



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 03:08 PM 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

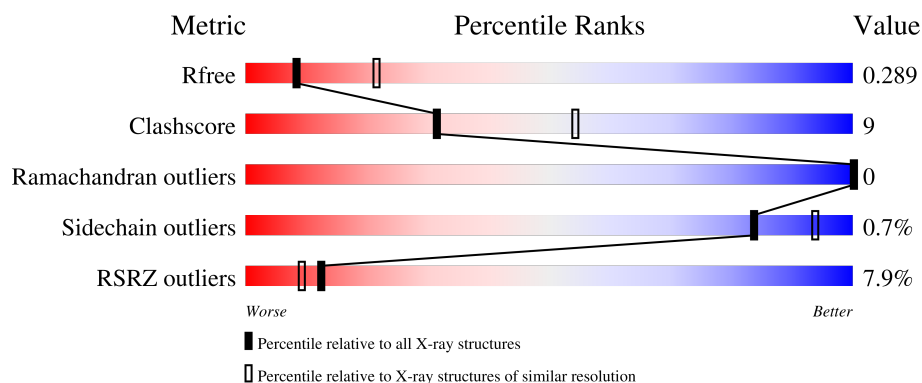
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>23%</div> </div> </div>
1	B	241	<div> <div></div> <div> <div>79%</div> <div>20%</div> </div> </div>
2	C	191	<div> <div>18%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• 9%</div> </div> </div>
3	F	366	<div> <div>11%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>7%</div> </div> </div>
4	G	356	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>22%</div> <div>•</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	PG4	A	308	-	-	-	X
8	PG4	B	302	-	-	-	X
9	PEG	B	303	-	-	-	X

## 2 Entry composition

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			

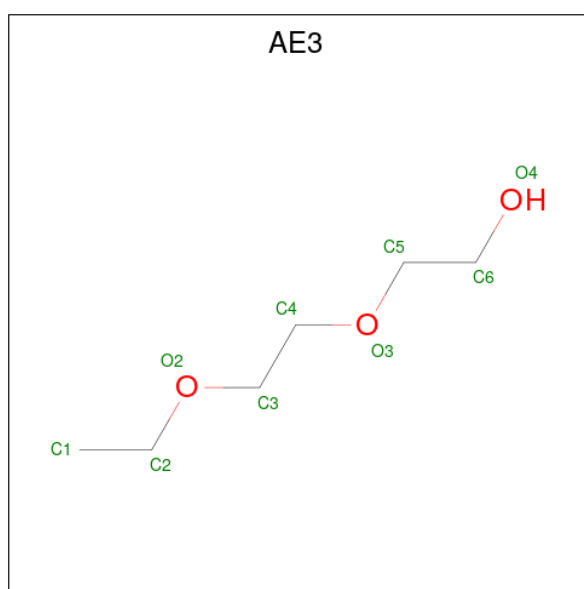
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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<sub>6</sub>H<sub>14</sub>O<sub>3</sub>).



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<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



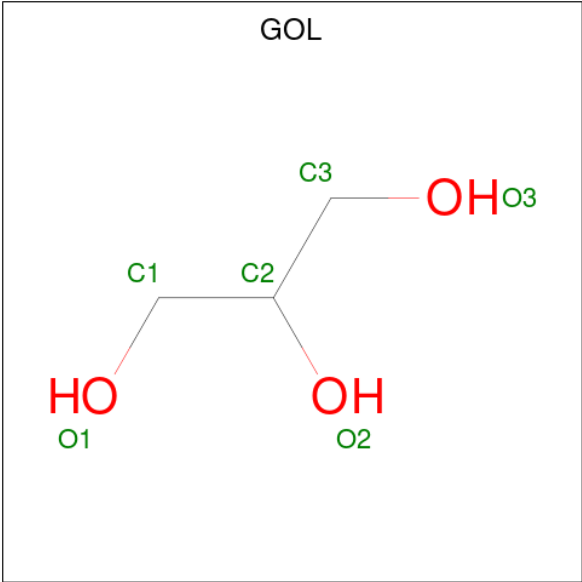
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	8	5		
8	B	1	Total	C	O	0	0
			13	8	5		

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



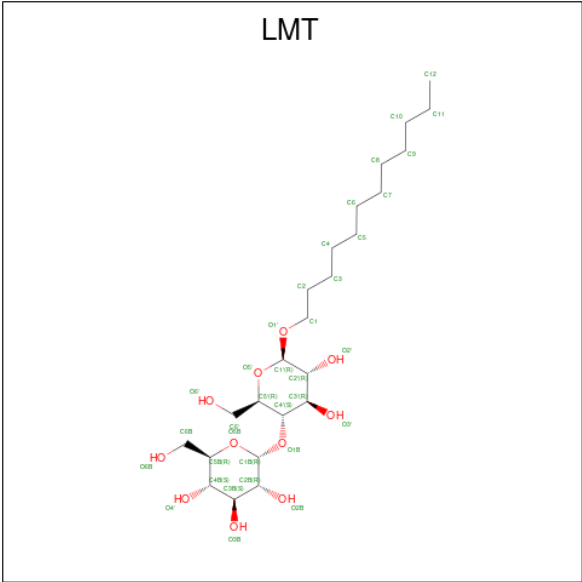
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		

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



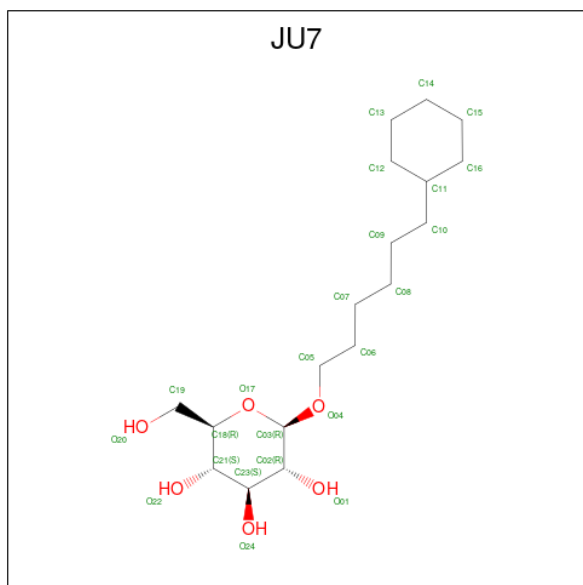
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	G	1	Total	C	O	0	0
			6	3	3		

- 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		

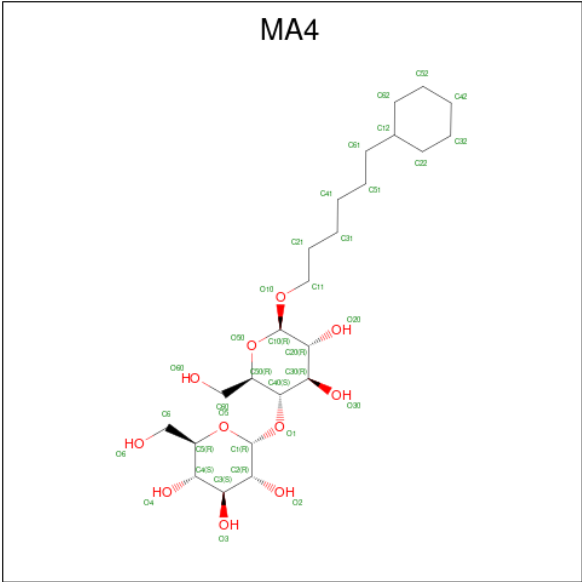
- Molecule 12 is 6-cyclohexylhexyl beta-D-glucopyranoside (three-letter code: JU7) (formula:  $C_{18}H_{34}O_6$ ).



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

- Molecule 13 is CYCLOHEXYL-HEXYL-BETA-D-MALTOSIDE (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		

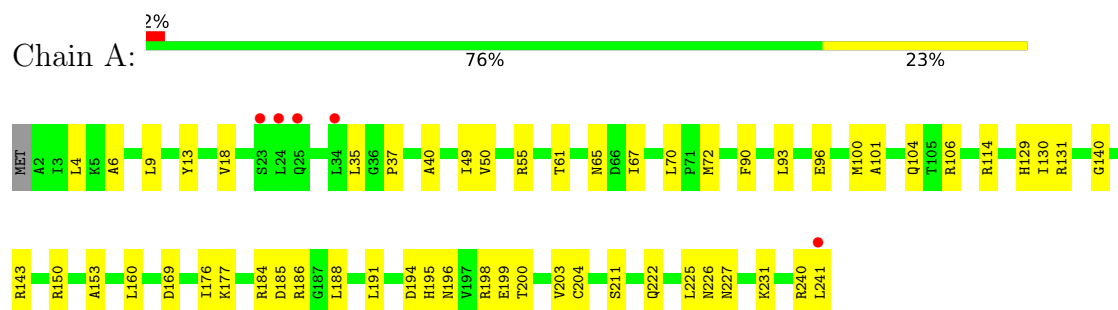
- Molecule 14 is water.

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		

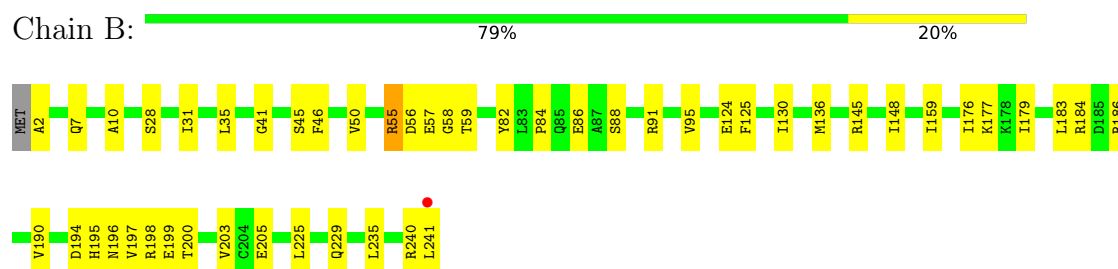
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

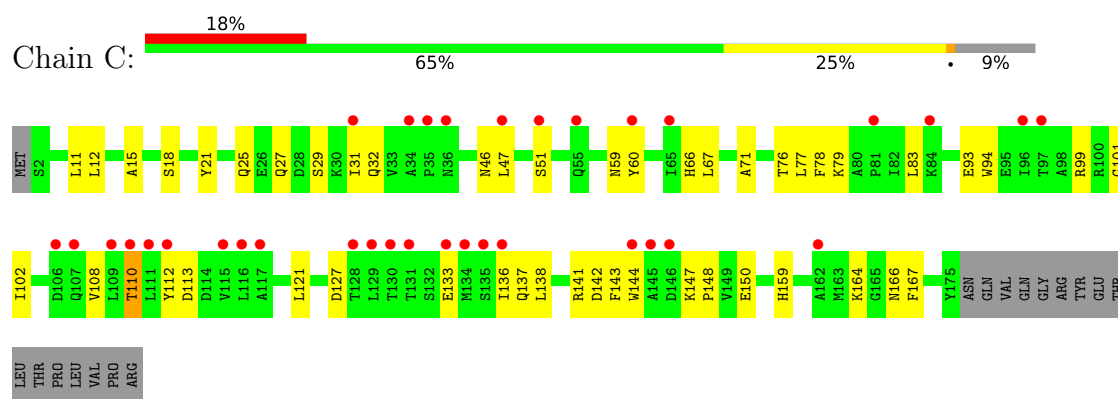
- Molecule 1: ABC transporter ATP-binding protein



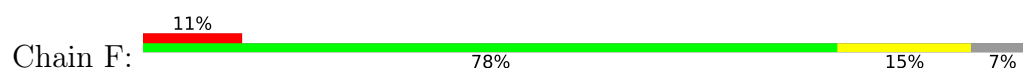
- Molecule 1: ABC transporter ATP-binding protein

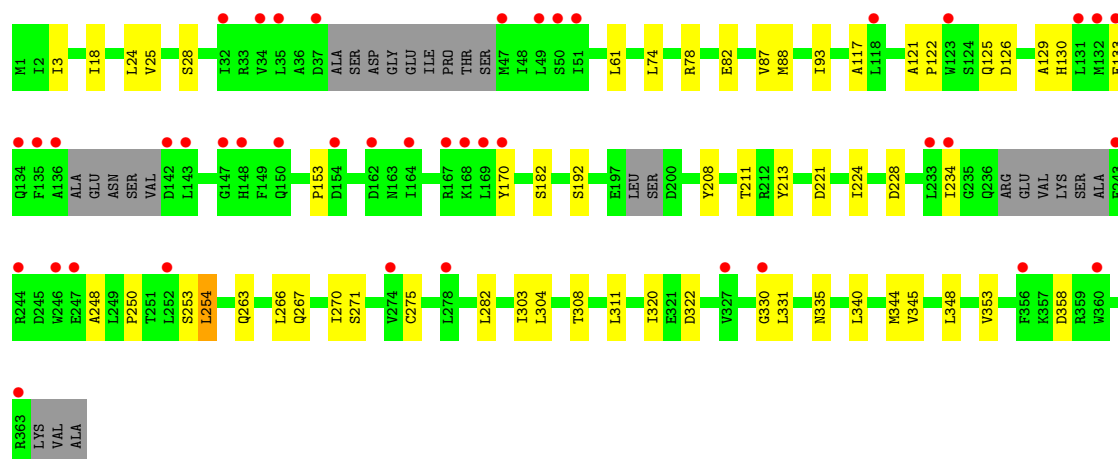


- Molecule 2: Lipopolysaccharide export system protein LptC

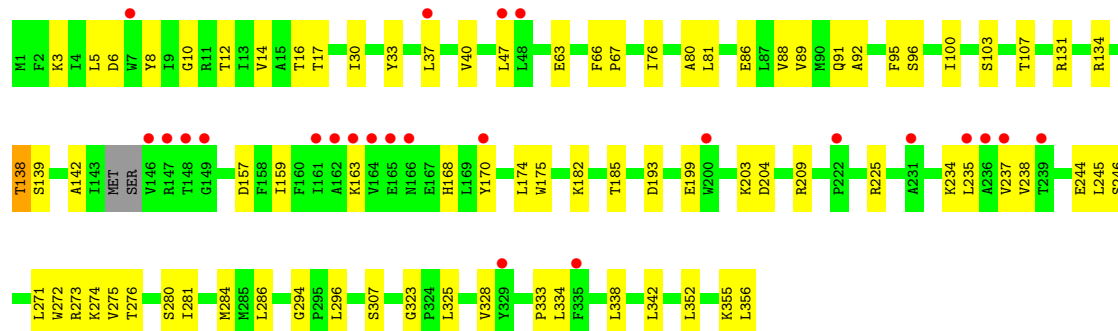
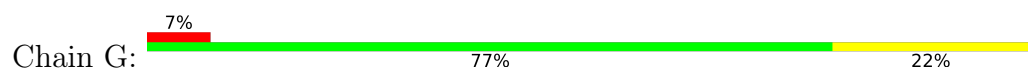


- Molecule 3: FIG000988: Predicted permease





• Molecule 4: LPS export ABC transporter permease LptG



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.35Å 80.73Å 202.99Å 90.00° 112.18° 90.00°	Depositor
Resolution (Å)	49.27 – 2.85 49.26 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.27-2.85) 99.5 (49.26-2.85)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.242 , 0.292 0.240 , 0.289	Depositor DCC
$R_{free}$ test set	1533 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.8	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 79.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PEG, CA, CL, JU7, MA4, LMT, GOL, AE3

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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	0/1897	0.63	0/2558
1	B	0.42	0/1887	0.62	0/2546
2	C	0.40	0/1327	0.60	0/1813
3	F	0.31	0/2554	0.48	0/3494
4	G	0.36	0/2729	0.55	1/3710 (0.0%)
All	All	0.37	0/10394	0.57	1/14121 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	296	LEU	CB-CG-CD1	-5.61	101.47	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1873	0	1904	40	0
1	B	1863	0	1884	33	0
2	C	1299	0	1176	39	0
3	F	2504	0	2419	38	0
4	G	2673	0	2716	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	3	0	0	1	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
7	A	18	0	28	0	0
8	A	13	0	18	3	0
8	B	13	0	18	1	0
9	B	7	0	10	1	0
10	B	12	0	16	0	0
10	G	6	0	8	0	0
11	F	64	0	76	3	0
11	G	35	0	46	1	0
12	F	24	0	0	1	0
13	G	35	0	44	3	0
14	A	27	0	0	4	1
14	B	18	0	0	1	1
14	C	2	0	0	2	0
14	F	1	0	0	0	0
14	G	5	0	0	0	0
All	All	10498	0	10363	188	1

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 9.

The worst 5 of 188 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)
4:G:307:SER:HB3	13:G:401:MA4:H322	1.44	0.99
1:B:184:ARG:NH1	1:B:205:GLU:OE2	2.12	0.83
1:B:91:ARG:HB3	1:B:136:MET:HB3	1.64	0.80
1:A:106:ARG:NH1	1:A:153:ALA:O	2.16	0.79
2:C:15:ALA:HB2	3:F:308:THR:HG22	1.63	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:424:HOH:O	14:B:403:HOH:O[4_545]	2.01	0.19

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	238/241 (99%)	228 (96%)	10 (4%)	0	100	100
1	B	238/241 (99%)	229 (96%)	9 (4%)	0	100	100
2	C	172/191 (90%)	161 (94%)	11 (6%)	0	100	100
3	F	331/366 (90%)	317 (96%)	14 (4%)	0	100	100
4	G	350/356 (98%)	336 (96%)	14 (4%)	0	100	100
All	All	1329/1395 (95%)	1271 (96%)	58 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	203/207 (98%)	201 (99%)	2 (1%)	76	91
1	B	199/207 (96%)	198 (100%)	1 (0%)	88	96
2	C	124/170 (73%)	123 (99%)	1 (1%)	81	93
3	F	244/312 (78%)	243 (100%)	1 (0%)	91	96
4	G	274/296 (93%)	272 (99%)	2 (1%)	84	94
All	All	1044/1192 (88%)	1037 (99%)	7 (1%)	84	94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	110	THR
3	F	254	LEU
4	G	138	THR
4	G	66	PHE
1	B	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	25	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 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	$\# Z  > 2$
9	PEG	B	303	-	6,6,6	0.72	0	5,5,5	0.58	0
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
7	AE3	A	307	-	8,8,8	0.56	0	7,7,7	0.74	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PG4	B	302	-	12,12,12	0.52	0	11,11,11	0.50	0
13	MA4	G	401	-	37,37,37	1.08	1 (2%)	50,50,50	1.40	7 (14%)
10	GOL	B	305	-	5,5,5	0.90	0	5,5,5	1.01	0
11	LMT	F	401	-	36,36,36	1.13	4 (11%)	47,47,47	1.01	2 (4%)
11	LMT	F	403	-	30,30,36	1.21	4 (13%)	41,41,47	1.02	2 (4%)
8	PG4	A	308	-	12,12,12	0.56	0	11,11,11	0.45	0
12	JU7	F	402	-	25,25,25	1.00	1 (4%)	32,32,32	1.34	5 (15%)
10	GOL	G	403	-	5,5,5	0.92	0	5,5,5	1.04	0
11	LMT	G	402	-	36,36,36	1.14	4 (11%)	47,47,47	1.17	3 (6%)

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
9	PEG	B	303	-	-	1/4/4/4	-
10	GOL	B	304	-	-	1/4/4/4	-
7	AE3	A	306	-	-	2/6/6/6	-
7	AE3	A	307	-	-	2/6/6/6	-
8	PG4	B	302	-	-	6/10/10/10	-
13	MA4	G	401	-	-	6/18/66/66	0/3/3/3
10	GOL	B	305	-	-	0/4/4/4	-
11	LMT	F	401	-	-	5/21/61/61	0/2/2/2
11	LMT	F	403	-	-	1/15/55/61	0/2/2/2
8	PG4	A	308	-	-	7/10/10/10	-
12	JU7	F	402	-	-	5/12/40/40	0/2/2/2
10	GOL	G	403	-	-	0/4/4/4	-
11	LMT	G	402	-	-	13/21/61/61	0/2/2/2

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(°)	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

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

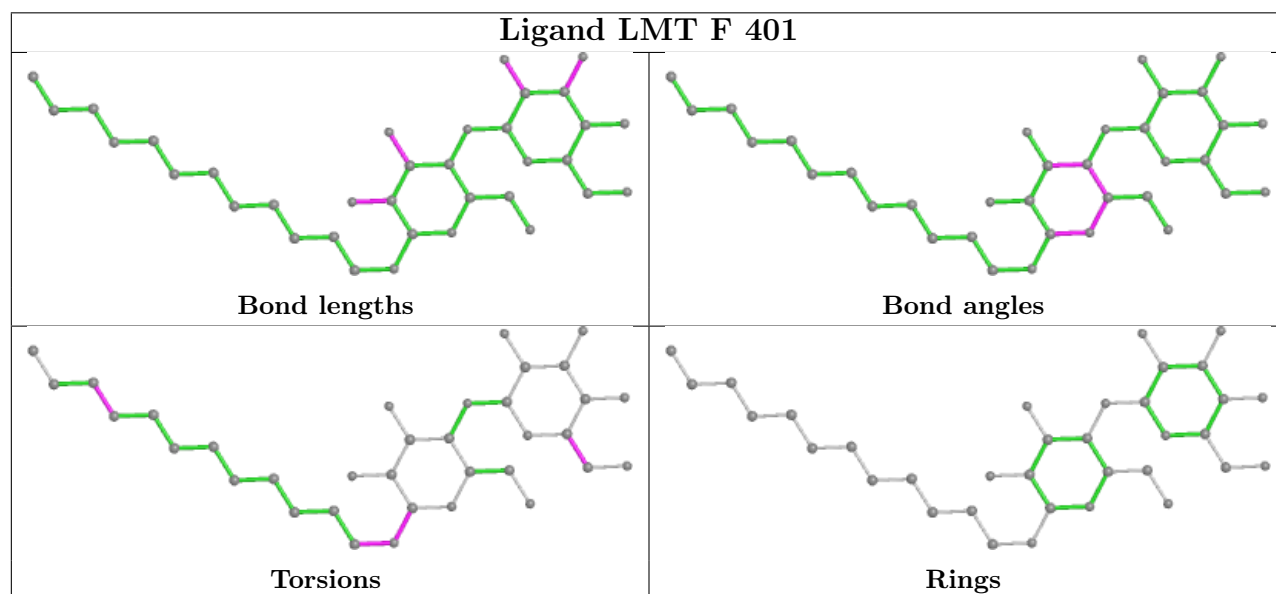
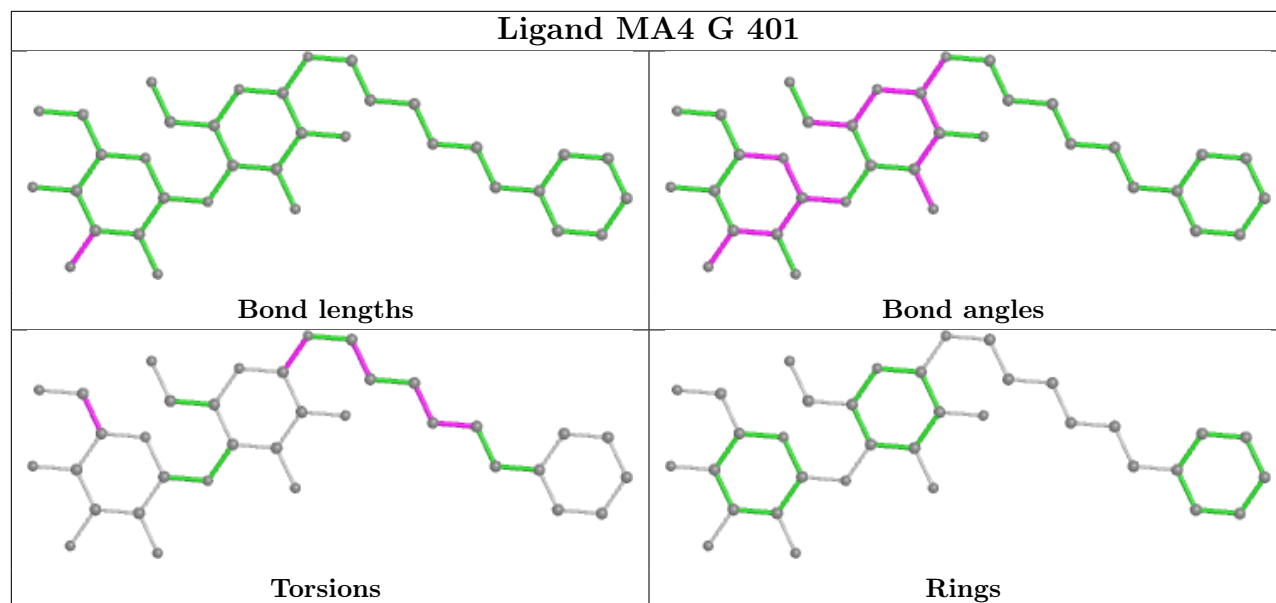
Mol	Chain	Res	Type	Atoms
11	F	401	LMT	C2'-C1'-O1'-C1
11	G	402	LMT	C2'-C1'-O1'-C1
11	G	402	LMT	O5'-C1'-O1'-C1
12	F	402	JU7	O17-C03-O04-C05
13	G	401	MA4	C31-C41-C51-C61

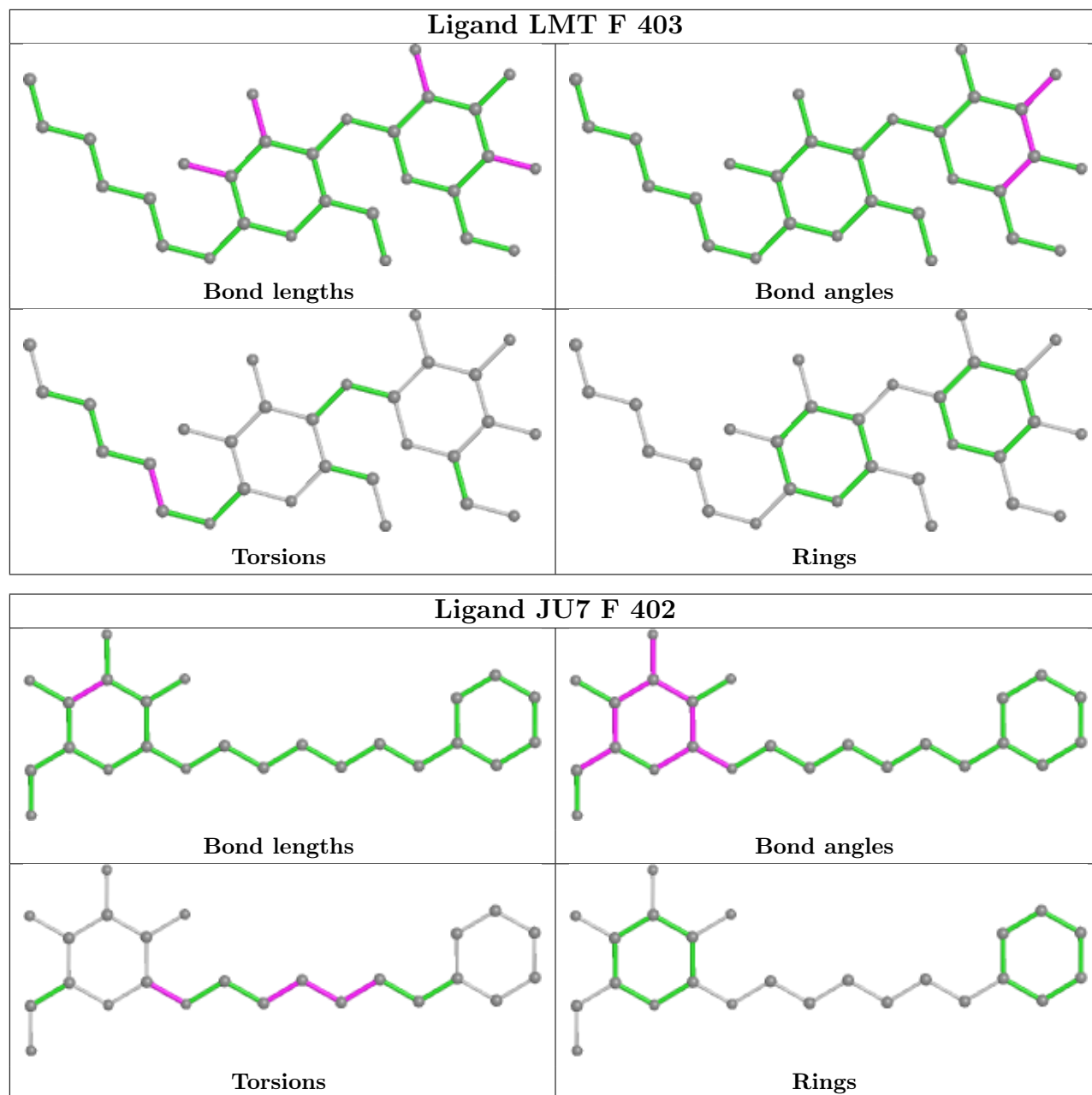
There are no ring outliers.

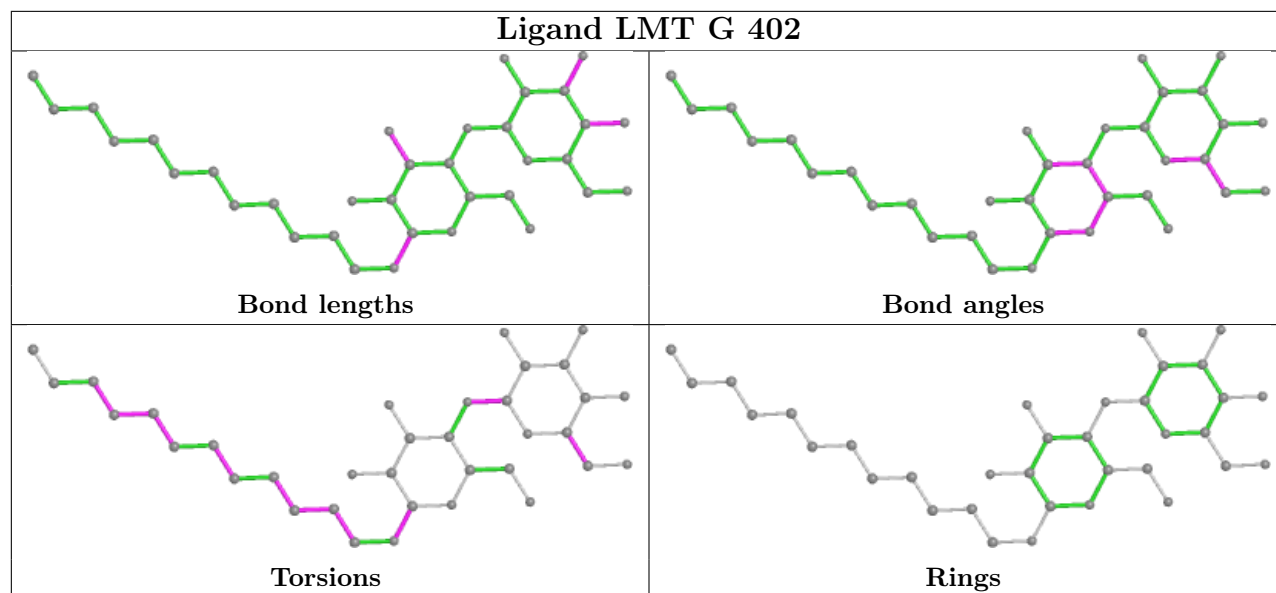
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	303	PEG	1	0
8	B	302	PG4	1	0
13	G	401	MA4	3	0
11	F	401	LMT	1	0
11	F	403	LMT	2	0
8	A	308	PG4	3	0
12	F	402	JU7	1	0
11	G	402	LMT	1	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.







## 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.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	240/241 (99%)	0.28	5 (2%) 63 60	45, 81, 110, 137	0
1	B	240/241 (99%)	0.13	1 (0%) 92 92	57, 88, 117, 150	0
2	C	174/191 (91%)	0.92	34 (19%) 1 1	75, 148, 191, 220	0
3	F	341/366 (93%)	0.62	42 (12%) 4 2	71, 131, 191, 221	0
4	G	354/356 (99%)	0.40	24 (6%) 17 13	57, 105, 150, 178	0
All	All	1349/1395 (96%)	0.45	106 (7%) 12 9	45, 103, 173, 221	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	47	MET	10.3
4	G	146	VAL	9.1
2	C	134	MET	8.6
4	G	147	ARG	8.3
3	F	134	GLN	6.9

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

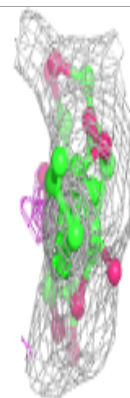
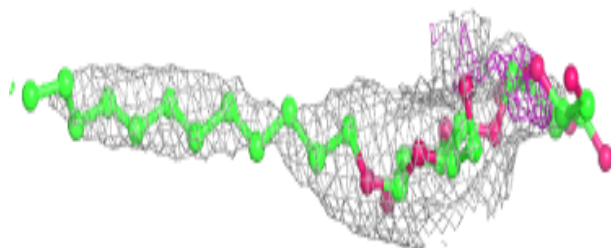
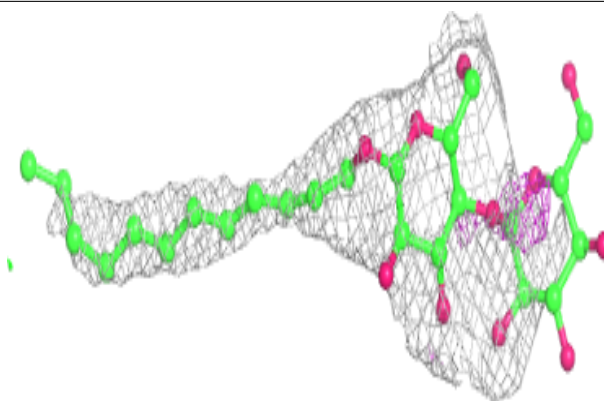
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	PEG	B	303	7/7	0.27	0.62	142,144,152,154	0
10	GOL	B	304	6/6	0.45	0.31	117,120,124,125	0
8	PG4	B	302	13/13	0.61	0.46	94,102,111,114	0
6	CA	A	303	1/1	0.62	0.20	127,127,127,127	0
10	GOL	B	305	6/6	0.73	0.30	103,120,125,127	0
11	LMT	F	401	35/35	0.75	0.36	96,143,175,176	0
8	PG4	A	308	13/13	0.77	0.51	100,103,127,130	0
5	CL	A	301	1/1	0.81	0.19	85,85,85,85	0
12	JU7	F	402	24/24	0.81	0.24	81,110,130,147	0
13	MA4	G	401	35/35	0.81	0.26	91,156,183,185	0
11	LMT	G	402	35/35	0.84	0.25	68,122,136,139	0
7	AE3	A	307	9/9	0.86	0.24	87,93,101,102	0
6	CA	A	304	1/1	0.87	0.23	98,98,98,98	0
10	GOL	G	403	6/6	0.87	0.13	105,106,111,111	0
7	AE3	A	306	9/9	0.88	0.27	75,80,83,85	0
11	LMT	F	403	29/35	0.90	0.21	87,94,107,109	0
5	CL	A	305	1/1	0.93	0.56	142,142,142,142	0
5	CL	A	302	1/1	0.93	0.29	103,103,103,103	0
5	CL	B	301	1/1	0.97	0.31	96,96,96,96	0

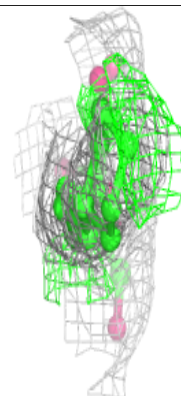
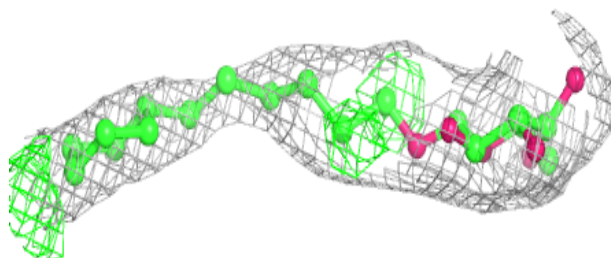
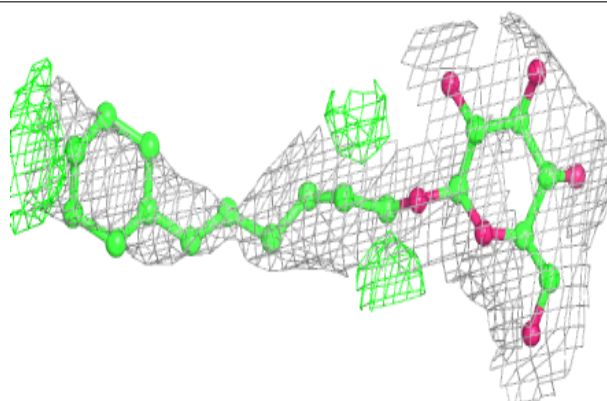
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around LMT F 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around JU7 F 402:**

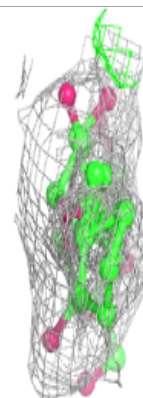
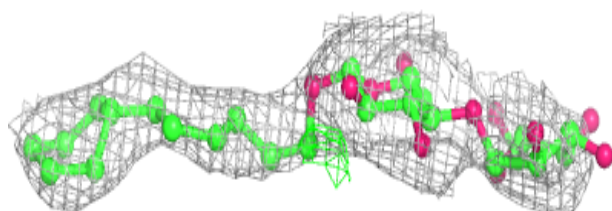
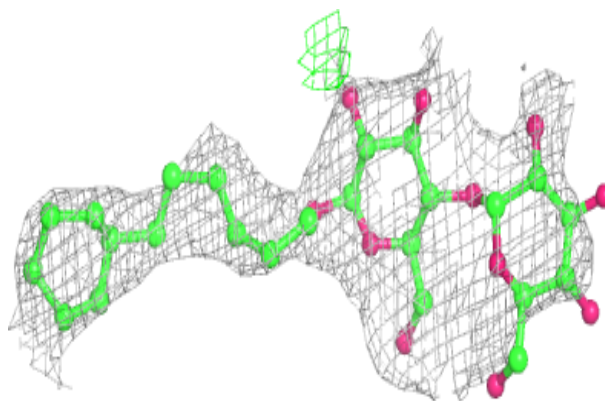
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



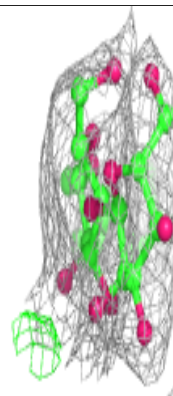
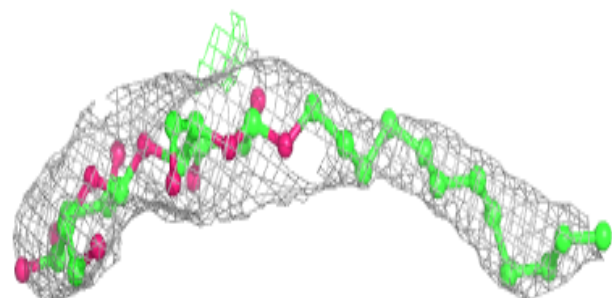
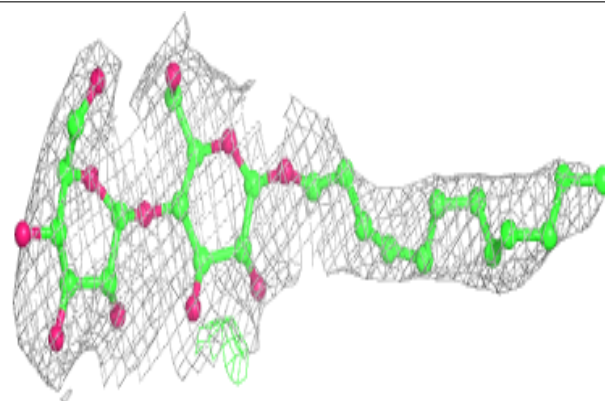


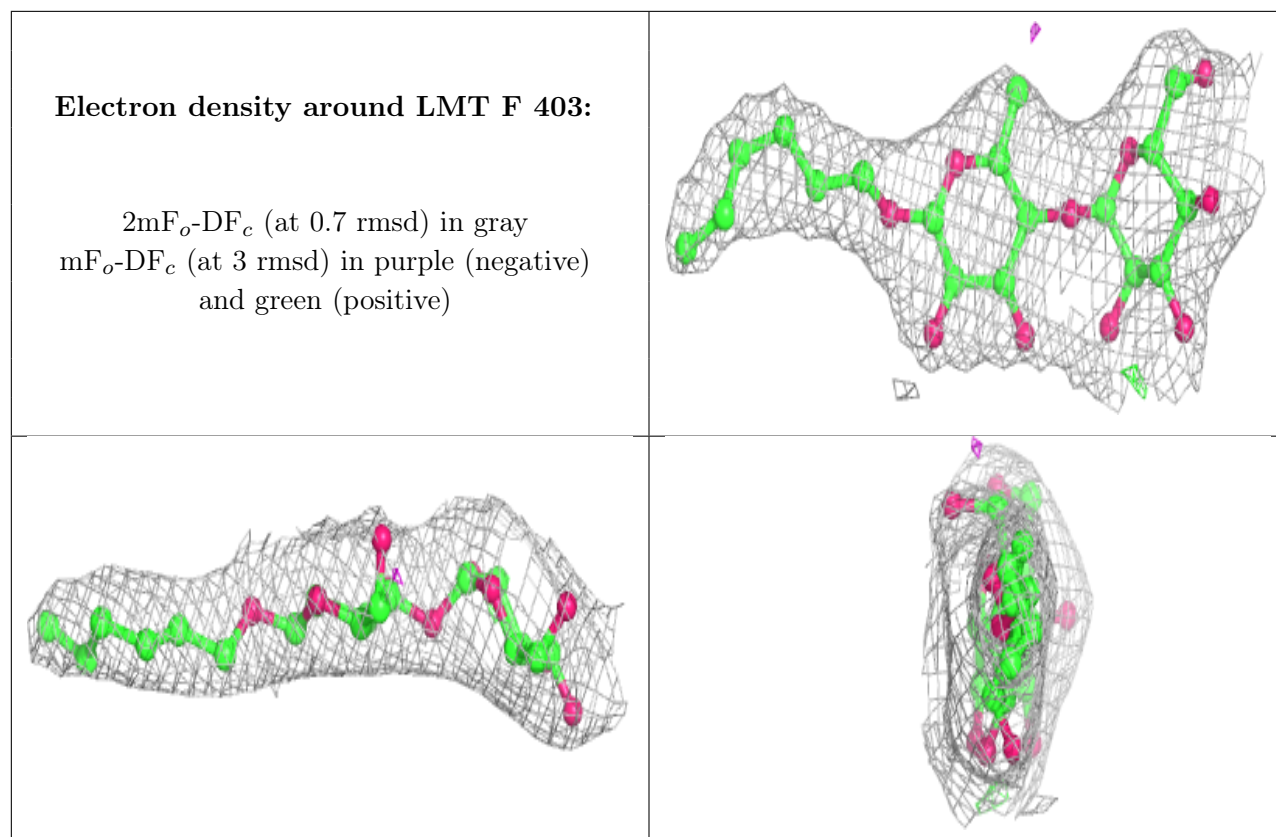
**Electron density around MA4 G 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMT G 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.