



Full wwPDB X-ray Structure Validation Report ⓘ

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 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)
Xtrriage (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 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
			Total	C	N	O	S			
1	A	240	1873	1174	337	356	6	0	0	0
1	B	240	1863	1170	334	353	6	0	0	0

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
			Total	C	N	O	S			
2	C	174	1299	834	210	253	2	0	0	0

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
			Total	C	N	O	S			
3	F	341	2504	1640	402	452	10	0	0	0

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

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

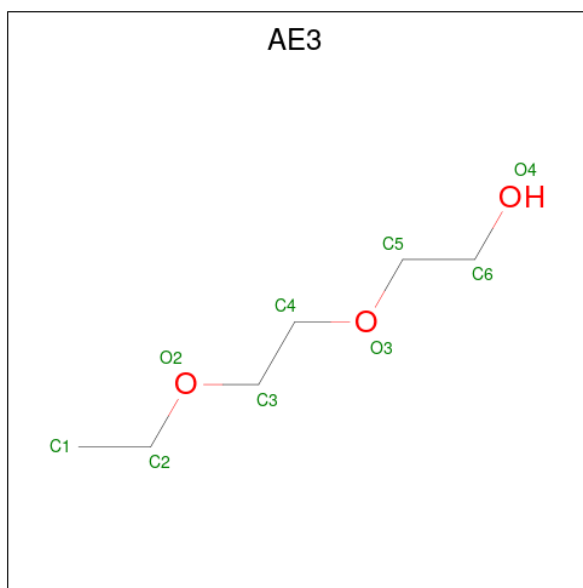
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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).

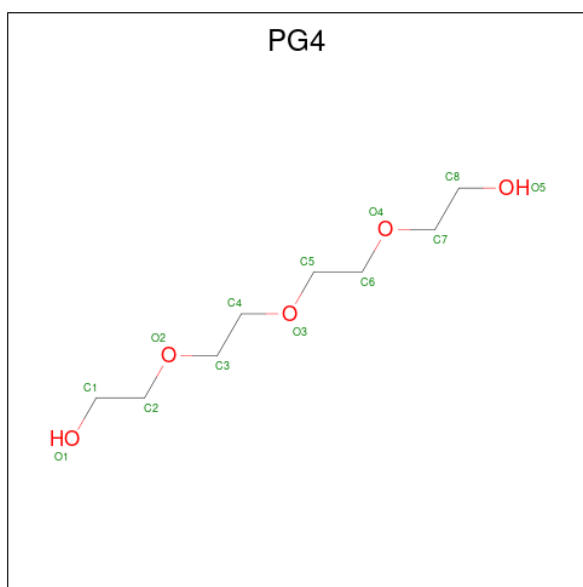
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ca	0	0
			2	2		

- Molecule 7 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: C₆H₁₄O₃).



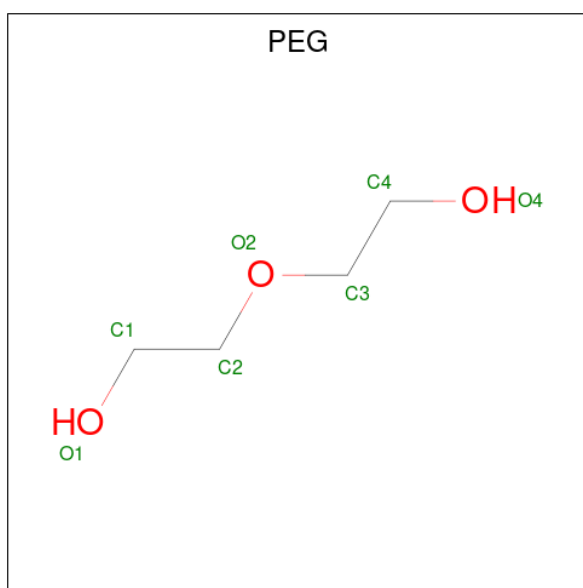
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	6	3		
7	A	1	Total	C	O	0	0
			9	6	3		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

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



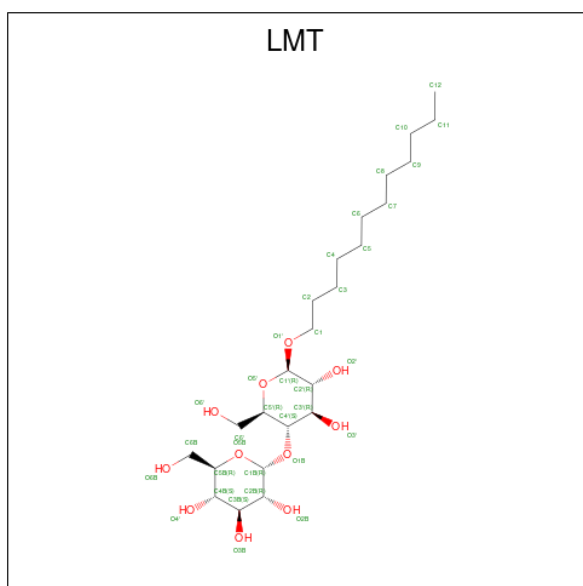
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		

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



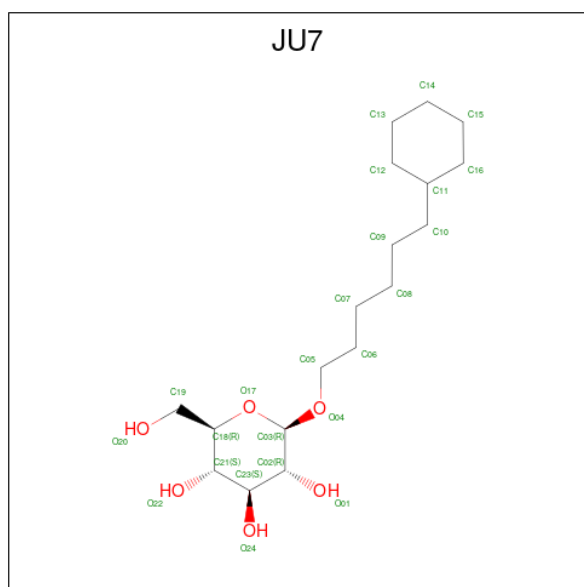
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 6 3 3	0	0
10	B	1	Total C O 6 3 3	0	0
10	G	1	Total C O 6 3 3	0	0

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



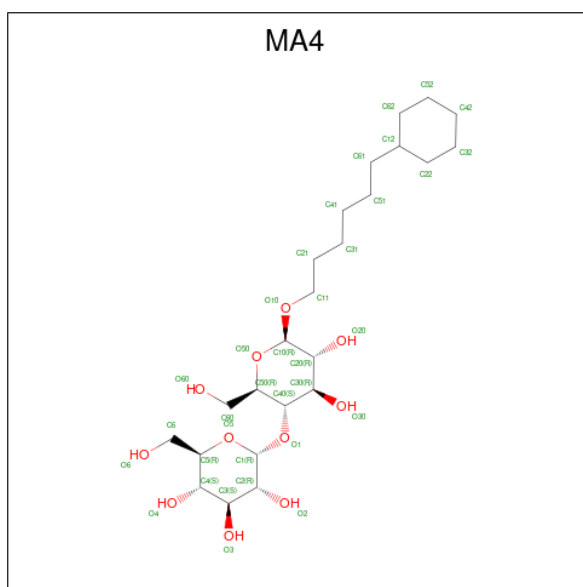
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	F	1	Total	C	O	0	0
			35	24	11		
11	F	1	Total	C	O	0	0
			29	18	11		
11	G	1	Total	C	O	0	0
			35	24	11		

- 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	0	0
			24	18	6		

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



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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	27	Total	O	0	0
			27	27		
14	B	18	Total	O	0	0
			18	18		
14	C	2	Total	O	0	0
			2	2		
14	F	1	Total	O	0	0
			1	1		
14	G	5	Total	O	0	0
			5	5		

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
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.242 , 0.292	Depositor
Wilson B-factor (Å ²)	82.8	Xtrriage
Anisotropy	0.406	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
Total number of atoms	10498	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtrriage'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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

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	-

All (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
13	G	401	MA4	O3-C3	-2.35	1.37	1.43
11	F	403	LMT	O4'-C4B	-2.35	1.37	1.43
11	G	402	LMT	O3'-C3'	-2.26	1.37	1.43
11	G	402	LMT	O1'-C1'	-2.23	1.36	1.40
11	F	403	LMT	O3'-C3'	-2.14	1.37	1.43
11	G	402	LMT	O3B-C3B	-2.12	1.38	1.43
11	F	401	LMT	O2B-C2B	-2.12	1.38	1.43
11	F	403	LMT	O2B-C2B	-2.12	1.38	1.43
12	F	402	JU7	C23-C21	2.09	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
11	F	403	LMT	C3B-C4B-C5B	-2.70	105.42	110.24
11	F	401	LMT	C1'-O5'-C5'	-2.68	108.44	113.69
11	G	402	LMT	C1'-O5'-C5'	-2.63	108.52	113.69
11	F	401	LMT	C3'-C4'-C5'	-2.60	104.97	110.93
11	G	402	LMT	C3'-C4'-C5'	-2.57	105.03	110.93
13	G	401	MA4	O1-C1-C2	2.38	114.27	108.10
13	G	401	MA4	O3-C3-C2	-2.33	104.96	110.35
12	F	402	JU7	O24-C23-C02	-2.32	104.99	110.35
12	F	402	JU7	O04-C03-C02	2.27	111.85	108.30
13	G	401	MA4	O50-C50-C60	-2.21	100.93	106.44
13	G	401	MA4	O30-C30-C20	-2.10	105.48	110.35
13	G	401	MA4	O50-C10-C20	-2.10	105.90	110.35
12	F	402	JU7	C23-C21-C18	2.07	113.94	110.24
11	F	403	LMT	O3B-C3B-C4B	2.07	115.13	110.35

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	401	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
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
8	A	308	PG4	O2-C3-C4-O3
11	G	402	LMT	O5B-C5B-C6B-O6B
13	G	401	MA4	C4-C5-C6-O6
11	F	401	LMT	O5B-C5B-C6B-O6B
13	G	401	MA4	O5-C5-C6-O6
7	A	306	AE3	O3-C5-C6-O4
8	A	308	PG4	O1-C1-C2-O2
8	B	302	PG4	O1-C1-C2-O2
11	G	402	LMT	O1'-C1-C2-C3
12	F	402	JU7	C02-C03-O04-C05
11	G	402	LMT	C6-C7-C8-C9
11	G	402	LMT	C7-C8-C9-C10
11	F	401	LMT	C2-C1-O1'-C1'
12	F	402	JU7	C05-C06-C07-C08
11	G	402	LMT	C2-C3-C4-C5
8	B	302	PG4	C1-C2-O2-C3
8	A	308	PG4	O3-C5-C6-O4
8	B	302	PG4	C8-C7-O4-C6
11	G	402	LMT	C4B-C5B-C6B-O6B
13	G	401	MA4	C20-C10-O10-C11
12	F	402	JU7	C06-C07-C08-C09
7	A	307	AE3	C1-C2-O2-C3
7	A	307	AE3	O2-C3-C4-O3
11	F	401	LMT	C4B-C5B-C6B-O6B
13	G	401	MA4	C21-C31-C41-C51
8	A	308	PG4	C5-C6-O4-C7
7	A	306	AE3	C3-C4-O3-C5
11	G	402	LMT	C4-C5-C6-C7
8	B	302	PG4	C6-C5-O3-C4
11	F	403	LMT	O1'-C1-C2-C3
11	F	401	LMT	C11-C10-C9-C8
11	G	402	LMT	C2B-C1B-O1B-C4'
8	A	308	PG4	C4-C3-O2-C2
11	G	402	LMT	C1-C2-C3-C4
9	B	303	PEG	C1-C2-O2-C3
8	B	302	PG4	O2-C3-C4-O3
8	A	308	PG4	C3-C4-O3-C5
13	G	401	MA4	O10-C11-C21-C31

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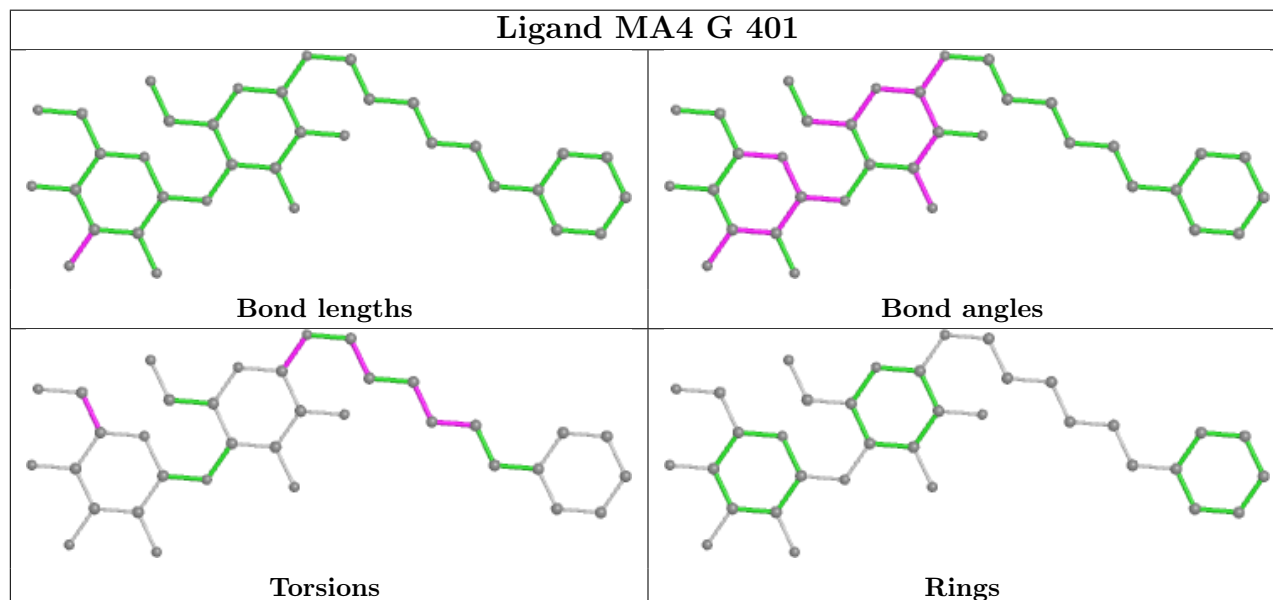
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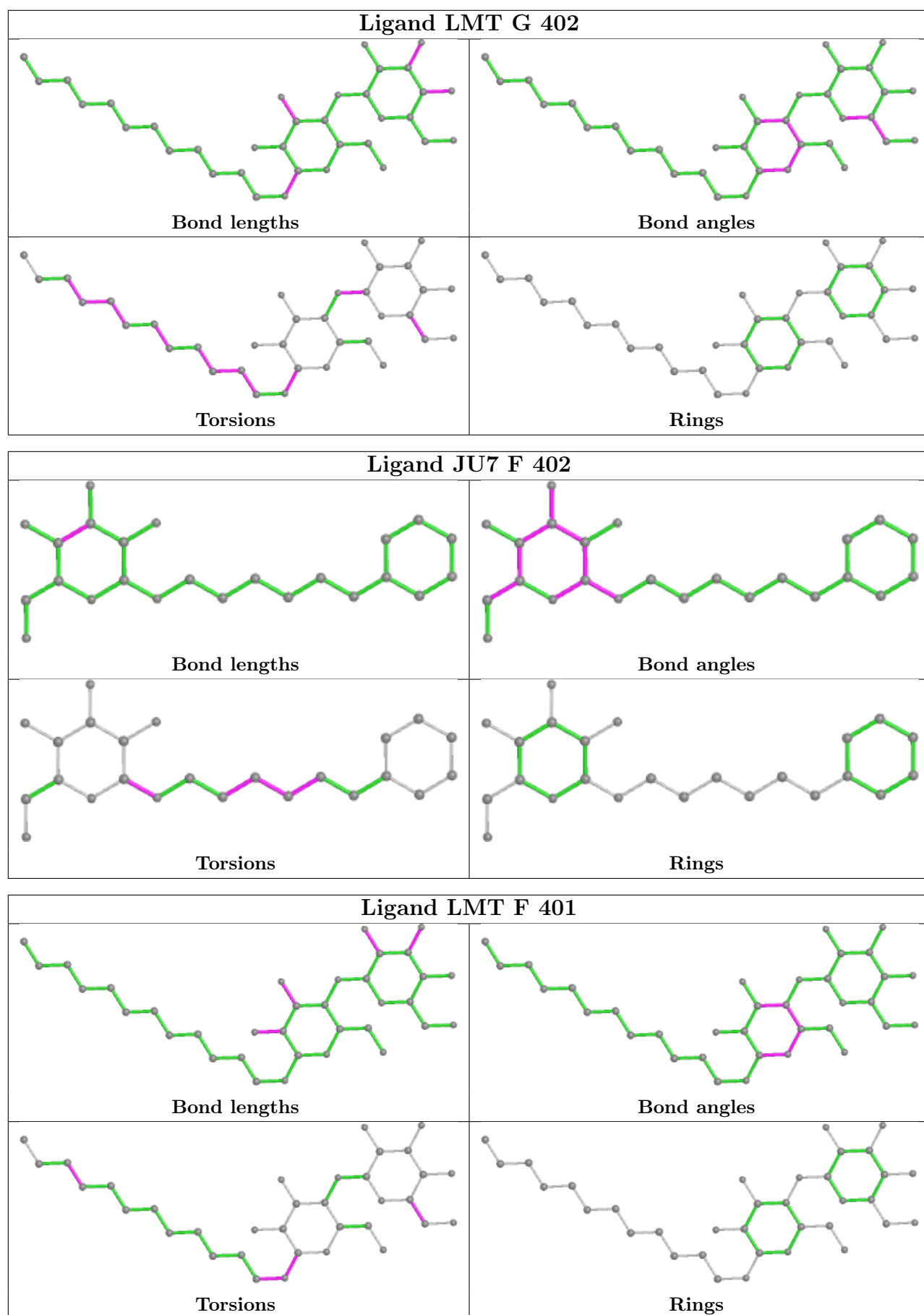
Mol	Chain	Res	Type	Atoms
11	G	402	LMT	C11-C10-C9-C8
11	G	402	LMT	O5B-C1B-O1B-C4'
8	B	302	PG4	O3-C5-C6-O4
10	B	304	GOL	O1-C1-C2-C3
8	A	308	PG4	C6-C5-O3-C4
12	F	402	JU7	C07-C08-C09-C10

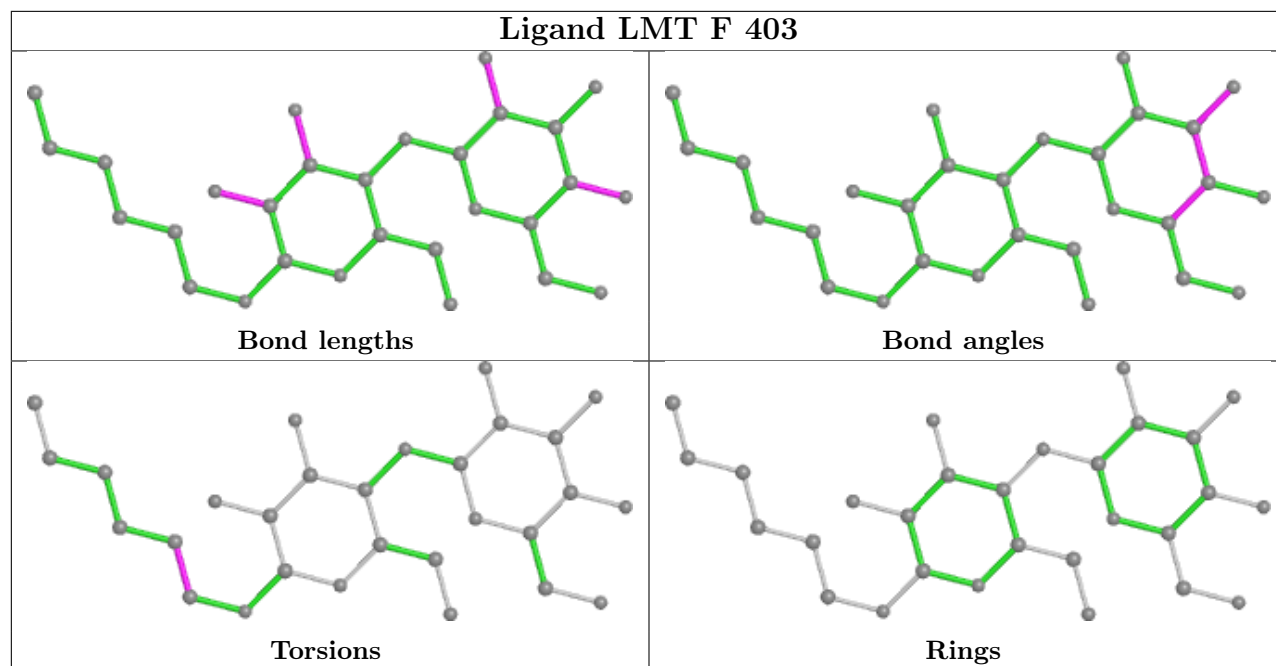
There are no ring outliers.

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 than 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.







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.