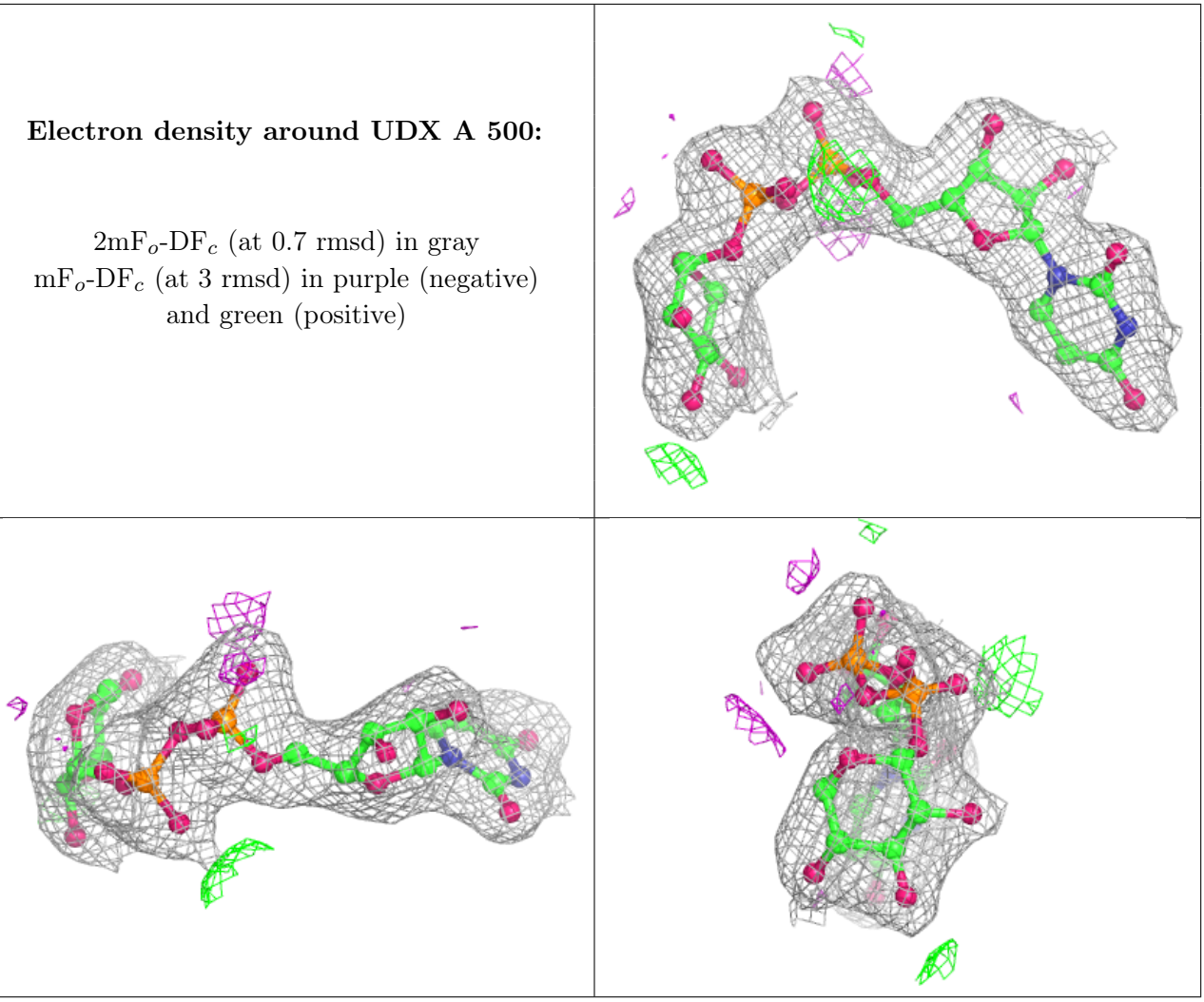






Electron density around UDX A 500:

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



Electron density around UDX G 501:

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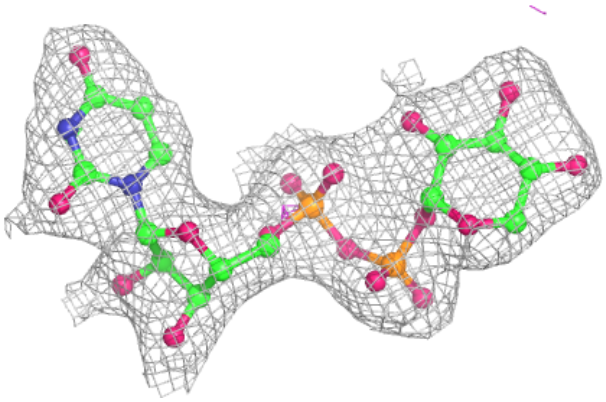
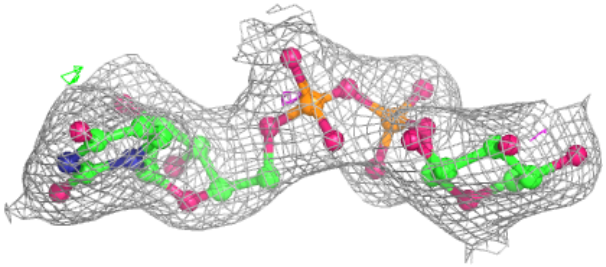
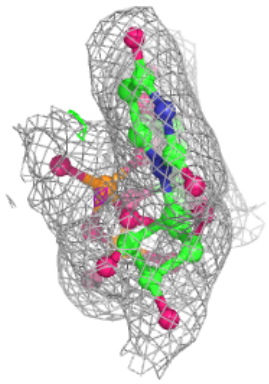
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around UDX H 500:

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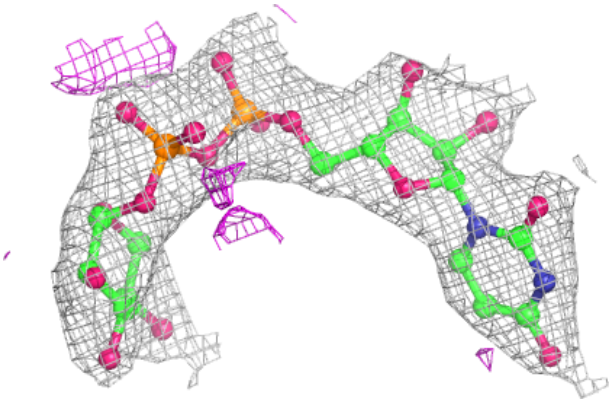
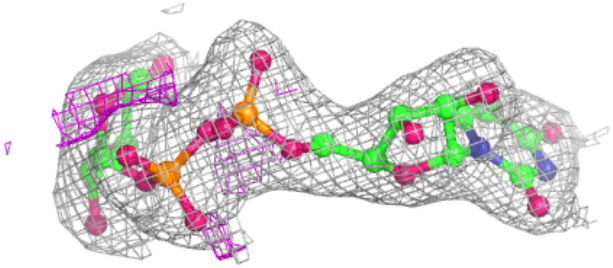
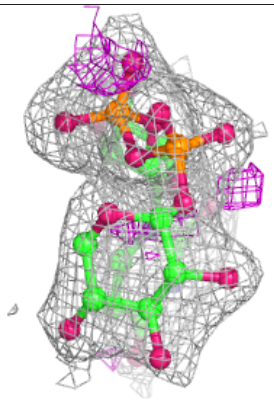
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

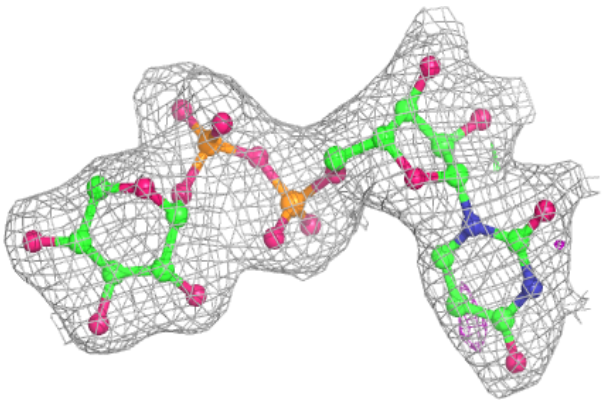


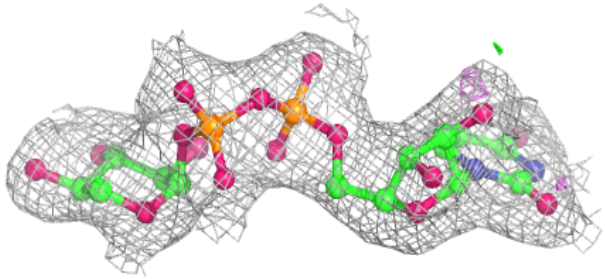


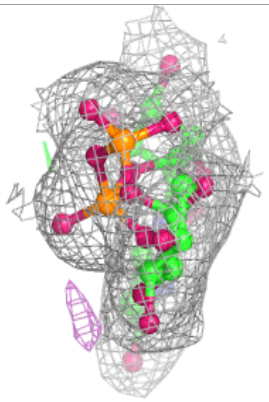


Electron density around UDX H 501:

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

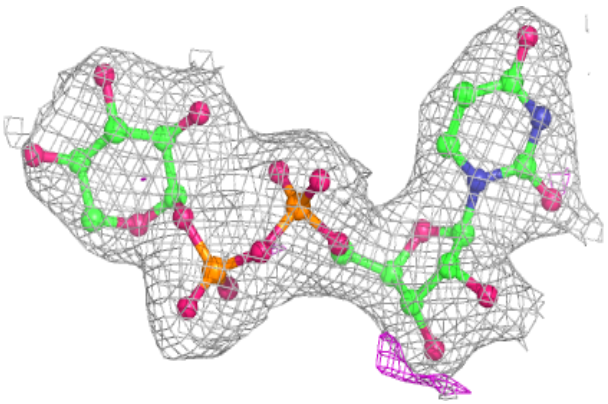


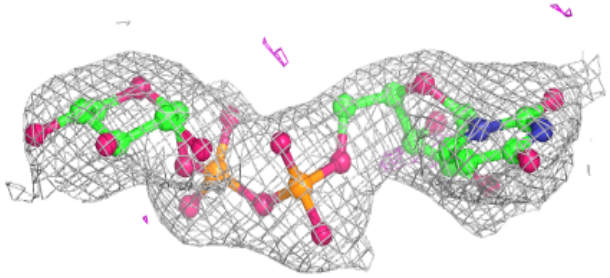


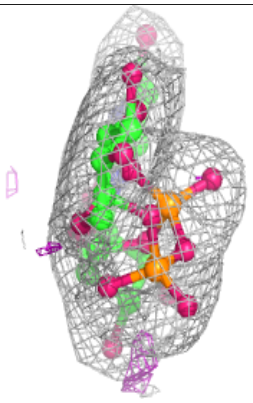


Electron density around UDX B 501:

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

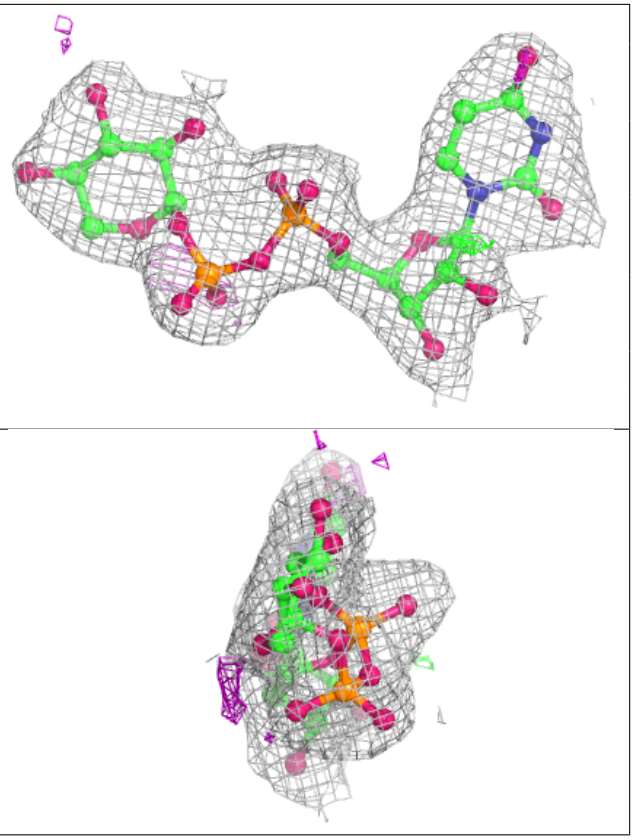






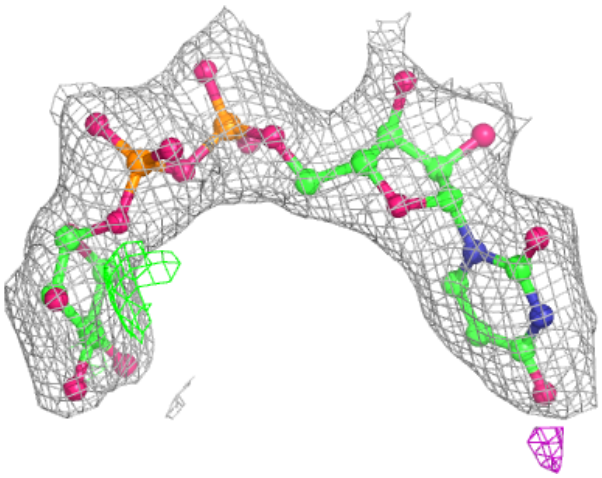
Electron density around UDX I 501:

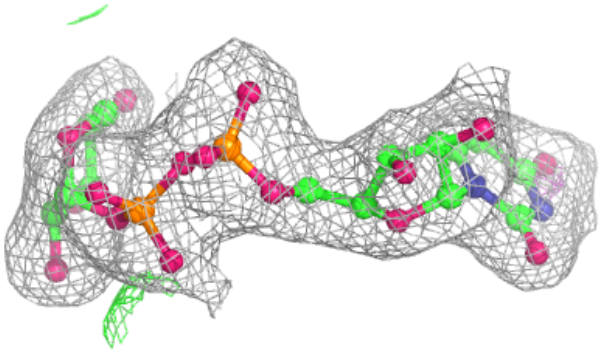
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

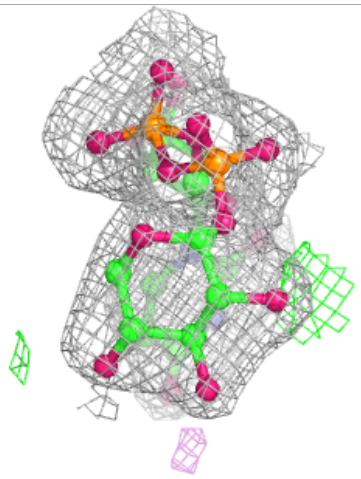


Electron density around UDX C 500:

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

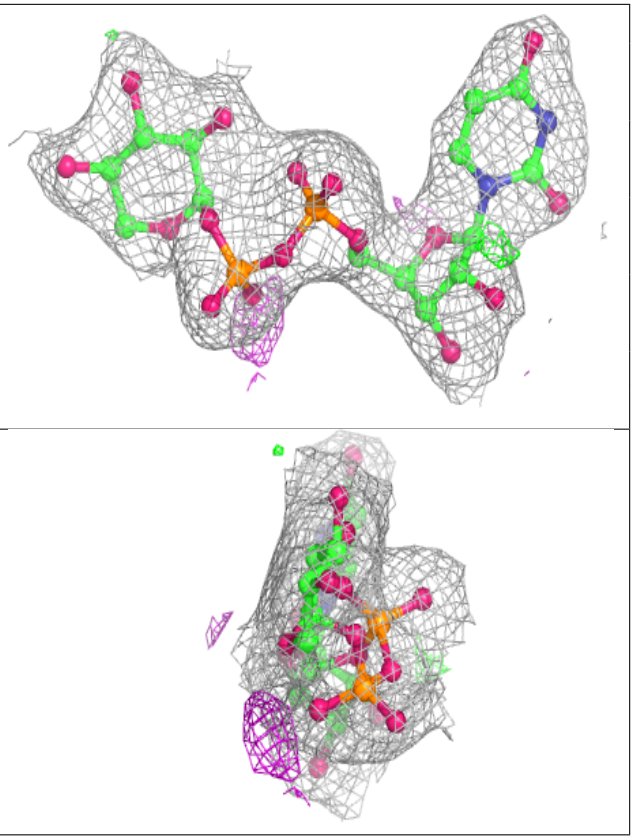






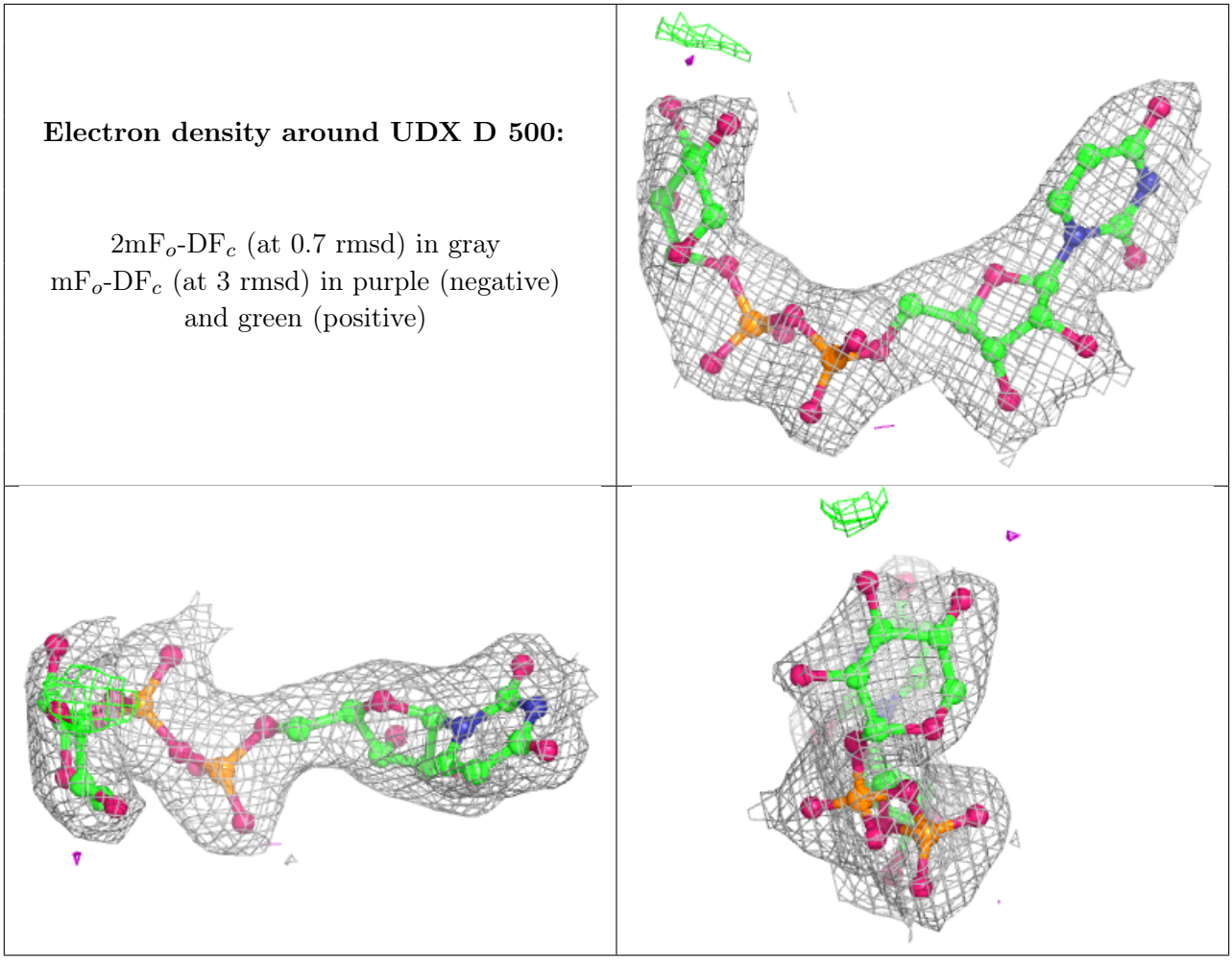
Electron density around UDX J 501:

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



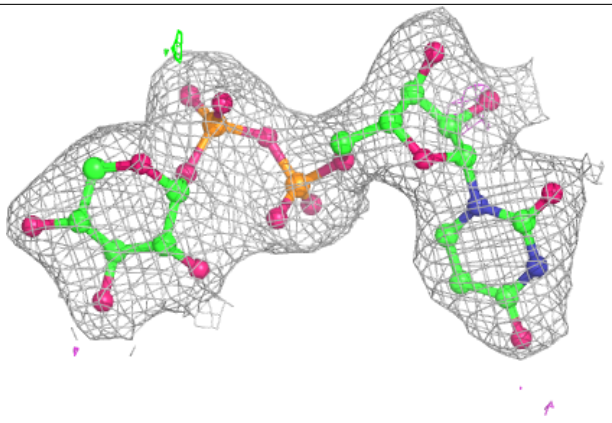
Electron density around UDX D 500:

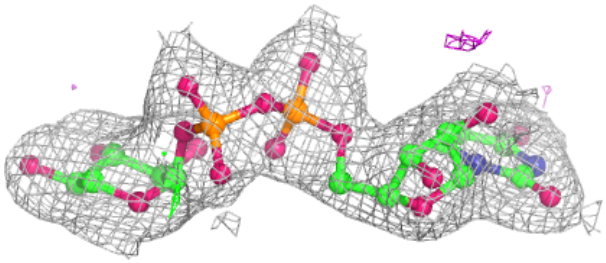
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

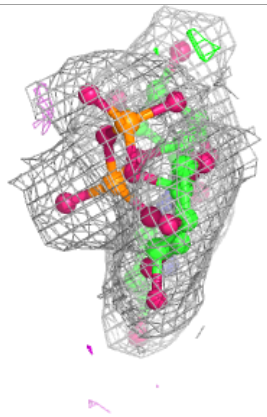


Electron density around UDX K 501:

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

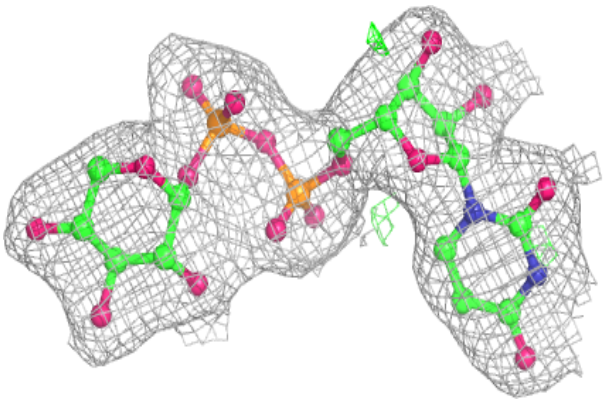


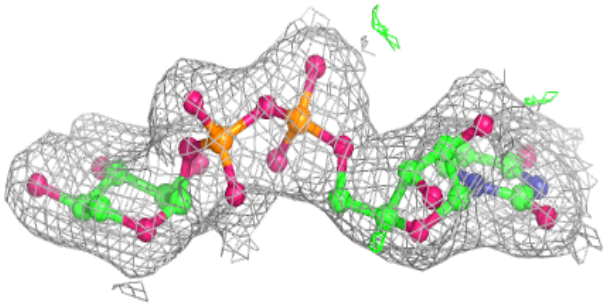


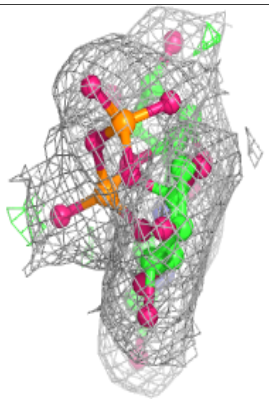


Electron density around UDX A 501:

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

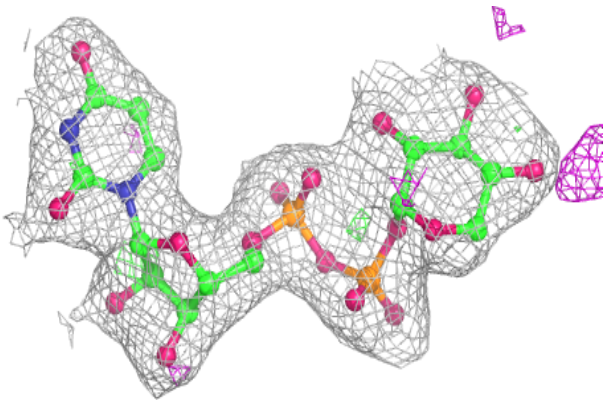


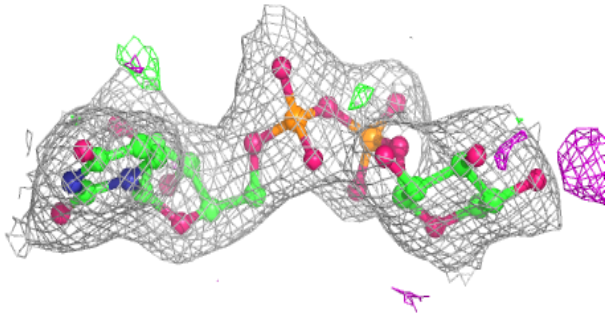


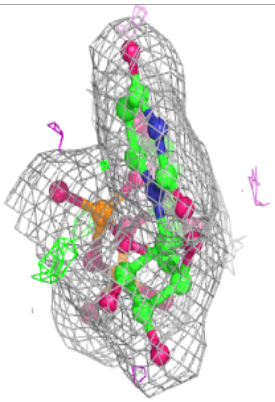


Electron density around UDX L 501:

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

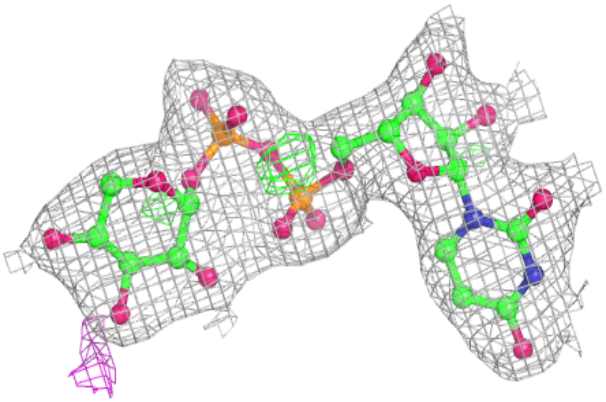


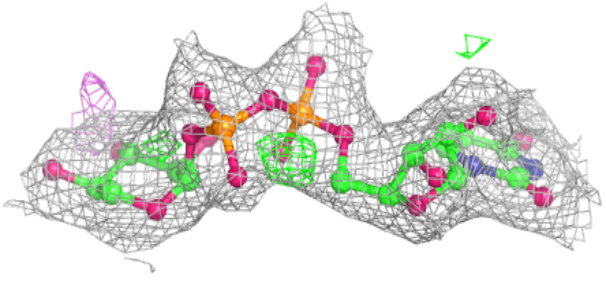


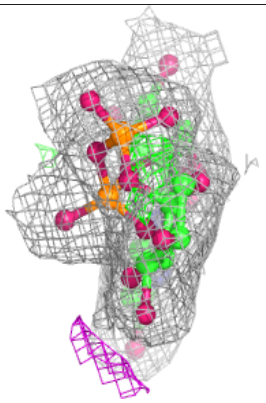


Electron density around UDX C 501:

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

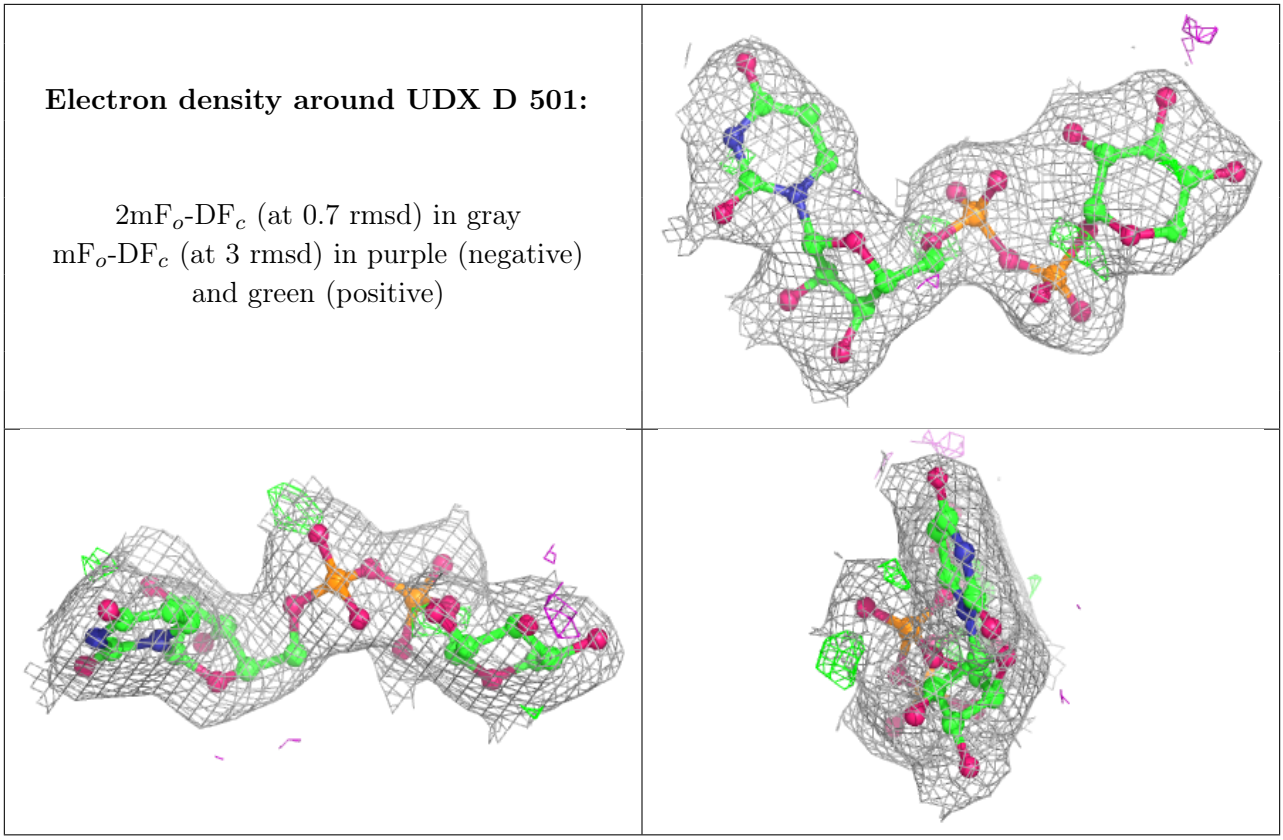






Electron density around UDX D 501:

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



6.5 Other polymers

There are no such residues in this entry.