



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 06:35 PM BST

PDB ID : 6OR2  
Title : MmpL3 is a lipid transporter that binds trehalose monomycolate and phosphatidylethanolamine  
Authors : Su, C.-C.  
Deposited on : 2019-04-29  
Resolution : 2.59 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](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.

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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 : 2.13.1  
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) : 2.13.1

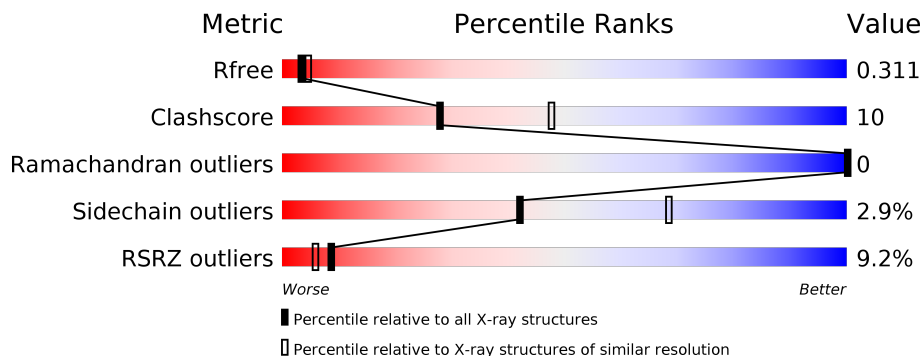
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	779	

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
2	L9Q	A	801	-	-	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5685 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.

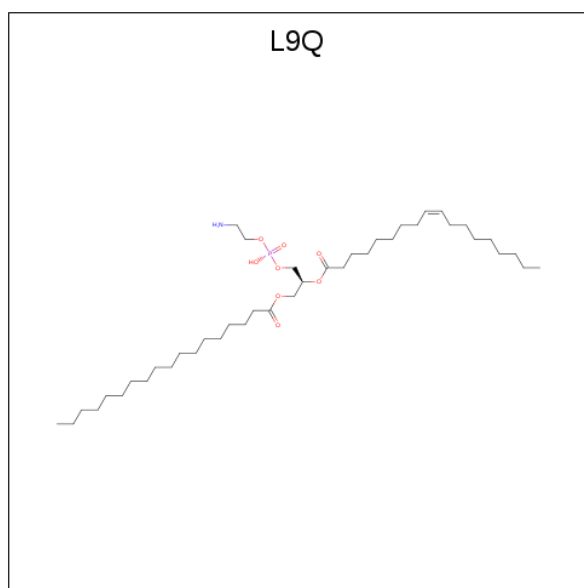
- Molecule 1 is a protein called Membrane protein, MmpL family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	732	5589	3618	925	1018	28	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

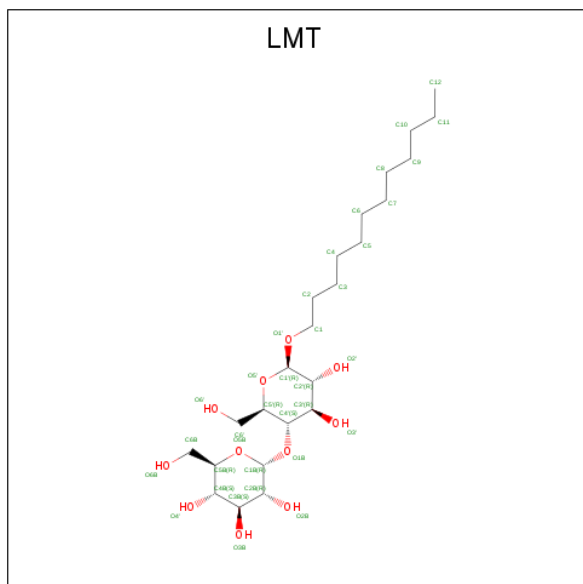
Chain	Residue	Modelled	Actual	Comment	Reference
A	774	HIS	-	expression tag	UNP A0QP27
A	775	HIS	-	expression tag	UNP A0QP27
A	776	HIS	-	expression tag	UNP A0QP27
A	777	HIS	-	expression tag	UNP A0QP27
A	778	HIS	-	expression tag	UNP A0QP27
A	779	HIS	-	expression tag	UNP A0QP27

- Molecule 2 is (1S)-2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-1-[(octadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: L9Q) (formula: C<sub>41</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	50	40	1	8	1	0	0

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	35	24	11	0	0

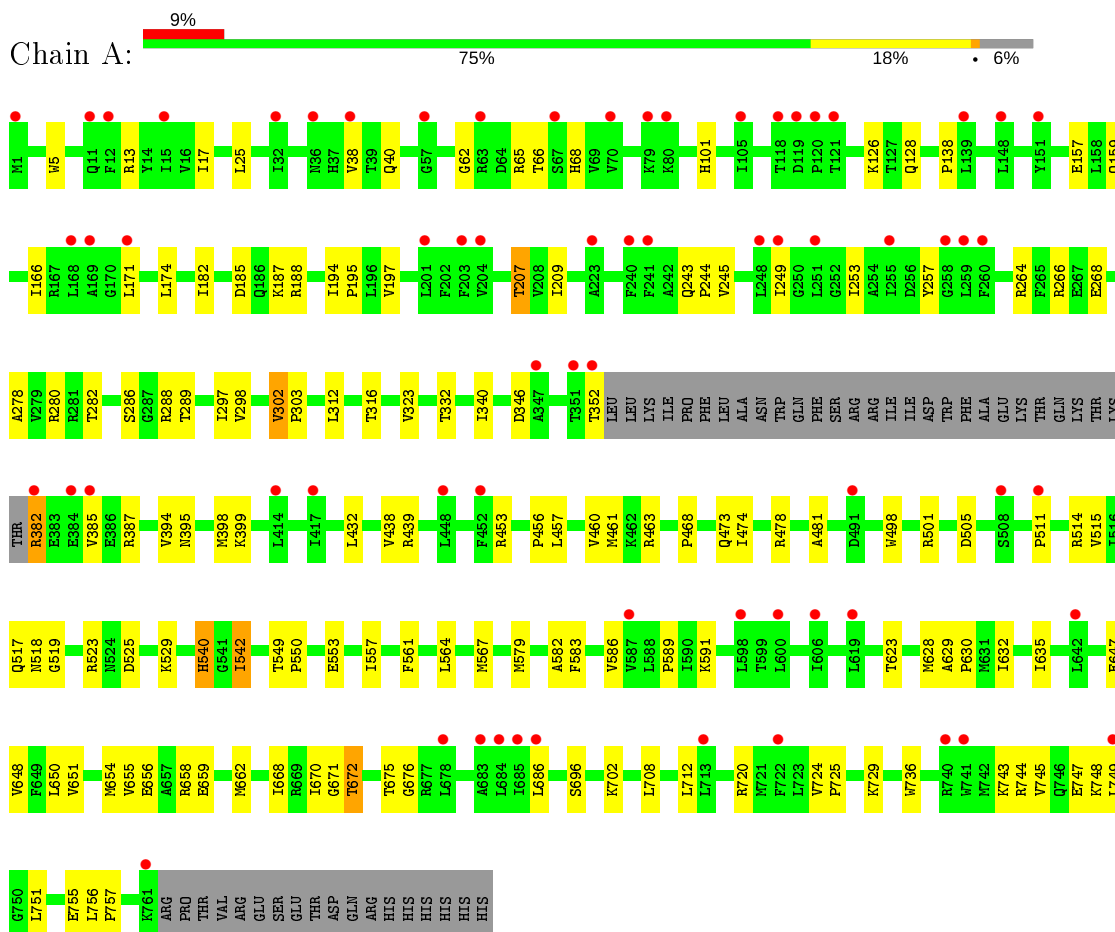
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	11	11	11	0	0

### 3 Residue-property plots

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: Membrane protein, MmpL family protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.81Å 129.46Å 154.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.25 – 2.59 99.25 – 2.56	Depositor EDS
% Data completeness (in resolution range)	92.9 (99.25-2.59) 77.9 (99.25-2.56)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.35 (at 2.55Å)	Xtrriage
Refinement program	PHENIX (dev_3318: ???)	Depositor
R, $R_{free}$	0.249 , 0.290 0.272 , 0.311	Depositor DCC
$R_{free}$ test set	1945 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.0	Xtrriage
Anisotropy	0.200	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	5685	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: LMT, L9Q

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	0.25	0/5704	0.42	0/7762

There are no bond length outliers.

There are no bond angle outliers.

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	5589	0	5748	96	0
2	A	50	0	74	19	0
3	A	35	0	46	8	0
4	A	11	0	0	2	0
All	All	5685	0	5868	114	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 10.

All (114) 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:A:801:L9Q:H37	2:A:801:L9Q:H16A	1.17	1.16
2:A:801:L9Q:H4	2:A:801:L9Q:H1A	1.31	1.06
2:A:801:L9Q:C37	2:A:801:L9Q:H16A	1.99	0.92
1:A:745:VAL:O	1:A:749:LEU:HD13	1.72	0.90
2:A:801:L9Q:HN	2:A:801:L9Q:H1A	1.37	0.90
1:A:743:LYS:O	1:A:747:GLU:HG3	1.72	0.90
2:A:801:L9Q:H36	2:A:801:L9Q:H41A	1.59	0.85
2:A:801:L9Q:H4	2:A:801:L9Q:C1	2.07	0.84
2:A:801:L9Q:C4	2:A:801:L9Q:H1A	2.07	0.81
2:A:801:L9Q:C16	2:A:801:L9Q:H37	2.08	0.78
3:A:802:LMT:H6'	3:A:802:LMT:H4O1	0.72	0.72
1:A:171:LEU:HD12	2:A:801:L9Q:H15A	1.72	0.71
1:A:264:ARG:NH1	1:A:268:GLU:OE2	2.23	0.71
1:A:207:THR:HG21	1:A:346:ASP:HA	1.72	0.71
1:A:280:ARG:NH1	4:A:901:HOH:O	2.23	0.71
1:A:439:ARG:HH12	1:A:623:THR:HG21	1.56	0.71
3:A:802:LMT:O6'	3:A:802:LMT:O4'	2.02	0.70
1:A:264:ARG:NH2	1:A:656:GLU:OE2	2.25	0.70
1:A:65:ARG:HB2	1:A:138:PRO:HB3	1.74	0.69
1:A:171:LEU:CD1	2:A:801:L9Q:H15A	2.23	0.69
1:A:744:ARG:HD2	1:A:747:GLU:OE1	1.94	0.68
1:A:266:ARG:NH1	1:A:346:ASP:OD1	2.28	0.67
2:A:801:L9Q:N	2:A:801:L9Q:H1A	2.07	0.67
3:A:802:LMT:O1B	3:A:802:LMT:O4'	2.13	0.67
1:A:473:GLN:HE21	1:A:540:HIS:HE1	1.40	0.66
1:A:549:THR:HG21	2:A:801:L9Q:H32A	1.78	0.66
2:A:801:L9Q:C41	2:A:801:L9Q:H36	2.27	0.65
3:A:802:LMT:H1B	3:A:802:LMT:O3'	1.97	0.64
1:A:473:GLN:HE21	1:A:540:HIS:CE1	2.16	0.63
1:A:185:ASP:OD1	1:A:188:ARG:NH2	2.32	0.62
3:A:802:LMT:H5B	3:A:802:LMT:O6'	1.98	0.62
2:A:801:L9Q:C36	2:A:801:L9Q:H41A	2.28	0.62
1:A:66:THR:HB	2:A:801:L9Q:H24	1.82	0.62
1:A:696:SER:O	1:A:702:LYS:NZ	2.27	0.61
1:A:756:LEU:HB3	1:A:757:PRO:HD2	1.81	0.61
1:A:461:MET:HB3	1:A:542:ILE:HD12	1.83	0.60
1:A:174:LEU:HD23	1:A:438:VAL:HG12	1.83	0.60
1:A:245:VAL:HG13	1:A:249:ILE:HD12	1.82	0.59
1:A:302:VAL:HG23	1:A:303:PRO:HD3	1.85	0.58
1:A:517:GLN:HE22	2:A:801:L9Q:H44	1.68	0.57
1:A:394:VAL:HG13	1:A:725:PRO:HB3	1.87	0.57
1:A:288:ARG:NH2	1:A:582:ALA:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HD23	3:A:802:LMT:H71	1.88	0.55
1:A:686:LEU:HB3	1:A:712:LEU:HD21	1.89	0.55
1:A:460:VAL:HA	1:A:515:VAL:HG12	1.89	0.55
1:A:463:ARG:NH1	1:A:468:PRO:O	2.40	0.53
1:A:557:ILE:HD13	3:A:802:LMT:H6'1	1.91	0.53
1:A:40:GLN:NE2	4:A:902:HOH:O	2.31	0.53
1:A:749:LEU:N	1:A:749:LEU:CD1	2.73	0.52
1:A:668:ILE:O	1:A:672:THR:HG22	2.08	0.52
1:A:194:ILE:HA	1:A:197:VAL:HG22	1.92	0.52
1:A:297:ILE:HG21	1:A:323:VAL:HG11	1.91	0.52
2:A:801:L9Q:HN	2:A:801:L9Q:C1	2.18	0.52
1:A:579:MET:HE3	1:A:589:PRO:HA	1.92	0.52
1:A:182:ILE:HD12	1:A:244:PRO:HG2	1.92	0.51
1:A:749:LEU:HD12	1:A:749:LEU:N	2.26	0.51
1:A:398:MET:HG2	1:A:729:LYS:HB2	1.93	0.50
1:A:312:LEU:O	1:A:316:THR:HG23	2.12	0.50
1:A:468:PRO:HB3	1:A:511:PRO:HB2	1.94	0.50
1:A:591:LYS:NZ	1:A:647:GLU:OE1	2.45	0.49
1:A:289:THR:HG23	1:A:648:VAL:HG12	1.95	0.49
1:A:453:ARG:HG3	2:A:801:L9Q:H16	1.95	0.49
1:A:463:ARG:HG2	1:A:542:ILE:HG22	1.95	0.49
1:A:658:ARG:NH1	1:A:662:MET:O	2.39	0.49
1:A:658:ARG:HG2	1:A:736:TRP:CD2	2.48	0.49
1:A:662:MET:HE1	1:A:670:ILE:HG13	1.94	0.49
1:A:583:PHE:HZ	1:A:648:VAL:HA	1.78	0.48
1:A:474:ILE:HD11	1:A:514:ARG:HE	1.79	0.48
1:A:724:VAL:HB	1:A:725:PRO:HD3	1.96	0.47
1:A:182:ILE:HG23	1:A:244:PRO:HG3	1.96	0.47
1:A:288:ARG:NH1	1:A:751:LEU:O	2.47	0.47
1:A:457:LEU:HD21	1:A:550:PRO:HB2	1.96	0.47
1:A:561:PHE:HB3	3:A:802:LMT:H22	1.97	0.46
1:A:243:GLN:HB2	1:A:244:PRO:HD3	1.98	0.46
1:A:278:ALA:O	1:A:282:THR:HG23	2.16	0.46
1:A:101:HIS:NE2	1:A:157:GLU:OE1	2.42	0.46
1:A:671:GLY:O	1:A:675:THR:HG22	2.17	0.45
1:A:708:LEU:O	1:A:712:LEU:HB2	2.17	0.45
1:A:62:GLY:O	1:A:501:ARG:NH2	2.50	0.44
1:A:481:ALA:HB1	1:A:498:TRP:CE2	2.51	0.44
1:A:478:ARG:HG3	1:A:498:TRP:HB2	1.99	0.44
1:A:632:ILE:HA	1:A:635:ILE:HG22	1.98	0.44
1:A:650:LEU:HD11	1:A:672:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:THR:O	1:A:286:SER:N	2.51	0.44
1:A:298:VAL:O	1:A:302:VAL:HG22	2.18	0.44
1:A:540:HIS:ND1	1:A:540:HIS:N	2.65	0.44
1:A:557:ILE:HG12	1:A:629:ALA:HB2	2.00	0.43
1:A:432:LEU:O	1:A:439:ARG:NH2	2.52	0.43
1:A:583:PHE:CZ	1:A:648:VAL:HA	2.53	0.43
1:A:744:ARG:O	1:A:748:LYS:N	2.47	0.43
1:A:194:ILE:HG13	1:A:195:PRO:HD3	2.00	0.43
1:A:253:ILE:HD12	1:A:257:TYR:CZ	2.54	0.43
1:A:523:ARG:NH2	1:A:553:GLU:OE1	2.39	0.42
1:A:13:ARG:HD2	1:A:340:ILE:HG13	2.01	0.42
1:A:676:GLY:O	1:A:720:ARG:NH2	2.51	0.42
1:A:628:MET:HG2	1:A:630:PRO:HG2	2.02	0.42
1:A:650:LEU:HD22	1:A:720:ARG:HG3	2.01	0.42
1:A:194:ILE:N	1:A:195:PRO:HD2	2.35	0.42
1:A:525:ASP:HB3	1:A:529:LYS:HG2	2.02	0.42
1:A:712:LEU:HD12	1:A:712:LEU:HA	1.89	0.42
1:A:65:ARG:HB3	1:A:68:HIS:CE1	2.55	0.42
1:A:655:VAL:O	1:A:659:GLU:HG2	2.20	0.42
1:A:659:GLU:HB3	1:A:755:GLU:HB2	2.01	0.42
1:A:382:ARG:O	1:A:385:VAL:HG22	2.20	0.41
2:A:801:L9Q:H12A	2:A:801:L9Q:H15	1.81	0.41
1:A:17:ILE:HD12	1:A:340:ILE:HD13	2.02	0.41
1:A:128:GLN:N	1:A:128:GLN:OE1	2.44	0.41
1:A:549:THR:OG1	1:A:550:PRO:HD3	2.19	0.41
1:A:456:PRO:HA	1:A:519:GLY:HA2	2.02	0.41
1:A:654:MET:HG2	1:A:671:GLY:HA3	2.03	0.41
1:A:583:PHE:CZ	1:A:651:VAL:HB	2.55	0.40
1:A:159:GLN:NE2	1:A:166:ILE:O	2.44	0.40
1:A:5:TRP:HZ2	1:A:332:THR:HG22	1.85	0.40
1:A:395:ASN:O	1:A:399:LYS:HB2	2.22	0.40

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 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	729/779 (94%)	705 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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 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	596/643 (93%)	579 (97%)	17 (3%)	42	68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	38	VAL
1	A	126	LYS
1	A	187	LYS
1	A	207	THR
1	A	209	ILE
1	A	302	VAL
1	A	352	THR
1	A	382	ARG
1	A	387	ARG
1	A	505	ASP
1	A	518	ASN
1	A	540	HIS
1	A	542	ILE
1	A	567	MET
1	A	586	VAL
1	A	672	THR

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

Mol	Chain	Res	Type
1	A	540	HIS

### 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](#)

2 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	L9Q	A	801	-	49,49,50	1.26	5 (10%)	52,54,55	1.02	3 (5%)
3	LMT	A	802	-	36,36,36	0.39	0	47,47,47	1.41	9 (19%)

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	L9Q	A	801	-	-	27/53/53/54	-
3	LMT	A	802	-	-	8/21/61/61	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	L9Q	C40-C39	3.81	1.53	1.31
2	A	801	L9Q	O3-C11	3.34	1.43	1.33
2	A	801	L9Q	O2-C2	-3.07	1.38	1.46
2	A	801	L9Q	O2-C31	2.82	1.42	1.34
2	A	801	L9Q	O4P-C4	-2.00	1.36	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	LMT	C1B-O1B-C4'	-4.21	107.55	117.96
2	A	801	L9Q	O2-C31-C32	3.44	118.91	111.50
3	A	802	LMT	O1'-C1'-C2'	-2.87	103.83	108.30
2	A	801	L9Q	O3-C11-C12	2.77	120.61	111.91
3	A	802	LMT	C4B-C3B-C2B	-2.69	106.12	110.82
3	A	802	LMT	C1-O1'-C1'	-2.68	109.39	113.84
3	A	802	LMT	C1'-O5'-C5'	-2.39	108.99	113.69
3	A	802	LMT	O2'-C2'-C1'	-2.38	104.26	110.05
3	A	802	LMT	O3B-C3B-C2B	-2.20	105.26	110.35
3	A	802	LMT	O5'-C5'-C6'	2.19	111.89	106.44
3	A	802	LMT	O1B-C1B-O5B	-2.11	104.79	110.67
2	A	801	L9Q	C2-O2-C31	-2.08	112.66	117.79

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	L9Q	C1-O3P-P-O2P
2	A	801	L9Q	C4-O4P-P-O2P
2	A	801	L9Q	O31-C31-O2-C2
2	A	801	L9Q	C32-C31-O2-C2
2	A	801	L9Q	O4P-C4-C5-N
2	A	801	L9Q	C38-C39-C40-C41
3	A	802	LMT	C2'-C1'-O1'-C1
3	A	802	LMT	O5'-C1'-O1'-C1
2	A	801	L9Q	C12-C13-C14-C15
3	A	802	LMT	C2-C3-C4-C5
2	A	801	L9Q	C14-C15-C16-C17
2	A	801	L9Q	C1-O3P-P-O4P
2	A	801	L9Q	C21-C22-C23-C24
2	A	801	L9Q	C32-C33-C34-C35
2	A	801	L9Q	C33-C34-C35-C36

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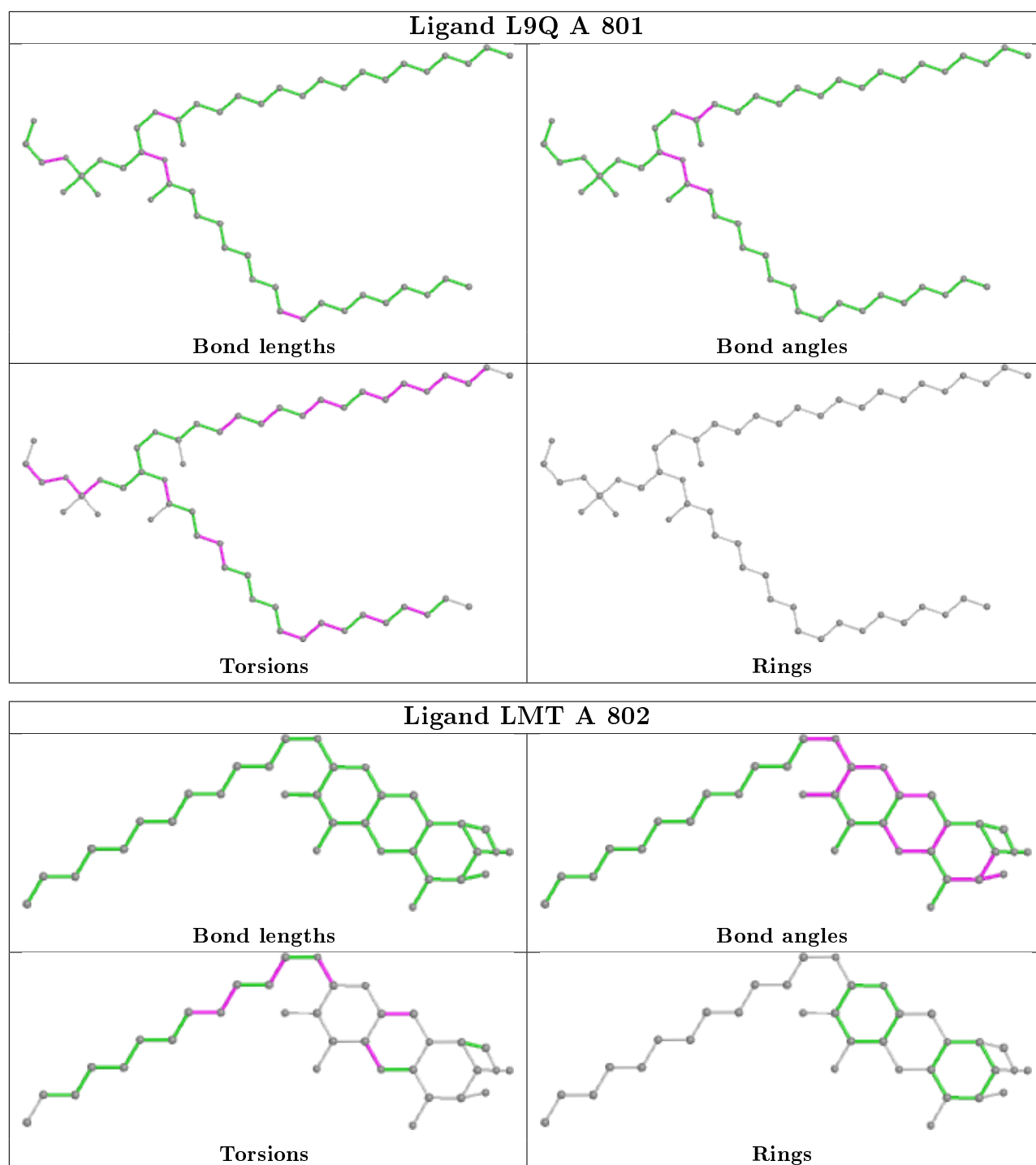
Mol	Chain	Res	Type	Atoms
2	A	801	L9Q	C23-C24-C25-C26
2	A	801	L9Q	C16-C17-C18-C19
2	A	801	L9Q	C17-C18-C19-C20
2	A	801	L9Q	C20-C21-C22-C23
2	A	801	L9Q	C22-C23-C24-C25
2	A	801	L9Q	C4-O4P-P-O3P
2	A	801	L9Q	C40-C41-C42-C43
3	A	802	LMT	O5'-C5'-C6'-O6'
3	A	802	LMT	O1'-C1-C2-C3
2	A	801	L9Q	C44-C45-C46-C47
2	A	801	L9Q	C42-C43-C44-C45
2	A	801	L9Q	C24-C25-C26-C27
2	A	801	L9Q	C19-C20-C21-C22
3	A	802	LMT	C3-C4-C5-C6
3	A	802	LMT	C5'-C4'-O1B-C1B
3	A	802	LMT	C3'-C4'-O1B-C1B
2	A	801	L9Q	C39-C40-C41-C42
2	A	801	L9Q	C1-O3P-P-O1P
2	A	801	L9Q	C4-O4P-P-O1P
2	A	801	L9Q	C5-C4-O4P-P

There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	L9Q	19	0
3	A	802	LMT	8	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	732/779 (93%)	0.83	67 (9%) <b>9</b> <b>6</b>	30, 99, 146, 203	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240[A]	PHE	6.2
1	A	63	ARG	5.2
1	A	385	VAL	5.2
1	A	452	PHE	4.0
1	A	642	LEU	3.9
1	A	1	MET	3.8
1	A	203	PHE	3.8
1	A	201	LEU	3.7
1	A	598	LEU	3.7
1	A	38	VAL	3.7
1	A	79	LYS	3.6
1	A	171	LEU	3.5
1	A	749	LEU	3.3
1	A	491	ASP	3.2
1	A	678	LEU	3.2
1	A	382	ARG	3.2
1	A	260	PHE	3.1
1	A	259	LEU	3.1
1	A	686	LEU	3.0
1	A	148	LEU	3.0
1	A	248	LEU	2.9
1	A	685	ILE	2.8
1	A	417	ILE	2.8
1	A	508	SER	2.8
1	A	713	LEU	2.8
1	A	36	ASN	2.7
1	A	70	VAL	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	121	THR	2.7
1	A	255	ILE	2.6
1	A	722	PHE	2.6
1	A	587	VAL	2.5
1	A	169	ALA	2.5
1	A	80	LYS	2.5
1	A	204	VAL	2.4
1	A	119	ASP	2.4
1	A	241	PHE	2.4
1	A	414	LEU	2.4
1	A	11	GLN	2.3
1	A	105	ILE	2.3
1	A	15	ILE	2.3
1	A	740	ARG	2.3
1	A	12	PHE	2.3
1	A	384	GLU	2.3
1	A	249	ILE	2.3
1	A	600	LEU	2.3
1	A	684	LEU	2.3
1	A	120	PRO	2.3
1	A	511	PRO	2.3
1	A	352	THR	2.3
1	A	448	LEU	2.2
1	A	32	ILE	2.2
1	A	351	THR	2.2
1	A	67	SER	2.2
1	A	258	GLY	2.1
1	A	168	LEU	2.1
1	A	251	LEU	2.1
1	A	118	THR	2.1
1	A	741	TRP	2.1
1	A	619	LEU	2.1
1	A	57	GLY	2.1
1	A	151	TYR	2.1
1	A	761	LYS	2.1
1	A	223	ALA	2.0
1	A	347	ALA	2.0
1	A	139	LEU	2.0
1	A	683	ALA	2.0
1	A	606	ILE	2.0

## 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](#)

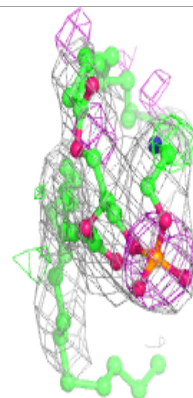
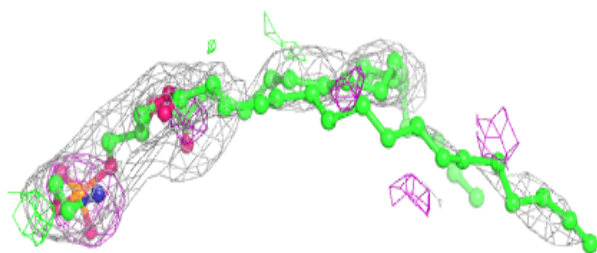
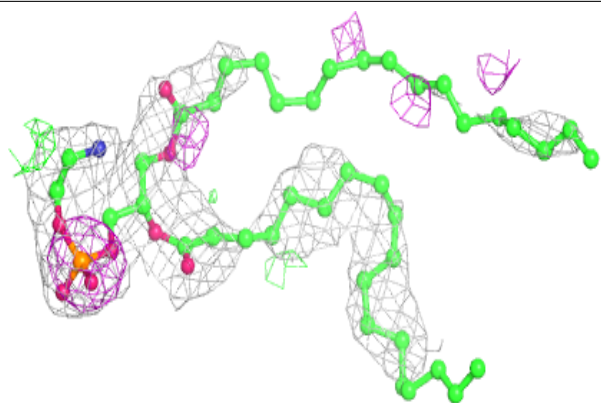
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	L9Q	A	801	50/51	0.78	0.56	81,104,129,139	0
3	LMT	A	802	35/35	0.91	0.20	73,101,128,132	0

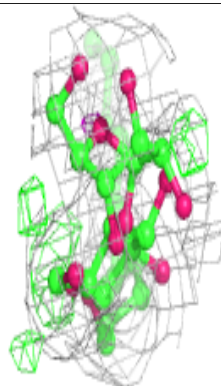
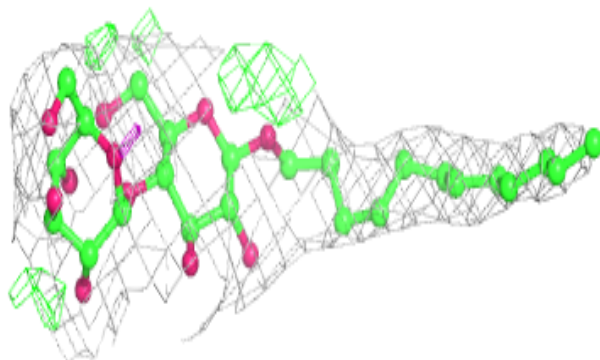
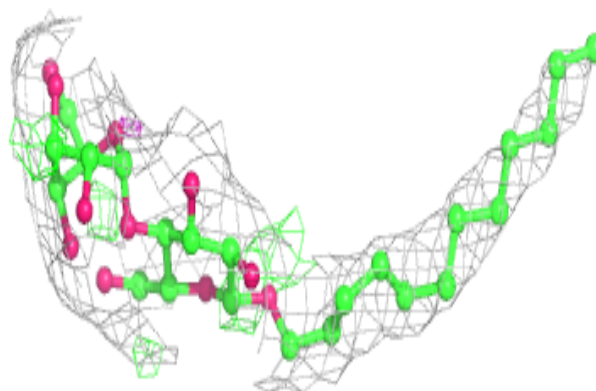
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around L9Q A 801:**

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

**Electron density around LMT A 802:**

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



## 6.5 Other polymers

There are no such residues in this entry.