



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 17, 2019 – 01:48 PM EDT

PDB ID : 6S8H
EMDB ID: : EMD-10122
Title : Cryo-EM structure of LptB2FG in complex with LPS
Authors : Tang, X.D.; Chang, S.H.; Luo, Q.H.; Zhang, Z.Y.; Qiao, W.; Xu, C.H.; Zhang, C.B.; Niu, Y.; Yang, W.X.; Wang, T.; Zhang, Z.B.; Zhu, X.F.; Dong, C.J.; Zhang, X.; Dong, H.H.
Deposited on : 2019-07-10
Resolution : 3.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

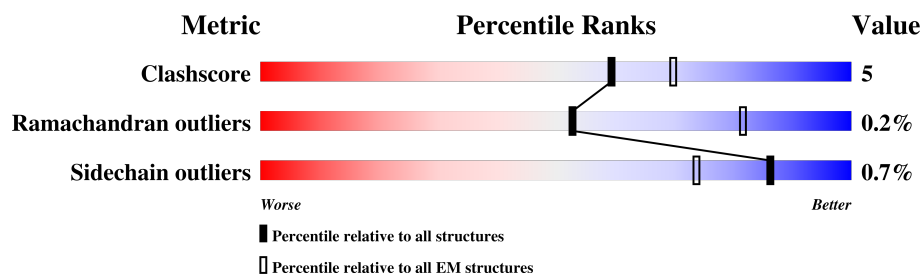
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	241	79% 20% .
1	B	241	85% 14% .
2	F	366	55% 10% 35%
3	G	360	63% 5% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7818 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Lipopolysaccharide ABC transporter, ATP-binding protein LptB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1868	1168	342	353	5		
1	B	238	Total	C	N	O	S	0	0
			1857	1162	338	352	5		

- Molecule 2 is a protein called Lipopolysaccharide export system permease protein LptF.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	239	Total	C	N	O	S	0	0
			1864	1233	303	313	15		

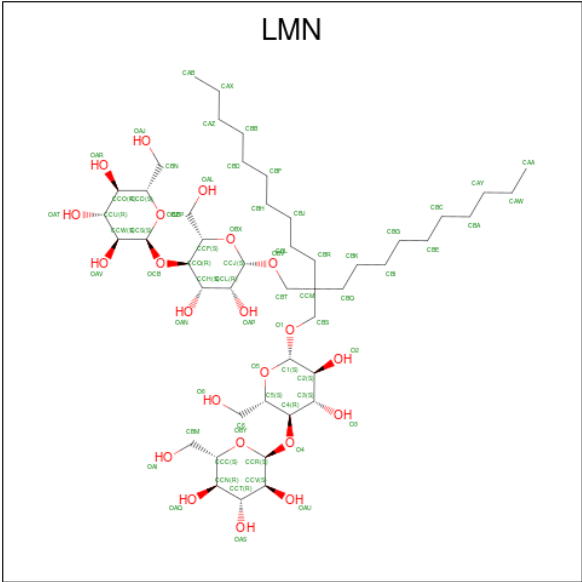
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	274	VAL	PHE	conflict	UNP P0AFA1

- Molecule 3 is a protein called Inner membrane protein yjgQ.

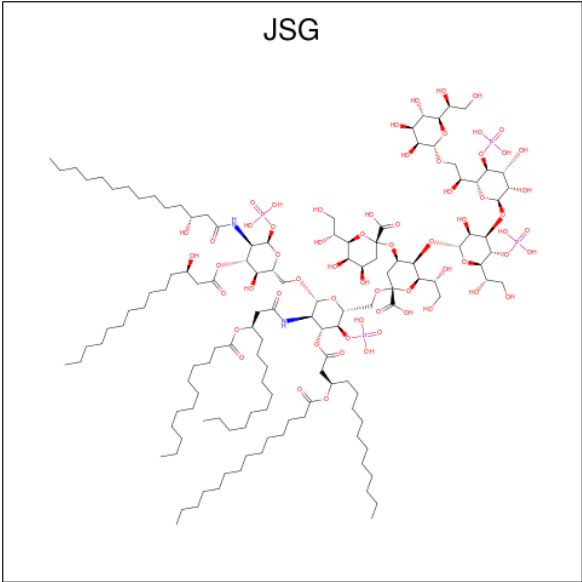
Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	243	Total	C	N	O	S	0	0
			1876	1247	300	311	18		

- Molecule 4 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: C₄₇H₈₈O₂₂) (labeled as "Ligand of Interest" by author).



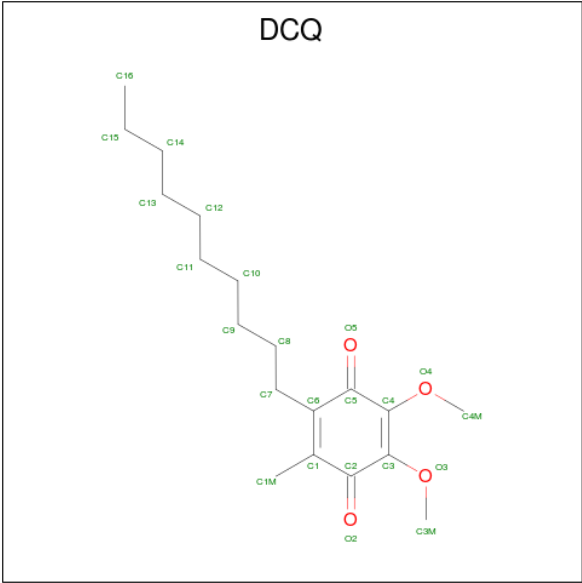
Mol	Chain	Residues	Atoms			AltConf
4	F	1	Total	C	O	0
			34	29	5	
4	G	1	Total	C	O	0
			35	29	6	

- Molecule 5 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-[(2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-5-[(2 {S},3 {S},4 {R},5 {R},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-4-[(2 {R},3 {S},4 {R},5 {S},6 {R})-6-[(1 {S})-2-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-1-oxidanyl-ethyl]-3,4-bis(oxidanyl)-5-phosphonooxy-oxan-2-yl]oxy-3-oxidanyl-5-phosphonooxy-oxan-2-yl]oxy-2-carboxy-2-[[[(2 {R},3 {S},4 {R},5 {R},6 {R})-5-[[[(3 {R})-3-dodecanoyloxytetradecanoyl]amino]-6-[[[(2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[[[(3 {R})-3-oxidanyltetradecanoyl]amino]-4-[[[(3 {R})-3-oxidanyltetradecanoyl]oxy-6-phosphonooxy-oxan-2-yl]methoxy]-3-phosphonooxy-4-[[[(3 {R})-3-tetradecanoyloxytetradecanoyl]oxy-oxan-2-yl]methoxy]oxan-4-yl]oxy-4,5-bis(oxidanyl)oxane-2-carboxylic acid (three-letter code: JSG) (formula: C₁₃₁H₂₄₀N₂O₆₃P₄) (labeled as "Ligand of Interest" by author).



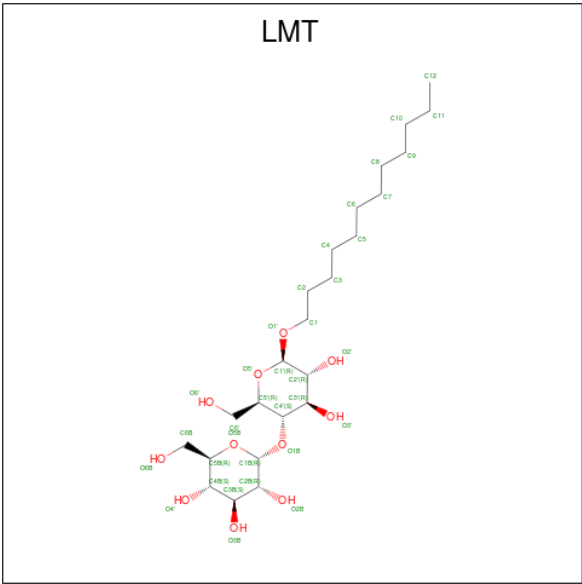
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	F	1	200	131	2	63	4	0

- Molecule 6 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: DCQ) (formula: C₁₉H₃₀O₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	F	1	23	19	4	0
6	G	1	23	19	4	0

- Molecule 7 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by author).

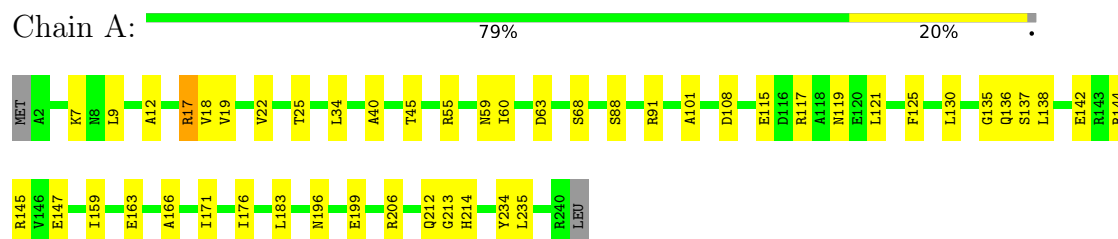


Mol	Chain	Residues	Atoms			AltConf
7	F	1	Total	C	O	0
			24	18	6	
7	G	1	Total	C	O	0
			14	13	1	

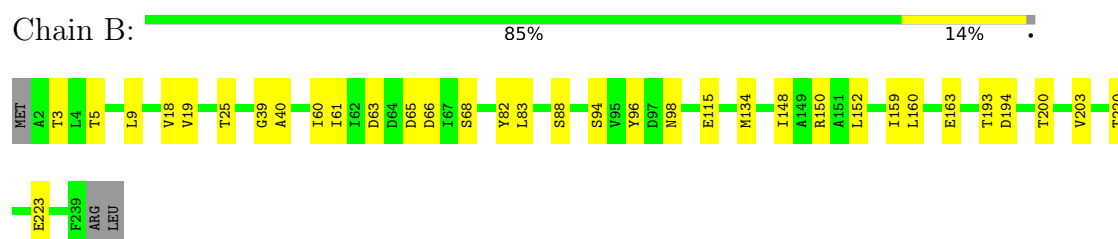
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

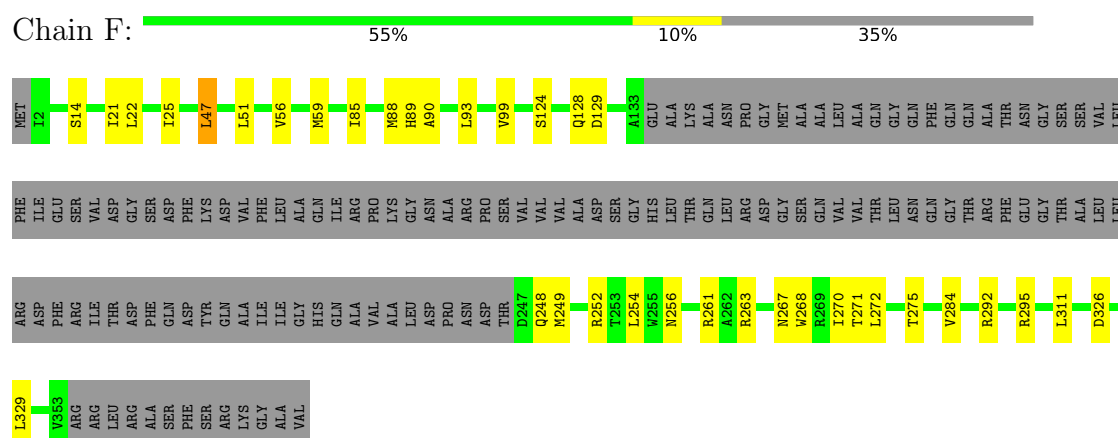
- Molecule 1: Lipopolysaccharide ABC transporter, ATP-binding protein LptB



- Molecule 1: Lipopolysaccharide ABC transporter, ATP-binding protein LptB



- Molecule 2: Lipopolysaccharide export system permease protein LptF



- Molecule 3: Inner membrane protein yjgQ



MET	ALA	LEU
GLN	PHE	GLY
P3	ASN	VAL
L7	GLU	VAL
	ALA	ALA
T22	ASN	LEU
	ARG	ASP
I33	ARG	PRO
	LEU	ASP
D48	GLN	ALA
	SER	LEU
A52	VAL	S250
	ARG	I251
N70	TYR	
	ALA	R262
L74	ALA	SER
	THR	SER
T98	LYS	GLY
R99	PHE	GLN
	ASP	ASP
M140	PRO	ALA
	GLU	G269
TYR	HIS	
GLY	LYS	S277
GLY	VAL	
SER	TRP	V307
LEU	ARG	
LEU	LEU	V310
SER	SER	
THR	GLN	I313
GLN	VAL	
GLN	ASP	V318
GLY	GLU	
LEU	SER	F348
TRP	ASP	
ALA	LEU	S360
LYS	THR	
ASP	ASN	
GLY	PRO	
ASN	LYS	
ASN	GLN	
PHE	ILE	
VAL	THR	
TYR	GLY	
ILE	SER	
GLU	GLN	
ARG	THR	
VAL	VAL	
LYS	SER	
GLY	GLY	
ASP	THR	
GLU	TRP	
VAL	LYS	
LEU	THR	
GLY	ASP	
GLY	LEU	
ILE	THR	
SER	PRO	
ILE	ASP	
TYR	LYS	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	95887	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40, 40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JSG, LMT, LMN, DCQ

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.30	0/1895	0.59	2/2562 (0.1%)
1	B	0.30	0/1884	0.62	1/2548 (0.0%)
2	F	0.32	0/1899	0.67	1/2588 (0.0%)
3	G	0.32	0/1917	0.58	0/2589
All	All	0.31	0/7595	0.61	4/10287 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	LEU	CA-CB-CG	7.13	131.71	115.30
2	F	329	LEU	CA-CB-CG	6.51	130.27	115.30
1	A	130	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	235	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	TYR	Peptide
1	B	39	GLY	Peptide
1	B	40	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1868	0	1888	25	0
1	B	1857	0	1875	18	0
2	F	1864	0	2002	20	0
3	G	1876	0	1985	12	0
4	F	34	0	52	4	0
4	G	35	0	53	6	0
5	F	200	0	0	2	0
6	F	23	0	26	2	0
6	G	23	0	28	2	0
7	F	24	0	32	2	0
7	G	14	0	24	0	0
All	All	7818	0	7965	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 82 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:248:GLN:HE21	2:F:263:ARG:HE	1.37	0.71
1:A:101:ALA:HB1	3:G:7:LEU:HG	1.81	0.62
1:A:25:THR:O	1:A:206:ARG:NH1	2.35	0.60
2:F:311:LEU:HD21	3:G:33:ILE:HG22	1.85	0.59
1:B:60:ILE:H	1:B:68:SER:HB2	1.68	0.58

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/241 (98%)	208 (88%)	28 (12%)	1 (0%)	36	75
1	B	236/241 (98%)	212 (90%)	24 (10%)	0	100	100
2	F	235/366 (64%)	212 (90%)	22 (9%)	1 (0%)	36	75
3	G	237/360 (66%)	217 (92%)	20 (8%)	0	100	100
All	All	945/1208 (78%)	849 (90%)	94 (10%)	2 (0%)	53	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	47	LEU
1	A	213	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/202 (99%)	199 (100%)	1 (0%)	90	96
1	B	199/202 (98%)	198 (100%)	1 (0%)	90	96
2	F	206/307 (67%)	203 (98%)	3 (2%)	67	86
3	G	202/300 (67%)	201 (100%)	1 (0%)	90	96
All	All	807/1011 (80%)	801 (99%)	6 (1%)	86	93

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	261	ARG
3	G	70	MET
2	F	292	ARG
1	B	193	THR
2	F	295	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	196	ASN
1	B	8	ASN
2	F	248	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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
4	LMN	F	401	-	34,34,72	1.00	3 (8%)	38,41,98	2.46	11 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	JSG	F	402	-	197,206,206	1.10	17 (8%)	251,278,278	2.08	55 (21%)
6	DCQ	F	403	-	23,23,23	1.75	5 (21%)	24,29,29	2.53	6 (25%)
7	LMT	F	404	-	24,24,36	1.07	2 (8%)	29,29,47	1.03	1 (3%)
4	LMN	G	401	-	35,35,72	0.97	2 (5%)	40,43,98	2.30	10 (25%)
7	LMT	G	402	-	13,13,36	0.40	0	12,12,47	0.86	0
6	DCQ	G	403	-	23,23,23	1.53	5 (21%)	24,29,29	2.42	7 (29%)

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	LMN	F	401	-	-	3/30/46/130	0/1/1/4
5	JSG	F	402	-	-	34/182/333/333	0/7/7/7
6	DCQ	F	403	-	-	4/14/38/38	0/1/1/1
7	LMT	F	404	-	-	6/15/35/61	0/1/1/2
4	LMN	G	401	-	-	3/30/50/130	0/1/1/4
7	LMT	G	402	-	-	6/11/11/61	-
6	DCQ	G	403	-	-	3/14/38/38	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	402	JSG	CBQ-CBP	4.27	1.56	1.52
6	F	403	DCQ	C1M-C1	-4.00	1.42	1.50
5	F	402	JSG	OBW-CBP	4.00	1.47	1.42
6	F	403	DCQ	C3-C2	-3.86	1.37	1.48
5	F	402	JSG	OCL-CCB	3.51	1.50	1.41

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	LMN	CBR-CCM-CBQ	8.74	127.43	108.54
4	F	401	LMN	CBL-CBR-CCM	7.92	126.62	116.66
5	F	402	JSG	OFZ-CFM-CFL	7.79	121.96	106.65
5	F	402	JSG	CBI-CBG-CBE	7.70	127.48	114.30
4	F	401	LMN	CBR-CBL-CBJ	7.20	135.01	113.21

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

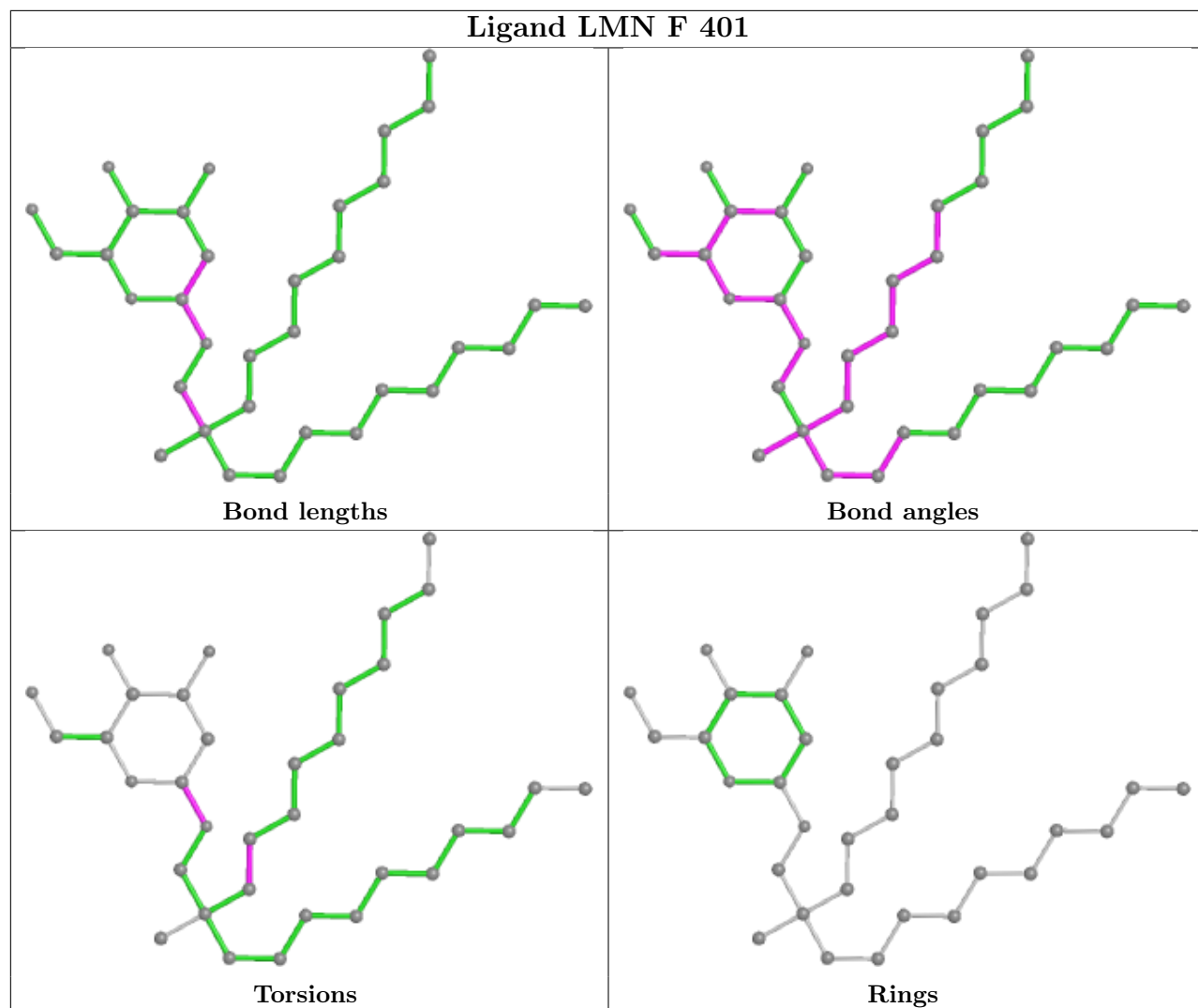
Mol	Chain	Res	Type	Atoms
4	G	401	LMN	OBX-CCJ-OBV-CBT
5	F	402	JSG	C7-C8-CEW-CEX
5	F	402	JSG	OAU-CAL-OAM-PHG
5	F	402	JSG	CBE-CBG-CBI-CBK
5	F	402	JSG	CBE-CBG-CBI-OBJ

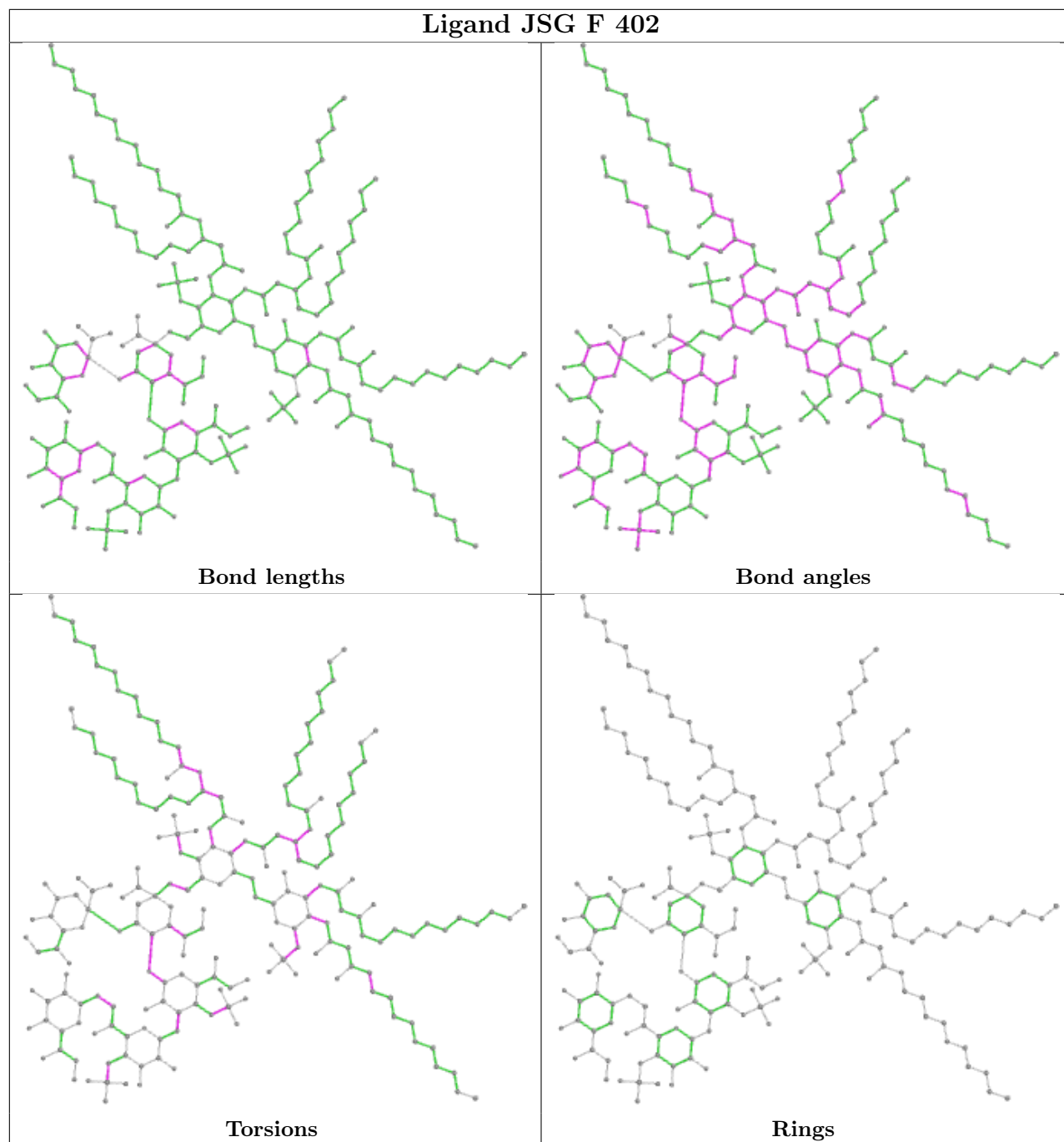
There are no ring outliers.

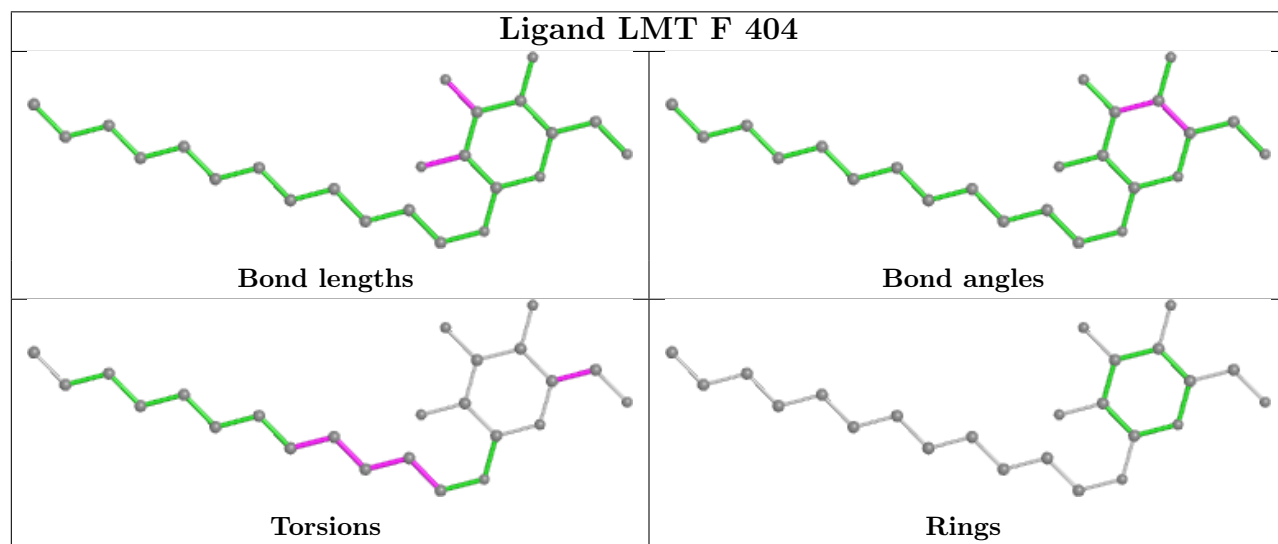
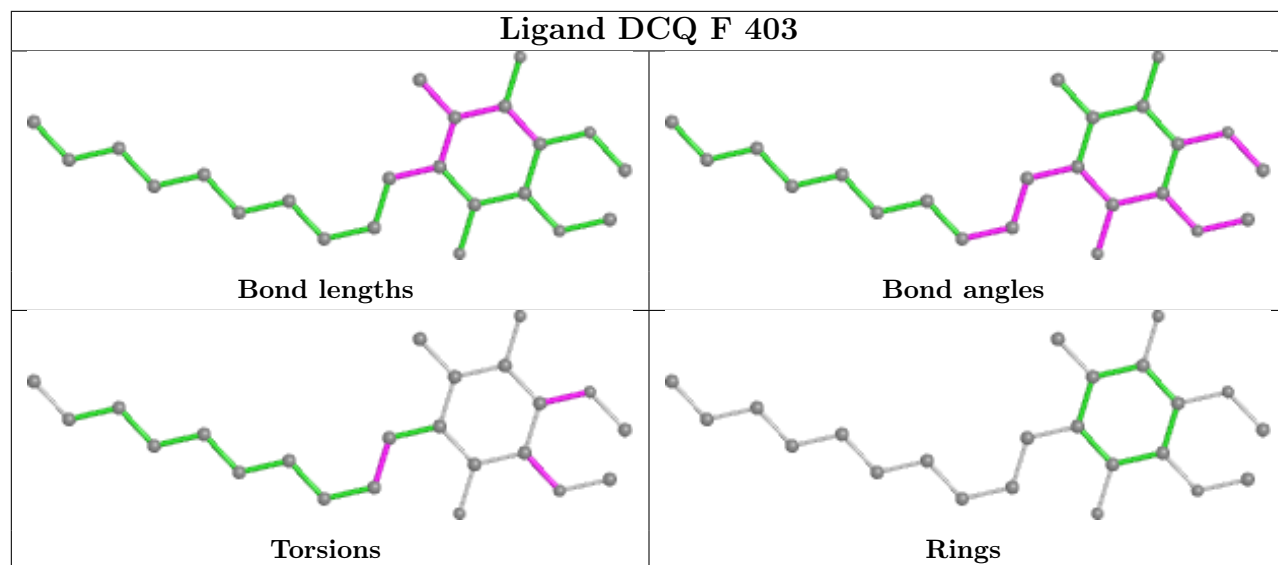
6 monomers are involved in 16 short contacts:

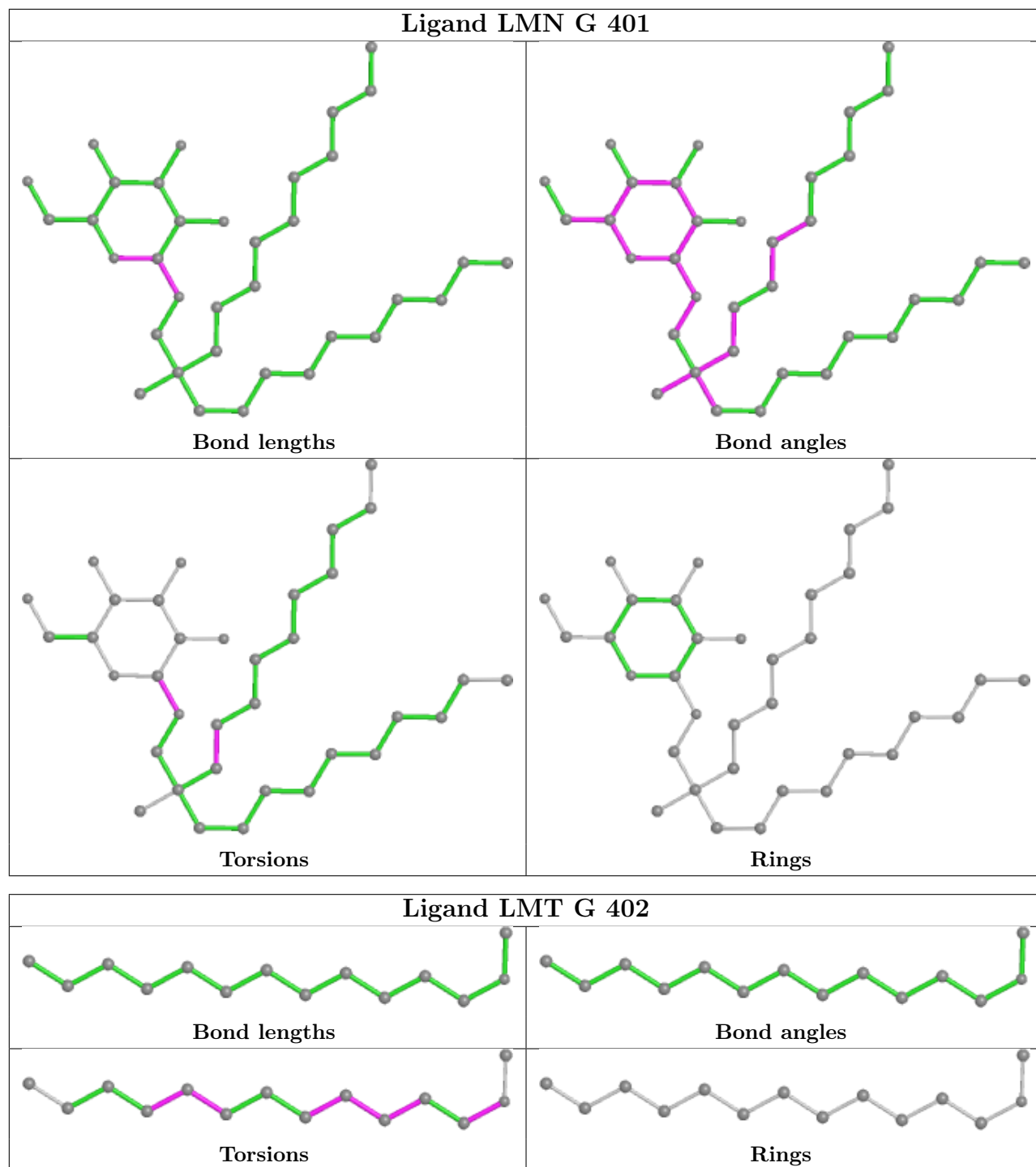
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	401	LMN	4	0
5	F	402	JSG	2	0
6	F	403	DCQ	2	0
7	F	404	LMT	2	0
4	G	401	LMN	6	0
6	G	403	DCQ	2	0

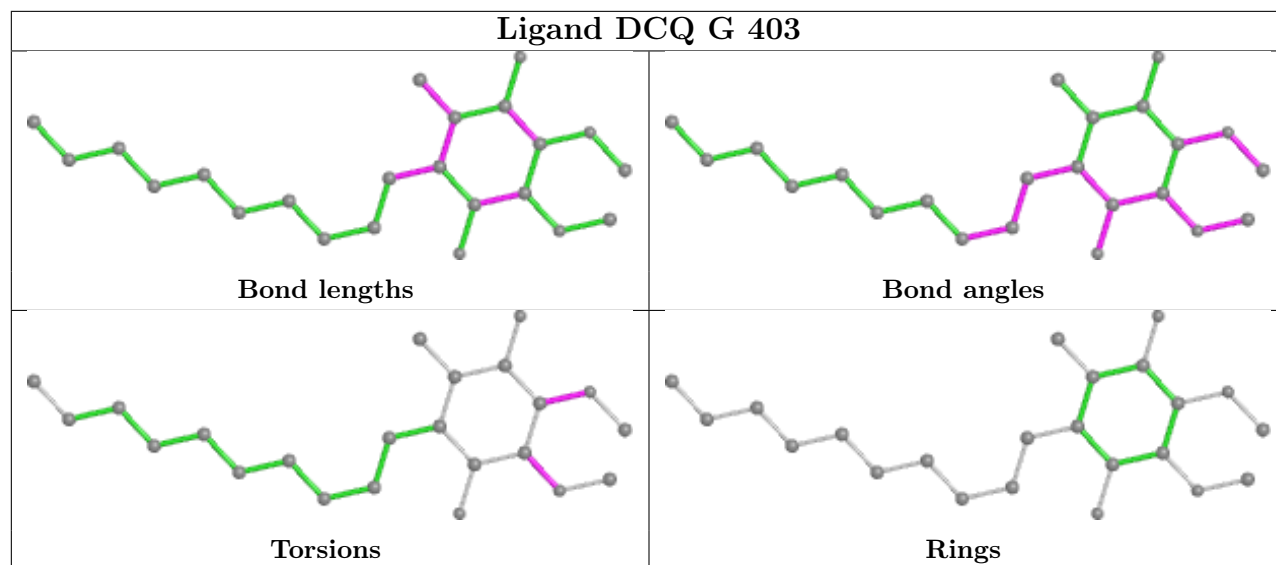
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand JSG F 402







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.