Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 08:17 AM EDT

PDB ID	:	6N1T
Title	:	Toxoplasma gondii TS-DHFR in complex with selective inhibitor 3
Authors	:	Hopper, A.T.; Brockman, A.; Wise, A.; Gould, J.; Barks, J.; Radke, J.B.; Sibley, L.D.; Zou, Y.; Thomas, S.B.
Deposited on	:	2018-11-11
Resolution	:	3.50 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 3.50 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 5 unique types of molecules in this entry. The entry contains 8452 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	511	Total	C	N	O	S	0	1	0
			4095	2618	717	735	25			
1	B	511	Total	C	N	O	S	0	1	0
			4095	2617	716	737	25			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q07422
A	?	-	ASN	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	TRP	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	THR	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	ASP	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	GLU	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	CYS	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	GLU	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	ASN	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	TRP	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422
B	?	-	LYS	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	LYS	deletion	UNP Q07422
B	?	-	THR	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	ASP	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422

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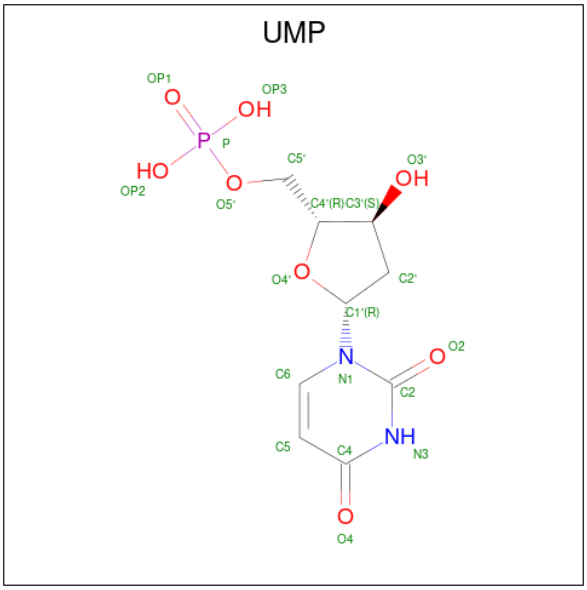
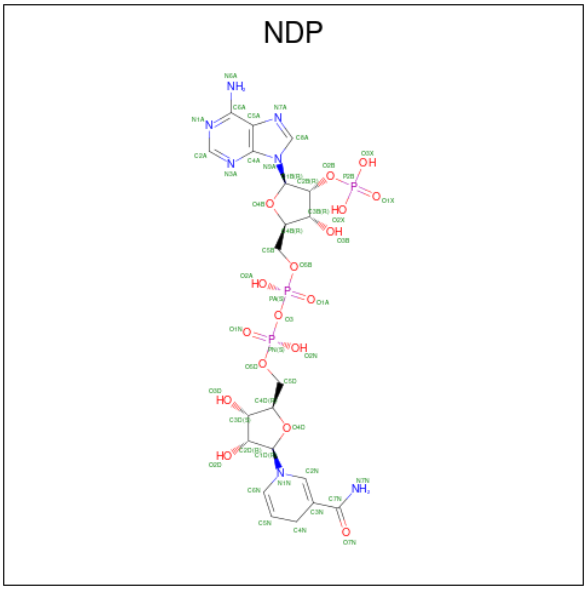
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422
B	?	-	GLN	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	GLU	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	CYS	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	GLU	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



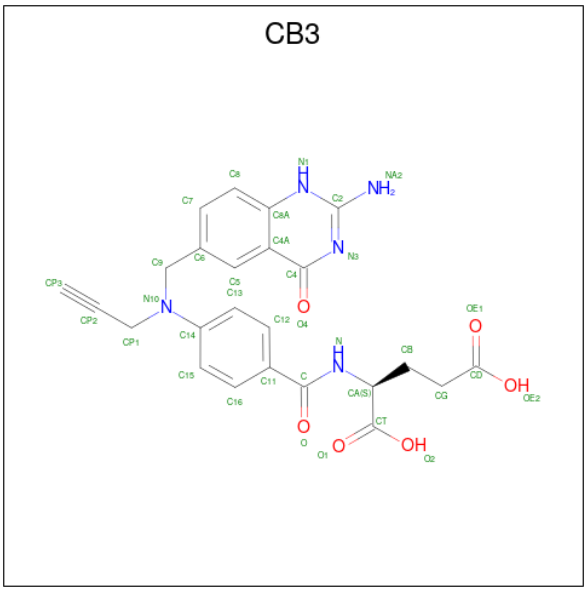
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



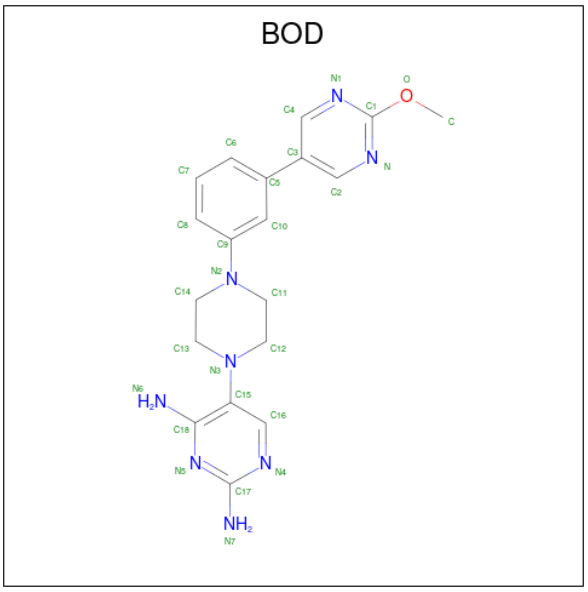
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 35 24 5 6	0	0
4	B	1	Total C N O 35 24 5 6	0	0

- Molecule 5 is 5-{4-[3-(2-methoxypyrimidin-5-yl)phenyl]piperazin-1-yl}pyrimidine-2,4-diamine (three-letter code: BOD) (formula: $C_{19}H_{22}N_8O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 28 19 8 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			28	19	8	1		

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	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.21Å 144.34Å 174.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50	Depositor
% Data completeness (in resolution range)	62.1 (50.00-3.50)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.35 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.198 , 0.264	Depositor
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.073	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8452	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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

8 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	UMP	B	701	-	21,21,21	1.21	2 (9%)	31,31,31	1.62	5 (16%)
5	BOD	A	704	-	31,31,31	1.15	3 (9%)	39,43,43	2.44	17 (43%)
3	NDP	B	702	-	45,52,52	1.04	2 (4%)	53,80,80	1.13	4 (7%)
2	UMP	A	701	-	21,21,21	1.22	3 (14%)	31,31,31	1.71	6 (19%)
3	NDP	A	702	-	45,52,52	1.06	3 (6%)	53,80,80	1.15	5 (9%)
4	CB3	A	703	-	36,37,37	1.16	3 (8%)	46,51,51	2.44	8 (17%)
4	CB3	B	703	-	36,37,37	1.18	3 (8%)	46,51,51	2.40	8 (17%)
5	BOD	B	704	-	31,31,31	1.19	4 (12%)	39,43,43	2.34	12 (30%)

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	UMP	B	701	-	-	4/10/22/22	0/2/2/2
5	BOD	A	704	-	-	8/14/24/24	0/4/4/4
3	NDP	B	702	-	-	6/30/77/77	0/5/5/5
2	UMP	A	701	-	-	4/10/22/22	0/2/2/2
3	NDP	A	702	-	-	2/30/77/77	0/5/5/5
4	CB3	A	703	-	-	10/27/28/28	0/3/3/3
4	CB3	B	703	-	-	10/27/28/28	0/3/3/3
5	BOD	B	704	-	-	6/14/24/24	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	BOD	C5-C3	-3.80	1.39	1.49
4	B	703	CB3	CP2-CP3	3.69	1.29	1.18
3	B	702	NDP	C6N-C5N	3.65	1.39	1.33
3	A	702	NDP	C6N-C5N	3.59	1.39	1.33
4	A	703	CB3	C4A-C8A	3.51	1.48	1.41
4	B	703	CB3	C4A-C8A	3.44	1.48	1.41
5	B	704	BOD	C1-N	3.43	1.37	1.32
4	A	703	CB3	CP2-CP3	3.27	1.27	1.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	BOD	C1-N1	3.13	1.36	1.32
2	A	701	UMP	C2-N1	3.02	1.43	1.38
5	B	704	BOD	C5-C3	-3.02	1.41	1.49
5	A	704	BOD	C1-N1	3.02	1.36	1.32
3	A	702	NDP	C5A-C4A	2.76	1.48	1.40
2	B	701	UMP	C2-N1	2.68	1.42	1.38
3	B	702	NDP	C5A-C4A	2.62	1.47	1.40
5	A	704	BOD	C1-N	2.48	1.35	1.32
2	B	701	UMP	C4-N3	-2.33	1.34	1.38
5	B	704	BOD	O-C1	2.16	1.38	1.33
4	A	703	CB3	C8A-N1	-2.16	1.34	1.37
3	A	702	NDP	C2A-N3A	2.13	1.35	1.32
2	A	701	UMP	C6-C5	2.06	1.39	1.35
4	B	703	CB3	C8A-N1	-2.05	1.34	1.37
2	A	701	UMP	C4-N3	-2.02	1.34	1.38

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	CB3	C4A-C4-N3	-10.04	117.40	124.40
4	B	703	CB3	C4A-C4-N3	-9.89	117.50	124.40
4	B	703	CB3	C4A-C8A-N1	-9.05	118.69	123.60
4	A	703	CB3	C4A-C8A-N1	-8.79	118.83	123.60
5	A	704	BOD	C13-N3-C12	6.36	125.56	111.52
5	B	704	BOD	N-C1-N1	-6.15	119.66	127.99
5	A	704	BOD	N-C1-N1	-5.11	121.06	127.99
5	B	704	BOD	C2-N-C1	5.06	121.12	114.97
5	A	704	BOD	C4-N1-C1	4.87	120.89	114.97
5	B	704	BOD	C4-N1-C1	4.77	120.77	114.97
5	B	704	BOD	C13-N3-C12	4.74	121.99	111.52
5	A	704	BOD	C12-C11-N2	-4.40	102.15	110.70
4	A	703	CB3	C6-C9-N10	-4.31	107.26	114.18
5	B	704	BOD	N4-C17-N5	-4.25	120.52	125.70
5	A	704	BOD	N4-C17-N5	-4.09	120.72	125.70
4	B	703	CB3	C6-C9-N10	-4.03	107.71	114.18
2	B	701	UMP	C4-N3-C2	-3.97	121.34	126.58
5	A	704	BOD	C2-N-C1	3.92	119.73	114.97
4	A	703	CB3	C2-N3-C4	3.87	122.08	115.93
4	B	703	CB3	C2-N3-C4	3.80	121.96	115.93
2	A	701	UMP	N3-C2-N1	3.74	119.86	114.89
2	A	701	UMP	C4-N3-C2	-3.70	121.70	126.58
2	B	701	UMP	N3-C2-N1	3.69	119.79	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	UMP	C5-C4-N3	3.68	120.35	114.84
5	B	704	BOD	C14-N2-C11	3.50	119.24	111.52
5	A	704	BOD	C17-N5-C18	3.48	120.84	116.99
2	A	701	UMP	C5-C4-N3	3.34	119.83	114.84
3	B	702	NDP	N3A-C2A-N1A	-3.31	123.50	128.68
4	A	703	CB3	N1-C2-N3	-3.31	122.81	127.22
2	A	701	UMP	C1'-N1-C2	3.30	124.14	117.64
5	B	704	BOD	C17-N5-C18	3.28	120.61	116.99
4	B	703	CB3	N1-C2-N3	-3.25	122.89	127.22
3	A	702	NDP	N3A-C2A-N1A	-3.21	123.67	128.68
2	A	701	UMP	O4-C4-C5	-3.20	119.54	125.16
5	B	704	BOD	C12-C11-N2	-3.19	104.51	110.70
5	A	704	BOD	C3-C4-N1	-3.12	119.17	124.32
3	B	702	NDP	PN-O3-PA	-3.03	122.42	132.83
5	B	704	BOD	C-O-C1	3.02	122.41	117.58
2	B	701	UMP	O4-C4-C5	-2.99	119.90	125.16
3	A	702	NDP	PN-O3-PA	-2.93	122.77	132.83
3	A	702	NDP	C4A-C5A-N7A	-2.72	106.56	109.40
5	A	704	BOD	C14-N2-C11	2.70	117.48	111.52
3	B	702	NDP	C4A-C5A-N7A	-2.70	106.58	109.40
5	A	704	BOD	C-O-C1	2.59	121.72	117.58
4	A	703	CB3	C6-C5-C4A	-2.55	118.83	122.65
5	A	704	BOD	C2-C3-C4	2.55	118.64	114.66
5	A	704	BOD	C8-C9-N2	-2.46	117.99	121.38
3	B	702	NDP	C1D-N1N-C2N	-2.44	117.05	121.11
5	B	704	BOD	C3-C2-N	-2.43	120.32	124.32
2	B	701	UMP	C1'-N1-C2	2.42	122.41	117.64
5	B	704	BOD	C16-N4-C17	2.41	120.91	116.44
4	B	703	CB3	C6-C5-C4A	-2.39	119.08	122.65
5	A	704	BOD	C3-C2-N	-2.32	120.50	124.32
3	A	702	NDP	C1D-N1N-C2N	-2.29	117.30	121.11
4	B	703	CB3	C8-C8A-N1	2.29	122.18	118.69
3	A	702	NDP	O4D-C1D-N1N	2.27	112.49	108.06
5	B	704	BOD	N7-C17-N4	2.27	119.74	117.44
5	A	704	BOD	C6-C5-C3	-2.24	117.47	121.36
4	A	703	CB3	C8-C8A-N1	2.23	122.10	118.69
2	A	701	UMP	C6-N1-C2	-2.16	118.22	120.99
4	B	703	CB3	C2-N1-C8A	2.13	121.60	116.33
5	A	704	BOD	C16-N4-C17	2.13	120.38	116.44
4	A	703	CB3	C2-N1-C8A	2.11	121.55	116.33
5	A	704	BOD	N7-C17-N4	2.09	119.56	117.44
5	A	704	BOD	C14-C13-N3	2.02	114.62	110.70

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	CB3	C11-C-N-CA
4	B	703	CB3	C11-C-N-CA
4	A	703	CB3	O-C-N-CA
4	B	703	CB3	O-C-N-CA
4	A	703	CB3	CB-CA-CT-O2
4	B	703	CB3	CB-CA-CT-O2
3	B	702	NDP	O4B-C4B-C5B-O5B
4	A	703	CB3	CB-CA-CT-O1
4	B	703	CB3	CB-CA-CT-O1
3	B	702	NDP	C3B-C4B-C5B-O5B
4	A	703	CB3	CT-CA-CB-CG
4	B	703	CB3	CT-CA-CB-CG
4	B	703	CB3	N-CA-CB-CG
2	A	701	UMP	C2'-C1'-N1-C2
2	A	701	UMP	C2'-C1'-N1-C6
4	B	703	CB3	N-CA-CT-O2
4	A	703	CB3	N-CA-CB-CG
5	A	704	BOD	N-C1-O-C
3	A	702	NDP	C4D-C5D-O5D-PN
4	B	703	CB3	N-CA-CT-O1
2	B	701	UMP	O4'-C4'-C5'-O5'
3	B	702	NDP	C4D-C5D-O5D-PN
2	A	701	UMP	O4'-C4'-C5'-O5'
3	A	702	NDP	O4D-C1D-N1N-C2N
5	A	704	BOD	N1-C1-O-C
2	B	701	UMP	C2'-C1'-N1-C2
4	A	703	CB3	N-CA-CT-O2
3	B	702	NDP	O4D-C1D-N1N-C2N
5	B	704	BOD	C18-C15-N3-C13
3	B	702	NDP	C2D-C1D-N1N-C2N
4	B	703	CB3	OE2-CD-CG-CB
5	A	704	BOD	C16-C15-N3-C12
4	B	703	CB3	OE1-CD-CG-CB
5	B	704	BOD	C16-C15-N3-C12
4	A	703	CB3	N-CA-CT-O1
5	A	704	BOD	C18-C15-N3-C13
5	A	704	BOD	C2-C3-C5-C10
5	B	704	BOD	C2-C3-C5-C10
5	B	704	BOD	C4-C3-C5-C10
5	A	704	BOD	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

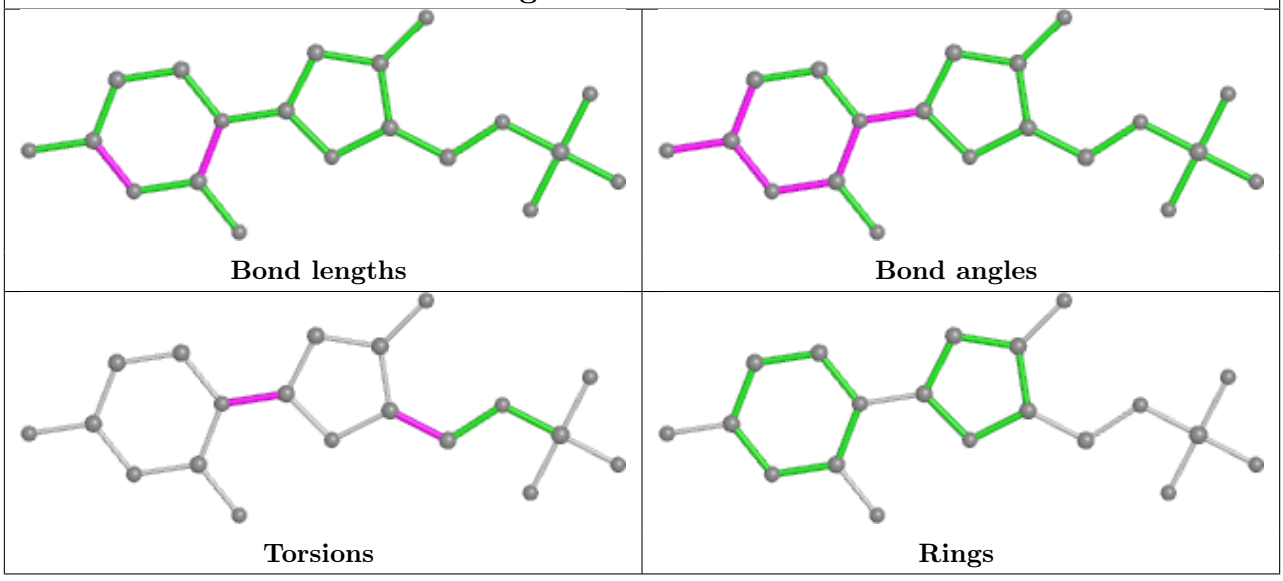
Mol	Chain	Res	Type	Atoms
5	A	704	BOD	C4-C3-C5-C10
5	B	704	BOD	C4-C3-C5-C6
2	B	701	UMP	C3'-C4'-C5'-O5'
5	A	704	BOD	C2-C3-C5-C6
5	B	704	BOD	C2-C3-C5-C6
2	A	701	UMP	C3'-C4'-C5'-O5'
4	A	703	CB3	OE1-CD-CG-CB
3	B	702	NDP	O4D-C1D-N1N-C6N
2	B	701	UMP	C2'-C1'-N1-C6
4	A	703	CB3	OE2-CD-CG-CB

There are no ring outliers.

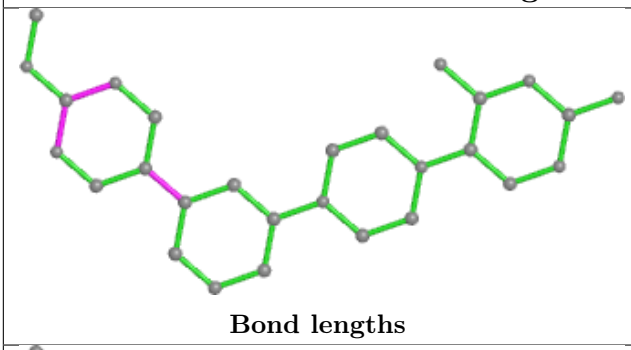
No monomer is involved in short contacts.

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.

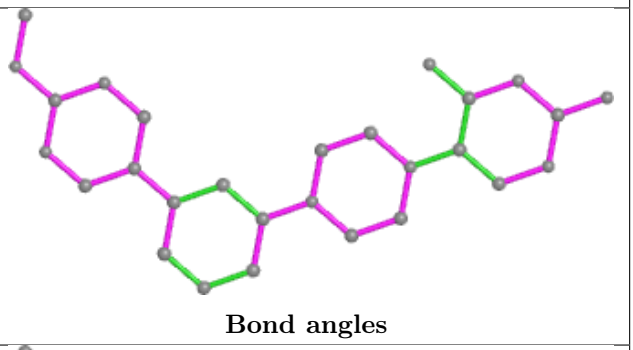
Ligand UMP B 701



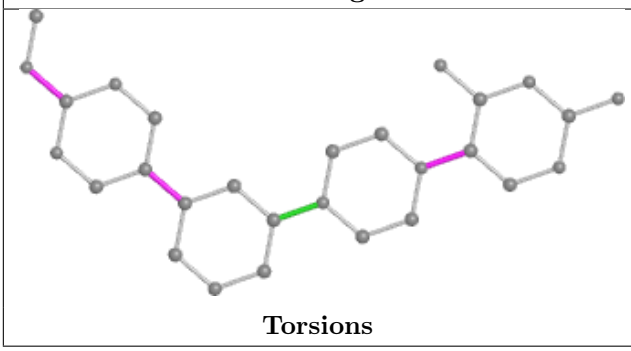
Ligand BOD A 704



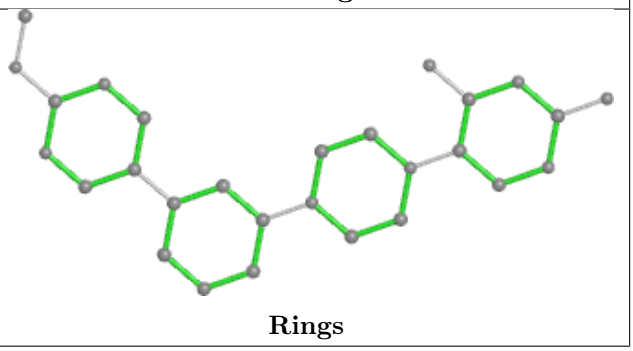
Bond lengths



Bond angles

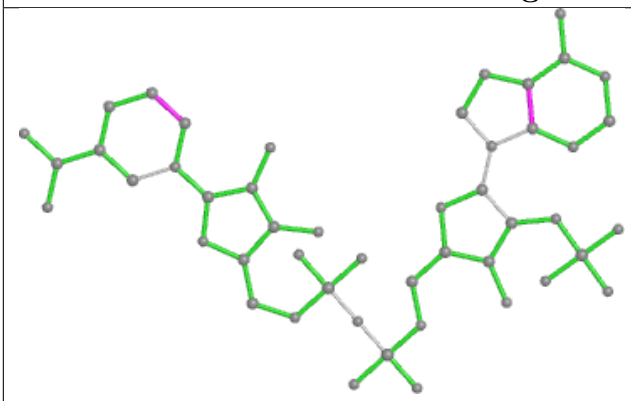


Torsions



Rings

Ligand NDP B 702



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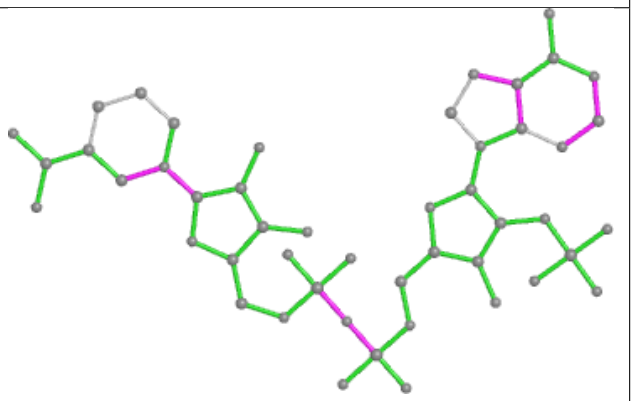
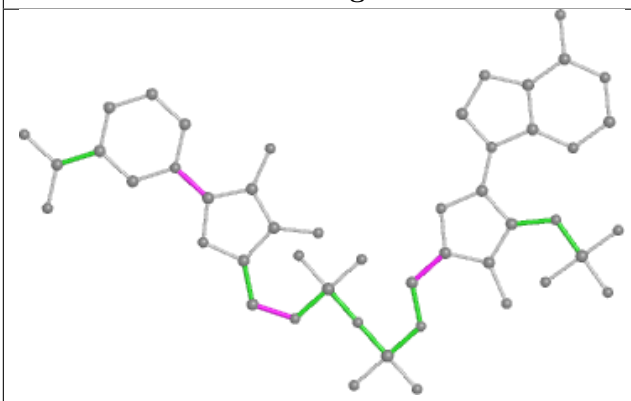


Bond angles



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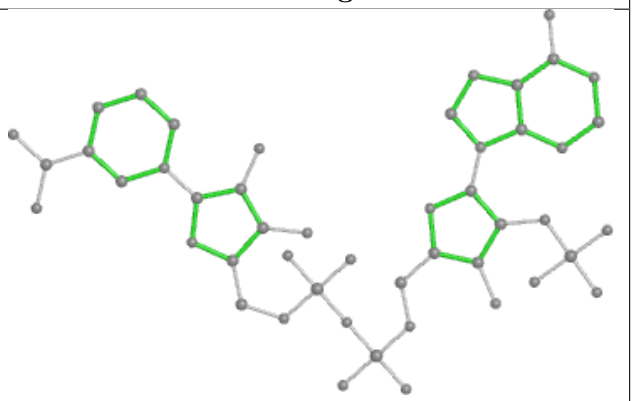
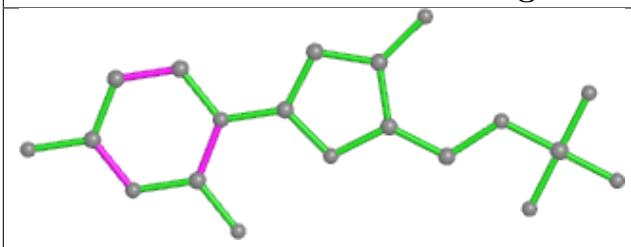


Rings

Ligand UMP A 701



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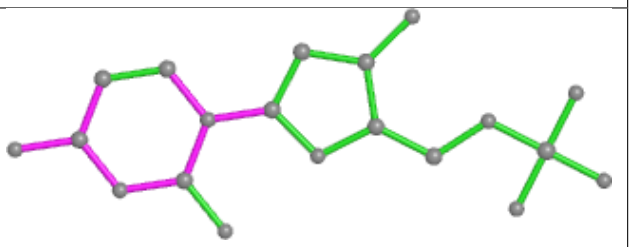
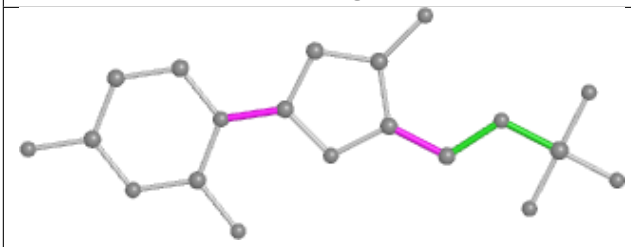


Bond angles



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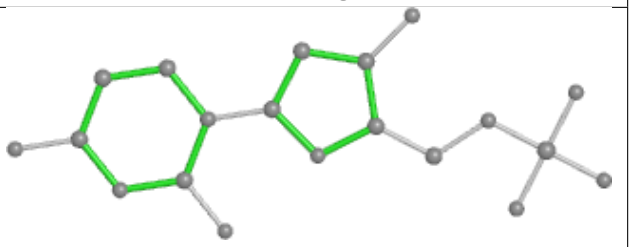
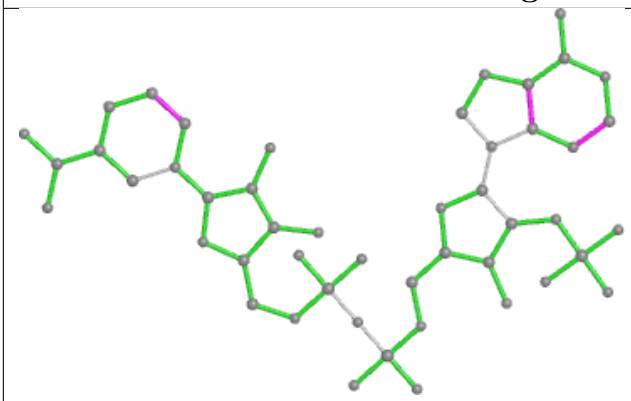


Rings

Ligand NDP A 702



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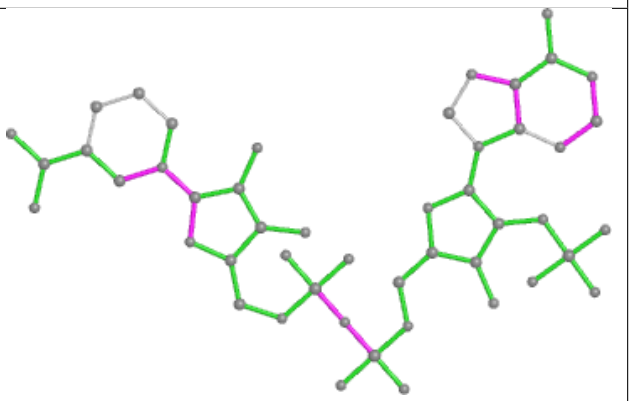
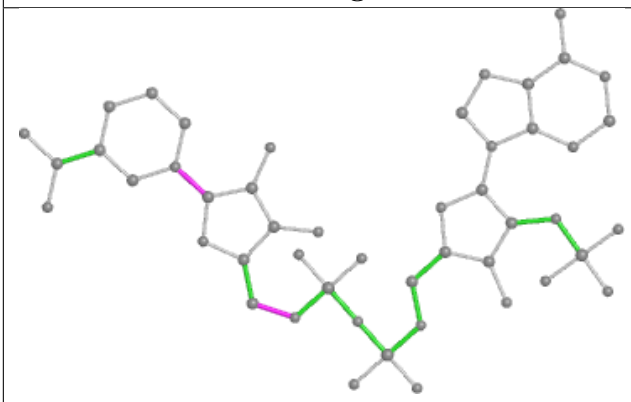
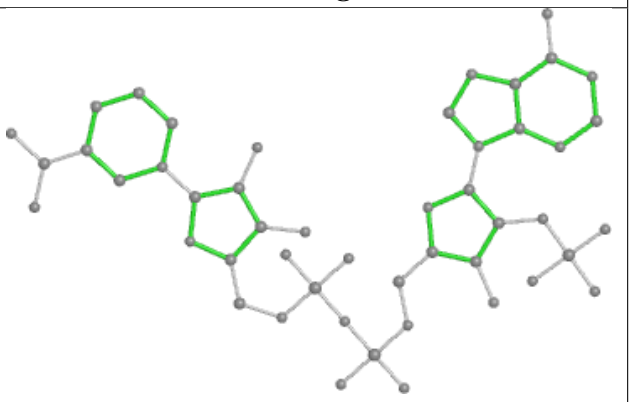


Bond angles

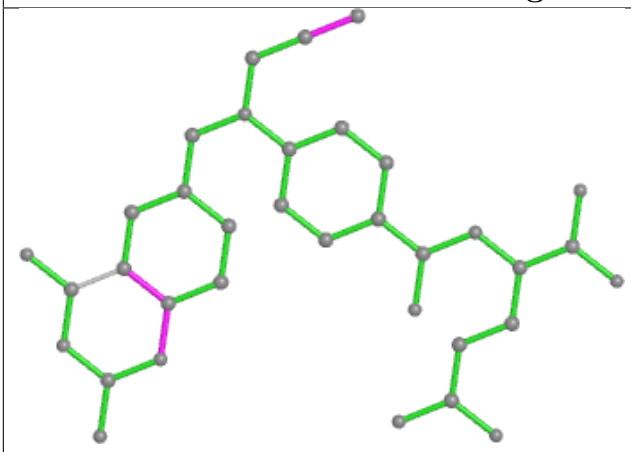


Torsions



Rings

Ligand CB3 A 703



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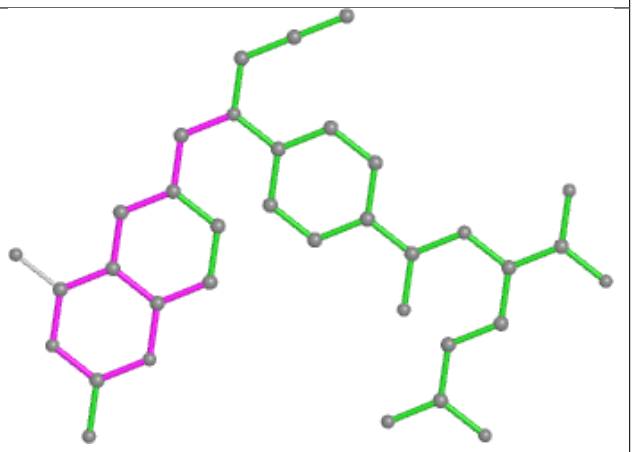

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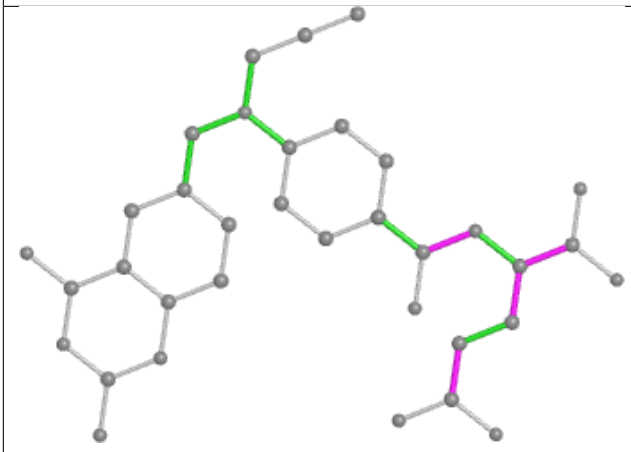

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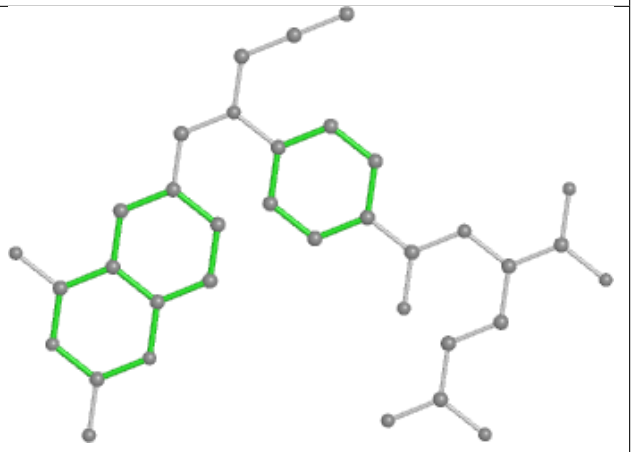
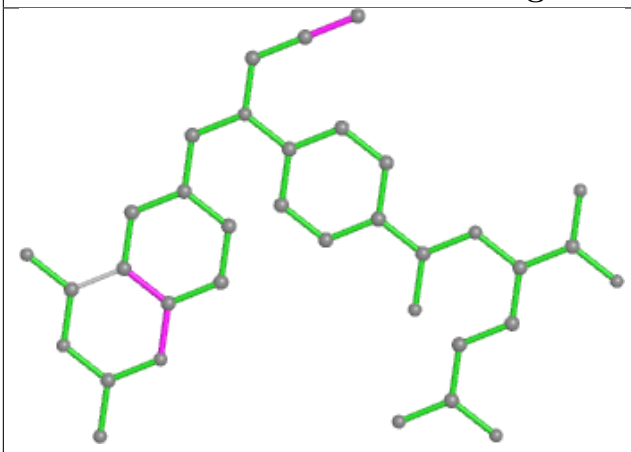


Rings

Ligand CB3 B 703



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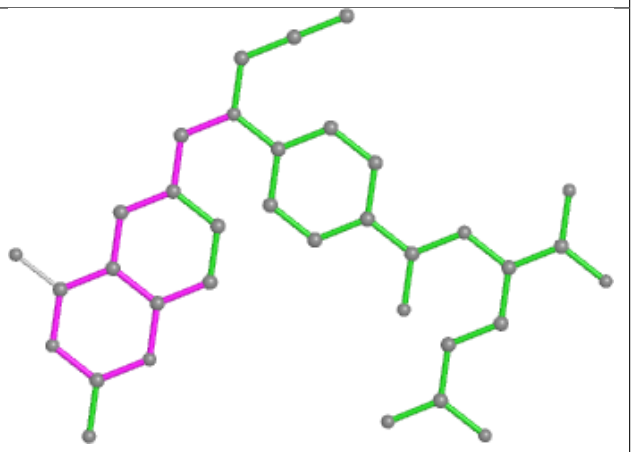

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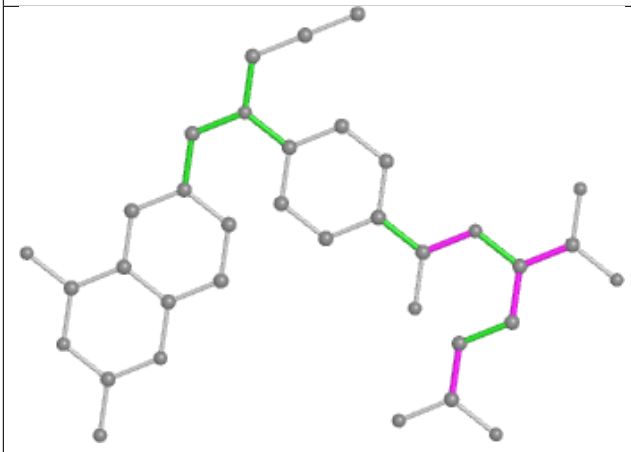

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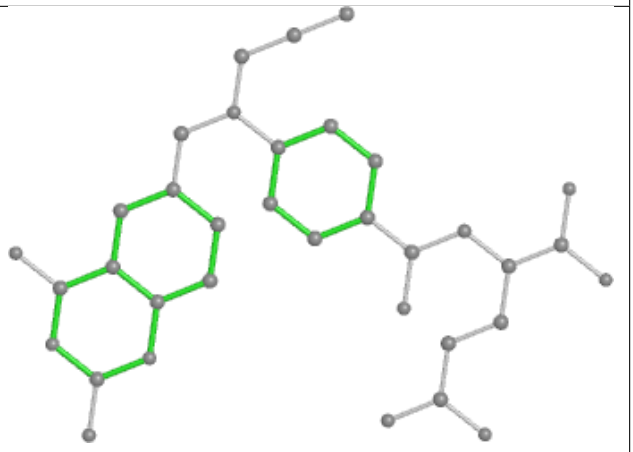
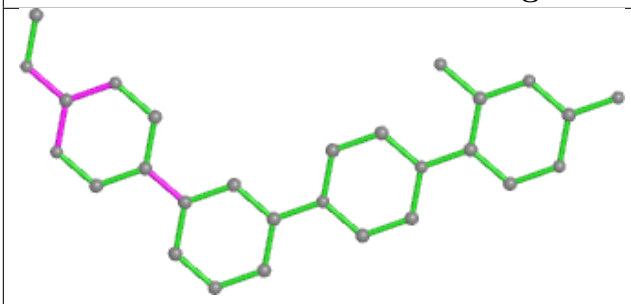


Rings

Ligand BOD B 704



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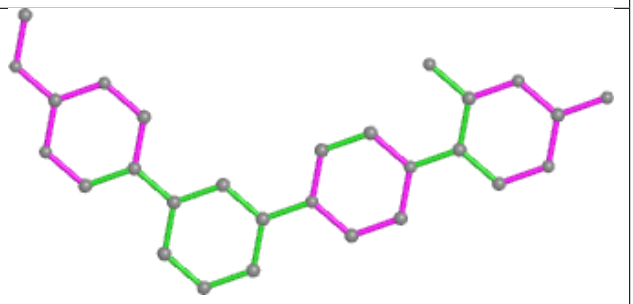
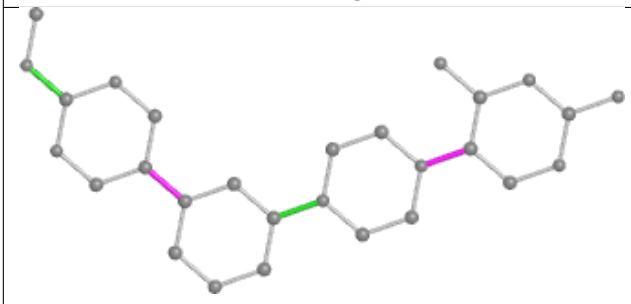


Bond angles



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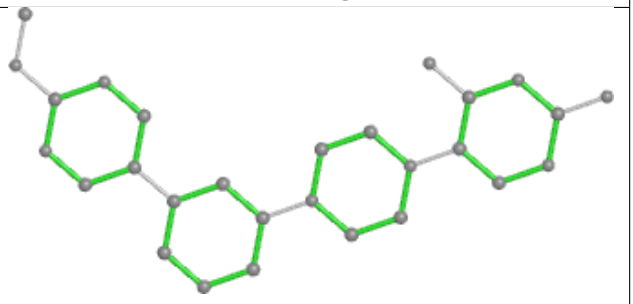

Rings

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.