wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 07:18 AM EDT

PDB ID	:	6MJP
Title	:	LptB(E163Q)FGC from Vibrio cholerae
Authors	:	Owens, T.W.; Kahne, D.; Kruse, A.C.
Deposited on	:	2018-09-21
Resolution	:	2.85 Å(reported)

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

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

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

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

MolProbity	:	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 2.85 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 14 unique types of molecules in this entry. The entry contains 10498 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 ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1873	1174	337	356	6			
1	B	240	Total	C	N	O	S	0	0	0
			1863	1170	334	353	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	GLN	GLU	engineered mutation	UNP O30650
B	163	GLN	GLU	engineered mutation	UNP O30650

- Molecule 2 is a protein called Lipopolysaccharide export system protein LptC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1299	834	210	253	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	188	LEU	-	expression tag	UNP A0A085S5D1
C	189	VAL	-	expression tag	UNP A0A085S5D1
C	190	PRO	-	expression tag	UNP A0A085S5D1
C	191	ARG	-	expression tag	UNP A0A085S5D1

- Molecule 3 is a protein called FIG000988: Predicted permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	341	Total	C	N	O	S	0	0	0
			2504	1640	402	452	10			

- Molecule 4 is a protein called LPS export ABC transporter permease LptG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	354	Total	C	N	O	S	0	0	0
			2673	1759	427	476	11			

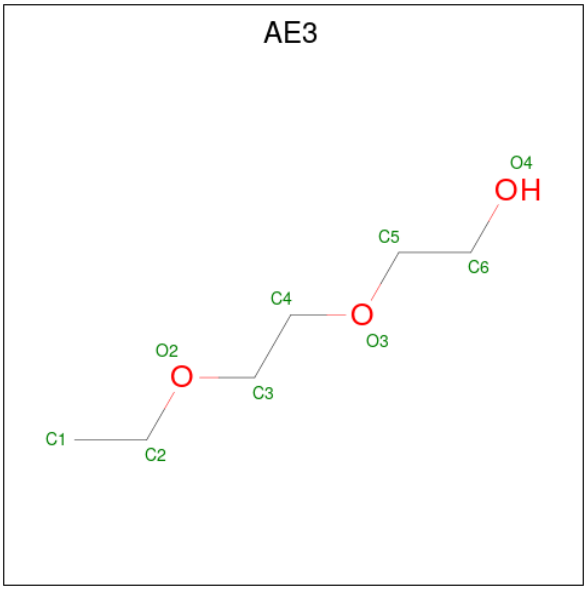
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

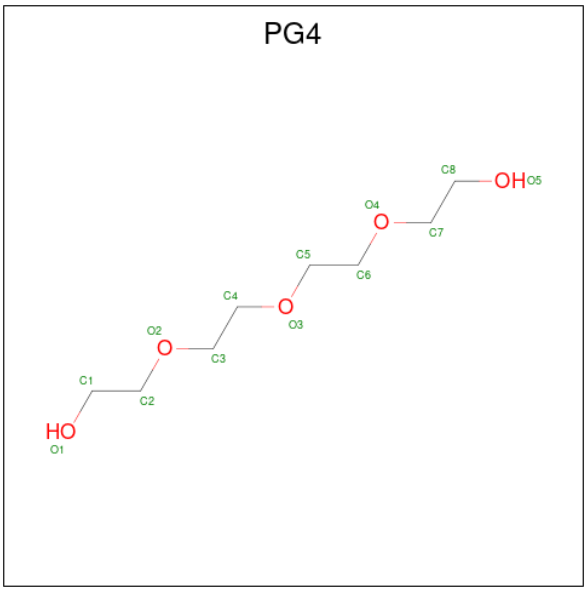
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ca	0	0
			2	2		

- Molecule 7 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: $C_6H_{14}O_3$).



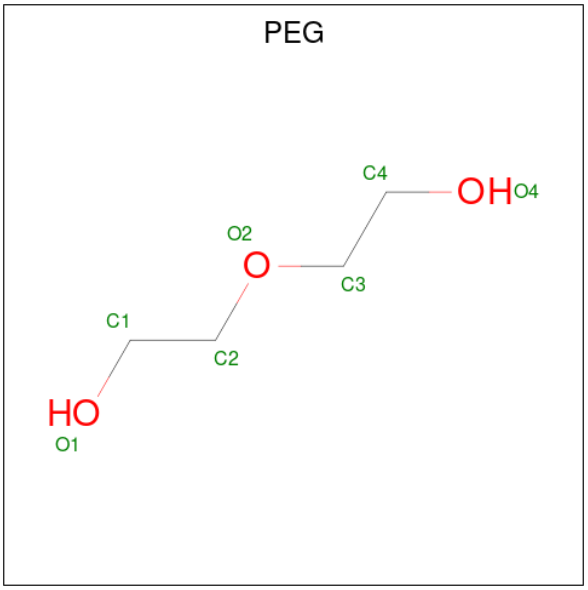
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	6	3		
7	A	1	Total	C	O	0	0
			9	6	3		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



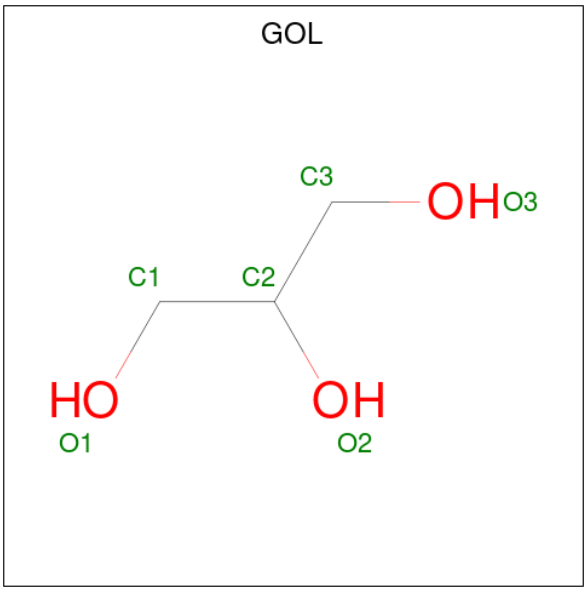
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 13 8 5	0	0
8	B	1	Total C O 13 8 5	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



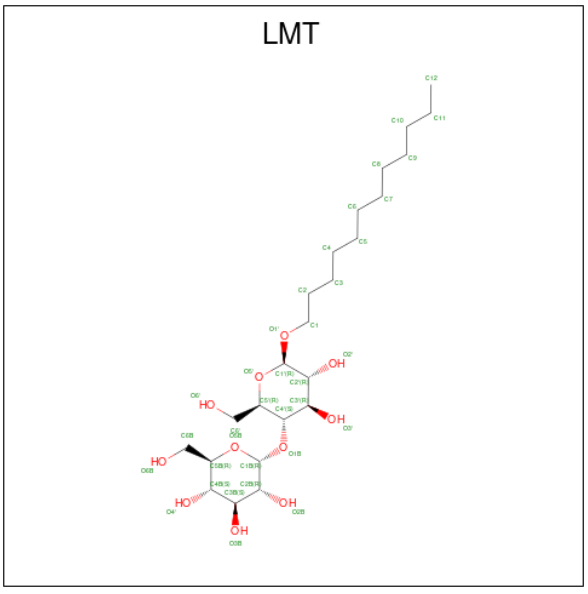
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 7 4 3	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



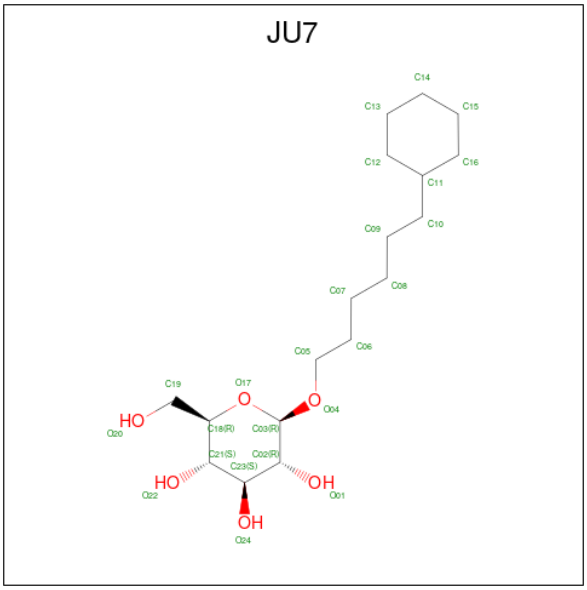
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 6 3 3	0	0
10	B	1	Total C O 6 3 3	0	0
10	G	1	Total C O 6 3 3	0	0

- Molecule 11 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



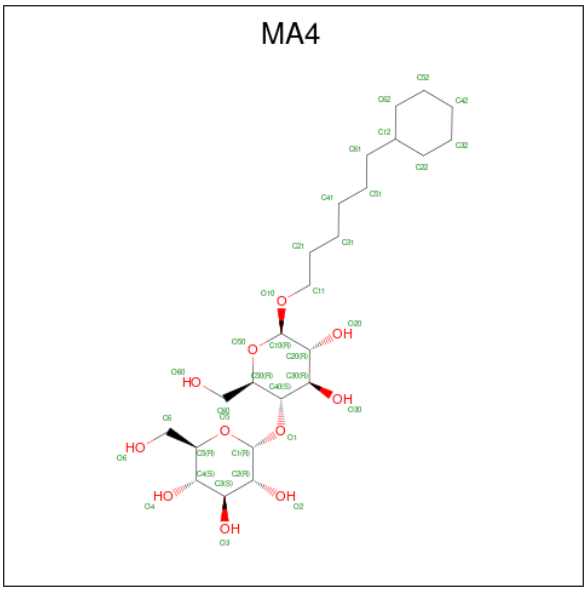
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	1	Total C O 35 24 11	0	0
11	F	1	Total C O 29 18 11	0	0
11	G	1	Total C O 35 24 11	0	0

- Molecule 12 is 6-cyclohexylhexyl beta-D-glucopyranoside (three-letter code: JU7) (formula: $C_{18}H_{34}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	F	1	Total C O 24 18 6	0	0

- Molecule 13 is CYCLOHEXYL-HEXYL-BETA-D-MALTOSIDE (three-letter code: MA4) (formula: $C_{24}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	G	1	Total C O 35 24 11	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	27	Total O 27 27	0	0
14	B	18	Total O 18 18	0	0
14	C	2	Total O 2 2	0	0
14	F	1	Total O 1 1	0	0
14	G	5	Total O 5 5	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	167.35Å 80.73Å 202.99Å 90.00° 112.18° 90.00°	Depositor
Resolution (Å)	49.27 – 2.85	Depositor
% Data completeness (in resolution range)	99.5 (49.27-2.85)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.242 , 0.292	Depositor
Wilson B-factor (Å^2)	82.8	Xtriage
Anisotropy	0.406	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Total number of atoms	10498	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
13	MA4	G	401	-	37,37,37	1.08	1 (2%)	50,50,50	1.40	7 (14%)
11	LMT	G	402	-	36,36,36	1.14	4 (11%)	47,47,47	1.17	3 (6%)
12	JU7	F	402	-	25,25,25	1.00	1 (4%)	32,32,32	1.34	5 (15%)
9	PEG	B	303	-	6,6,6	0.72	0	5,5,5	0.58	0
11	LMT	F	401	-	36,36,36	1.13	4 (11%)	47,47,47	1.01	2 (4%)
10	GOL	B	304	-	5,5,5	1.07	0	5,5,5	0.89	0
7	AE3	A	306	-	8,8,8	0.74	0	7,7,7	0.52	0
11	LMT	F	403	-	30,30,36	1.21	4 (13%)	41,41,47	1.02	2 (4%)
10	GOL	G	403	-	5,5,5	0.92	0	5,5,5	1.04	0
10	GOL	B	305	-	5,5,5	0.90	0	5,5,5	1.01	0
7	AE3	A	307	-	8,8,8	0.56	0	7,7,7	0.74	0
8	PG4	A	308	-	12,12,12	0.56	0	11,11,11	0.45	0
8	PG4	B	302	-	12,12,12	0.52	0	11,11,11	0.50	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
13	MA4	G	401	-	-	6/18/66/66	0/3/3/3
11	LMT	G	402	-	-	13/21/61/61	0/2/2/2
12	JU7	F	402	-	-	5/12/40/40	0/2/2/2
9	PEG	B	303	-	-	1/4/4/4	-
11	LMT	F	401	-	-	5/21/61/61	0/2/2/2
10	GOL	B	304	-	-	1/4/4/4	-
7	AE3	A	306	-	-	2/6/6/6	-
11	LMT	F	403	-	-	1/15/55/61	0/2/2/2
10	GOL	G	403	-	-	0/4/4/4	-
10	GOL	B	305	-	-	0/4/4/4	-
7	AE3	A	307	-	-	2/6/6/6	-
8	PG4	A	308	-	-	7/10/10/10	-
8	PG4	B	302	-	-	6/10/10/10	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	LMT	O3'-C3'	-2.68	1.36	1.43
11	G	402	LMT	O4'-C4B	-2.54	1.37	1.43
11	F	403	LMT	O2'-C2'	-2.52	1.37	1.43
11	F	401	LMT	O2'-C2'	-2.51	1.37	1.43
11	F	401	LMT	O3B-C3B	-2.37	1.37	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	401	MA4	O50-C10-O10	-4.92	98.31	109.97
12	F	402	JU7	C19-C18-C21	-3.60	104.58	113.00
13	G	401	MA4	C1-O5-C5	2.84	119.26	113.69
12	F	402	JU7	O17-C03-C02	-2.77	104.50	110.35
11	G	402	LMT	O5B-C5B-C6B	2.75	113.28	106.44

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

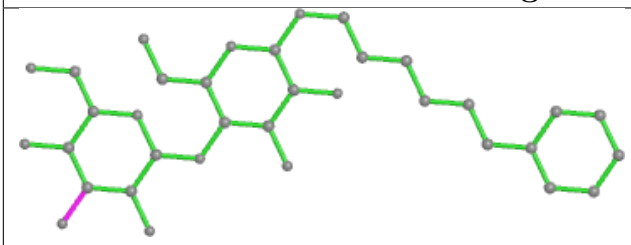
Mol	Chain	Res	Type	Atoms
11	F	401	LMT	C2'-C1'-O1'-C1
11	G	402	LMT	C2'-C1'-O1'-C1
11	G	402	LMT	O5'-C1'-O1'-C1
12	F	402	JU7	O17-C03-O04-C05
13	G	401	MA4	C31-C41-C51-C61

There are no ring outliers.

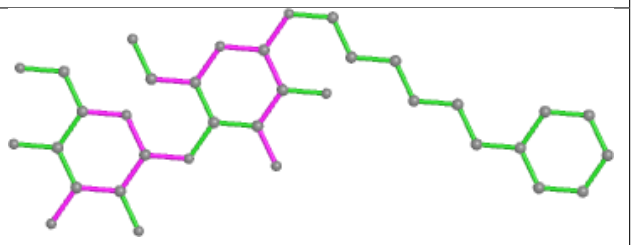
No monomer is involved in short contacts.

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.

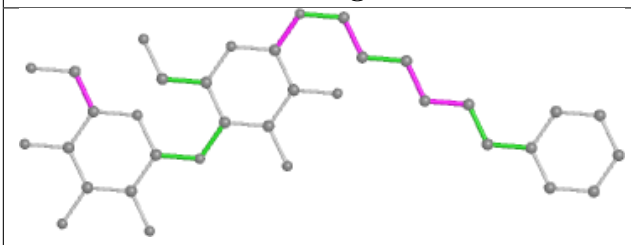
Ligand MA4 G 401



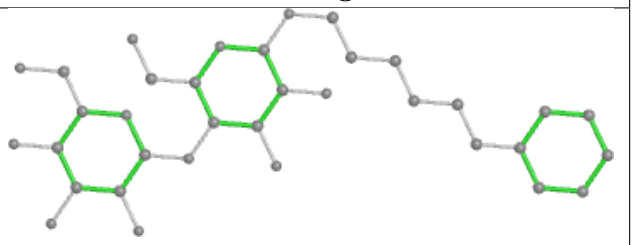
Bond lengths



Bond angles

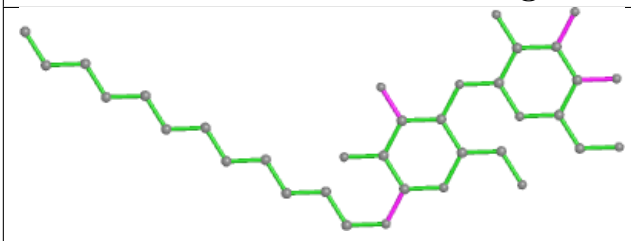


Torsions

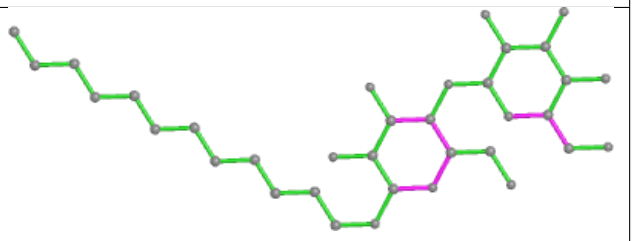


Rings

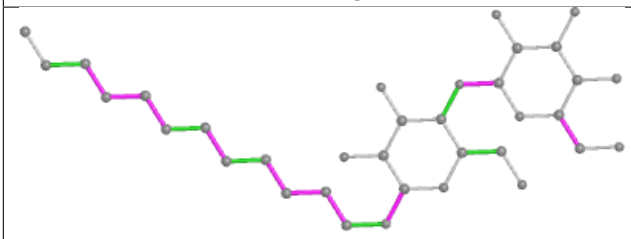
Ligand LMT G 402



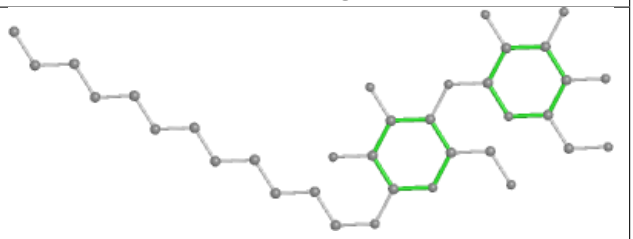
Bond lengths



Bond angles

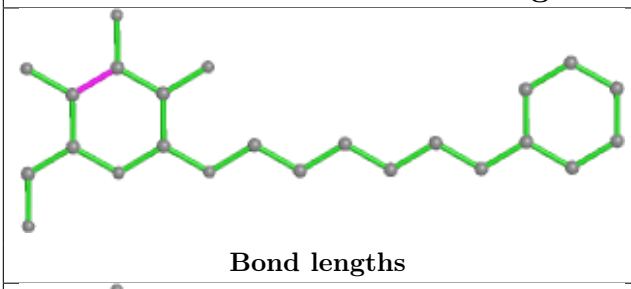


Torsions

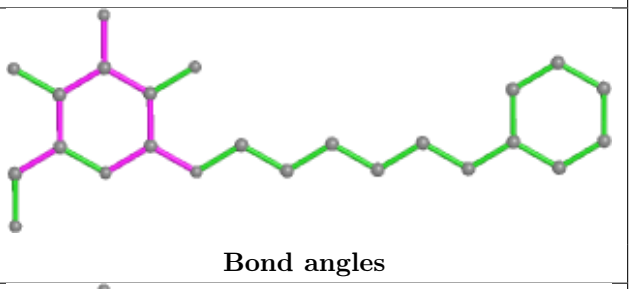


Rings

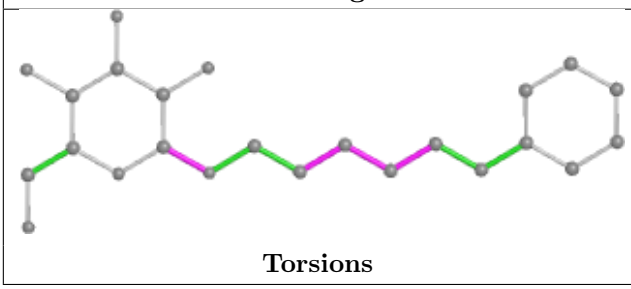
Ligand JU7 F 402



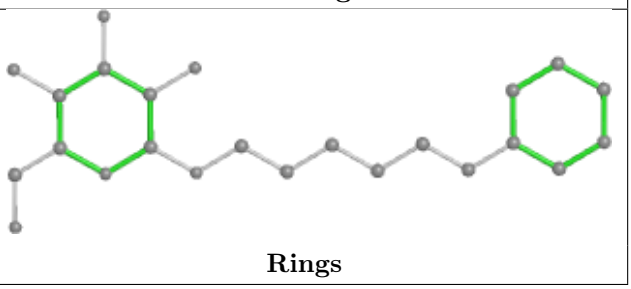
Bond lengths



Bond angles

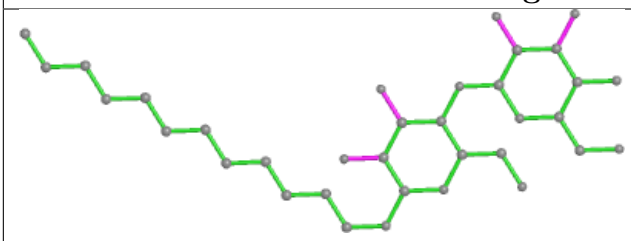


Torsions

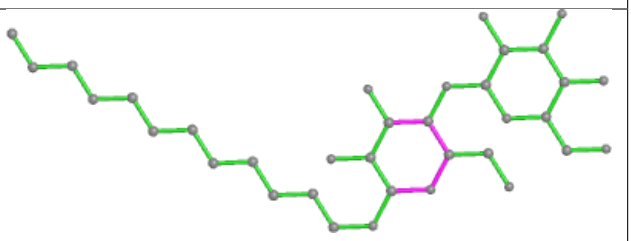


Rings

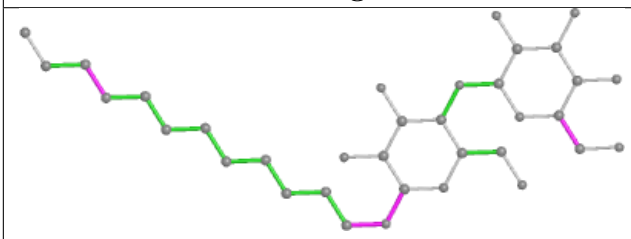
Ligand LMT F 401



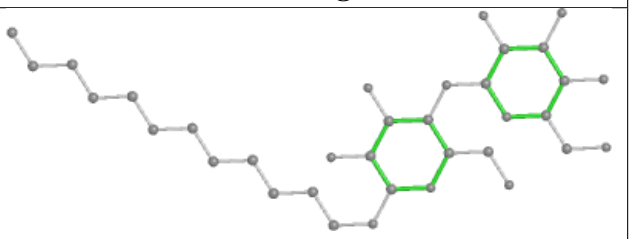
Bond lengths



Bond angles

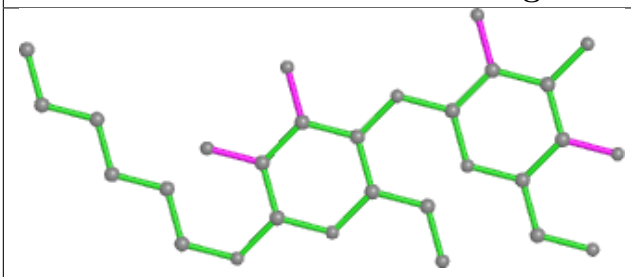


Torsions

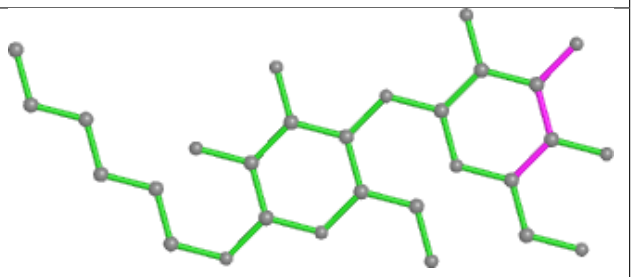


Rings

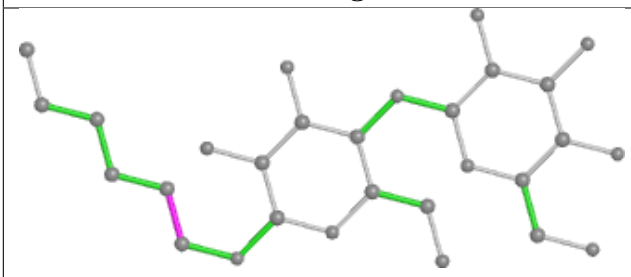
Ligand LMT F 403



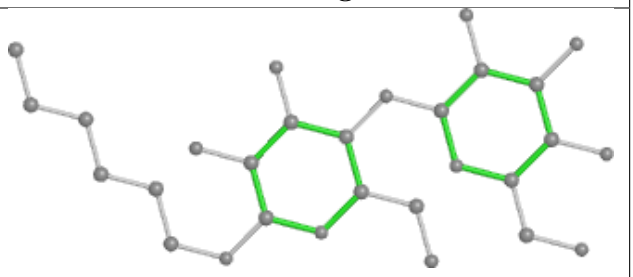
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

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.