wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 09:58 AM EDT

PDB ID	:	6NB1
Title	:	Crystal structure of Escherichia coli ClpP protease complexed with small molecule activator, ACP1-06
Authors	:	Mabanglo, M.F.; Houry, W.A.; Eger, B.T.; Bryson, S.; Pai, E.F.
Deposited on	:	2018-12-06
Resolution	:	1.90 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 (1)) 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

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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)

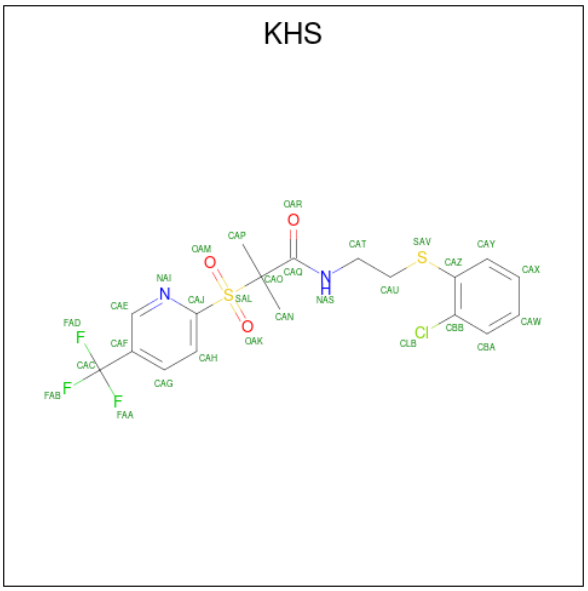
There are 4 unique types of molecules in this entry. The entry contains 21848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent Clp protease proteolytic subunit.

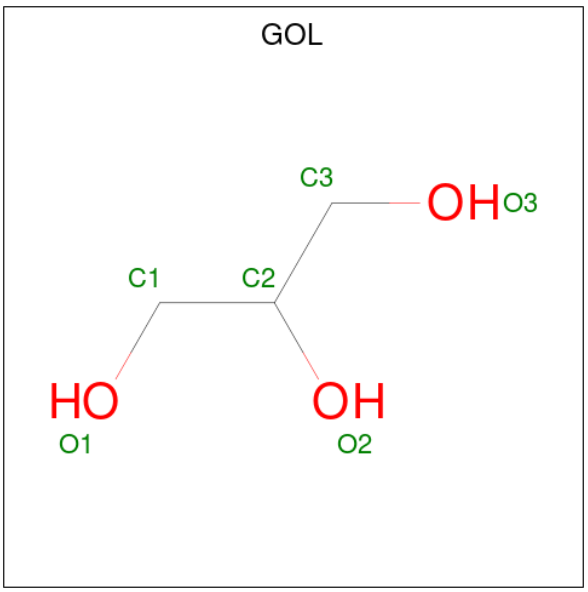
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1472	930	253	277	12			
1	B	193	Total	C	N	O	S	0	0	0
			1509	950	262	285	12			
1	C	184	Total	C	N	O	S	0	0	0
			1441	910	247	272	12			
1	D	184	Total	C	N	O	S	0	0	0
			1442	910	249	271	12			
1	E	186	Total	C	N	O	S	0	0	0
			1458	922	251	273	12			
1	F	183	Total	C	N	O	S	0	0	0
			1429	905	245	267	12			
1	G	183	Total	C	N	O	S	0	0	0
			1428	903	245	268	12			
1	H	181	Total	C	N	O	S	0	0	0
			1416	896	243	265	12			
1	I	176	Total	C	N	O	S	0	0	0
			1376	867	238	260	11			
1	J	180	Total	C	N	O	S	0	0	0
			1403	885	242	264	12			
1	K	181	Total	C	N	O	S	0	0	0
			1413	893	243	265	12			
1	L	182	Total	C	N	O	S	0	0	0
			1424	902	244	266	12			
1	M	180	Total	C	N	O	S	0	0	0
			1409	891	242	264	12			
1	N	180	Total	C	N	O	S	0	0	0
			1409	891	242	264	12			

- Molecule 2 is N-{2-[(2-chlorophenyl)sulfanyl]ethyl}-2-methyl-2-{[5-(trifluoromethyl)pyridin-2-yl]sulfonyl}propanamide (three-letter code: KHS) (formula: $C_{18}H_{18}ClF_3N_2O_3S_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	B	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	C	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	D	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	E	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	F	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	G	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	H	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	I	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	J	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	K	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	L	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	M	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	N	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	72	Total O 72 72	0	0
4	B	65	Total O 65 65	0	0
4	C	44	Total O 44 44	0	0
4	D	43	Total O 43 43	0	0
4	E	64	Total O 64 64	0	0
4	F	89	Total O 89 89	0	0
4	G	90	Total O 90 90	0	0
4	H	66	Total O 66 66	0	0
4	I	61	Total O 61 61	0	0
4	J	43	Total O 43 43	0	0
4	K	55	Total O 55 55	0	0
4	L	70	Total O 70 70	0	0
4	M	89	Total O 89 89	0	0
4	N	72	Total O 72 72	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	190.99Å 101.09Å 155.19Å 90.00° 98.29° 90.00°	Depositor
Resolution (Å)	48.00 – 1.90	Depositor
% Data completeness (in resolution range)	97.5 (48.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.209 , 0.244	Depositor
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.383	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	21848	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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

42 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	KHS	D	301[B]	-	28,30,30	3.21	5 (17%)	35,45,45	2.42	8 (22%)
2	KHS	I	301[B]	-	28,30,30	3.23	5 (17%)	35,45,45	2.39	8 (22%)
2	KHS	J	301[A]	-	28,30,30	3.24	5 (17%)	35,45,45	2.26	7 (20%)
3	GOL	M	302	-	5,5,5	0.54	0	5,5,5	0.20	0
2	KHS	M	301[A]	-	28,30,30	3.28	5 (17%)	35,45,45	2.39	10 (28%)
3	GOL	B	302	-	5,5,5	0.40	0	5,5,5	0.33	0
2	KHS	N	301[B]	-	28,30,30	3.16	5 (17%)	35,45,45	2.52	9 (25%)
2	KHS	F	301[B]	-	28,30,30	3.02	5 (17%)	35,45,45	2.80	12 (34%)
3	GOL	F	302	-	5,5,5	0.60	0	5,5,5	0.44	0
2	KHS	B	301[B]	-	28,30,30	3.26	6 (21%)	35,45,45	2.37	7 (20%)
3	GOL	A	302	-	5,5,5	0.41	0	5,5,5	0.54	0
2	KHS	L	301[B]	-	28,30,30	3.24	5 (17%)	35,45,45	2.41	8 (22%)
3	GOL	N	302	-	5,5,5	0.43	0	5,5,5	0.39	0
2	KHS	K	301[A]	-	28,30,30	3.30	5 (17%)	35,45,45	2.36	9 (25%)
3	GOL	D	302	-	5,5,5	0.47	0	5,5,5	0.17	0
2	KHS	J	301[B]	-	28,30,30	3.23	6 (21%)	35,45,45	2.45	7 (20%)
2	KHS	M	301[B]	-	28,30,30	3.18	5 (17%)	35,45,45	2.34	8 (22%)
2	KHS	C	301[A]	-	28,30,30	3.28	6 (21%)	35,45,45	2.27	9 (25%)
2	KHS	E	301[A]	-	28,30,30	3.39	5 (17%)	35,45,45	2.39	10 (28%)
2	KHS	A	301[A]	-	28,30,30	3.27	6 (21%)	35,45,45	2.35	9 (25%)
2	KHS	G	301[A]	-	28,30,30	3.34	5 (17%)	35,45,45	2.28	9 (25%)
3	GOL	H	302	-	5,5,5	0.40	0	5,5,5	0.23	0
2	KHS	K	301[B]	-	28,30,30	3.24	5 (17%)	35,45,45	2.54	9 (25%)
3	GOL	C	302	-	5,5,5	0.36	0	5,5,5	0.60	0
3	GOL	E	302	-	5,5,5	0.55	0	5,5,5	0.86	0
2	KHS	C	301[B]	-	28,30,30	3.16	5 (17%)	35,45,45	2.48	9 (25%)
2	KHS	E	301[B]	-	28,30,30	3.31	6 (21%)	35,45,45	2.42	8 (22%)
2	KHS	H	301[A]	-	28,30,30	3.24	5 (17%)	35,45,45	2.38	9 (25%)
2	KHS	A	301[B]	-	28,30,30	3.22	5 (17%)	35,45,45	2.40	8 (22%)
2	KHS	D	301[A]	-	28,30,30	3.28	5 (17%)	35,45,45	2.35	10 (28%)
2	KHS	G	301[B]	-	28,30,30	3.24	5 (17%)	35,45,45	2.50	10 (28%)
2	KHS	I	301[A]	-	28,30,30	3.29	5 (17%)	35,45,45	2.31	10 (28%)
2	KHS	H	301[B]	-	28,30,30	3.15	5 (17%)	35,45,45	2.42	8 (22%)
3	GOL	G	302	-	5,5,5	0.40	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	KHS	N	301[A]	-	28,30,30	3.26	5 (17%)	35,45,45	2.21	7 (20%)
3	GOL	L	302	-	5,5,5	0.41	0	5,5,5	0.11	0
2	KHS	B	301[A]	-	28,30,30	3.40	5 (17%)	35,45,45	2.38	10 (28%)
2	KHS	F	301[A]	-	28,30,30	3.33	4 (14%)	35,45,45	2.97	14 (40%)
3	GOL	J	302	-	5,5,5	0.47	0	5,5,5	0.67	0
3	GOL	I	302	-	5,5,5	0.54	0	5,5,5	0.33	0
3	GOL	K	302	-	5,5,5	0.40	0	5,5,5	0.45	0
2	KHS	L	301[A]	-	28,30,30	3.30	6 (21%)	35,45,45	2.34	8 (22%)

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	KHS	D	301[B]	-	-	5/30/34/34	0/2/2/2
2	KHS	I	301[B]	-	-	4/30/34/34	0/2/2/2
2	KHS	J	301[A]	-	-	5/30/34/34	0/2/2/2
3	GOL	M	302	-	-	2/4/4/4	-
2	KHS	M	301[A]	-	-	4/30/34/34	0/2/2/2
3	GOL	B	302	-	-	2/4/4/4	-
2	KHS	N	301[B]	-	-	5/30/34/34	0/2/2/2
2	KHS	F	301[B]	-	-	6/30/34/34	0/2/2/2
3	GOL	F	302	-	-	1/4/4/4	-
2	KHS	B	301[B]	-	-	5/30/34/34	0/2/2/2
3	GOL	A	302	-	-	2/4/4/4	-
2	KHS	L	301[B]	-	-	4/30/34/34	0/2/2/2
3	GOL	N	302	-	-	2/4/4/4	-
2	KHS	K	301[A]	-	-	4/30/34/34	0/2/2/2
3	GOL	D	302	-	-	2/4/4/4	-
2	KHS	J	301[B]	-	-	5/30/34/34	0/2/2/2
2	KHS	M	301[B]	-	-	4/30/34/34	0/2/2/2
2	KHS	C	301[A]	-	-	4/30/34/34	0/2/2/2
2	KHS	E	301[A]	-	-	4/30/34/34	0/2/2/2
2	KHS	A	301[A]	-	-	4/30/34/34	0/2/2/2
2	KHS	G	301[A]	-	-	5/30/34/34	0/2/2/2
3	GOL	H	302	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KHS	K	301[B]	-	-	2/30/34/34	0/2/2/2
3	GOL	C	302	-	-	2/4/4/4	-
3	GOL	E	302	-	-	4/4/4/4	-
2	KHS	C	301[B]	-	-	4/30/34/34	0/2/2/2
2	KHS	E	301[B]	-	-	5/30/34/34	0/2/2/2
2	KHS	H	301[A]	-	-	5/30/34/34	0/2/2/2
2	KHS	A	301[B]	-	-	4/30/34/34	0/2/2/2
2	KHS	D	301[A]	-	-	5/30/34/34	0/2/2/2
2	KHS	G	301[B]	-	-	5/30/34/34	0/2/2/2
2	KHS	I	301[A]	-	-	4/30/34/34	0/2/2/2
2	KHS	H	301[B]	-	-	5/30/34/34	0/2/2/2
3	GOL	G	302	-	-	4/4/4/4	-
2	KHS	N	301[A]	-	-	4/30/34/34	0/2/2/2
3	GOL	L	302	-	-	2/4/4/4	-
2	KHS	B	301[A]	-	-	5/30/34/34	0/2/2/2
2	KHS	F	301[A]	-	-	5/30/34/34	0/2/2/2
3	GOL	J	302	-	-	2/4/4/4	-
3	GOL	I	302	-	-	1/4/4/4	-
3	GOL	K	302	-	-	4/4/4/4	-
2	KHS	L	301[A]	-	-	4/30/34/34	0/2/2/2

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301[A]	KHS	OAM-SAL	11.41	1.54	1.44
2	B	301[A]	KHS	OAM-SAL	11.40	1.54	1.44
2	B	301[A]	KHS	OAK-SAL	11.19	1.53	1.44
2	G	301[A]	KHS	OAM-SAL	11.14	1.53	1.44
2	K	301[A]	KHS	OAM-SAL	11.09	1.53	1.44

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	301[B]	KHS	OAK-SAL-OAM	-9.07	109.01	118.98
2	F	301[A]	KHS	OAK-SAL-OAM	-9.03	109.05	118.98
2	B	301[A]	KHS	OAK-SAL-OAM	-8.90	109.20	118.98
2	N	301[B]	KHS	OAK-SAL-OAM	-8.86	109.24	118.98
2	E	301[B]	KHS	OAK-SAL-OAM	-8.84	109.26	118.98

There are no chirality outliers.

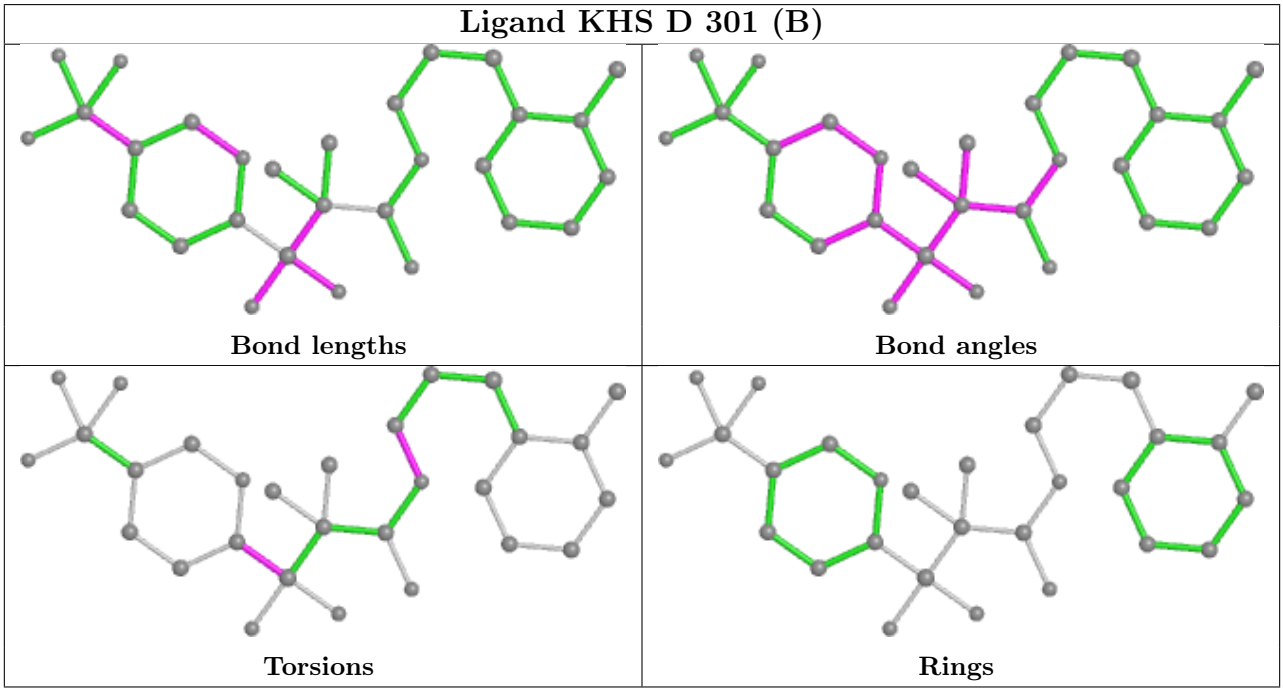
5 of 155 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[A]	KHS	NAI-CAJ-SAL-OAM
2	A	301[A]	KHS	CAH-CAJ-SAL-OAM
2	A	301[B]	KHS	NAI-CAJ-SAL-OAM
2	A	301[B]	KHS	CAH-CAJ-SAL-OAM
2	B	301[A]	KHS	NAI-CAJ-SAL-OAM

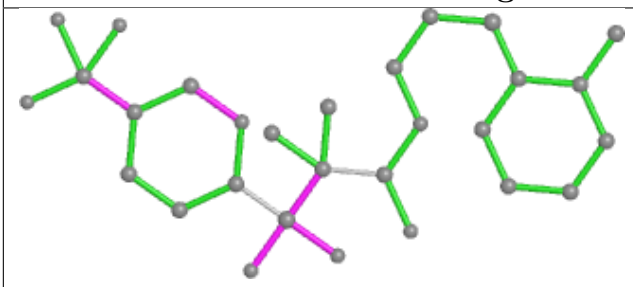
There are no ring outliers.

No monomer is involved in short contacts.

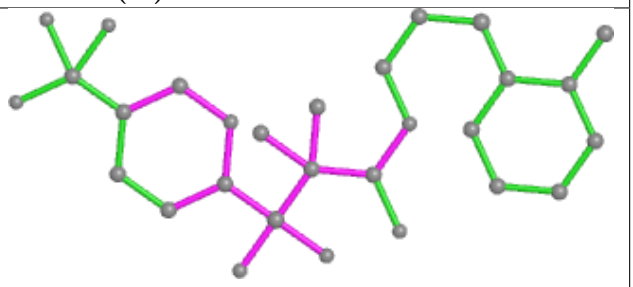
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



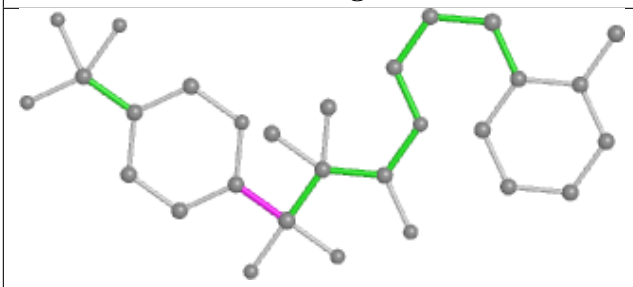
Ligand KHS I 301 (B)



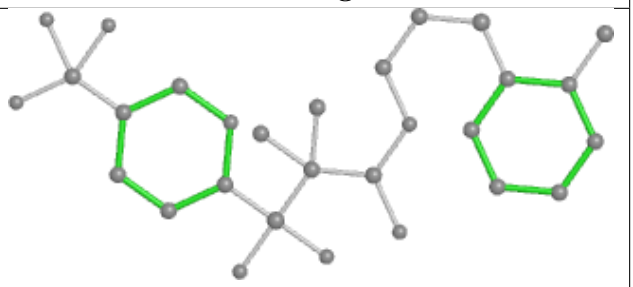
Bond lengths



Bond angles

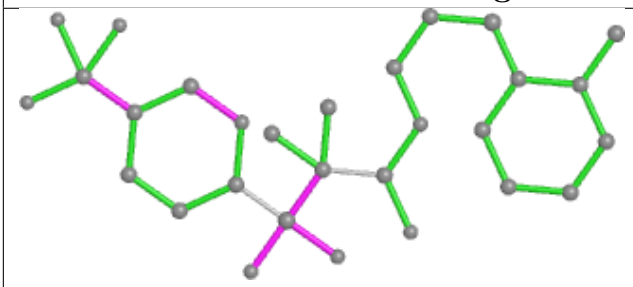


Torsions

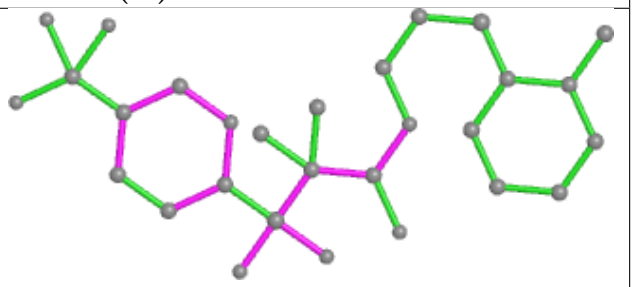


Rings

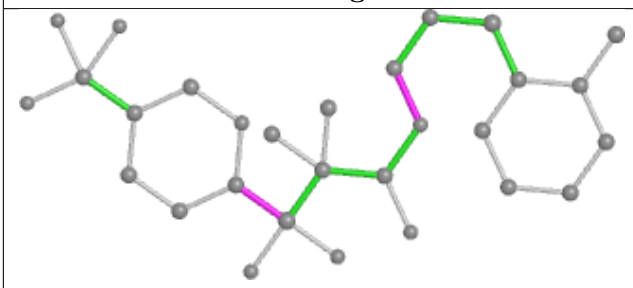
Ligand KHS J 301 (A)



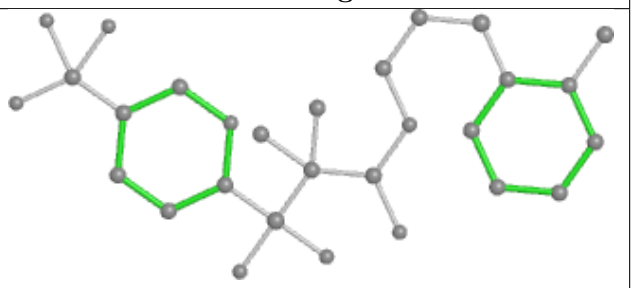
Bond lengths



Bond angles

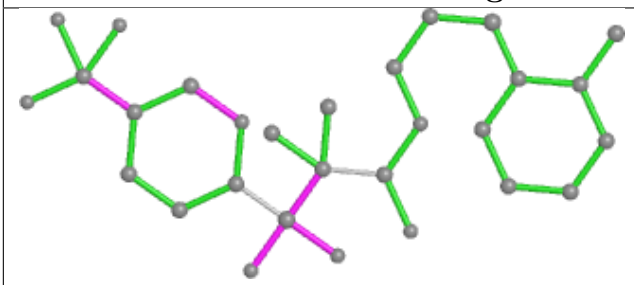


Torsions

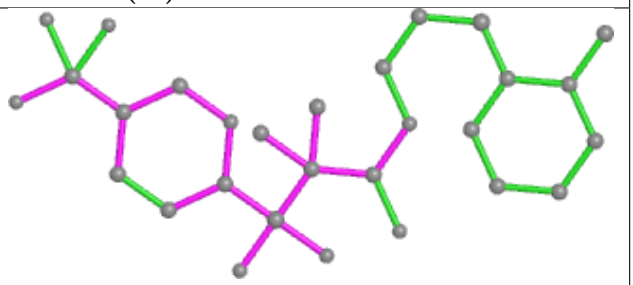


Rings

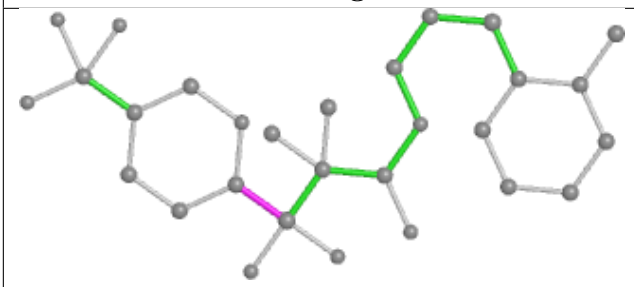
Ligand KHS M 301 (A)



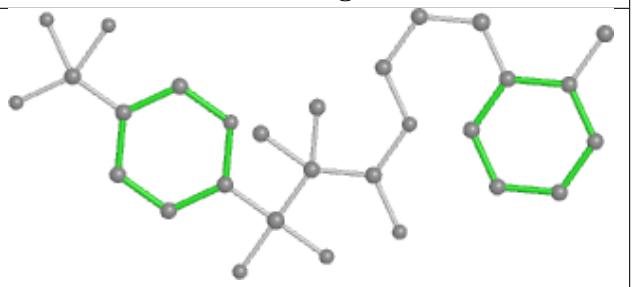
Bond lengths



Bond angles

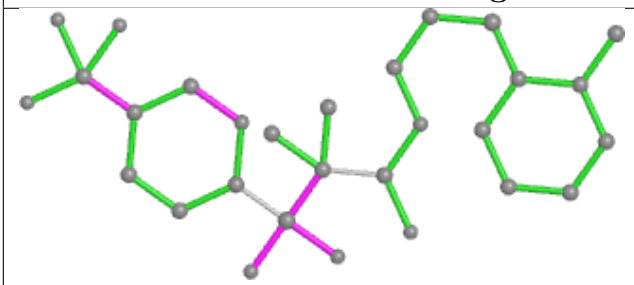


Torsions

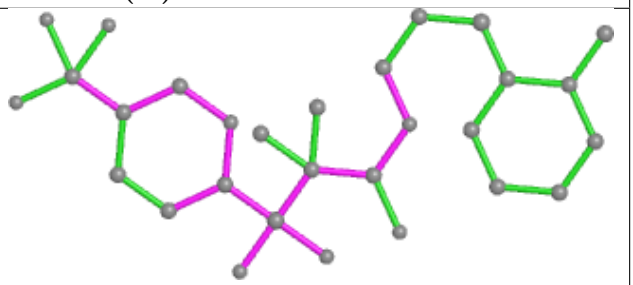


Rings

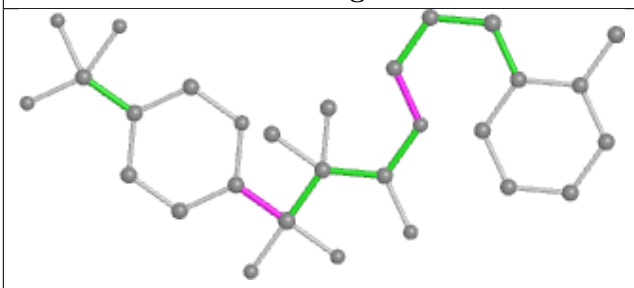
Ligand KHS N 301 (B)



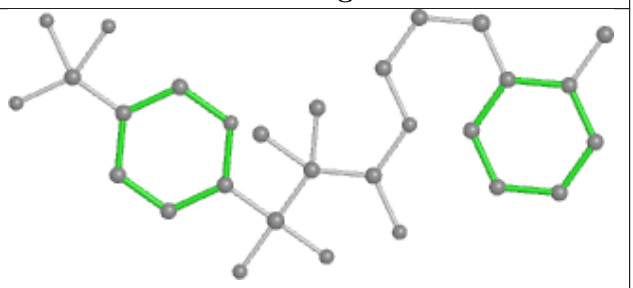
Bond lengths



Bond angles

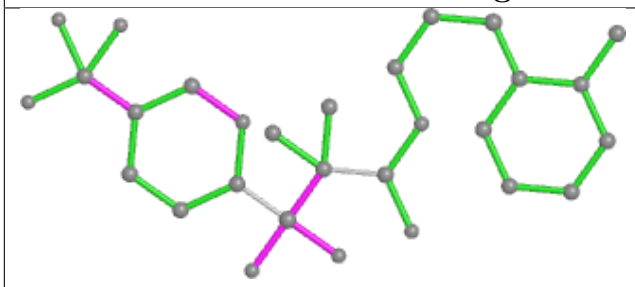


Torsions

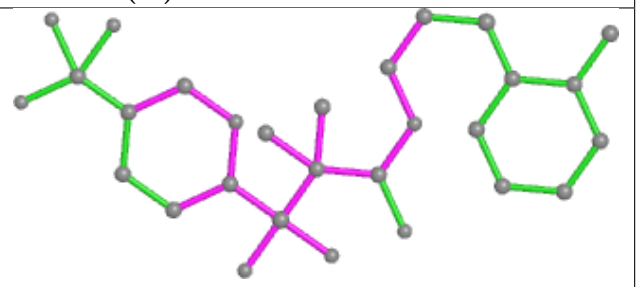


Rings

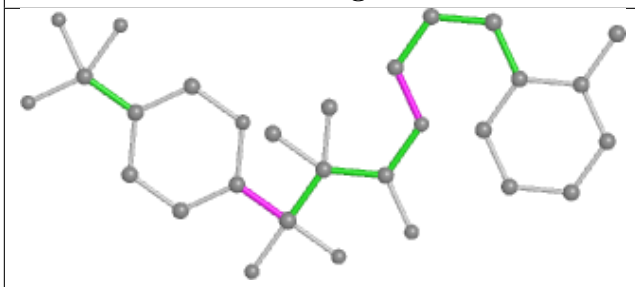
Ligand KHS F 301 (B)



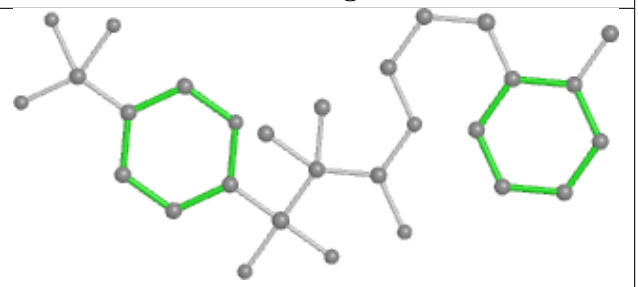
Bond lengths



Bond angles

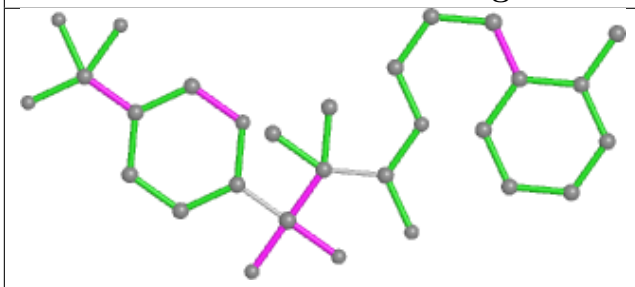


Torsions

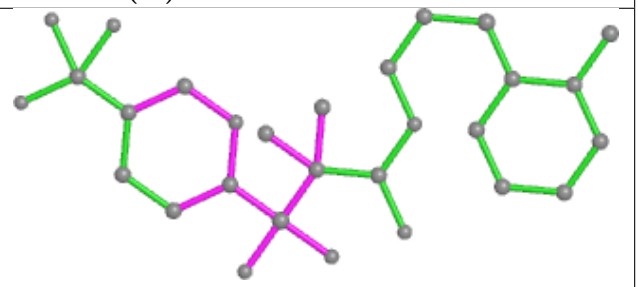


Rings

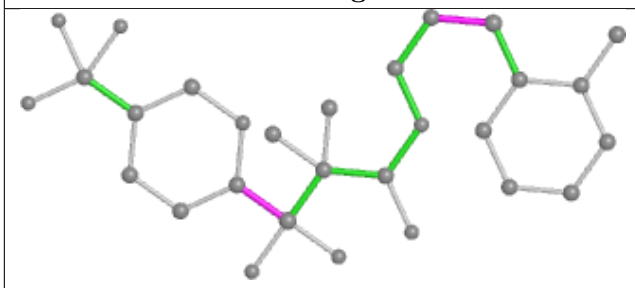
Ligand KHS B 301 (B)



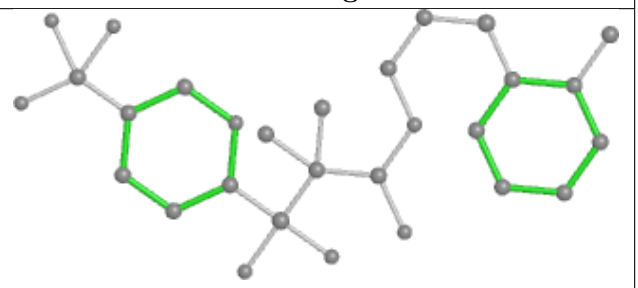
Bond lengths



Bond angles

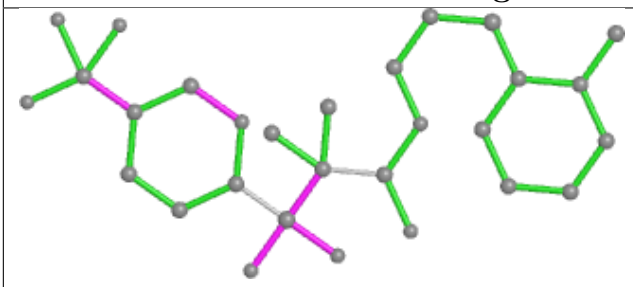


Torsions

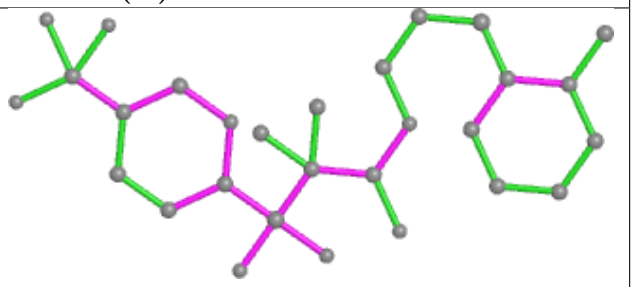


Rings

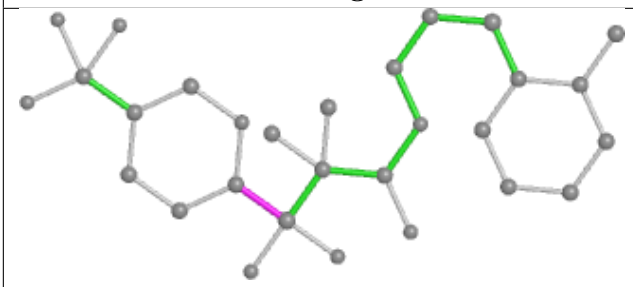
Ligand KHS L 301 (B)



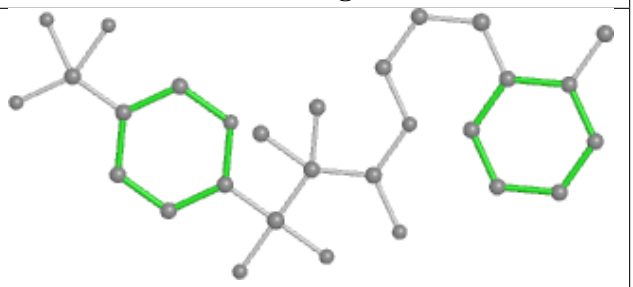
Bond lengths



Bond angles

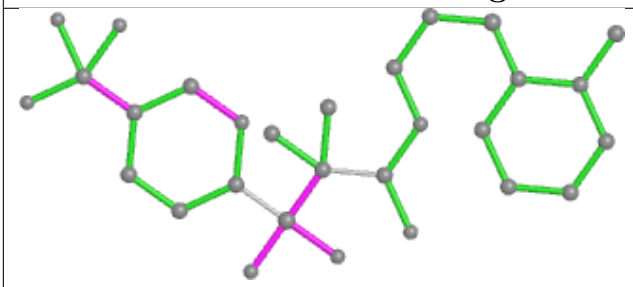


Torsions



Rings

Ligand KHS K 301 (A)



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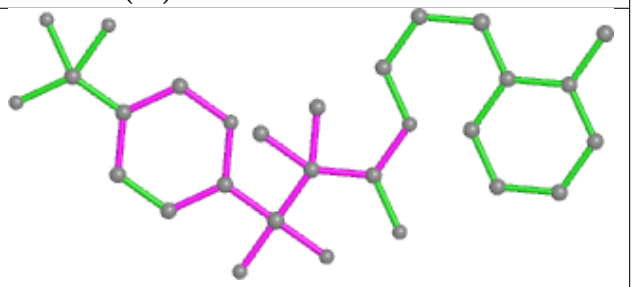
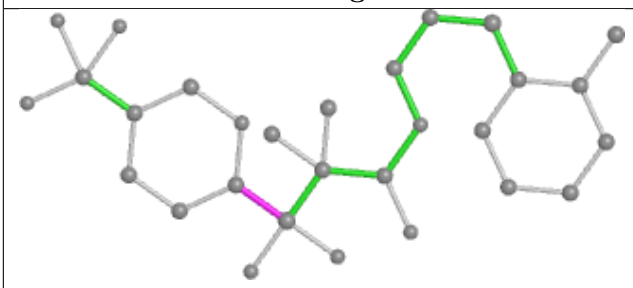
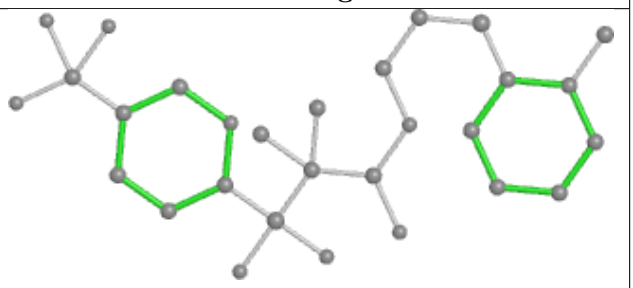


Bond angles

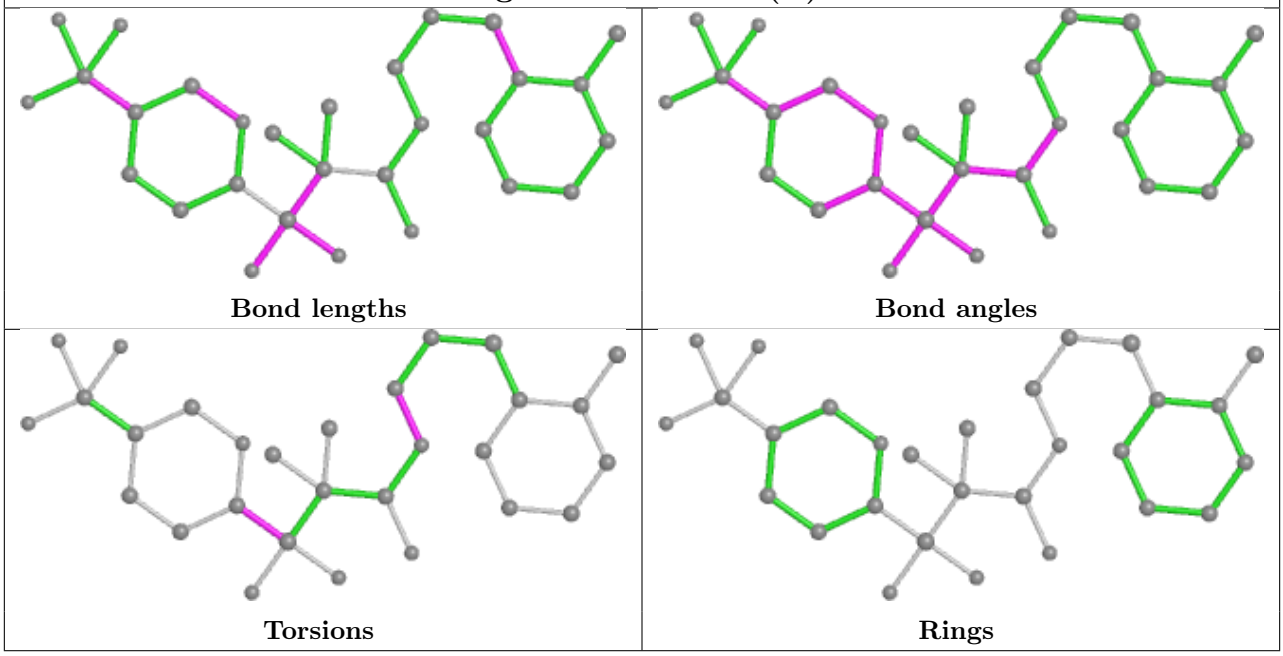


Torsions

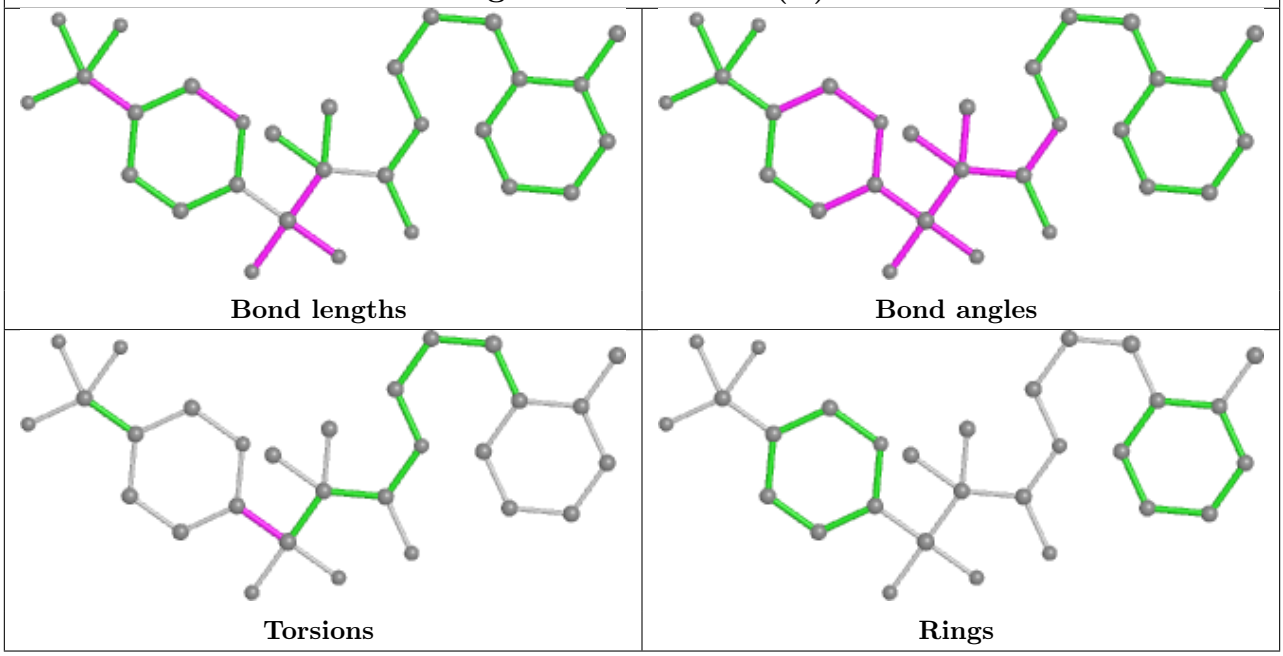


Rings

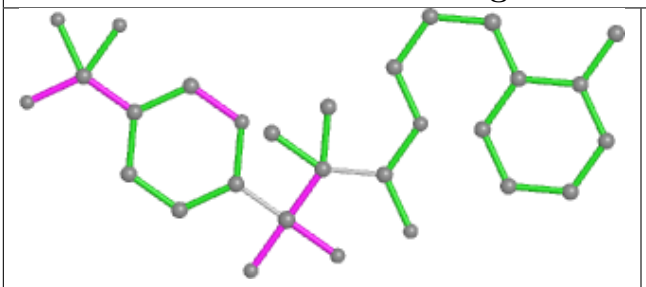
Ligand KHS J 301 (B)



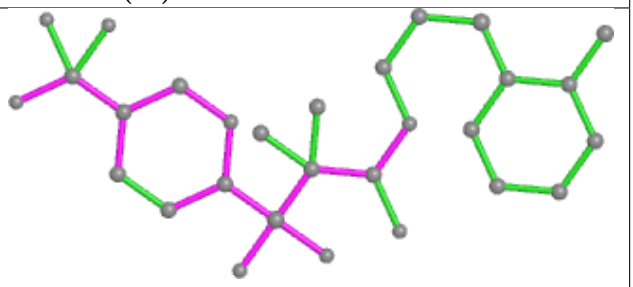
Ligand KHS M 301 (B)



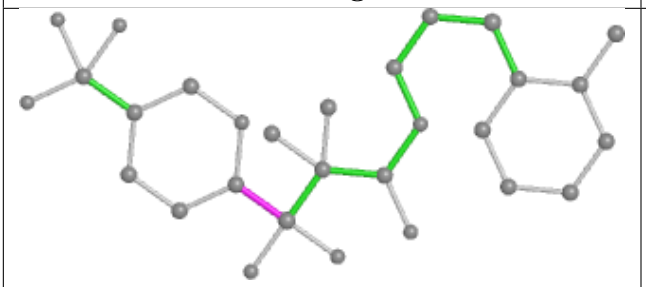
Ligand KHS C 301 (A)



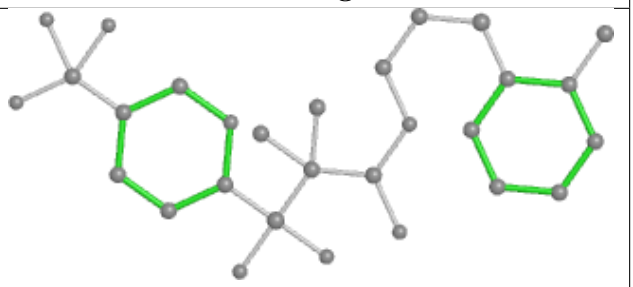
Bond lengths



Bond angles

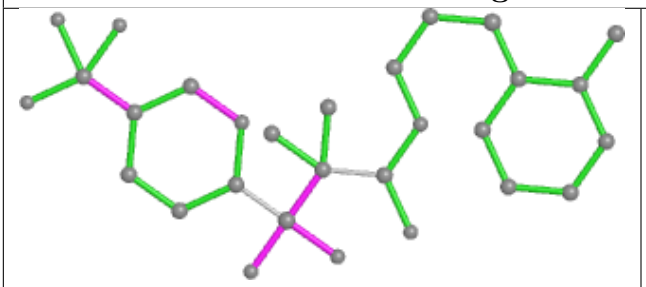


Torsions

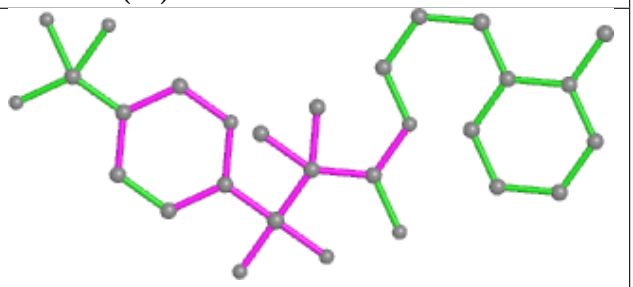


Rings

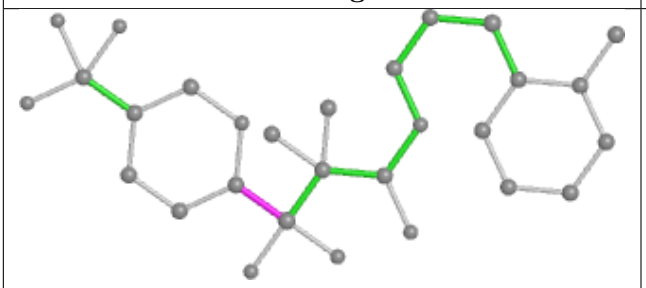
Ligand KHS E 301 (A)



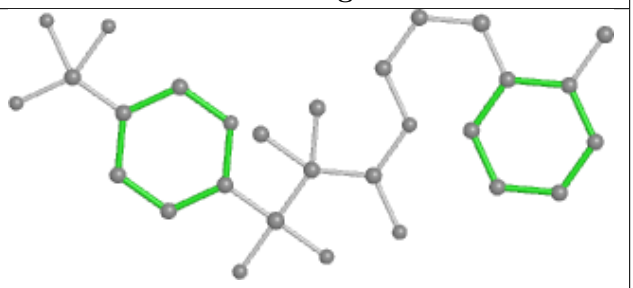
Bond lengths



Bond angles

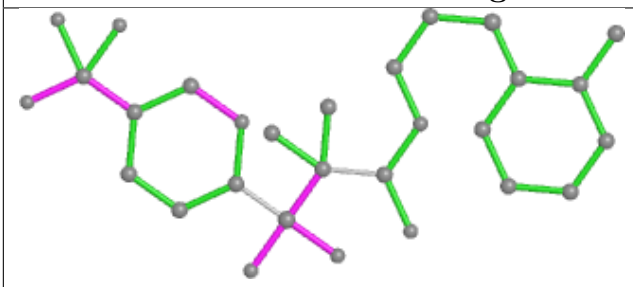


Torsions

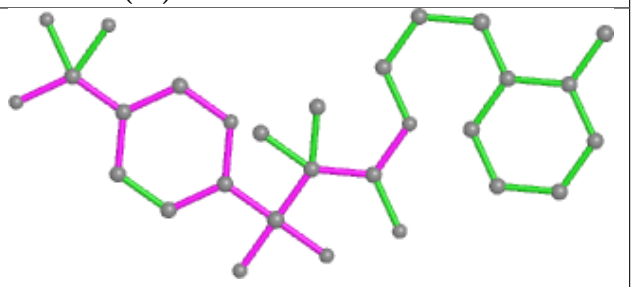


Rings

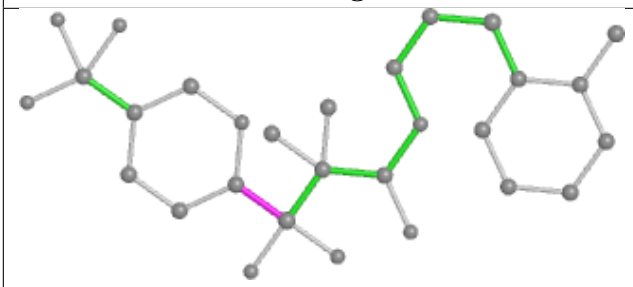
Ligand KHS A 301 (A)



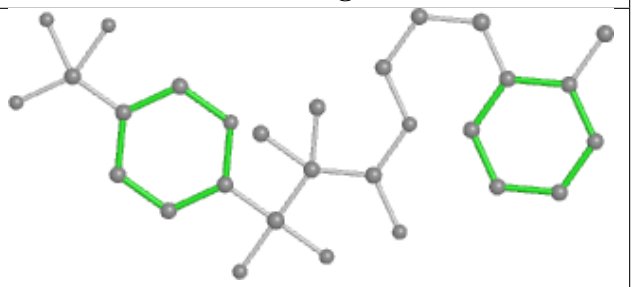
Bond lengths



Bond angles

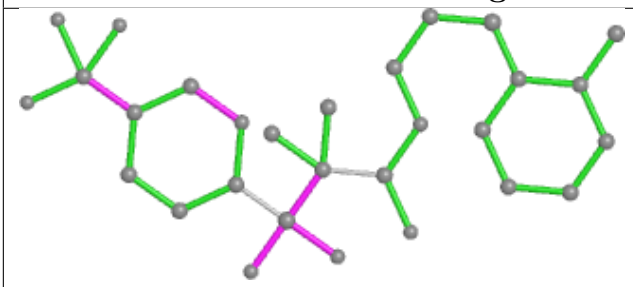


Torsions

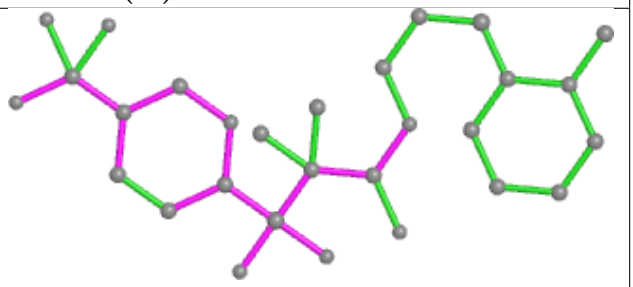


Rings

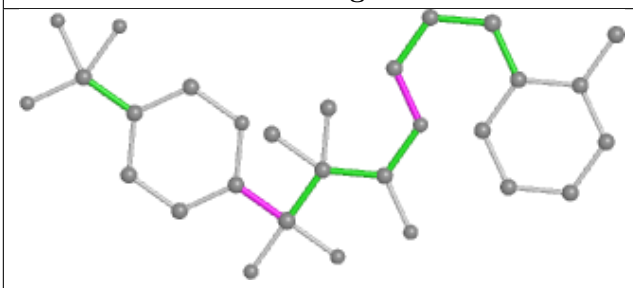
Ligand KHS G 301 (A)



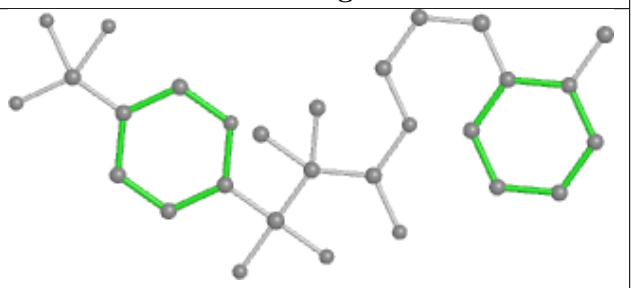
Bond lengths



Bond angles

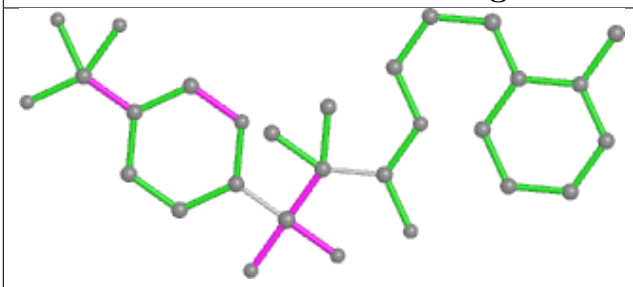


Torsions

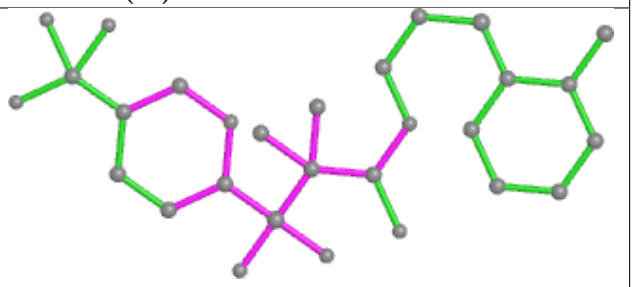


Rings

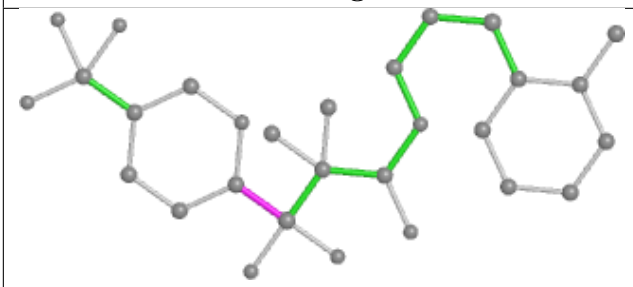
Ligand KHS K 301 (B)



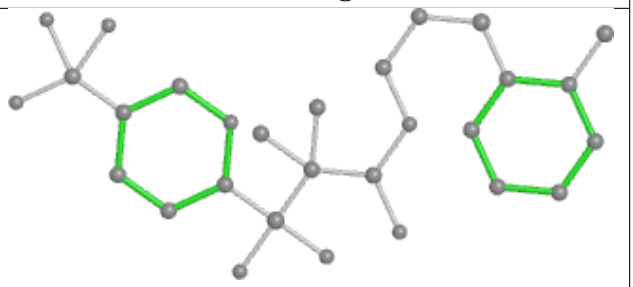
Bond lengths



Bond angles

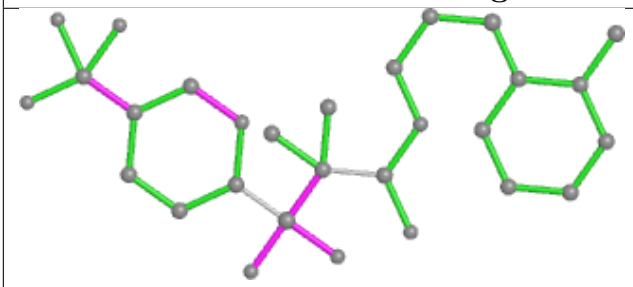


Torsions

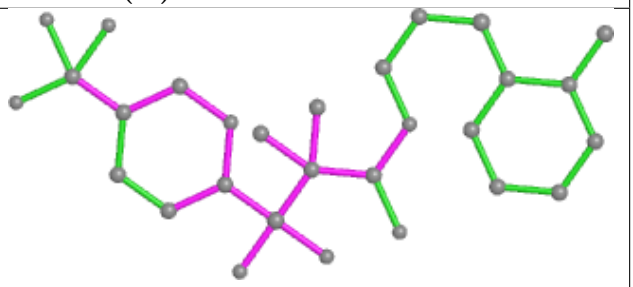


Rings

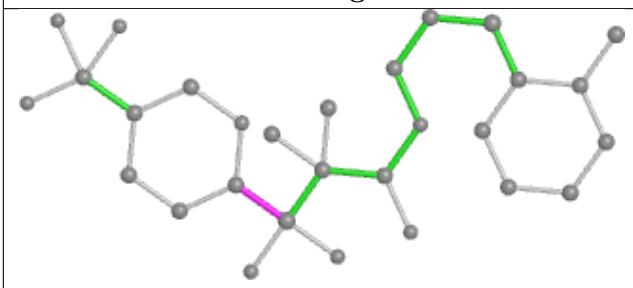
Ligand KHS C 301 (B)



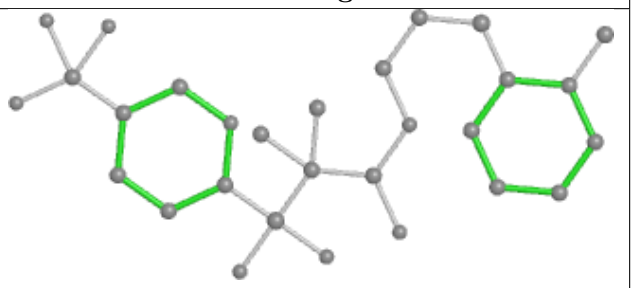
Bond lengths



Bond angles

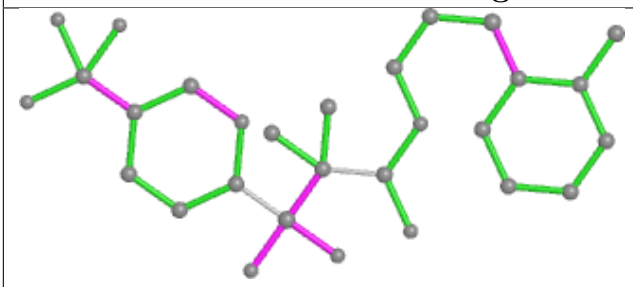


Torsions

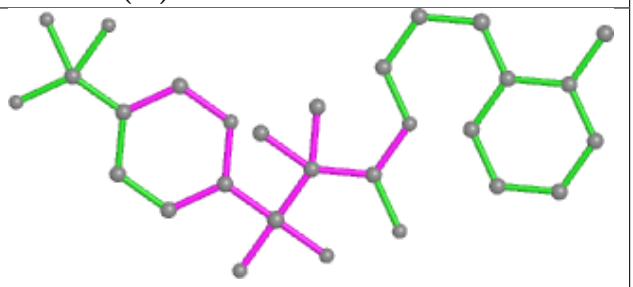


Rings

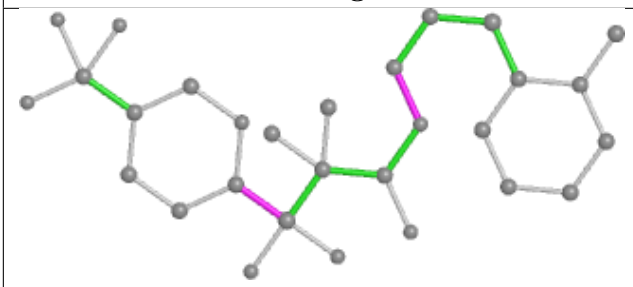
Ligand KHS E 301 (B)



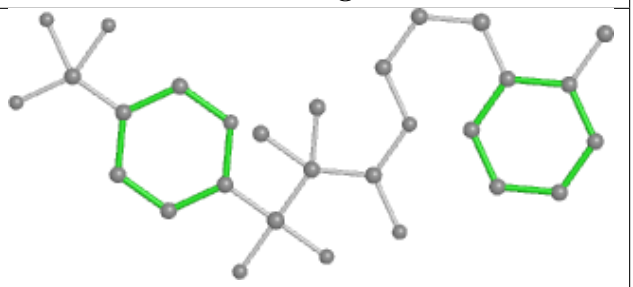
Bond lengths



Bond angles

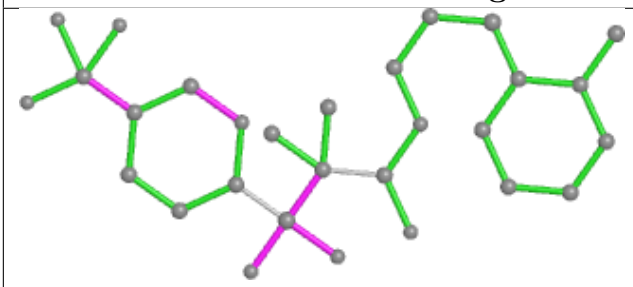


Torsions

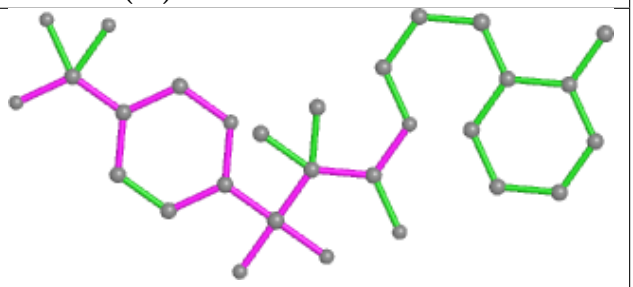


Rings

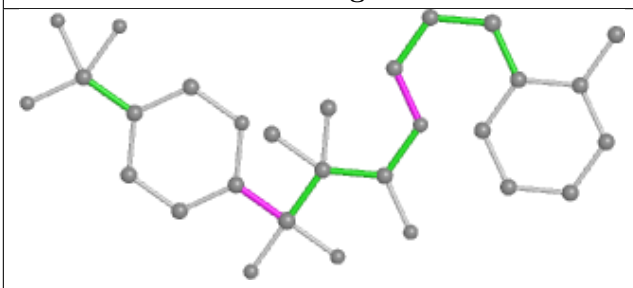
Ligand KHS H 301 (A)



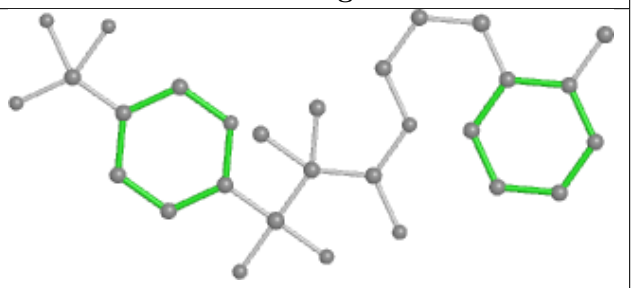
Bond lengths



Bond angles

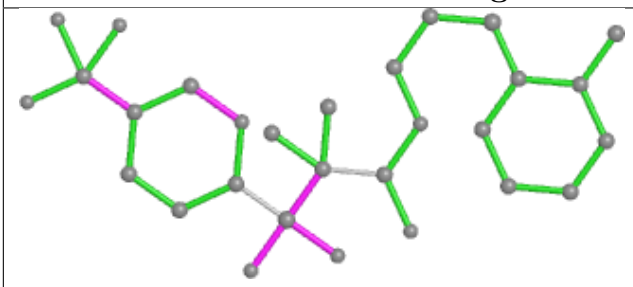


Torsions

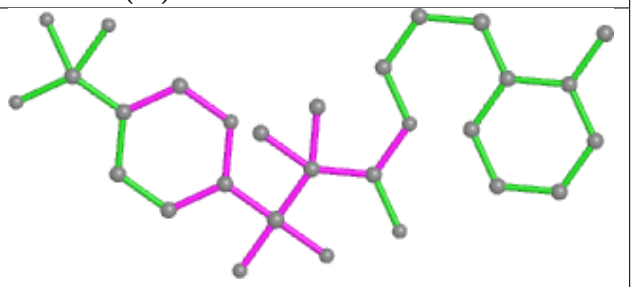


Rings

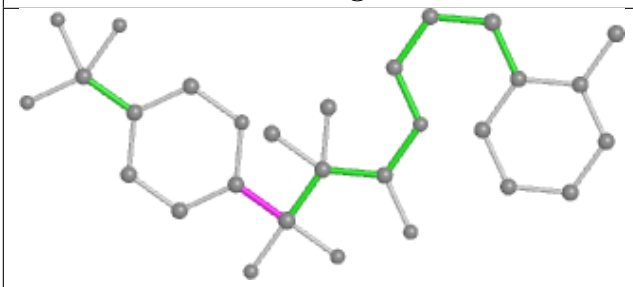
Ligand KHS A 301 (B)



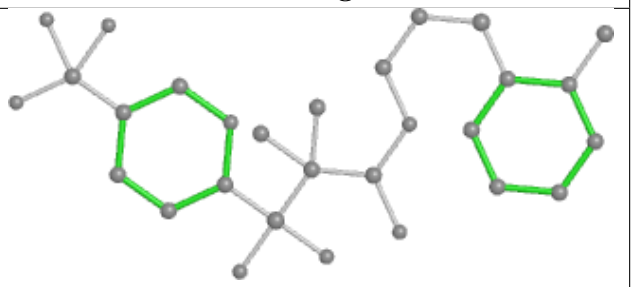
Bond lengths



Bond angles

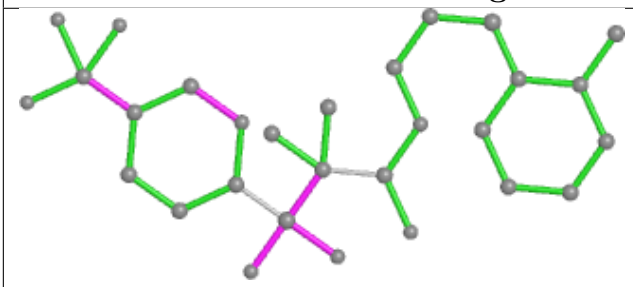


Torsions

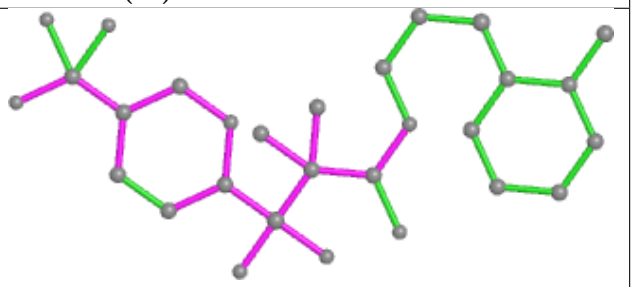


Rings

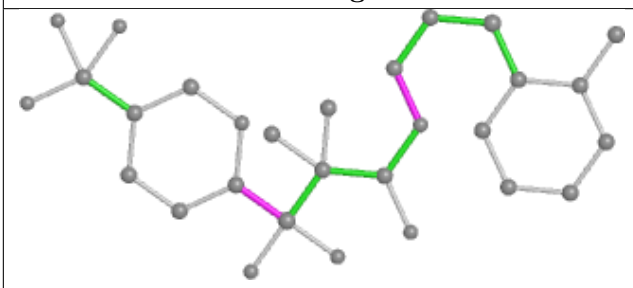
Ligand KHS D 301 (A)



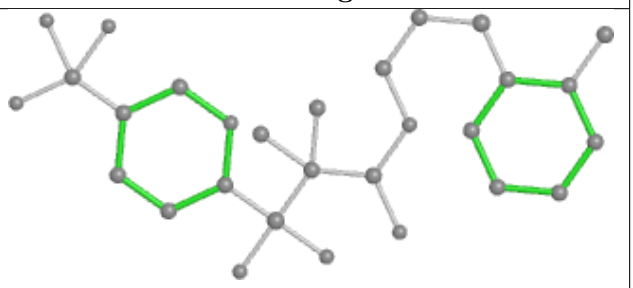
Bond lengths



Bond angles

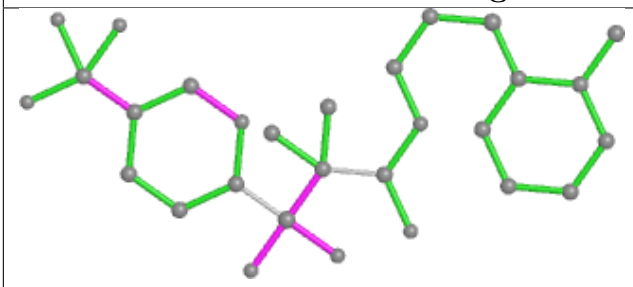


Torsions

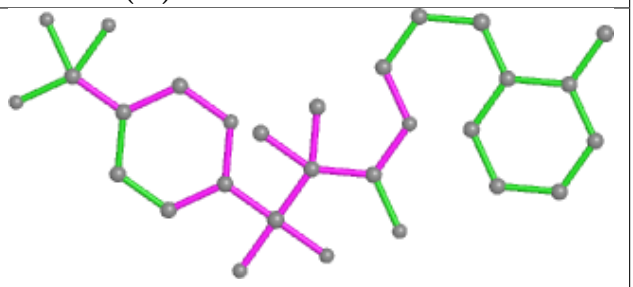


Rings

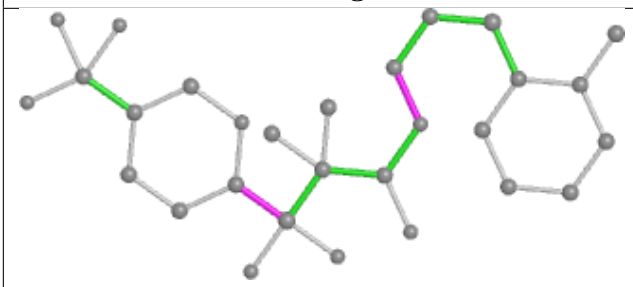
Ligand KHS G 301 (B)



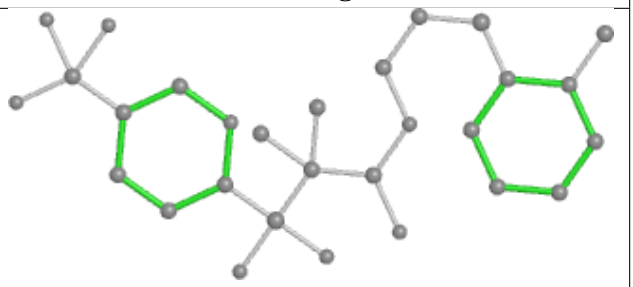
Bond lengths



Bond angles

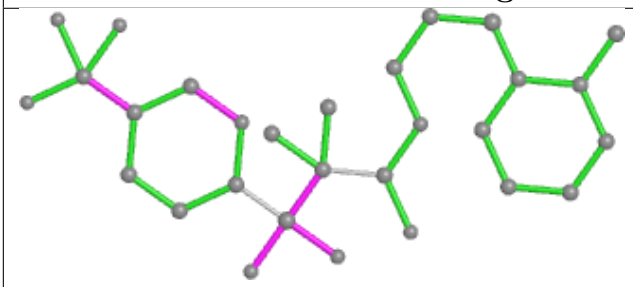


Torsions

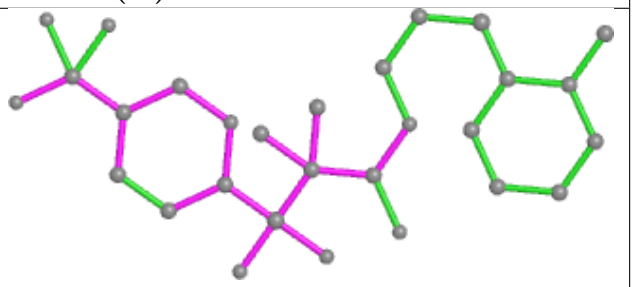


Rings

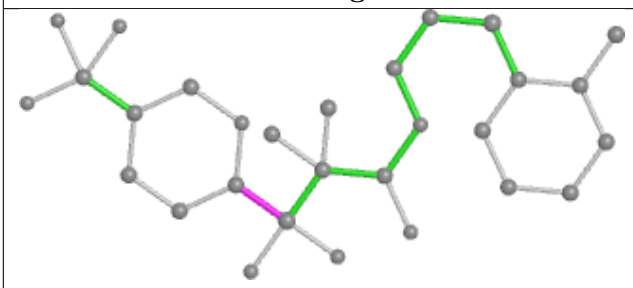
Ligand KHS I 301 (A)



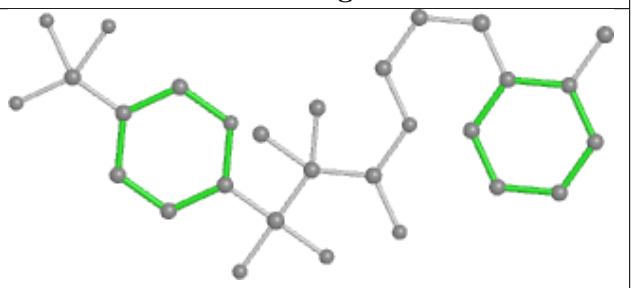
Bond lengths



Bond angles

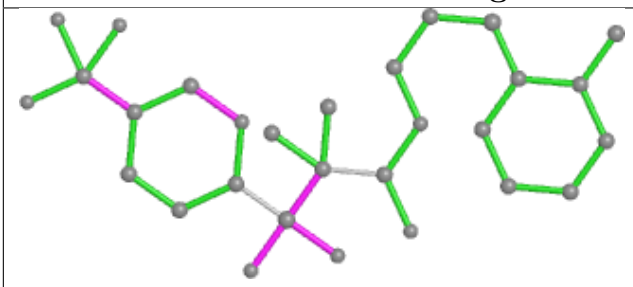


Torsions

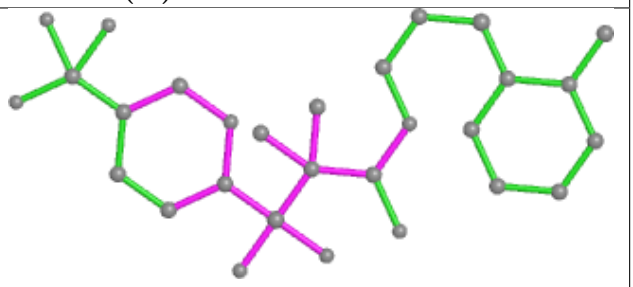


Rings

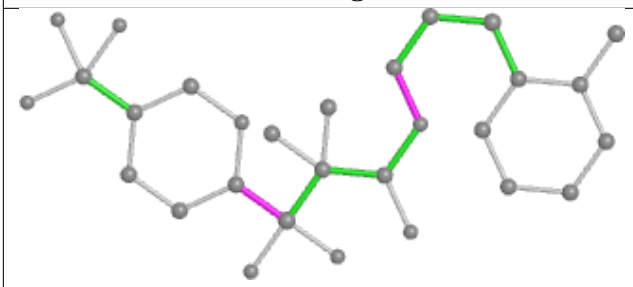
Ligand KHS H 301 (B)



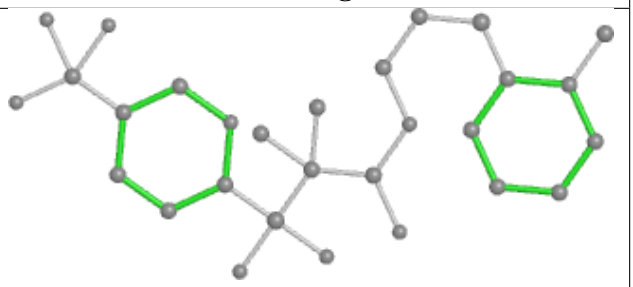
Bond lengths



Bond angles

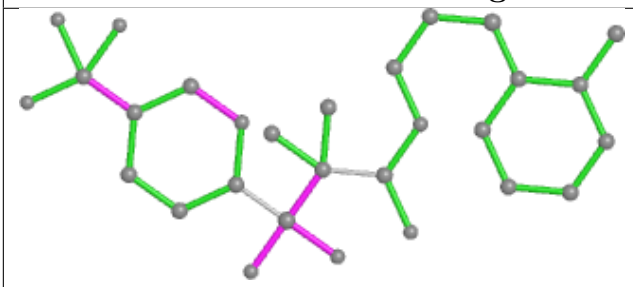


Torsions

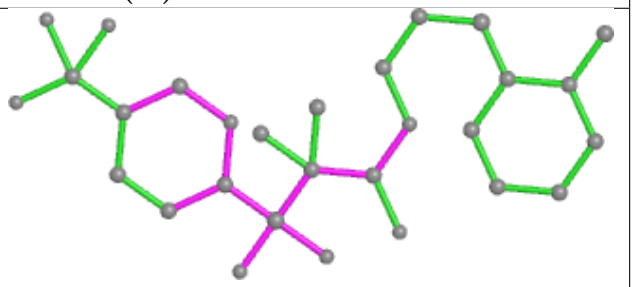


Rings

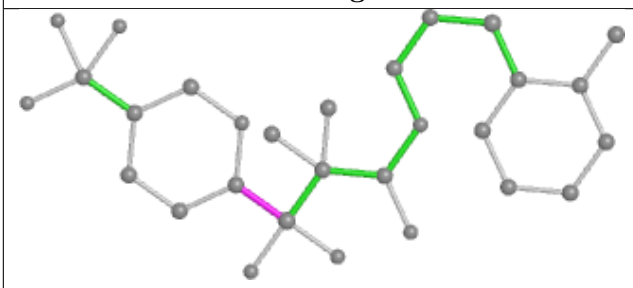
Ligand KHS N 301 (A)



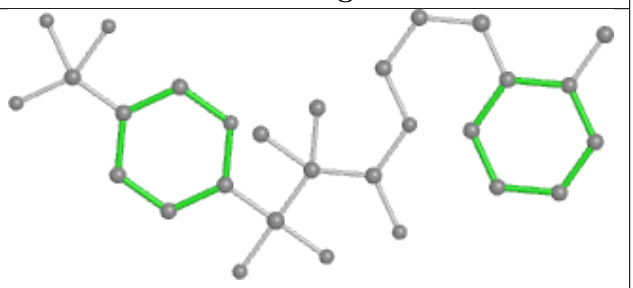
Bond lengths



Bond angles

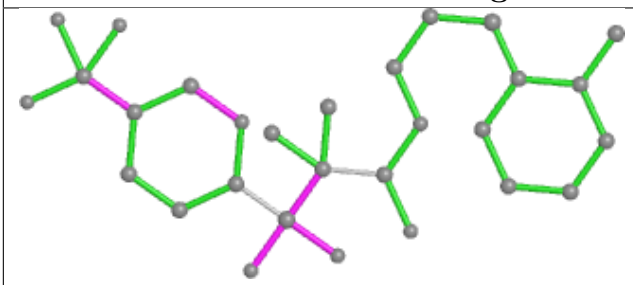


Torsions

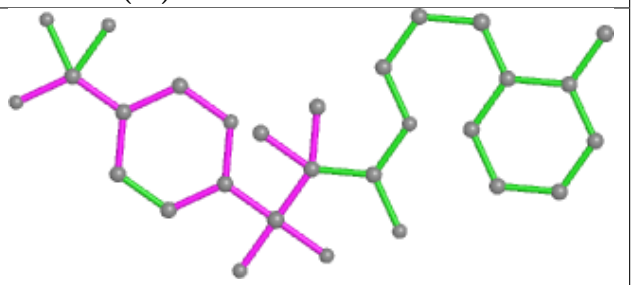


Rings

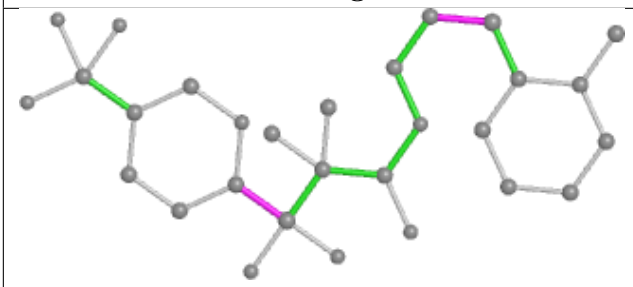
Ligand KHS B 301 (A)



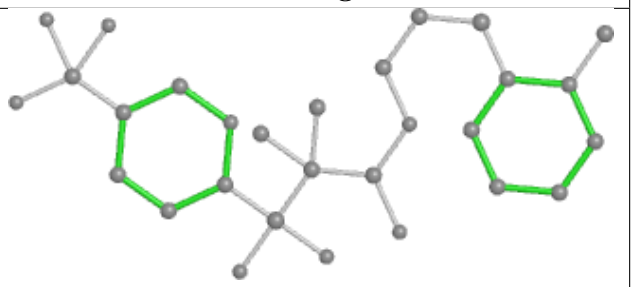
Bond lengths



Bond angles

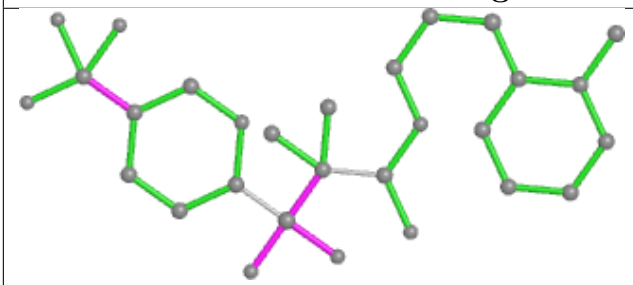


Torsions

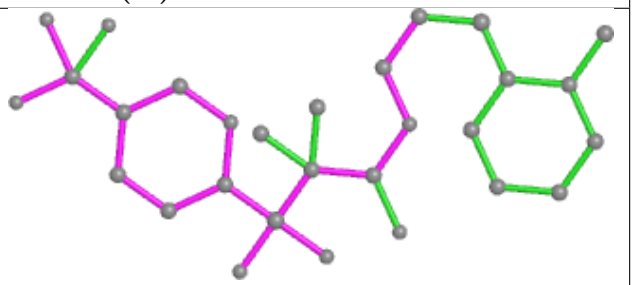


Rings

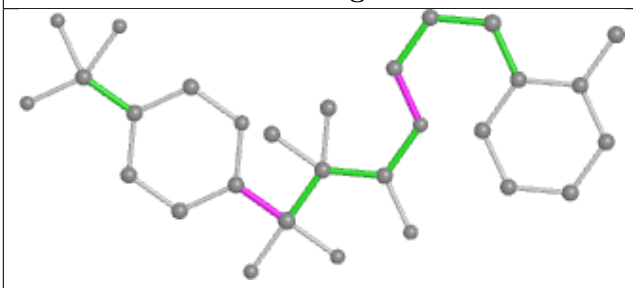
Ligand KHS F 301 (A)



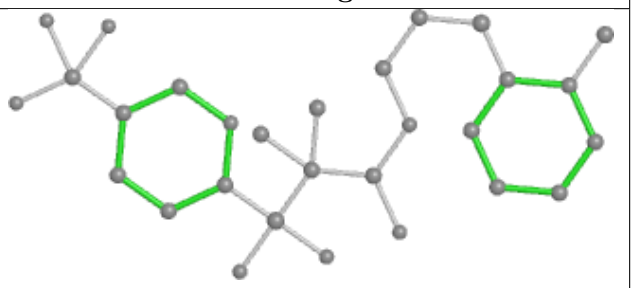
Bond lengths



Bond angles

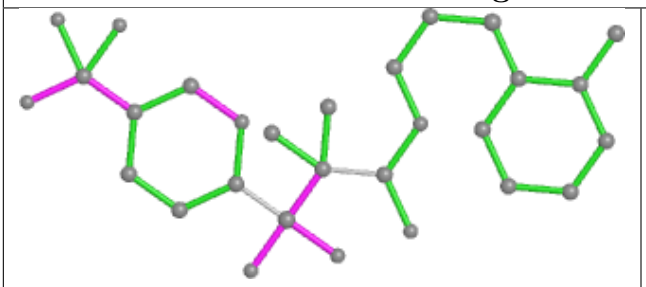


Torsions

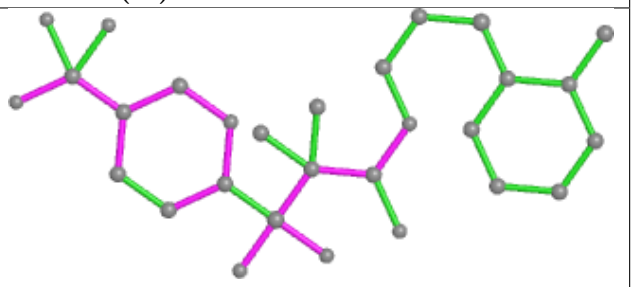


Rings

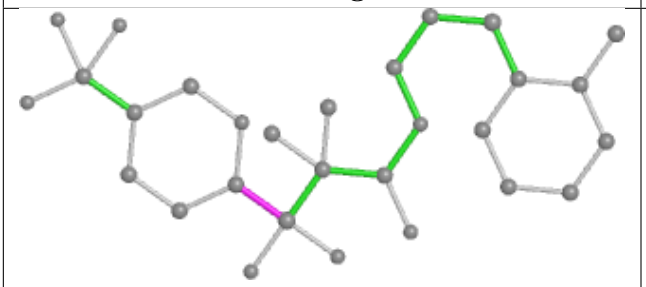
Ligand KHS L 301 (A)



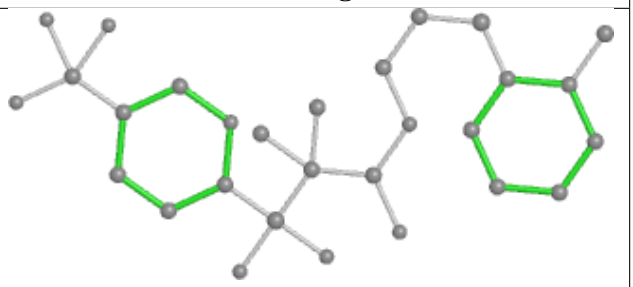
Bond lengths



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.