Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 07:30 AM EDT

PDB ID	:	6PFF
Title	:	Crystal structure of TS-DHFR from Cryptosporidium hominis in complex with NADPH, FdUMP and 2-(4-((2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl)benzamido)-4-cyanobenzoic acid.
Authors	:	Czyzyk, D.J.; Valhondo, M.; Jorgensen, W.L.; Anderson, K.S.
Deposited on	:	2019-06-21
Resolution	:	2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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 2.98 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

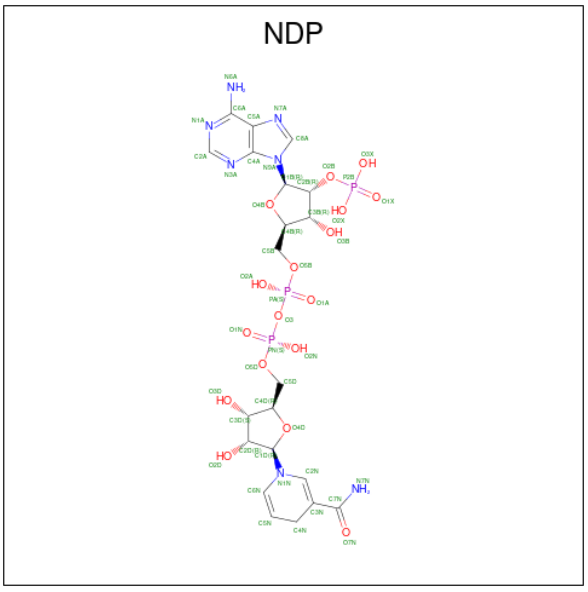
There are 7 unique types of molecules in this entry. The entry contains 20924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			4061	2598	685	757	21			
1	B	506	Total	C	N	O	S	0	0	0
			4085	2612	687	765	21			
1	C	506	Total	C	N	O	S	0	0	0
			4027	2576	676	754	21			
1	D	506	Total	C	N	O	S	0	0	0
			4069	2599	682	767	21			
1	E	506	Total	C	N	O	S	0	0	0
			3973	2532	667	753	21			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



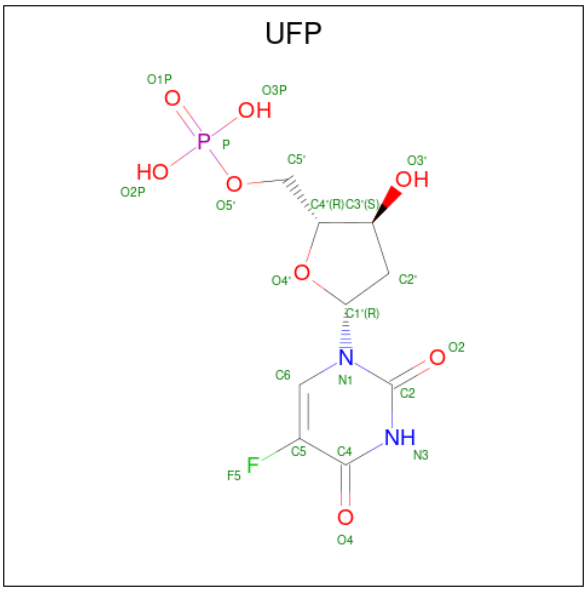
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

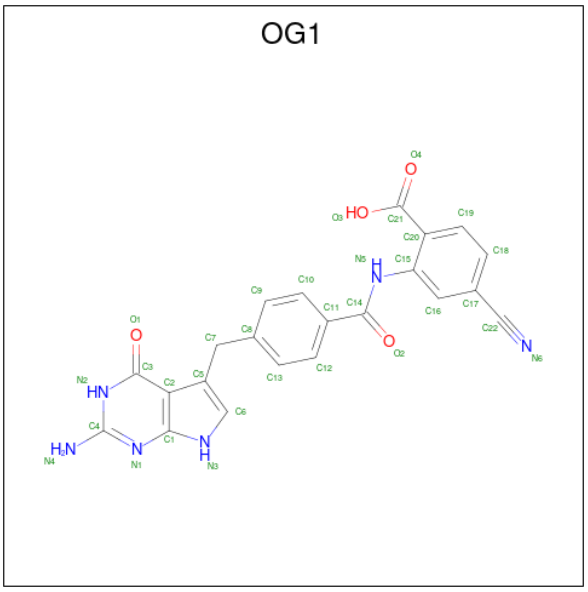
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: $C_9H_{12}FN_2O_8P$).



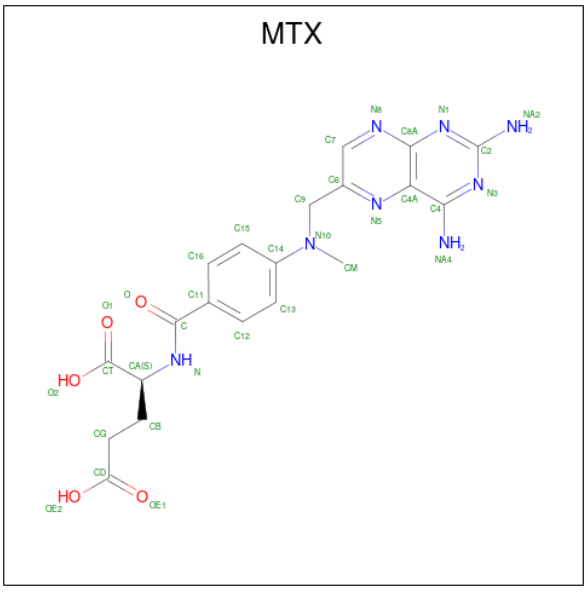
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		
3	B	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		
3	C	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		
3	D	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		
3	E	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		

- Molecule 4 is 2-({4-[(2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl]benzene-1-carbonyl}amino)-4-cyanobenzoic acid (three-letter code: OG1) (formula: $C_{22}H_{16}N_6O_4$) (labeled as "Ligand of Interest" by depositor).



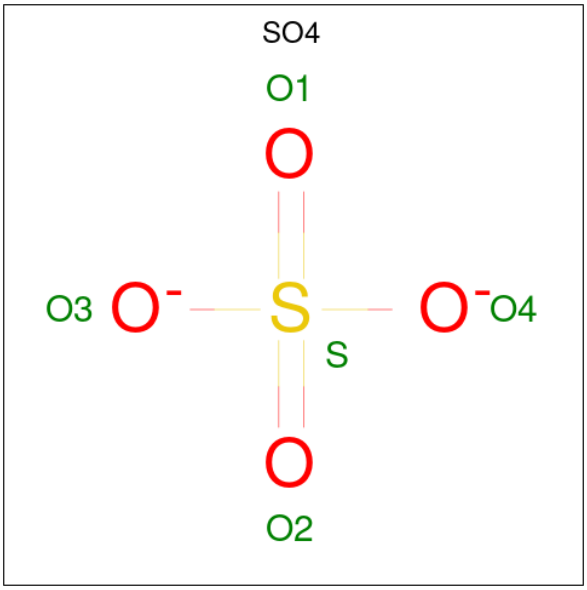
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 32 22 6 4	0	0
4	B	1	Total C N O 32 22 6 4	0	0
4	C	1	Total C N O 32 22 6 4	0	0
4	D	1	Total C N O 32 22 6 4	0	0
4	E	1	Total C N O 32 22 6 4	0	0

- Molecule 5 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 33 20 8 5	0	0
5	B	1	Total C N O 33 20 8 5	0	0
5	C	1	Total C N O 33 20 8 5	0	0
5	D	1	Total C N O 33 20 8 5	0	0
5	E	1	Total C N O 33 20 8 5	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	B	6	Total O 6 6	0	0
7	C	1	Total O 1 1	0	0
7	D	4	Total O 4 4	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	213.42Å 116.79Å 221.76Å 90.00° 95.69° 90.00°	Depositor
Resolution (Å)	48.82 – 2.98	Depositor
% Data completeness (in resolution range)	98.1 (48.82-2.98)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: 000)	Depositor
R, R_{free}	0.208 , 0.239	Depositor
Wilson B-factor (Å^2)	60.6	Xtriage
Anisotropy	0.420	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20924	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

25 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	$\#\|Z\| > 2$
3	UFP	A	602	-	22,22,22	1.04	1 (4%)	33,33,33	2.61	12 (36%)
4	OG1	C	603	-	34,35,35	1.29	3 (8%)	38,50,50	1.03	4 (10%)
6	SO4	C	605	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	B	605	-	4,4,4	0.15	0	6,6,6	0.06	0
3	UFP	C	602	-	22,22,22	1.25	1 (4%)	33,33,33	2.60	12 (36%)
5	MTX	C	604	-	35,35,35	1.61	5 (14%)	46,49,49	1.88	8 (17%)
4	OG1	A	603	-	34,35,35	1.29	3 (8%)	38,50,50	1.03	3 (7%)
6	SO4	E	605	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.06	0
3	UFP	B	602	-	22,22,22	1.23	2 (9%)	33,33,33	2.57	12 (36%)
3	UFP	E	602	-	22,22,22	1.04	0	33,33,33	2.62	12 (36%)
5	MTX	E	604	-	35,35,35	1.59	5 (14%)	46,49,49	1.85	11 (23%)
6	SO4	D	605	-	4,4,4	0.14	0	6,6,6	0.05	0
4	OG1	B	603	-	34,35,35	1.32	3 (8%)	38,50,50	1.16	6 (15%)
2	NDP	A	601	-	45,52,52	1.95	11 (24%)	53,80,80	1.12	7 (13%)
5	MTX	A	604	-	35,35,35	1.62	5 (14%)	46,49,49	1.96	11 (23%)
4	OG1	D	603	-	34,35,35	1.30	3 (8%)	38,50,50	1.13	6 (15%)
2	NDP	B	601	-	45,52,52	1.94	11 (24%)	53,80,80	1.09	6 (11%)
5	MTX	B	604	-	35,35,35	1.62	5 (14%)	46,49,49	1.84	10 (21%)
2	NDP	E	601	-	45,52,52	1.93	11 (24%)	53,80,80	1.10	6 (11%)
5	MTX	D	604	-	35,35,35	1.62	5 (14%)	46,49,49	1.81	8 (17%)
2	NDP	C	601	-	45,52,52	1.93	11 (24%)	53,80,80	1.09	6 (11%)
2	NDP	D	601	-	45,52,52	1.93	11 (24%)	53,80,80	1.11	5 (9%)
3	UFP	D	602	-	22,22,22	1.02	0	33,33,33	2.61	12 (36%)
4	OG1	E	603	-	34,35,35	1.29	3 (8%)	38,50,50	0.95	4 (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
3	UFP	A	602	-	-	4/10/22/22	0/2/2/2
4	OG1	C	603	-	-	2/18/18/18	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UFP	C	602	-	-	4/10/22/22	0/2/2/2
5	MTX	C	604	-	-	6/25/25/25	0/3/3/3
4	OG1	A	603	-	-	2/18/18/18	0/4/4/4
3	UFP	B	602	-	-	4/10/22/22	0/2/2/2
3	UFP	E	602	-	-	3/10/22/22	0/2/2/2
5	MTX	E	604	-	-	7/25/25/25	0/3/3/3
4	OG1	B	603	-	-	2/18/18/18	0/4/4/4
2	NDP	A	601	-	-	2/30/77/77	0/5/5/5
5	MTX	A	604	-	-	5/25/25/25	0/3/3/3
4	OG1	D	603	-	-	2/18/18/18	0/4/4/4
2	NDP	B	601	-	-	2/30/77/77	0/5/5/5
5	MTX	B	604	-	-	6/25/25/25	0/3/3/3
2	NDP	E	601	-	-	3/30/77/77	0/5/5/5
5	MTX	D	604	-	-	8/25/25/25	0/3/3/3
2	NDP	C	601	-	-	2/30/77/77	0/5/5/5
2	NDP	D	601	-	-	5/30/77/77	0/5/5/5
3	UFP	D	602	-	-	4/10/22/22	0/2/2/2
4	OG1	E	603	-	-	2/18/18/18	0/4/4/4

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	604	MTX	C2-NA2	5.31	1.44	1.33
5	D	604	MTX	C2-NA2	5.30	1.44	1.33
5	B	604	MTX	C2-NA2	5.29	1.44	1.33
5	A	604	MTX	C2-NA2	5.25	1.44	1.33
5	E	604	MTX	C2-NA2	5.19	1.44	1.33
5	D	604	MTX	C-N	5.15	1.45	1.34
5	B	604	MTX	C-N	5.08	1.45	1.34
5	A	604	MTX	C-N	5.00	1.45	1.34
5	C	604	MTX	C-N	4.95	1.44	1.34
5	E	604	MTX	C-N	4.92	1.44	1.34
2	D	601	NDP	C4N-C3N	-4.48	1.41	1.49
2	B	601	NDP	C4N-C3N	-4.47	1.41	1.49
2	E	601	NDP	C4N-C3N	-4.45	1.41	1.49
2	C	601	NDP	C4N-C3N	-4.44	1.41	1.49
2	A	601	NDP	C4N-C3N	-4.42	1.41	1.49
2	C	601	NDP	C6A-N6A	4.11	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NDP	C6A-N6A	4.09	1.49	1.34
2	A	601	NDP	C6A-N6A	4.08	1.49	1.34
2	E	601	NDP	C6A-N6A	4.07	1.48	1.34
2	D	601	NDP	C6A-N6A	4.06	1.48	1.34
2	A	601	NDP	C7N-N7N	4.04	1.44	1.33
2	B	601	NDP	C7N-N7N	4.01	1.44	1.33
2	D	601	NDP	C7N-N7N	4.00	1.44	1.33
2	E	601	NDP	C7N-N7N	4.00	1.44	1.33
2	C	601	NDP	C7N-N7N	3.97	1.44	1.33
2	A	601	NDP	C2D-C3D	-3.89	1.42	1.53
2	E	601	NDP	C2D-C3D	-3.88	1.42	1.53
2	B	601	NDP	C2D-C3D	-3.86	1.42	1.53
2	C	601	NDP	C2D-C3D	-3.86	1.42	1.53
2	D	601	NDP	C2D-C3D	-3.83	1.42	1.53
2	C	601	NDP	C3B-C2B	-3.79	1.44	1.52
2	A	601	NDP	C3B-C2B	-3.73	1.44	1.52
2	B	601	NDP	C3B-C2B	-3.70	1.44	1.52
2	E	601	NDP	C3B-C2B	-3.70	1.44	1.52
2	A	601	NDP	C6N-C5N	3.70	1.39	1.33
2	D	601	NDP	C3B-C2B	-3.69	1.44	1.52
2	B	601	NDP	C6N-C5N	3.64	1.39	1.33
2	C	601	NDP	C6N-C5N	3.63	1.39	1.33
2	D	601	NDP	C6N-C5N	3.61	1.39	1.33
2	E	601	NDP	C6N-C5N	3.60	1.39	1.33
3	C	602	UFP	P-O1P	3.26	1.61	1.50
4	B	603	OG1	C2-C1	-3.24	1.37	1.42
4	C	603	OG1	C2-C1	-3.24	1.37	1.42
2	A	601	NDP	C4N-C5N	-3.22	1.40	1.48
4	D	603	OG1	C2-C1	-3.20	1.37	1.42
2	C	601	NDP	C4N-C5N	-3.20	1.40	1.48
2	D	601	NDP	C4N-C5N	-3.20	1.40	1.48
4	A	603	OG1	C2-C1	-3.19	1.37	1.42
2	E	601	NDP	C4N-C5N	-3.19	1.40	1.48
2	B	601	NDP	C4N-C5N	-3.18	1.40	1.48
4	E	603	OG1	C2-C1	-3.16	1.37	1.42
3	B	602	UFP	P-O1P	3.12	1.60	1.50
5	E	604	MTX	C4-NA4	2.54	1.43	1.34
4	B	603	OG1	C2-C5	2.53	1.44	1.39
5	A	604	MTX	C4-NA4	2.53	1.43	1.34
5	D	604	MTX	C4-NA4	2.53	1.43	1.34
5	C	604	MTX	C4-NA4	2.53	1.43	1.34
5	B	604	MTX	C4-NA4	2.50	1.43	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	OG1	C2-C5	2.47	1.44	1.39
4	E	603	OG1	C2-C5	2.43	1.44	1.39
2	D	601	NDP	C3B-C4B	-2.42	1.46	1.53
2	E	601	NDP	C3B-C4B	-2.40	1.46	1.53
5	A	604	MTX	C7-N8	2.40	1.35	1.31
5	B	604	MTX	C7-N8	2.39	1.35	1.31
2	A	601	NDP	C3B-C4B	-2.39	1.46	1.53
2	C	601	NDP	C3B-C4B	-2.39	1.46	1.53
4	A	603	OG1	C2-C5	2.38	1.44	1.39
5	C	604	MTX	C7-N8	2.38	1.35	1.31
4	C	603	OG1	C2-C5	2.38	1.44	1.39
5	D	604	MTX	C14-N10	2.37	1.45	1.39
2	E	601	NDP	C4A-N3A	2.36	1.38	1.35
2	B	601	NDP	C3B-C4B	-2.34	1.47	1.53
2	D	601	NDP	C4A-N3A	2.33	1.38	1.35
2	A	601	NDP	C3D-C4D	-2.33	1.47	1.53
4	B	603	OG1	O3-C21	2.28	1.37	1.30
5	E	604	MTX	C7-N8	2.28	1.35	1.31
2	A	601	NDP	C4A-N3A	2.27	1.38	1.35
2	B	601	NDP	C3D-C4D	-2.26	1.47	1.53
5	E	604	MTX	C14-N10	2.26	1.45	1.39
2	E	601	NDP	C3D-C4D	-2.26	1.47	1.53
5	B	604	MTX	C14-N10	2.25	1.45	1.39
5	D	604	MTX	C7-N8	2.25	1.35	1.31
4	D	603	OG1	O3-C21	2.24	1.37	1.30
2	C	601	NDP	C4A-N3A	2.24	1.38	1.35
2	C	601	NDP	C3D-C4D	-2.24	1.47	1.53
4	C	603	OG1	O3-C21	2.23	1.37	1.30
2	B	601	NDP	C4A-N3A	2.23	1.38	1.35
5	C	604	MTX	C14-N10	2.22	1.45	1.39
4	A	603	OG1	O3-C21	2.22	1.37	1.30
2	D	601	NDP	C3D-C4D	-2.22	1.47	1.53
5	A	604	MTX	C14-N10	2.16	1.45	1.39
4	E	603	OG1	O3-C21	2.16	1.37	1.30
2	A	601	NDP	C2N-C3N	2.14	1.40	1.34
2	B	601	NDP	C2N-C3N	2.09	1.40	1.34
2	E	601	NDP	C2N-C3N	2.06	1.40	1.34
3	A	602	UFP	C4-C5	-2.06	1.41	1.44
2	C	601	NDP	C2N-C3N	2.05	1.40	1.34
3	B	602	UFP	C4-N3	-2.04	1.35	1.38
2	D	601	NDP	C2N-C3N	2.02	1.40	1.34

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	UFP	C5-C4-N3	6.51	118.97	112.56
3	E	602	UFP	C5-C4-N3	6.49	118.94	112.56
3	D	602	UFP	C5-C4-N3	6.46	118.92	112.56
3	C	602	UFP	C5-C4-N3	6.36	118.81	112.56
3	B	602	UFP	C5-C4-N3	6.34	118.80	112.56
3	A	602	UFP	O4-C4-C5	-5.90	120.40	125.72
3	E	602	UFP	O4-C4-C5	-5.87	120.43	125.72
3	C	602	UFP	O4-C4-C5	-5.78	120.50	125.72
3	D	602	UFP	O4-C4-C5	-5.68	120.59	125.72
3	B	602	UFP	O4-C4-C5	-5.46	120.79	125.72
5	A	604	MTX	C6-C7-N8	-5.30	117.93	123.13
3	D	602	UFP	F5-C5-C4	5.25	121.27	116.40
5	E	604	MTX	C6-C7-N8	-5.08	118.15	123.13
5	C	604	MTX	C6-C7-N8	-4.97	118.26	123.13
3	B	602	UFP	F5-C5-C4	4.95	120.99	116.40
3	A	602	UFP	F5-C5-C4	4.79	120.83	116.40
3	C	602	UFP	F5-C5-C4	4.73	120.78	116.40
5	D	604	MTX	C6-C7-N8	-4.73	118.50	123.13
3	E	602	UFP	F5-C5-C4	4.73	120.78	116.40
5	B	604	MTX	C6-C7-N8	-4.66	118.56	123.13
3	D	602	UFP	C4-N3-C2	-4.58	121.43	127.35
3	E	602	UFP	C4-N3-C2	-4.57	121.44	127.35
3	A	602	UFP	C4-N3-C2	-4.50	121.53	127.35
5	C	604	MTX	CG-CB-CA	4.49	121.55	113.16
3	B	602	UFP	C4-N3-C2	-4.44	121.61	127.35
3	C	602	UFP	C4-N3-C2	-4.42	121.63	127.35
3	C	602	UFP	C1'-N1-C2	4.40	126.31	117.64
3	E	602	UFP	C1'-N1-C2	4.37	126.25	117.64
3	D	602	UFP	C1'-N1-C2	4.33	126.17	117.64
3	A	602	UFP	C6-C5-C4	-4.32	118.57	122.60
3	A	602	UFP	C1'-N1-C2	4.32	126.15	117.64
3	C	602	UFP	C6-C5-C4	-4.22	118.66	122.60
3	B	602	UFP	C1'-N1-C2	4.19	125.90	117.64
3	E	602	UFP	N3-C2-N1	4.18	120.44	114.89
3	D	602	UFP	C6-C5-C4	-4.17	118.71	122.60
3	C	602	UFP	N3-C2-N1	4.16	120.41	114.89
3	E	602	UFP	C6-C5-C4	-4.16	118.72	122.60
3	B	602	UFP	C6-C5-C4	-4.13	118.75	122.60
3	B	602	UFP	N3-C2-N1	4.13	120.37	114.89
5	A	604	MTX	CG-CB-CA	4.10	120.82	113.16
3	A	602	UFP	N3-C2-N1	4.09	120.32	114.89
3	D	602	UFP	N3-C2-N1	4.09	120.31	114.89
5	A	604	MTX	N8-C8A-N1	4.04	120.43	115.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	604	MTX	C7-N8-C8A	4.02	120.73	116.69
5	D	604	MTX	C7-N8-C8A	3.96	120.67	116.69
5	B	604	MTX	N8-C8A-N1	3.93	120.30	115.82
5	D	604	MTX	N1-C2-N3	-3.90	122.02	127.22
3	E	602	UFP	P-O5'-C5'	-3.89	107.57	118.30
5	E	604	MTX	C7-N8-C8A	3.87	120.58	116.69
2	E	601	NDP	N3A-C2A-N1A	-3.82	122.70	128.68
5	C	604	MTX	N1-C2-N3	-3.82	122.13	127.22
5	A	604	MTX	C2-N1-C8A	3.81	119.71	115.36
2	C	601	NDP	N3A-C2A-N1A	-3.80	122.75	128.68
5	B	604	MTX	CG-CB-CA	3.79	120.24	113.16
5	D	604	MTX	N8-C8A-N1	3.75	120.11	115.82
5	A	604	MTX	N1-C2-N3	-3.74	122.23	127.22
5	A	604	MTX	C7-N8-C8A	3.74	120.45	116.69
5	B	604	MTX	N1-C2-N3	-3.72	122.26	127.22
2	A	601	NDP	N3A-C2A-N1A	-3.72	122.87	128.68
5	C	604	MTX	N8-C8A-N1	3.71	120.06	115.82
5	D	604	MTX	CG-CB-CA	3.66	120.00	113.16
3	D	602	UFP	P-O5'-C5'	-3.65	108.24	118.30
2	D	601	NDP	N3A-C2A-N1A	-3.65	122.97	128.68
5	D	604	MTX	C2-N1-C8A	3.65	119.52	115.36
5	B	604	MTX	C7-N8-C8A	3.63	120.34	116.69
2	B	601	NDP	N3A-C2A-N1A	-3.63	123.00	128.68
5	E	604	MTX	N1-C2-N3	-3.61	122.40	127.22
3	D	602	UFP	C1'-N1-C6	-3.57	114.61	120.77
3	C	602	UFP	P-O5'-C5'	-3.57	108.45	118.30
5	B	604	MTX	C2-N1-C8A	3.57	119.43	115.36
5	C	604	MTX	C2-N1-C8A	3.55	119.42	115.36
5	E	604	MTX	CG-CB-CA	3.55	119.79	113.16
3	A	602	UFP	P-O5'-C5'	-3.53	108.56	118.30
3	E	602	UFP	C1'-N1-C6	-3.52	114.70	120.77
5	E	604	MTX	N8-C8A-N1	3.51	119.83	115.82
3	B	602	UFP	P-O5'-C5'	-3.47	108.74	118.30
4	B	603	OG1	C20-C15-N5	3.46	124.94	118.69
3	A	602	UFP	C1'-N1-C6	-3.46	114.81	120.77
5	E	604	MTX	C2-N1-C8A	3.45	119.30	115.36
3	C	602	UFP	C1'-N1-C6	-3.43	114.85	120.77
3	B	602	UFP	C1'-N1-C6	-3.33	115.04	120.77
4	D	603	OG1	C20-C15-N5	3.28	124.62	118.69
3	C	602	UFP	O2-C2-N3	-2.95	116.00	121.50
2	B	601	NDP	PN-O3-PA	-2.94	122.73	132.83
2	D	601	NDP	PN-O3-PA	-2.93	122.77	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	NDP	PN-O3-PA	-2.93	122.77	132.83
3	E	602	UFP	O2-C2-N3	-2.92	116.06	121.50
3	B	602	UFP	O2-C2-N3	-2.89	116.12	121.50
3	A	602	UFP	O2-C2-N3	-2.87	116.16	121.50
2	A	601	NDP	PN-O3-PA	-2.86	123.03	132.83
4	A	603	OG1	C20-C15-N5	2.77	123.70	118.69
3	D	602	UFP	O2-C2-N3	-2.73	116.41	121.50
5	A	604	MTX	C6-C9-N10	-2.69	108.98	113.60
2	E	601	NDP	PN-O3-PA	-2.66	123.71	132.83
3	B	602	UFP	O4'-C1'-C2'	-2.64	101.26	106.25
5	E	604	MTX	C4A-C4-N3	-2.61	119.30	121.01
4	C	603	OG1	C20-C15-N5	2.59	123.37	118.69
5	C	604	MTX	C4A-C4-N3	-2.58	119.32	121.01
4	B	603	OG1	C5-C7-C8	-2.58	108.39	114.22
5	B	604	MTX	C4A-C4-N3	-2.54	119.34	121.01
2	E	601	NDP	O5D-C5D-C4D	2.52	117.68	108.99
5	A	604	MTX	C7-C6-N5	2.52	122.50	120.85
2	D	601	NDP	O5D-C5D-C4D	2.51	117.64	108.99
4	D	603	OG1	C5-C7-C8	-2.50	108.57	114.22
5	A	604	MTX	C4A-C4-N3	-2.46	119.39	121.01
3	C	602	UFP	C6-N1-C2	-2.43	118.84	121.30
4	D	603	OG1	N4-C4-N2	-2.42	111.55	116.71
4	B	603	OG1	C15-C20-C21	2.42	124.57	121.72
4	A	603	OG1	N4-C4-N2	-2.41	111.59	116.71
4	C	603	OG1	N4-C4-N2	-2.41	111.59	116.71
4	E	603	OG1	C20-C15-N5	2.40	123.03	118.69
2	E	601	NDP	O5B-C5B-C4B	2.39	117.21	108.99
2	D	601	NDP	O5B-C5B-C4B	2.36	117.12	108.99
2	A	601	NDP	C3N-C7N-N7N	2.36	121.85	117.67
2	C	601	NDP	O5D-C5D-C4D	2.34	117.05	108.99
4	E	603	OG1	N4-C4-N2	-2.34	111.73	116.71
5	C	604	MTX	O2-CT-CA	2.32	121.10	113.40
4	B	603	OG1	N4-C4-N2	-2.30	111.82	116.71
2	D	601	NDP	C4A-C5A-N7A	-2.30	107.01	109.40
4	D	603	OG1	N4-C4-N1	2.29	124.20	119.74
2	B	601	NDP	C3N-C7N-N7N	2.29	121.73	117.67
2	C	601	NDP	C4A-C5A-N7A	-2.28	107.03	109.40
4	A	603	OG1	N4-C4-N1	2.28	124.17	119.74
4	D	603	OG1	C15-C20-C21	2.27	124.40	121.72
5	A	604	MTX	CM-N10-C9	2.27	120.87	114.84
2	A	601	NDP	O5D-C5D-C4D	2.27	116.80	108.99
5	A	604	MTX	O2-CT-CA	2.26	120.90	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	NDP	C4A-C5A-N7A	-2.26	107.05	109.40
2	B	601	NDP	O5D-C5D-C4D	2.25	116.73	108.99
3	A	602	UFP	C6-N1-C2	-2.23	119.04	121.30
2	A	601	NDP	O4D-C1D-N1N	2.23	112.41	108.06
3	E	602	UFP	C6-N1-C2	-2.21	119.05	121.30
4	C	603	OG1	N4-C4-N1	2.21	124.05	119.74
2	B	601	NDP	C4A-C5A-N7A	-2.21	107.09	109.40
5	D	604	MTX	C4A-C4-N3	-2.21	119.56	121.01
2	C	601	NDP	O5B-C5B-C4B	2.21	116.59	108.99
5	E	604	MTX	CM-N10-C9	2.20	120.70	114.84
3	B	602	UFP	C6-N1-C2	-2.20	119.07	121.30
5	E	604	MTX	C7-C6-N5	2.20	122.28	120.85
2	A	601	NDP	C4A-C5A-N7A	-2.19	107.12	109.40
4	E	603	OG1	N4-C4-N1	2.18	123.98	119.74
5	B	604	MTX	O2-CT-CA	2.17	120.63	113.40
5	E	604	MTX	C6-C9-N10	-2.16	109.89	113.60
2	E	601	NDP	C3N-C7N-N7N	2.16	121.50	117.67
4	B	603	OG1	N4-C4-N1	2.16	123.93	119.74
2	A	601	NDP	O5B-C5B-C4B	2.15	116.40	108.99
4	B	603	OG1	C16-C15-N5	-2.15	116.22	121.90
3	C	602	UFP	O4'-C1'-C2'	-2.13	102.22	106.25
3	E	602	UFP	O4'-C1'-C2'	-2.13	102.23	106.25
4	E	603	OG1	C15-C20-C21	2.10	124.19	121.72
4	C	603	OG1	C15-C20-C21	2.08	124.17	121.72
2	B	601	NDP	O5B-C5B-C4B	2.07	116.12	108.99
3	A	602	UFP	O4'-C1'-C2'	-2.07	102.34	106.25
3	D	602	UFP	O4'-C1'-C2'	-2.06	102.36	106.25
5	D	604	MTX	O2-CT-CA	2.05	120.22	113.40
3	D	602	UFP	C6-N1-C2	-2.05	119.22	121.30
5	B	604	MTX	C6-C9-N10	-2.05	110.09	113.60
5	B	604	MTX	CM-N10-C9	2.04	120.27	114.84
5	E	604	MTX	OE2-CD-OE1	-2.03	118.23	123.30
4	D	603	OG1	C16-C15-N5	-2.01	116.59	121.90
2	C	601	NDP	C3N-C7N-N7N	2.01	121.23	117.67

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	604	MTX	N-CA-CB-CG
5	C	604	MTX	CT-CA-CB-CG
5	E	604	MTX	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	604	MTX	N-CA-CB-CG
2	D	601	NDP	C3D-C4D-C5D-O5D
3	C	602	UFP	C3'-C4'-C5'-O5'
3	C	602	UFP	O4'-C4'-C5'-O5'
5	C	604	MTX	C13-C14-N10-CM
5	D	604	MTX	C13-C14-N10-CM
5	D	604	MTX	CT-CA-CB-CG
5	E	604	MTX	CT-CA-CB-CG
2	D	601	NDP	O4D-C4D-C5D-O5D
3	D	602	UFP	C3'-C4'-C5'-O5'
3	D	602	UFP	O4'-C4'-C5'-O5'
5	B	604	MTX	C13-C14-N10-CM
5	C	604	MTX	C15-C14-N10-CM
5	D	604	MTX	C15-C14-N10-CM
5	B	604	MTX	C15-C14-N10-CM
3	A	602	UFP	O4'-C4'-C5'-O5'
3	B	602	UFP	C3'-C4'-C5'-O5'
3	B	602	UFP	O4'-C4'-C5'-O5'
5	A	604	MTX	C15-C14-N10-CM
5	E	604	MTX	C15-C14-N10-CM
3	A	602	UFP	C2'-C1'-N1-C2
3	B	602	UFP	C2'-C1'-N1-C2
3	C	602	UFP	C2'-C1'-N1-C2
3	E	602	UFP	C2'-C1'-N1-C2
5	A	604	MTX	C13-C14-N10-CM
5	E	604	MTX	C13-C14-N10-CM
3	D	602	UFP	C2'-C1'-N1-C2
3	A	602	UFP	C2'-C1'-N1-C6
3	E	602	UFP	C2'-C1'-N1-C6
4	C	603	OG1	C16-C15-N5-C14
4	E	603	OG1	C16-C15-N5-C14
4	B	603	OG1	C16-C15-N5-C14
3	A	602	UFP	C3'-C4'-C5'-O5'
4	D	603	OG1	C16-C15-N5-C14
3	B	602	UFP	C2'-C1'-N1-C6
3	C	602	UFP	C2'-C1'-N1-C6
4	A	603	OG1	C16-C15-N5-C14
5	A	604	MTX	C6-C9-N10-CM
5	B	604	MTX	C6-C9-N10-CM
5	C	604	MTX	C6-C9-N10-CM
5	D	604	MTX	C6-C9-N10-CM
5	E	604	MTX	C6-C9-N10-CM

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	602	UFP	C2'-C1'-N1-C6
4	E	603	OG1	C20-C15-N5-C14
4	C	603	OG1	C20-C15-N5-C14
4	D	603	OG1	C20-C15-N5-C14
5	B	604	MTX	CT-CA-CB-CG
2	A	601	NDP	O4D-C1D-N1N-C2N
2	C	601	NDP	O4D-C1D-N1N-C2N
2	E	601	NDP	O4D-C1D-N1N-C2N
4	B	603	OG1	C20-C15-N5-C14
5	A	604	MTX	OE1-CD-CG-CB
5	B	604	MTX	OE1-CD-CG-CB
2	B	601	NDP	O4D-C1D-N1N-C2N
2	D	601	NDP	O4D-C1D-N1N-C2N
4	A	603	OG1	C20-C15-N5-C14
5	B	604	MTX	OE2-CD-CG-CB
5	E	604	MTX	OE1-CD-CG-CB
2	A	601	NDP	C2D-C1D-N1N-C2N
2	B	601	NDP	C2D-C1D-N1N-C2N
2	C	601	NDP	C2D-C1D-N1N-C2N
5	E	604	MTX	OE2-CD-CG-CB
5	A	604	MTX	OE2-CD-CG-CB
2	E	601	NDP	C2D-C1D-N1N-C2N
2	E	601	NDP	C3D-C4D-C5D-O5D
5	C	604	MTX	C15-C14-N10-C9
5	D	604	MTX	OE1-CD-CG-CB
5	D	604	MTX	OE2-CD-CG-CB
5	D	604	MTX	C15-C14-N10-C9
3	E	602	UFP	O4'-C4'-C5'-O5'
2	D	601	NDP	C5D-O5D-PN-O2N
2	D	601	NDP	C2D-C1D-N1N-C2N

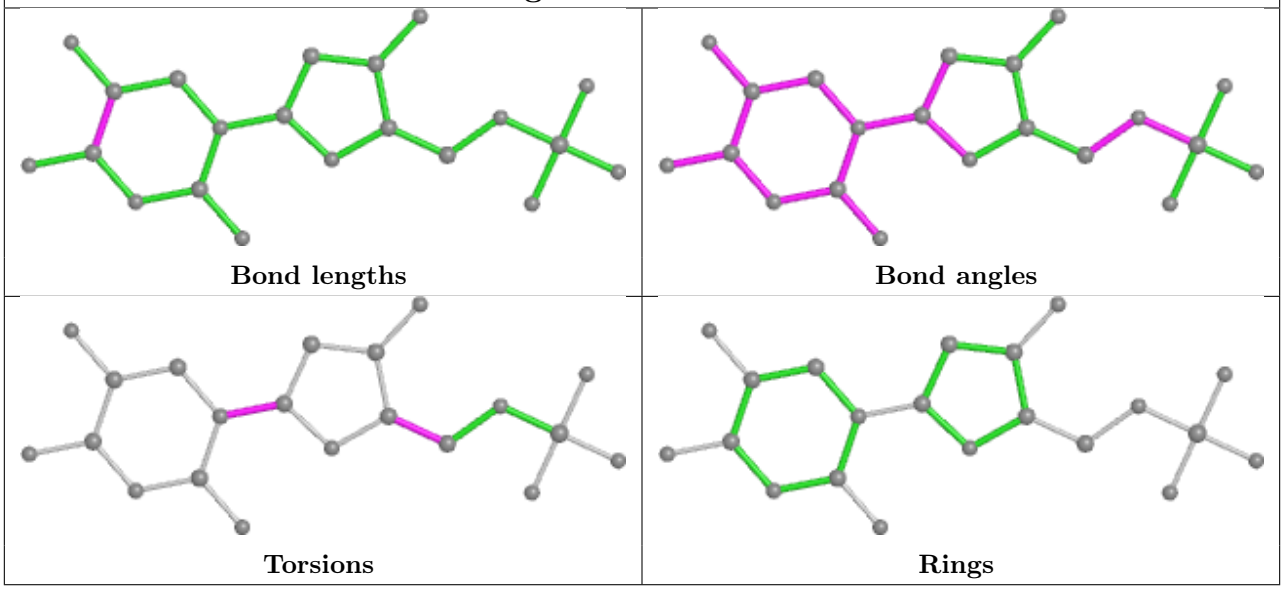
There are no ring outliers.

No monomer is involved in short contacts.

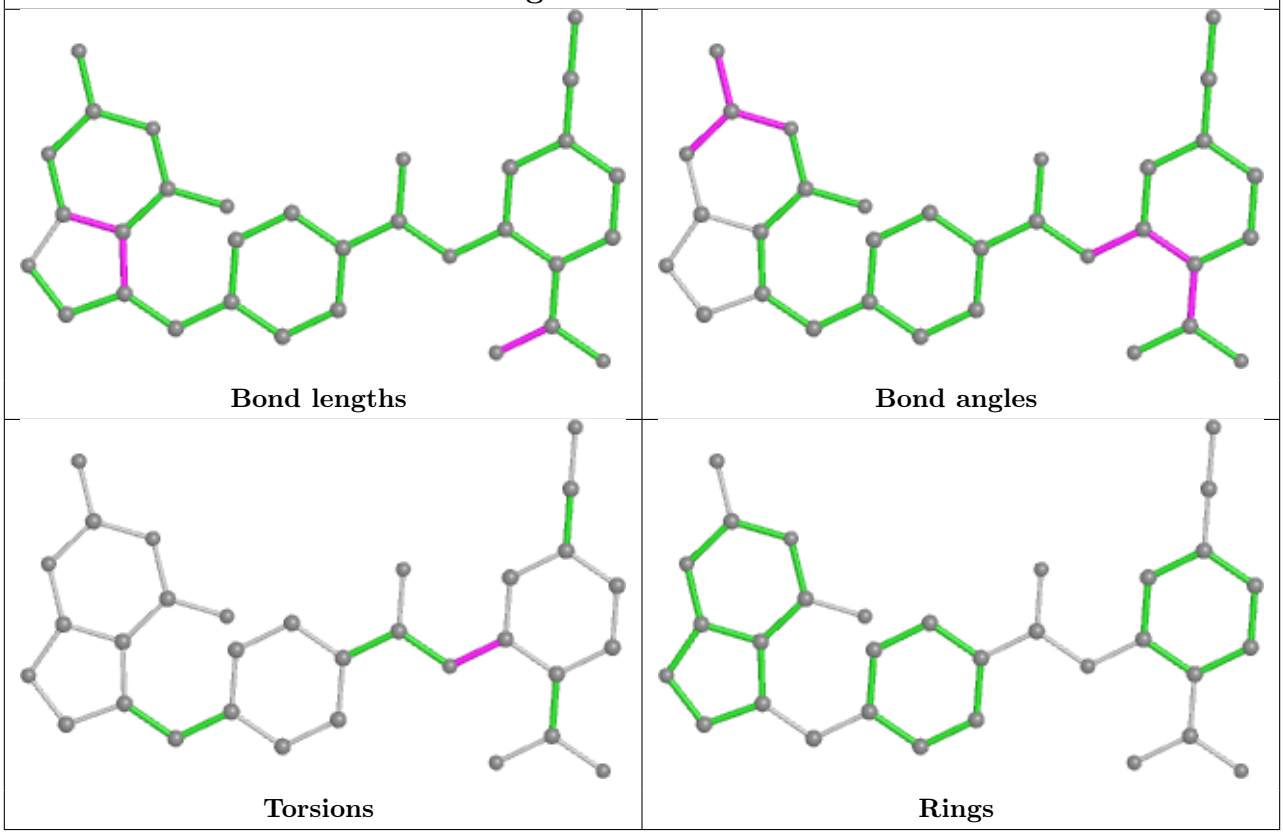
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

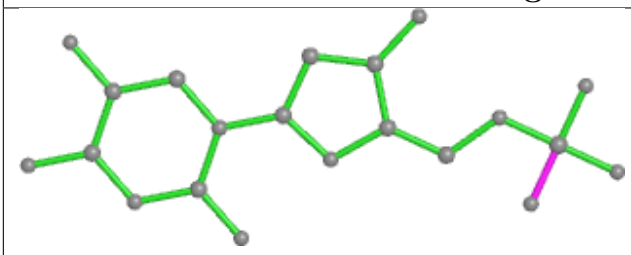
Ligand UFP A 602



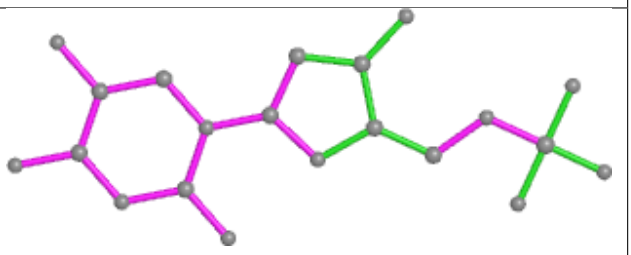
Ligand OG1 C 603



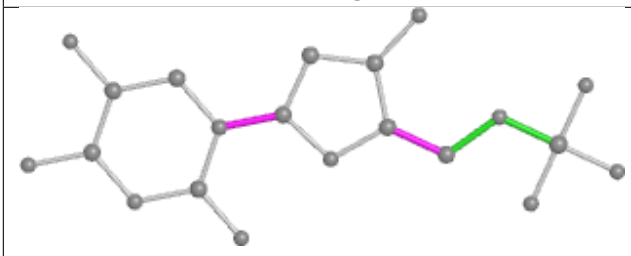
Ligand UFP C 602



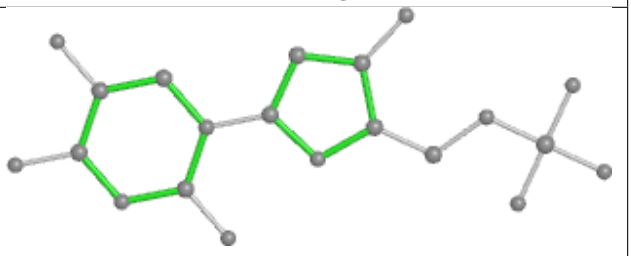
Bond lengths



Bond angles

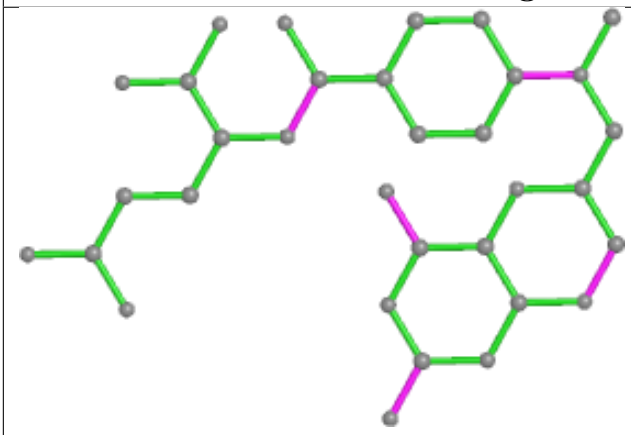


Torsions

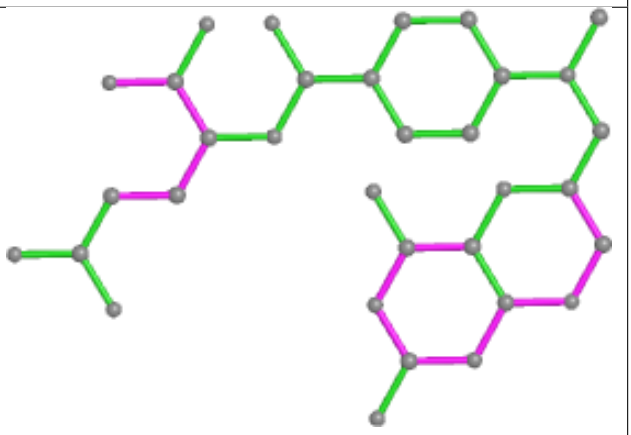


Rings

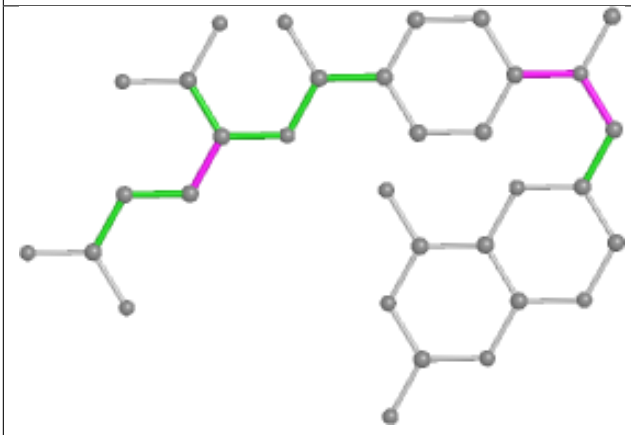
Ligand MTX C 604



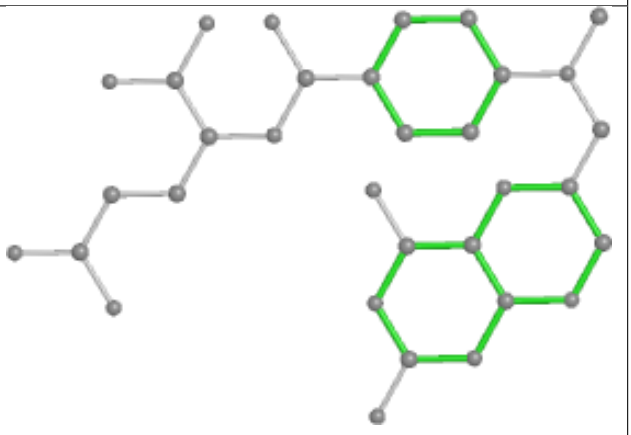
Bond lengths



Bond angles

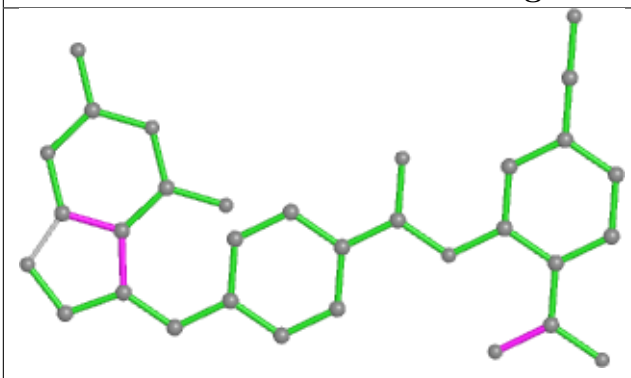


Torsions

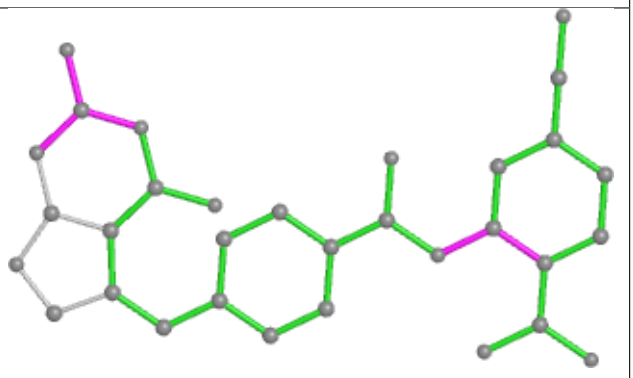


Rings

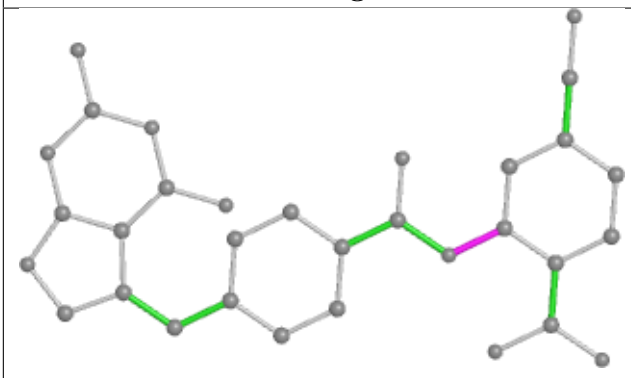
Ligand OG1 A 603



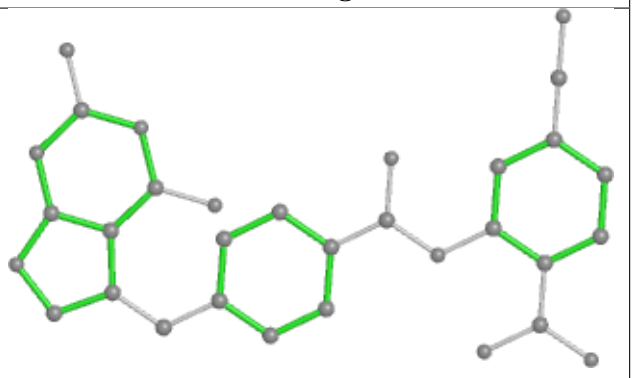
Bond lengths



Bond angles

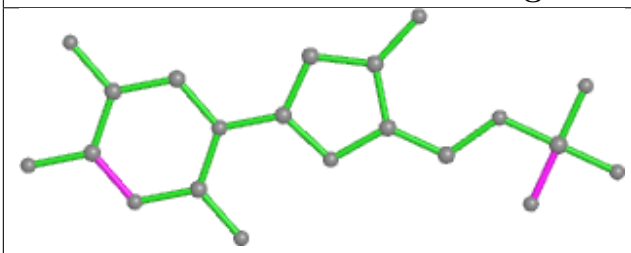


Torsions

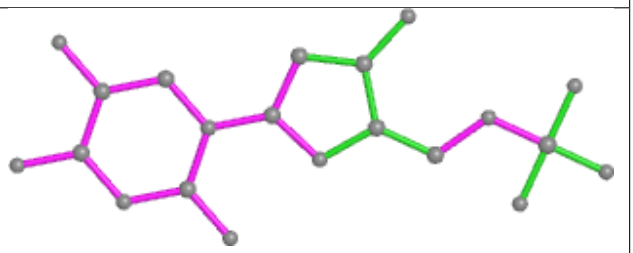


Rings

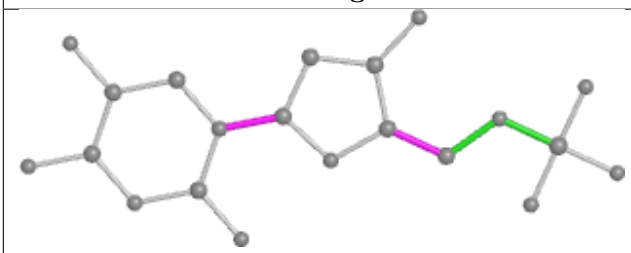
Ligand UFP B 602



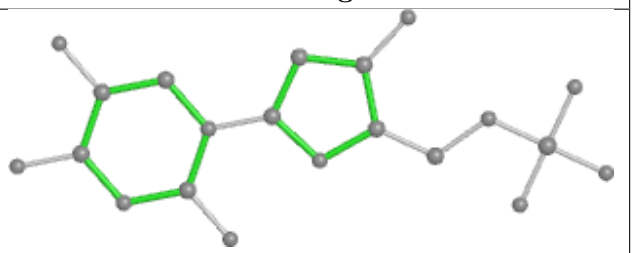
Bond lengths



Bond angles

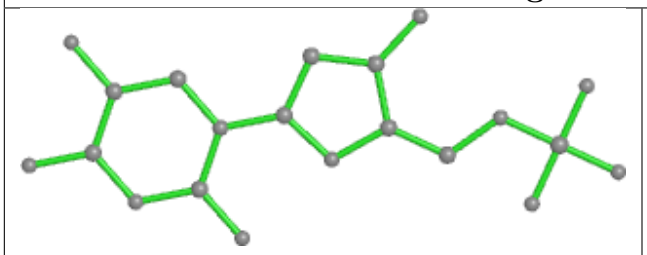


Torsions

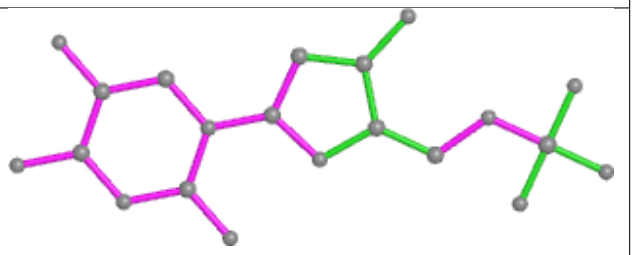


Rings

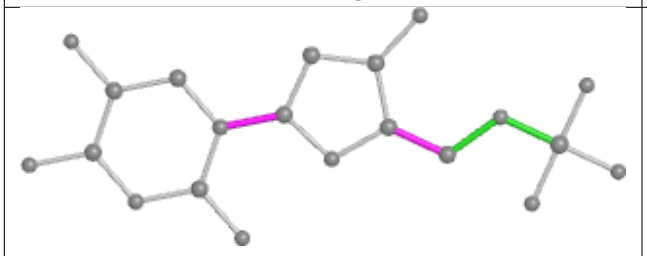
Ligand UFP E 602



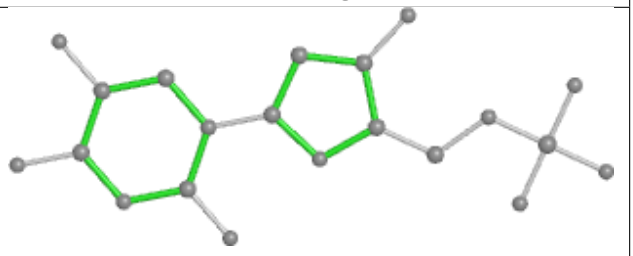
Bond lengths



Bond angles

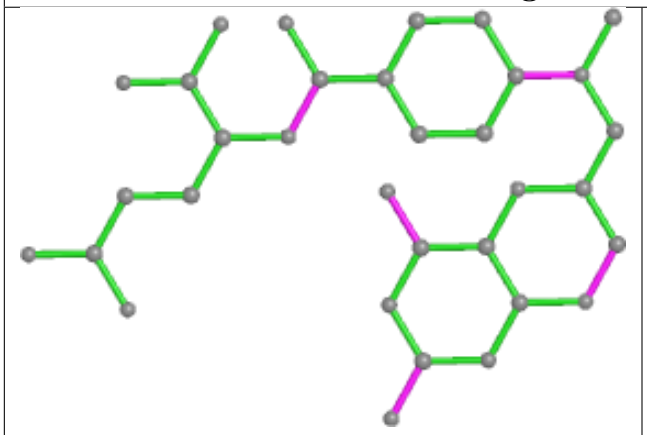


Torsions

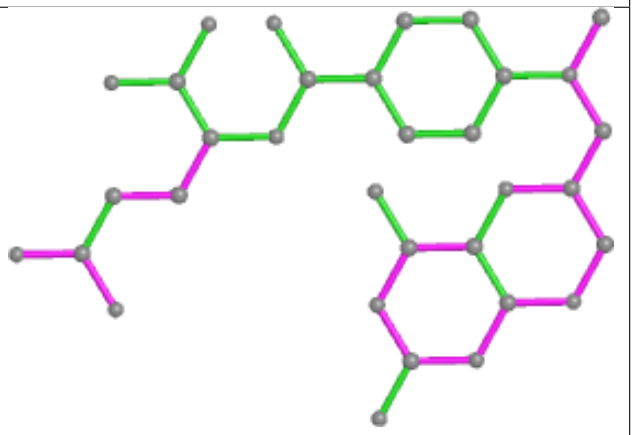


Rings

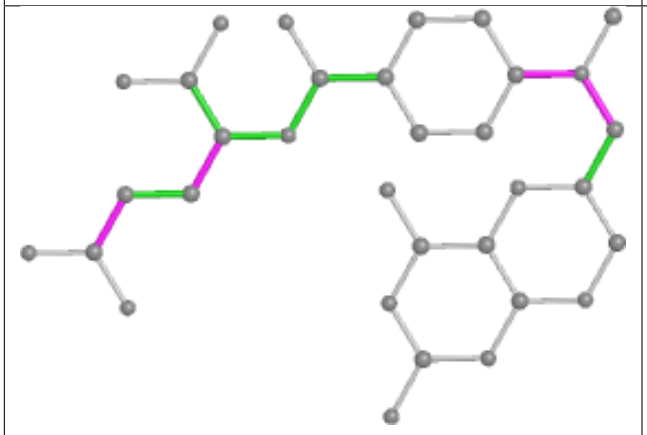
Ligand MTX E 604



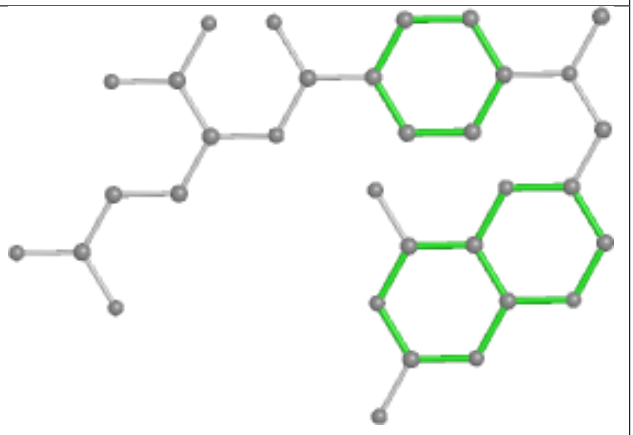
Bond lengths



Bond angles

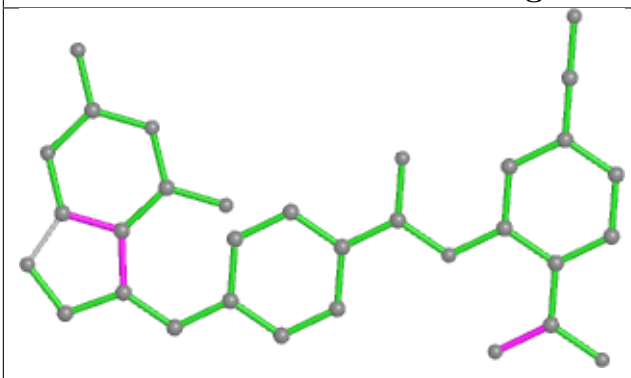


Torsions

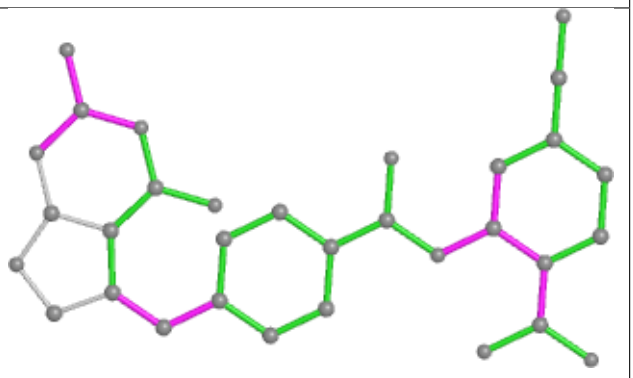


Rings

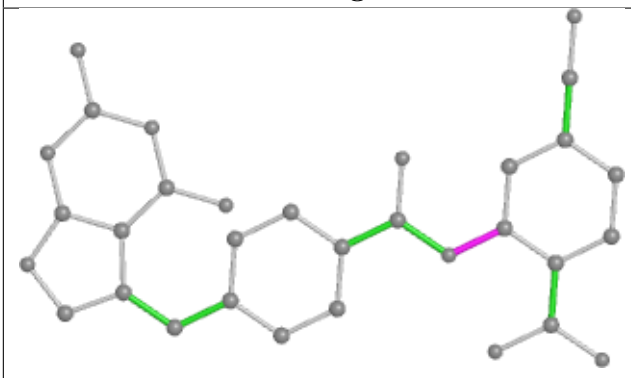
Ligand OG1 B 603



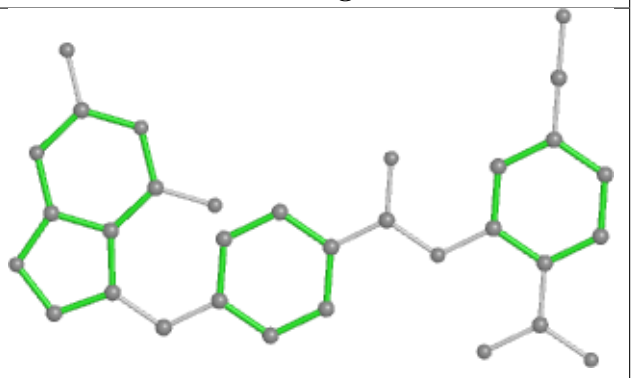
Bond lengths



Bond angles

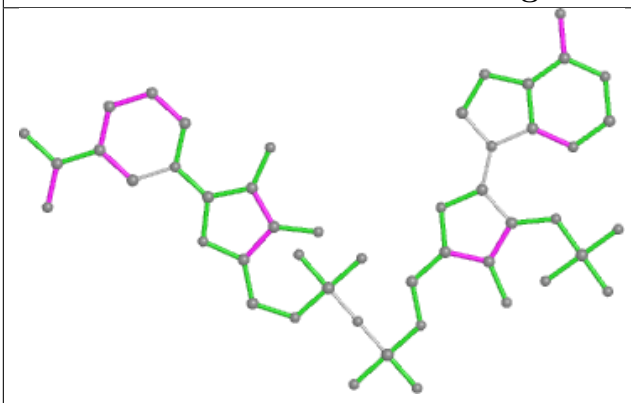


Torsions

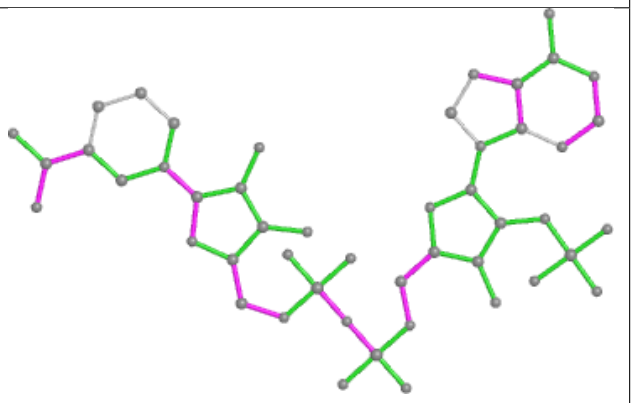


Rings

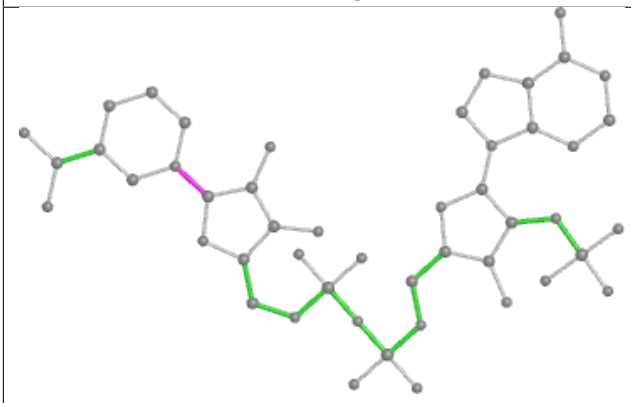
Ligand NDP A 601



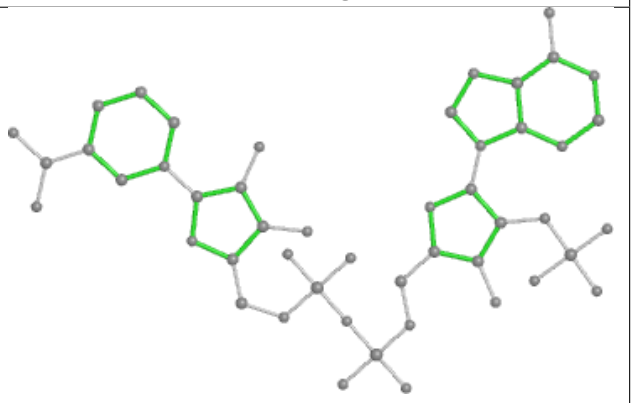
Bond lengths



Bond angles

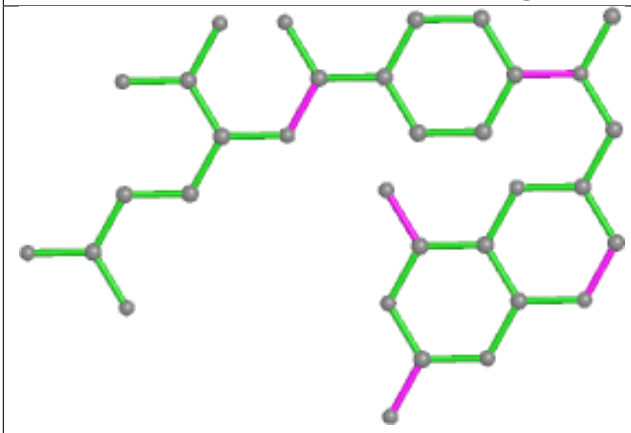


Torsions

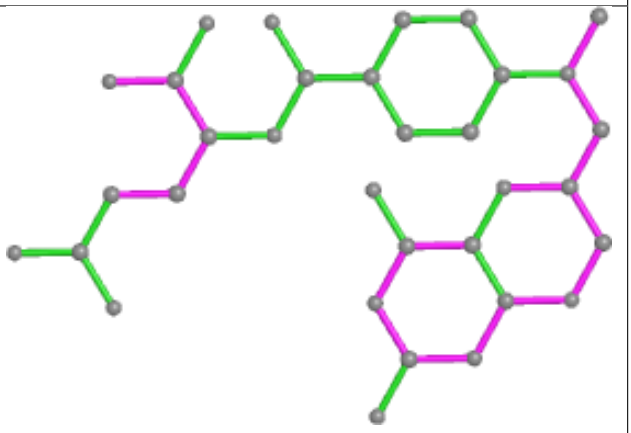


Rings

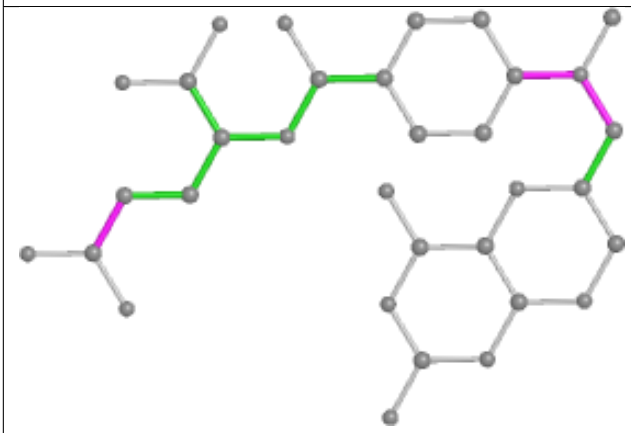
Ligand MTX A 604



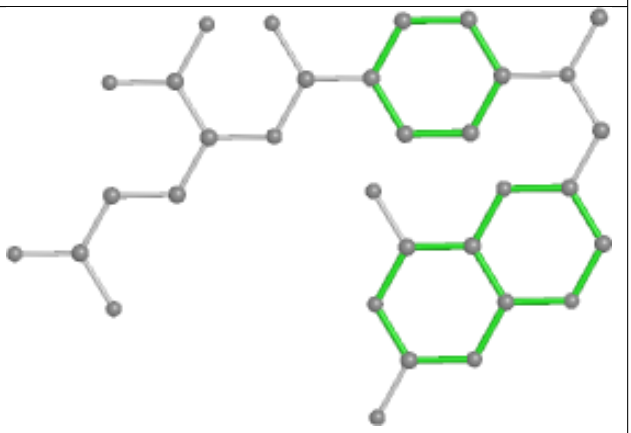
Bond lengths



Bond angles

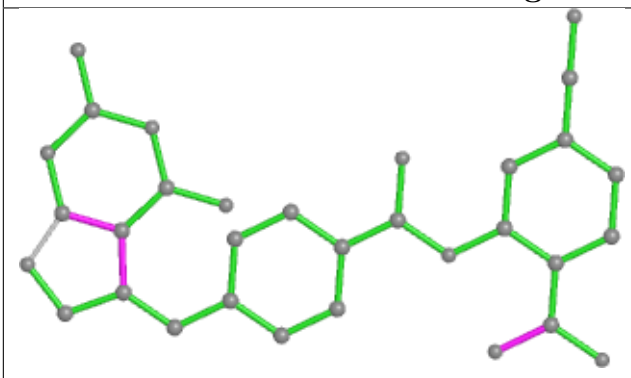


Torsions

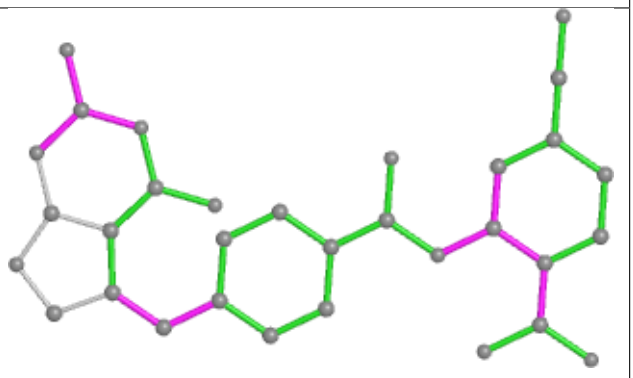


Rings

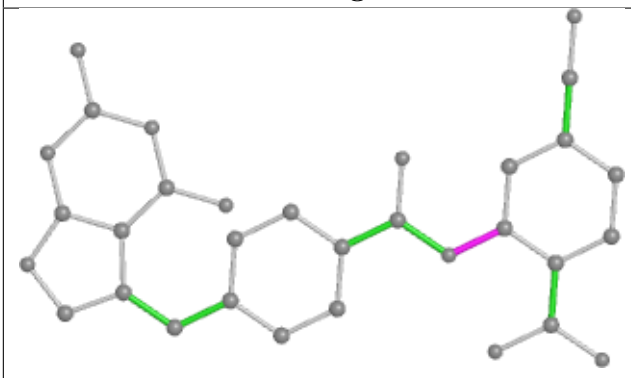
Ligand OG1 D 603



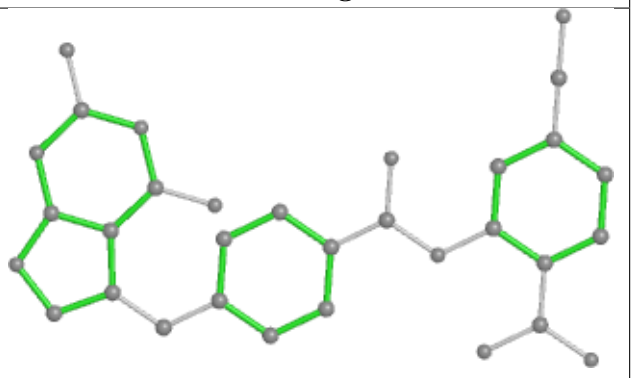
Bond lengths



Bond angles

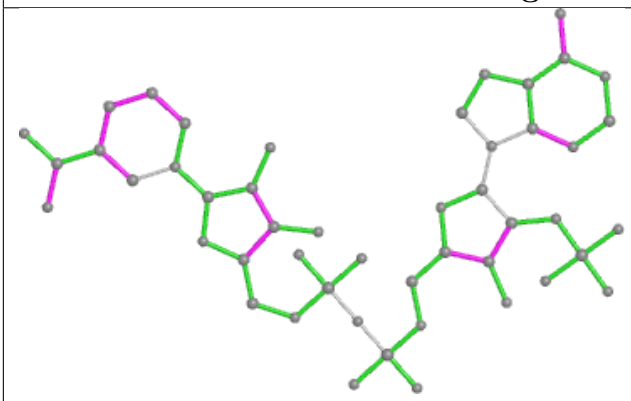


Torsions

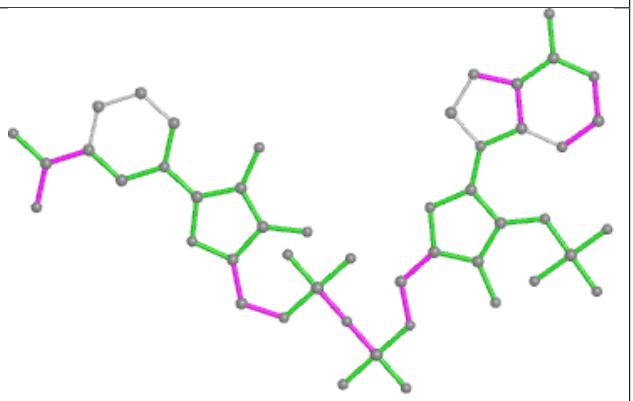


Rings

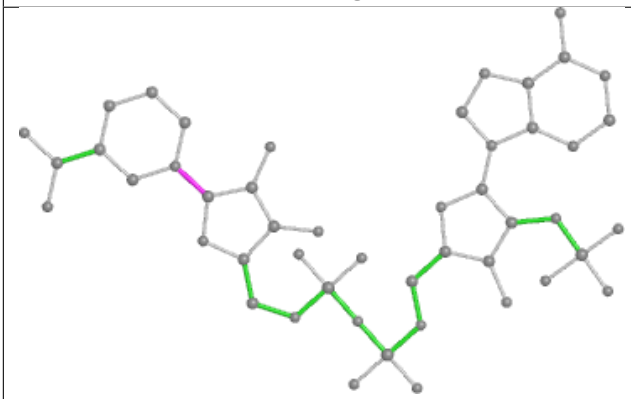
Ligand NDP B 601



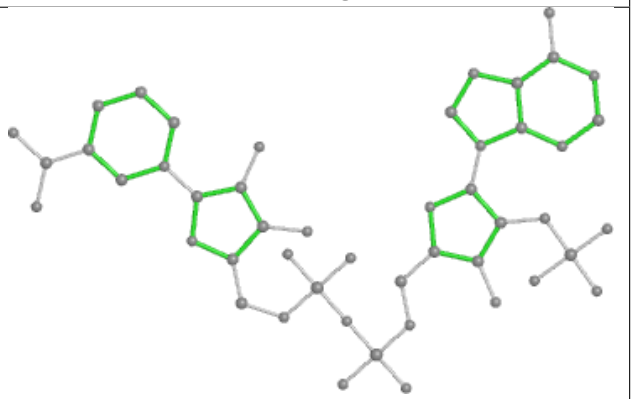
Bond lengths



Bond angles

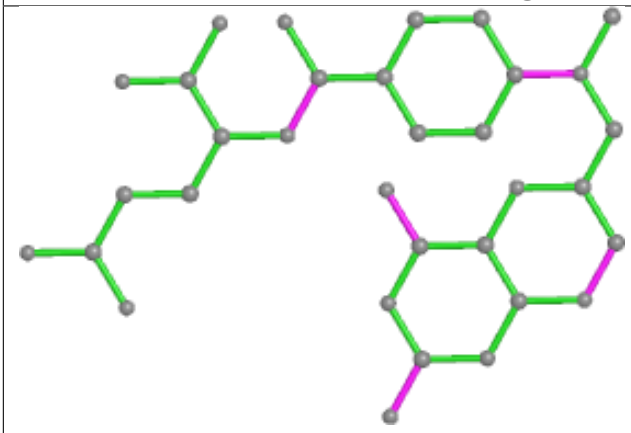


Torsions

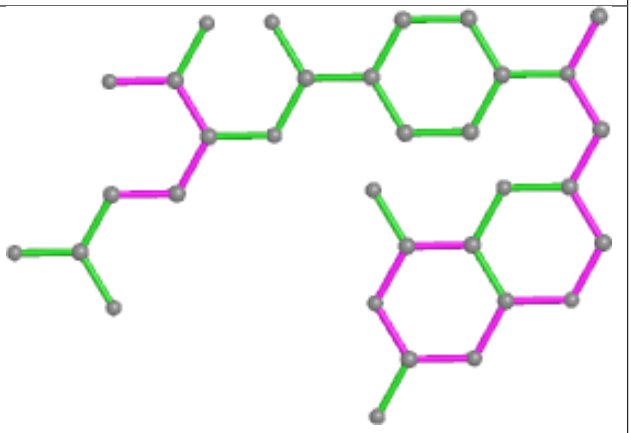


Rings

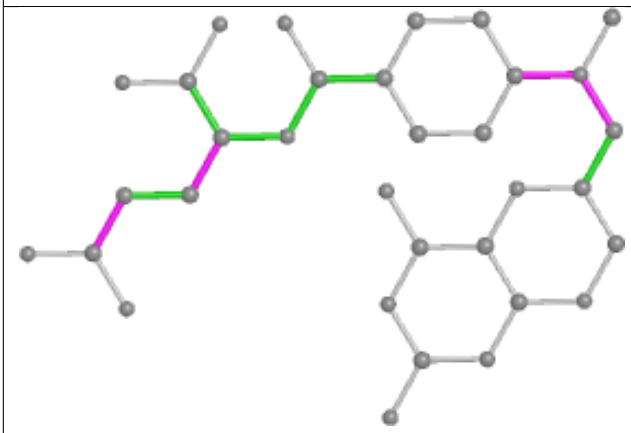
Ligand MTX B 604



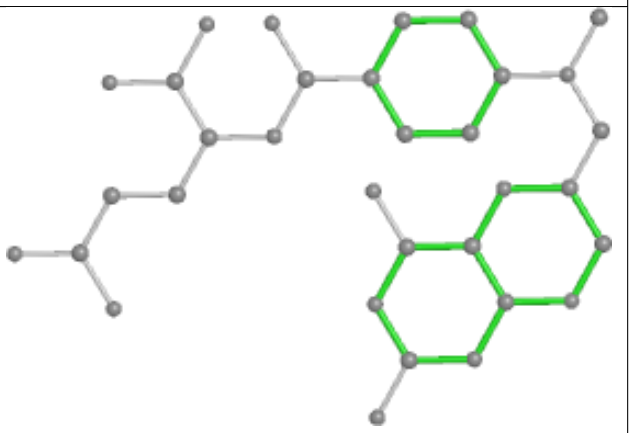
Bond lengths



Bond angles

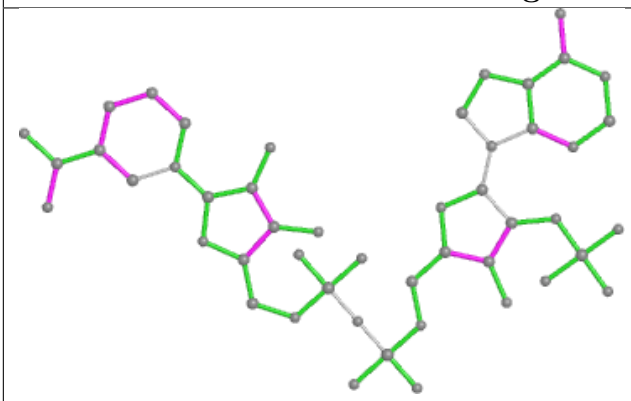


Torsions

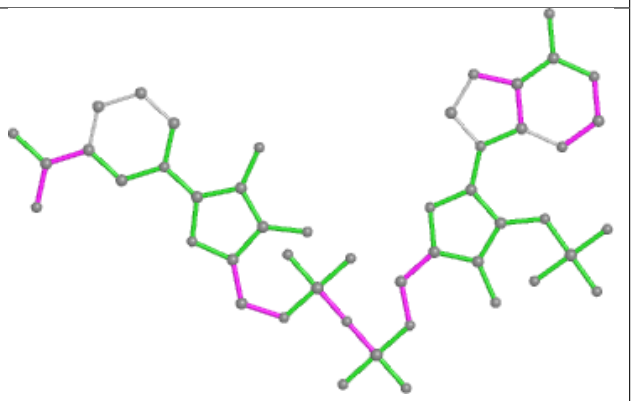


Rings

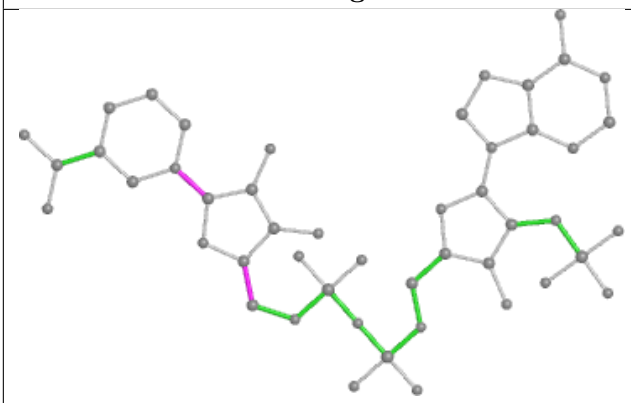
Ligand NDP E 601



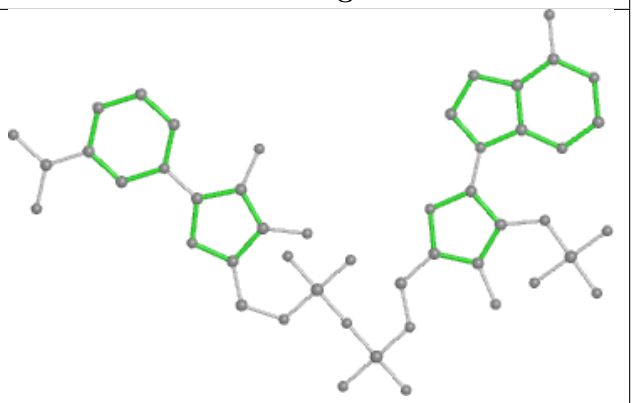
Bond lengths



Bond angles

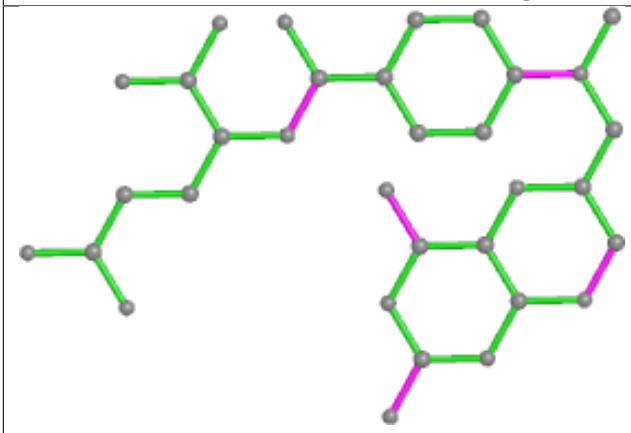


Torsions

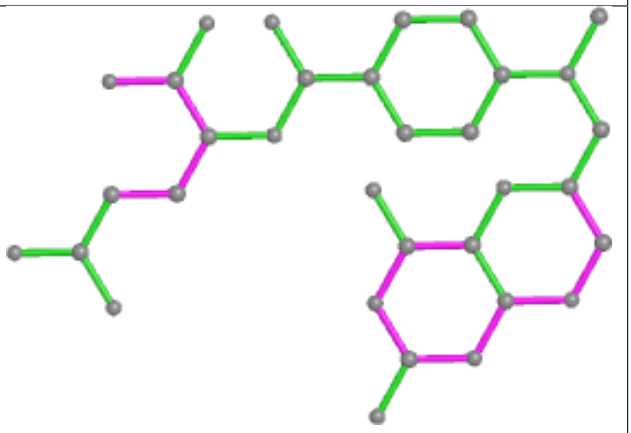


Rings

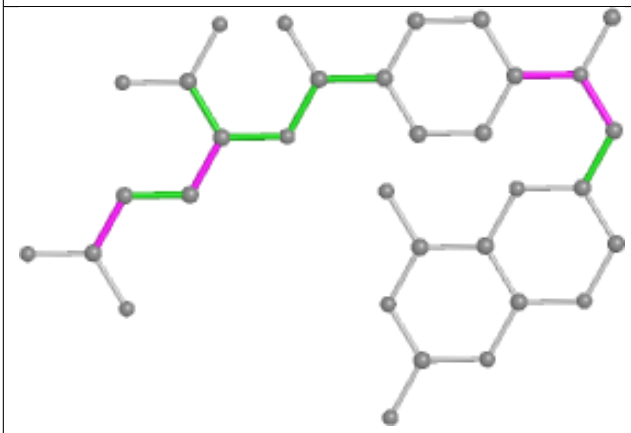
Ligand MTX D 604



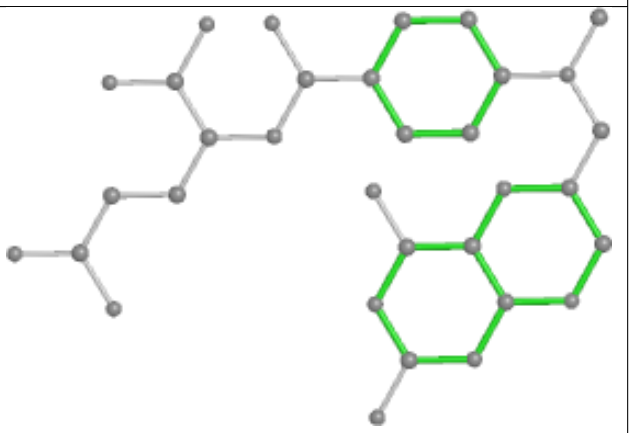
Bond lengths



Bond angles

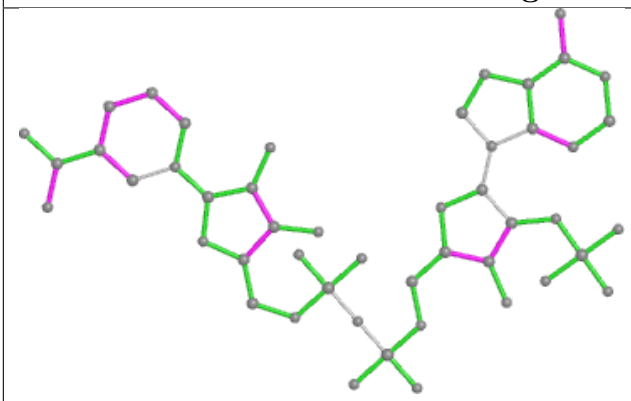


Torsions

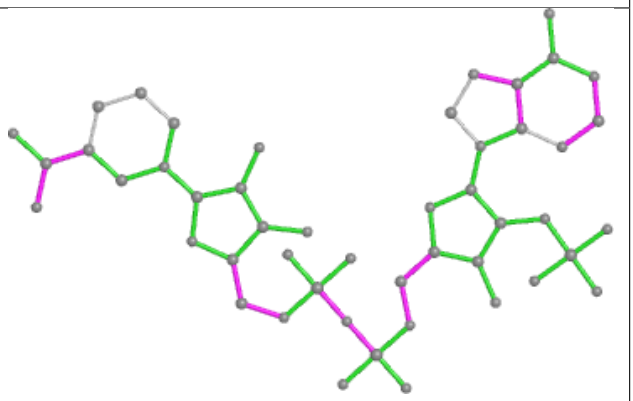


Rings

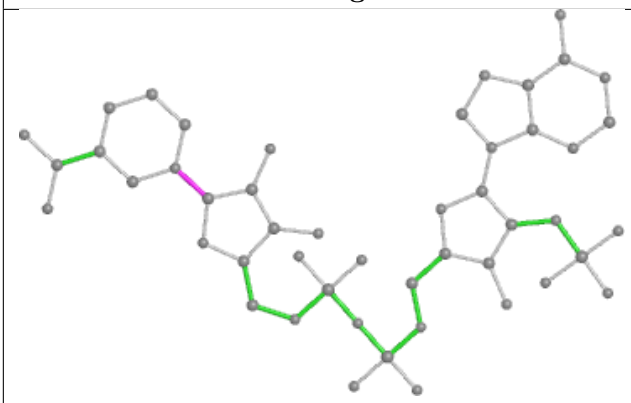
Ligand NDP C 601



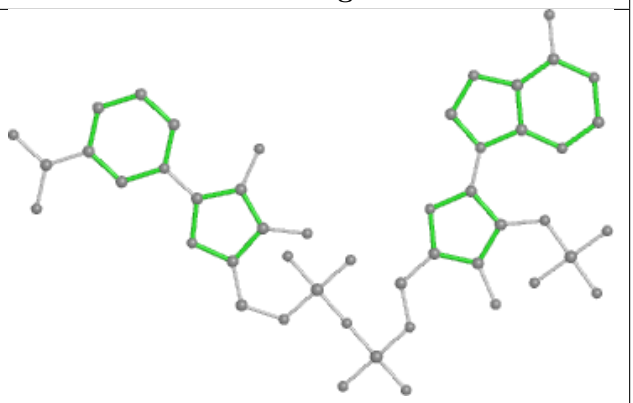
Bond lengths



Bond angles

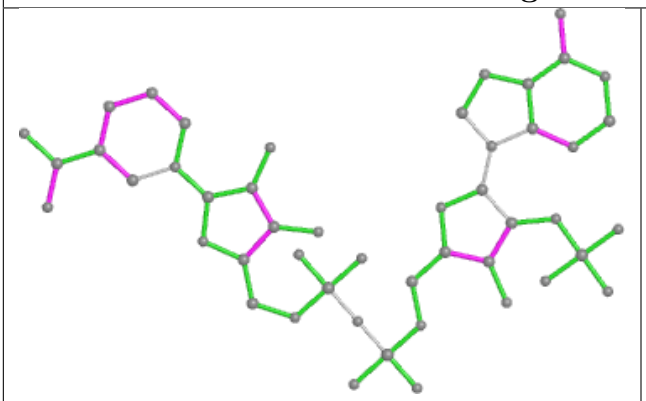


Torsions

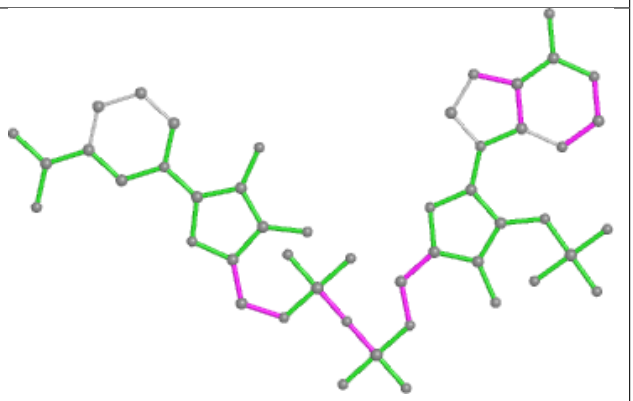


Rings

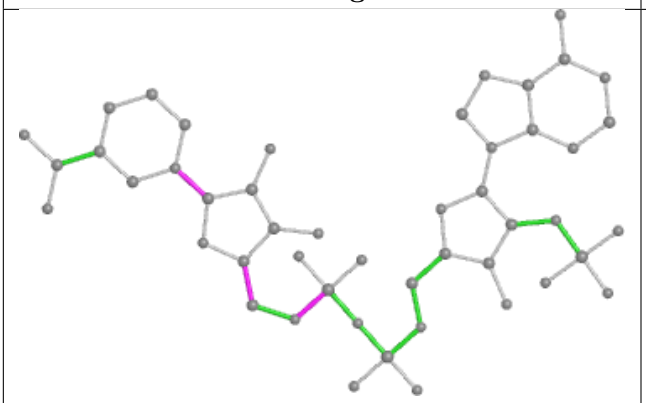
Ligand NDP D 601



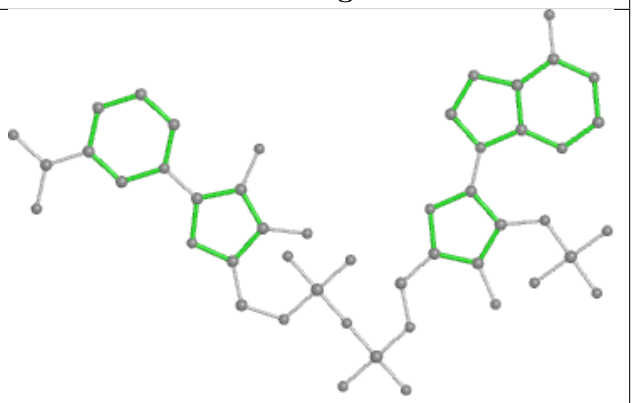
Bond lengths



Bond angles

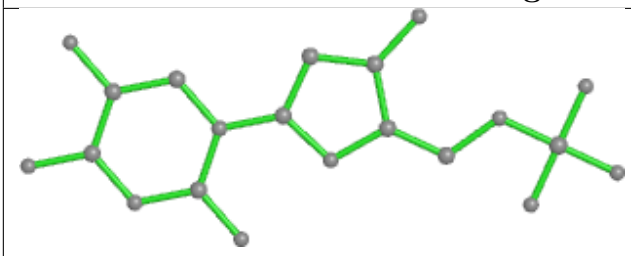


Torsions

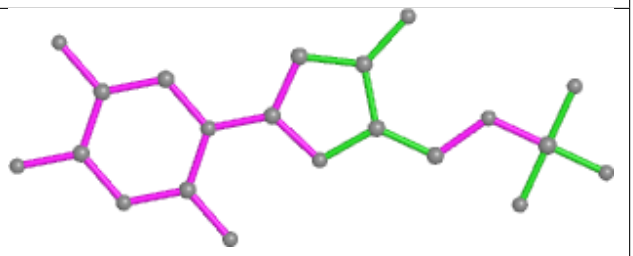


Rings

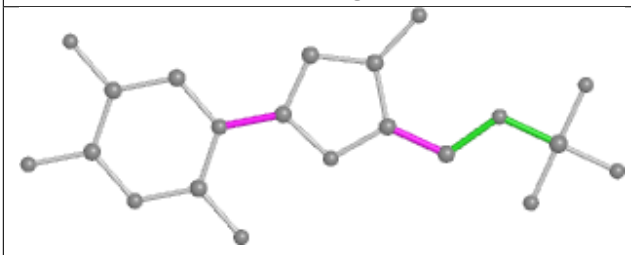
Ligand UFP D 602



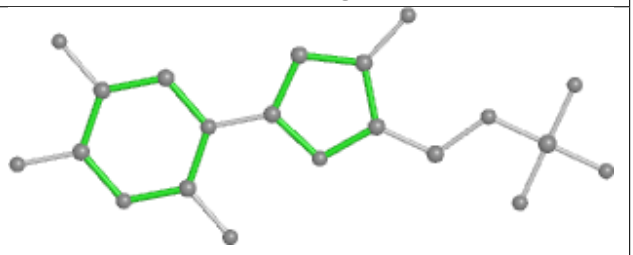
Bond lengths



Bond angles

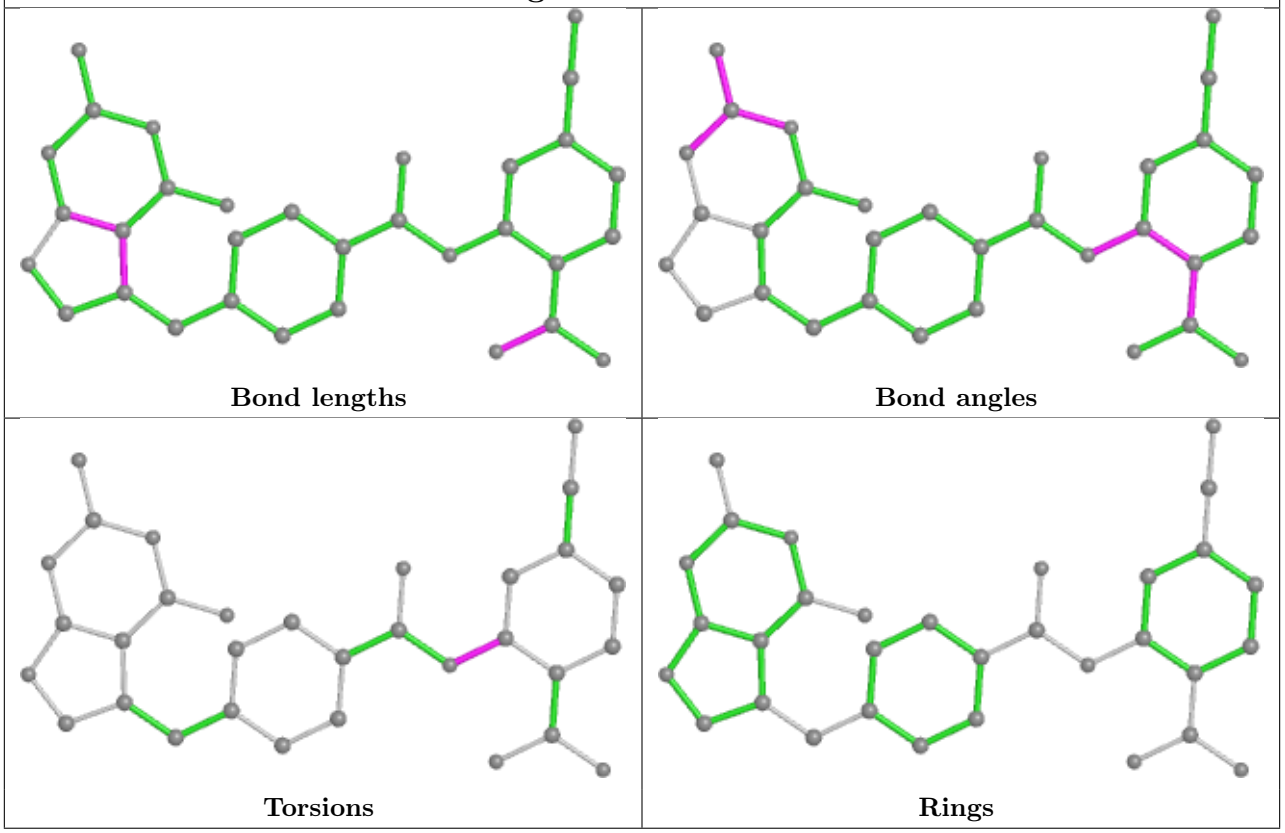


Torsions



Rings

Ligand OG1 E 603



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.