Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 10:28 AM EDT

PDB ID	:	6MVD
Title	:	Crystal structure of Lecithin:cholesterol acyltransferase (LCAT) in complex with isopropyl dodec-11-enylfluorophosphonate (IDFP) and a small molecule activator
Authors	:	Manthei, K.A.; Chang, L.; Tesmer, J.J.G.
Deposited on	:	2018-10-25
Resolution	:	3.10 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 3.10 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 6181 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.

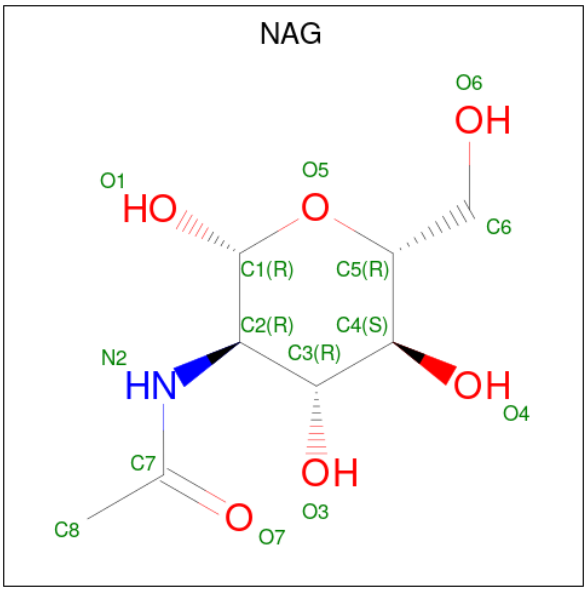
- Molecule 1 is a protein called Phosphatidylcholine-sterol acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			3019	1955	509	540	15			
1	B	368	Total	C	N	O	S	0	0	0
			2959	1919	498	527	15			

There are 12 discrepancies between the modelled and reference sequences:

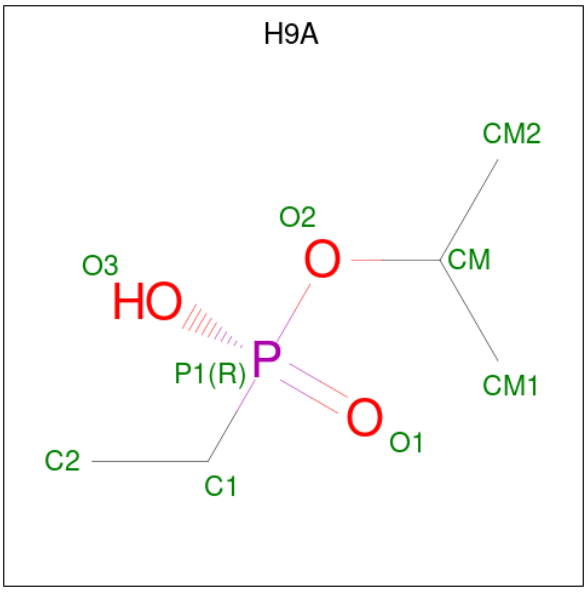
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	HIS	-	expression tag	UNP P04180
A	399	HIS	-	expression tag	UNP P04180
A	400	HIS	-	expression tag	UNP P04180
A	401	HIS	-	expression tag	UNP P04180
A	402	HIS	-	expression tag	UNP P04180
A	403	HIS	-	expression tag	UNP P04180
B	398	HIS	-	expression tag	UNP P04180
B	399	HIS	-	expression tag	UNP P04180
B	400	HIS	-	expression tag	UNP P04180
B	401	HIS	-	expression tag	UNP P04180
B	402	HIS	-	expression tag	UNP P04180
B	403	HIS	-	expression tag	UNP P04180

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



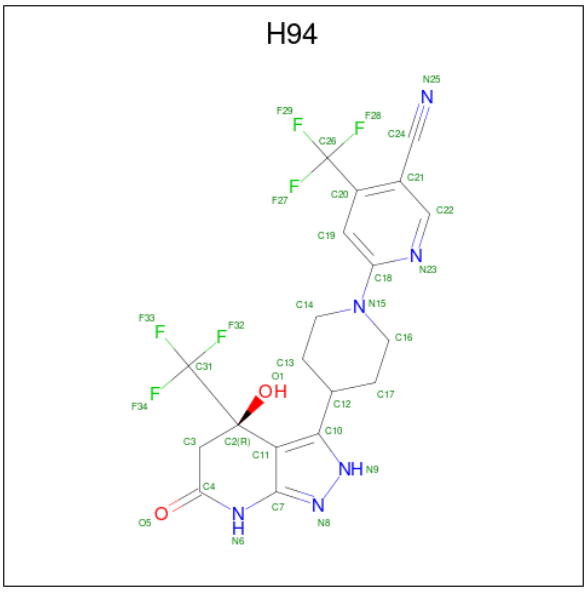
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is propan-2-yl hydrogen (R)-ethylphosphonate (three-letter code: H9A) (formula: $C_5H_{13}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	5	2	1		
3	B	1	Total	C	O	P	0	0
			8	5	2	1		

- Molecule 4 is 6-{4-[(4R)-4-hydroxy-6-oxo-4-(trifluoromethyl)-4,5,6,7-tetrahydro-2H-pyrazolo[3,4-b]pyridin-3-yl]piperidin-1-yl}-4-(trifluoromethyl)pyridine-3-carbonitrile (three-letter code: H94) (formula: $C_{19}H_{16}F_6N_6O_2$).



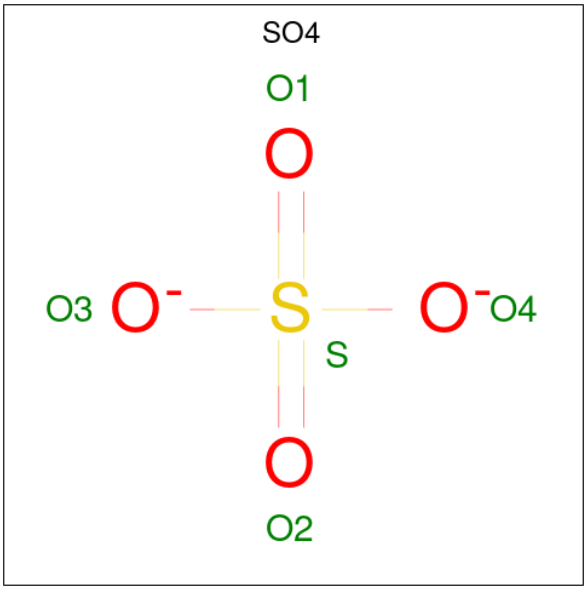
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			33	19	6	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C F N O 33 19 6 6 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ni 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	16	Total O 16 16	0	0
7	B	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	134.70Å 106.38Å 117.82Å 90.00° 125.45° 90.00°	Depositor
Resolution (Å)	28.80 – 3.10	Depositor
% Data completeness (in resolution range)	87.3 (28.80-3.10)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.193 , 0.239	Depositor
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.156	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
Total number of atoms	6181	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	A	508	-	4,4,4	0.47	0	6,6,6	0.41	0
4	H94	A	505	-	33,36,36	2.23	5 (15%)	41,57,57	2.17	9 (21%)
4	H94	B	504	-	33,36,36	2.12	6 (18%)	41,57,57	2.28	13 (31%)
2	NAG	B	501	1	14,14,15	0.59	0	17,19,21	1.38	3 (17%)
5	SO4	A	509	-	4,4,4	0.42	0	6,6,6	0.26	0
2	NAG	B	502	1	14,14,15	0.58	0	17,19,21	2.10	4 (23%)
2	NAG	A	502	1	14,14,15	0.41	0	17,19,21	1.12	1 (5%)
3	H9A	A	504	1	4,7,8	2.25	1 (25%)	3,8,11	0.74	0
5	SO4	A	507	-	4,4,4	0.34	0	6,6,6	0.16	0
2	NAG	A	501	1	14,14,15	0.52	0	17,19,21	1.44	3 (17%)
5	SO4	B	506	-	4,4,4	0.40	0	6,6,6	0.23	0
2	NAG	A	503	1	14,14,15	0.83	0	17,19,21	1.57	3 (17%)
5	SO4	A	506	-	4,4,4	0.44	0	6,6,6	0.37	0
3	H9A	B	503	1	4,7,8	2.59	1 (25%)	3,8,11	0.88	0
5	SO4	B	505	-	4,4,4	0.47	0	6,6,6	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H94	A	505	-	-	3/21/50/50	0/4/4/4
4	H94	B	504	-	-	2/21/50/50	0/4/4/4
2	NAG	B	501	1	-	2/6/23/26	0/1/1/1
2	NAG	B	502	1	-	3/6/23/26	0/1/1/1
2	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	H9A	A	504	1	-	0/2/6/8	-
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
2	NAG	A	503	1	-	3/6/23/26	0/1/1/1
3	H9A	B	503	1	-	0/2/6/8	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	H94	C21-C24	-10.62	1.28	1.44
4	B	504	H94	C21-C24	-10.11	1.29	1.44
3	B	503	H9A	O2-CM	-5.02	1.39	1.45
4	A	505	H94	C2-C11	-4.67	1.47	1.53
3	A	504	H9A	O2-CM	-4.11	1.40	1.45
4	B	504	H94	C7-N6	-3.20	1.34	1.38
4	B	504	H94	C2-C11	-2.41	1.50	1.53
4	B	504	H94	C18-N15	2.29	1.42	1.37
4	B	504	H94	C26-C20	2.21	1.55	1.50
4	B	504	H94	N8-N9	2.15	1.41	1.37
4	A	505	H94	C11-C7	-2.13	1.37	1.40
4	A	505	H94	C3-C4	2.11	1.52	1.50
4	A	505	H94	C7-N6	-2.05	1.35	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	505	H94	F34-C31-C2	-6.91	106.11	112.07
4	B	504	H94	C3-C4-N6	6.25	122.95	116.49
4	A	505	H94	C3-C4-N6	5.58	122.27	116.49
4	B	504	H94	F33-C31-C2	-5.31	107.49	112.07
2	B	502	NAG	C2-N2-C7	4.70	129.60	122.90
2	B	502	NAG	C8-C7-N2	4.42	123.58	116.10
4	B	504	H94	C7-N6-C4	-4.42	119.96	124.24
4	B	504	H94	C14-N15-C18	-4.30	110.41	120.39
2	A	503	NAG	C4-C3-C2	4.14	117.09	111.02
4	B	504	H94	C16-N15-C18	-4.01	111.08	120.39
4	B	504	H94	O5-C4-C3	-3.97	116.27	122.56
4	A	505	H94	C7-N6-C4	-3.90	120.47	124.24
2	A	501	NAG	C4-C3-C2	3.70	116.44	111.02
4	B	504	H94	F34-C31-C2	-3.54	109.02	112.07
4	A	505	H94	C13-C14-N15	-3.33	104.24	111.10
2	A	503	NAG	C1-O5-C5	-3.33	107.68	112.19
4	A	505	H94	O5-C4-C3	-3.24	117.42	122.56
4	B	504	H94	C14-C13-C12	2.78	114.33	111.04
4	A	505	H94	C16-N15-C18	-2.73	114.04	120.39
4	A	505	H94	F29-C26-C20	-2.70	107.99	112.70
2	B	501	NAG	O5-C5-C6	2.69	111.43	107.20
4	A	505	H94	C17-C12-C10	-2.69	107.58	111.44
4	A	505	H94	C21-C24-N25	-2.63	173.54	177.88
2	B	502	NAG	O7-C7-N2	-2.56	117.24	121.95
2	A	501	NAG	C3-C4-C5	2.52	114.74	110.24
2	B	502	NAG	C6-C5-C4	2.52	118.90	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	H94	C19-C18-N23	-2.43	118.52	122.73
4	B	504	H94	C22-N23-C18	2.39	121.66	117.30
2	B	501	NAG	C1-O5-C5	-2.34	109.02	112.19
2	B	501	NAG	O5-C1-C2	2.28	114.88	111.29
4	B	504	H94	C20-C21-C24	2.19	124.67	122.26
4	B	504	H94	C13-C12-C10	-2.16	108.33	111.44
2	A	503	NAG	C6-C5-C4	2.11	117.95	113.00
2	A	501	NAG	C1-O5-C5	2.11	115.05	112.19
4	B	504	H94	C19-C20-C21	-2.08	115.78	119.42
2	A	502	NAG	C4-C3-C2	-2.05	108.01	111.02

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	NAG	C1-C2-N2-C7
2	B	502	NAG	C8-C7-N2-C2
2	B	502	NAG	O7-C7-N2-C2
2	A	501	NAG	O5-C5-C6-O6
2	A	501	NAG	C4-C5-C6-O6
4	B	504	H94	N23-C18-N15-C14
4	A	505	H94	N23-C18-N15-C14
4	B	504	H94	C19-C18-N15-C14
2	A	502	NAG	C4-C5-C6-O6
2	A	503	NAG	C4-C5-C6-O6
4	A	505	H94	C20-C21-C24-N25
2	B	502	NAG	C1-C2-N2-C7
4	A	505	H94	C19-C18-N15-C14
2	B	501	NAG	C3-C2-N2-C7
2	A	503	NAG	C1-C2-N2-C7
2	A	503	NAG	O5-C5-C6-O6
2	A	502	NAG	O5-C5-C6-O6

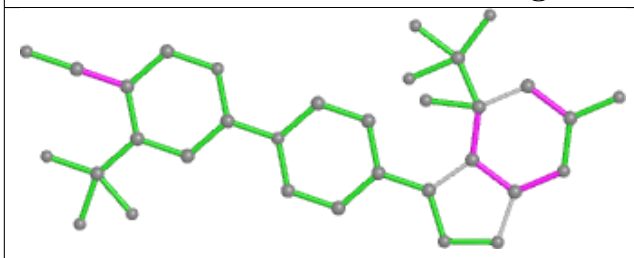
There are no ring outliers.

No monomer is involved in short contacts.

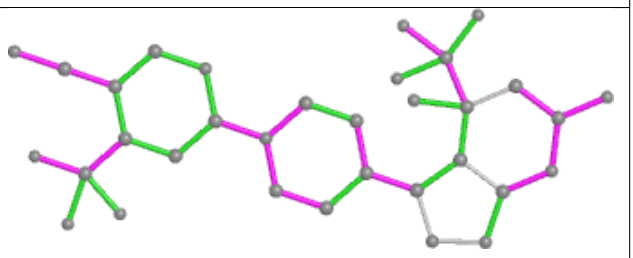
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

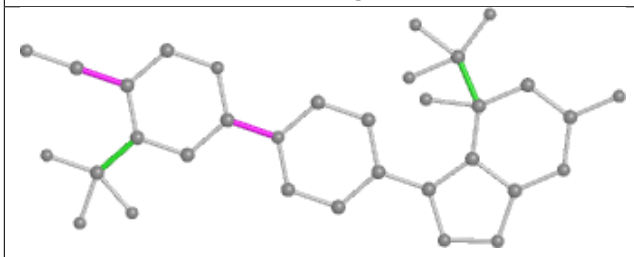
Ligand H94 A 505



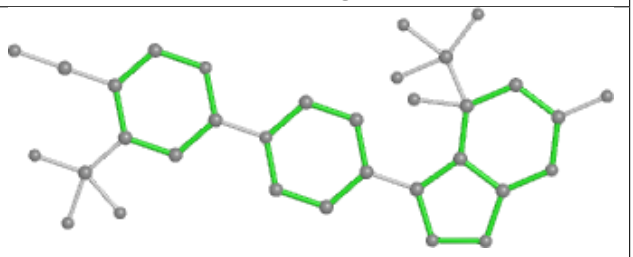
Bond lengths



Bond angles

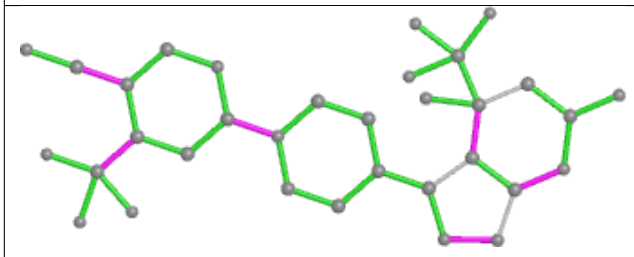


Torsions

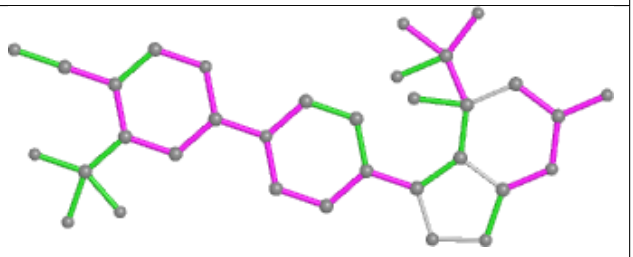


Rings

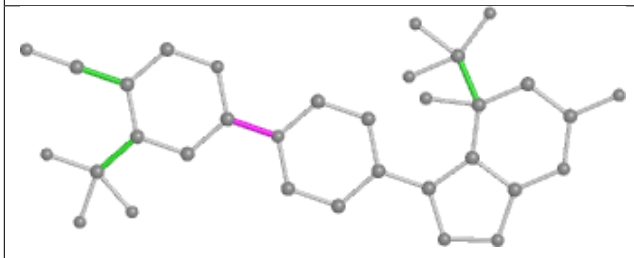
Ligand H94 B 504



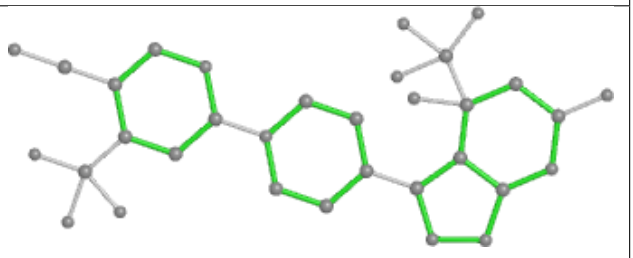
Bond lengths



Bond angles



Torsions



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.