



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:14 AM UTC

PDB ID : 6OR2 / pdb_00006or2
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

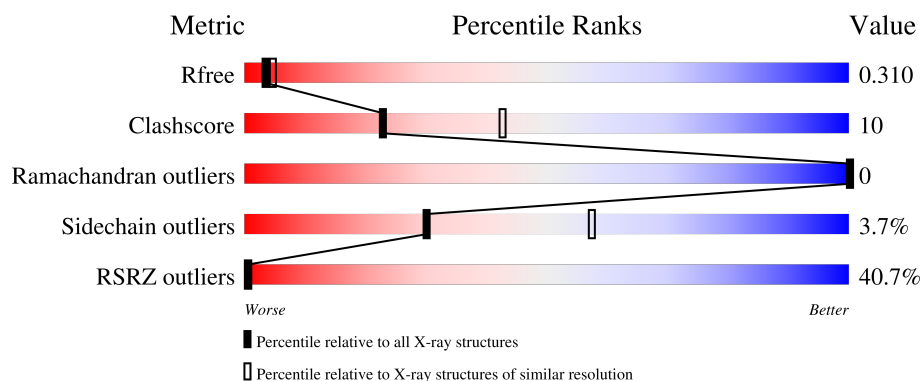
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	38% 75% 18% 6%

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.

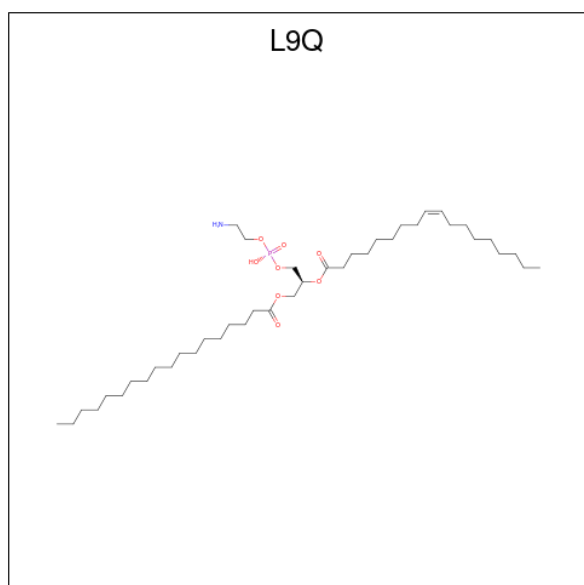
- Molecule 1 is a protein called Membrane protein, MmpL family protein.

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:

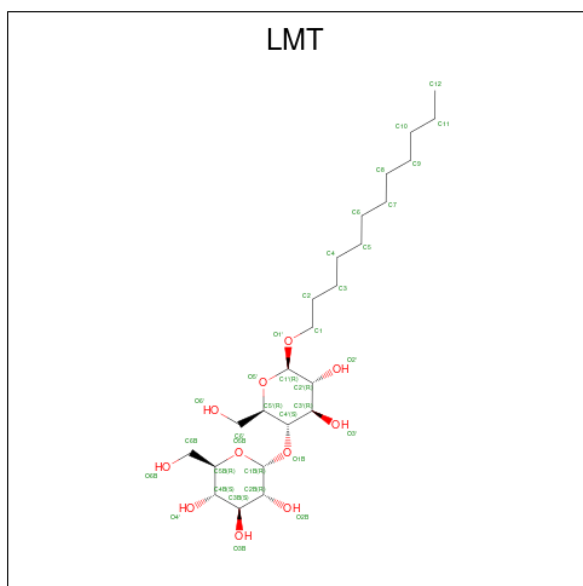
Chain	Residue	Modelled	Actual	Comment	Reference
A	774	HIS	-	expression tag	UNP A0QP27
A	775	HIS	-	expression tag	UNP A0QP27
A	776	HIS	-	expression tag	UNP A0QP27
A	777	HIS	-	expression tag	UNP A0QP27
A	778	HIS	-	expression tag	UNP A0QP27
A	779	HIS	-	expression tag	UNP A0QP27

- Molecule 2 is (1S)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(octadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: L9Q) (formula: C₄₁H₈₀NO₈P).



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

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



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

- Molecule 4 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.81Å 129.46Å 154.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.25 – 2.59 99.25 – 2.59	Depositor EDS
% Data completeness (in resolution range)	92.9 (99.25-2.59) 78.9 (99.25-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.35 (at 2.55Å)	Xtriage
Refinement program	PHENIX (dev_3318: ???)	Depositor
R, R_{free}	0.249 , 0.290 0.284 , 0.310	Depositor DCC
R_{free} test set	1945 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5685	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: L9Q, LMT

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	0.16	0/5704	0.39	3/7762 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	756	LEU	CA-C-N	12.51	132.91	120.52
1	A	756	LEU	C-N-CA	12.51	132.91	120.52
1	A	746	GLN	N-CA-C	-5.23	105.58	111.28

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	102	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	120	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 (120) 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:H16A	2:A:801:L9Q:H37	1.17	1.16
2:A:801:L9Q:H4	2:A:801:L9Q:H1A	1.31	1.06
2:A:801:L9Q:H16A	2:A:801:L9Q:C37	1.99	0.92
1:A:745:VAL:O	1:A:749:LEU:HD13	1.72	0.90
2:A:801:L9Q:H1A	2:A:801:L9Q:HN	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:H1A	2:A:801:L9Q:C4	2.07	0.81
2:A:801:L9Q:H37	2:A:801:L9Q:C16	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:394:VAL:HG12	1:A:398:MET:HE2	1.74	0.70
1:A:65:ARG:HB2	1:A:138:PRO:HB3	1.74	0.69
1:A:280:ARG:HG2	1:A:284:MET:HE2	1.75	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:H1A	2:A:801:L9Q:N	2.07	0.67
3:A:802:LMT:O4'	3:A:802:LMT:O1B	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:H36	2:A:801:L9Q:C41	2.27	0.65
1:A:461:MET:HE1	1:A:474:ILE:HA	1.78	0.64
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:O6'	3:A:802:LMT:H5B	1.98	0.62
2:A:801:L9Q:H41A	2:A:801:L9Q:C36	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:595:MET:HE3	1:A:719:ILE:HG23	1.88	0.55
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:CD1	1:A:749:LEU:N	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:662:MET:HE1	1:A:670:ILE:HG13	1.90	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:182:ILE:HD12	1:A:244:PRO:HG2	1.92	0.51
1:A:749:LEU:N	1:A:749:LEU:HD12	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:579:MET:HE1	1:A:592:ALA:HB3	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: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:281:ARG:HA	1:A:284:MET:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:A:540:HIS:ND1	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:H15	2:A:801:L9Q:H12A	1.81	0.41
1:A:17:ILE:HD12	1:A:340:ILE:HD13	2.02	0.41
1:A:128:GLN:OE1	1:A:128:GLN:N	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:5:TRP:HZ2	1:A:332:THR:HG22	1.85	0.40
1:A:159:GLN:NE2	1:A:166:ILE:O	2.44	0.40
1:A:241:PHE:CE2	1:A:631:MET:HE1	2.56	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

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	729/779 (94%)	705 (97%)	24 (3%)	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	596/643 (93%)	574 (96%)	22 (4%)	30	57

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	38	VAL
1	A	65	ARG
1	A	126	LYS
1	A	166	ILE
1	A	204	VAL
1	A	207	THR
1	A	209	ILE
1	A	253	ILE
1	A	302	VAL
1	A	340	ILE
1	A	352	THR
1	A	387	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	505	ASP
1	A	518	ASN
1	A	540	HIS
1	A	542	ILE
1	A	586	VAL
1	A	595	MET
1	A	632	ILE
1	A	672	THR
1	A	714	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	ASN
1	A	517	GLN
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 oligosaccharides 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	1.28	5 (10%)	52,54,55	1.04	3 (5%)
3	LMT	A	802	-	36,36,36	0.38	0	47,47,47	1.42	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	-	-	24/53/53/54	-
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	3.90	1.53	1.31
2	A	801	L9Q	O3-C11	3.34	1.43	1.33
2	A	801	L9Q	O2-C2	-3.27	1.38	1.46
2	A	801	L9Q	O2-C31	2.83	1.42	1.34
2	A	801	L9Q	O4P-C4	-2.05	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'	-4.40	107.55	117.98
2	A	801	L9Q	O2-C31-C32	3.44	118.91	111.48
3	A	802	LMT	O1'-C1'-C2'	-2.93	103.83	108.27
2	A	801	L9Q	O3-C11-C12	2.88	120.61	111.83
3	A	802	LMT	C4B-C3B-C2B	-2.68	106.12	110.83
3	A	802	LMT	C1-O1'-C1'	-2.51	109.39	113.68
3	A	802	LMT	O2'-C2'-C1'	-2.44	104.26	110.08
3	A	802	LMT	C1'-O5'-C5'	-2.42	108.99	113.72
3	A	802	LMT	O1B-C1B-O5B	-2.24	104.79	110.69
3	A	802	LMT	O5'-C5'-C6'	2.20	111.89	106.44
3	A	802	LMT	O3B-C3B-C2B	-2.17	105.26	110.38
2	A	801	L9Q	C2-O2-C31	-2.14	112.66	117.80

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	L9Q	C1-O3P-P-O2P
2	A	801	L9Q	C1-O3P-P-O4P
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	O5'-C1'-O1'-C1
3	A	802	LMT	C2'-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	C21-C22-C23-C24
2	A	801	L9Q	C32-C33-C34-C35
2	A	801	L9Q	C33-C34-C35-C36
2	A	801	L9Q	C23-C24-C25-C26
2	A	801	L9Q	C16-C17-C18-C19
2	A	801	L9Q	C17-C18-C19-C20
3	A	802	LMT	O5'-C5'-C6'-O6'
2	A	801	L9Q	C20-C21-C22-C23
2	A	801	L9Q	C22-C23-C24-C25
2	A	801	L9Q	C40-C41-C42-C43
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
2	A	801	L9Q	C4-O4P-P-O3P
3	A	802	LMT	C5'-C4'-O1B-C1B
3	A	802	LMT	C3-C4-C5-C6
3	A	802	LMT	C3'-C4'-O1B-C1B
2	A	801	L9Q	C39-C40-C41-C42

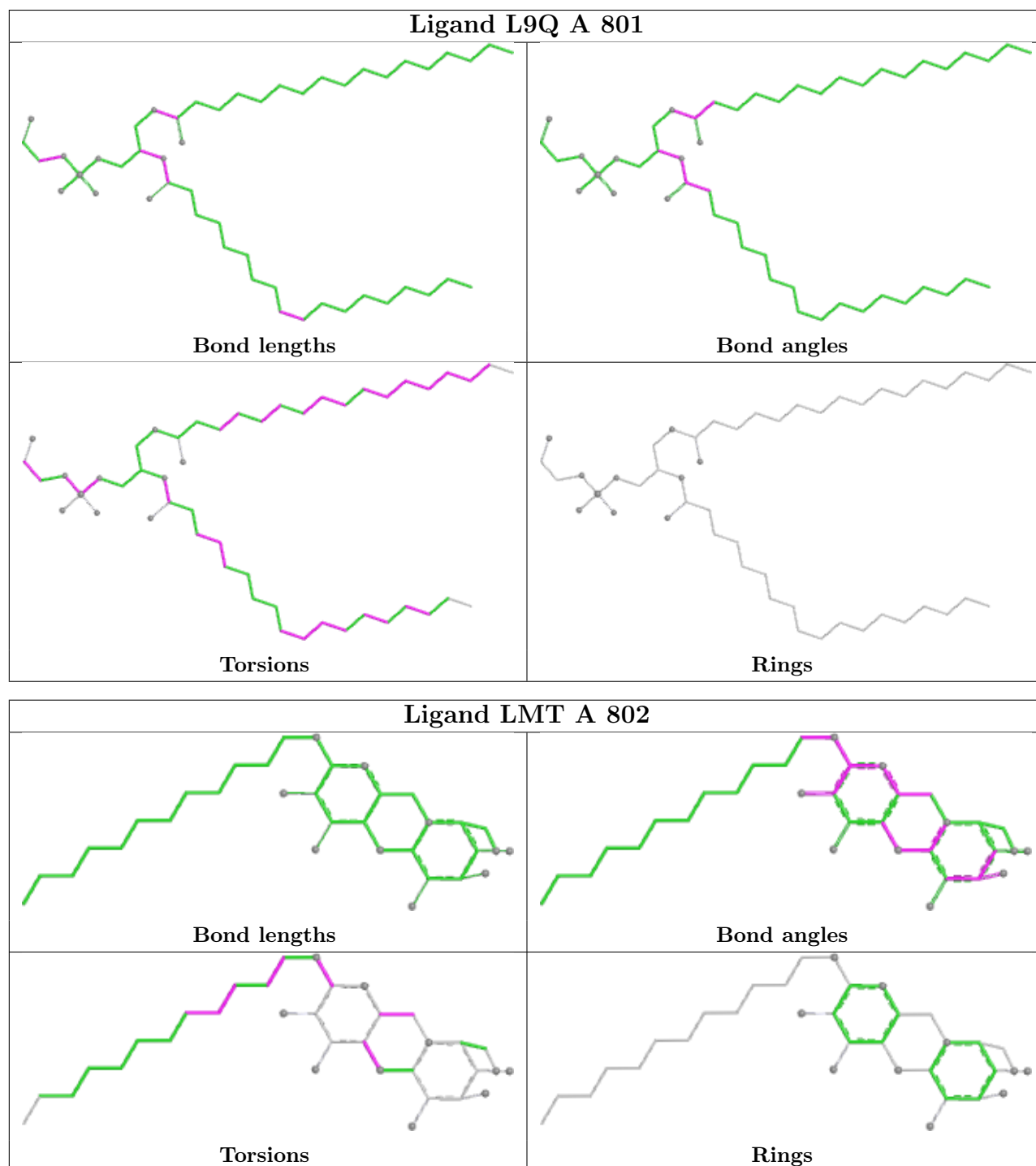
There are no ring outliers.

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

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q<0.9
1	A	732/779 (93%)	2.07	298 (40%) 0 0	30, 99, 146, 203	1 (0%)

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	ASP	11.1
1	A	67	SER	10.6
1	A	120	PRO	10.5
1	A	504	ASN	10.1
1	A	63	ARG	9.8
1	A	749	LEU	9.7
1	A	15	ILE	8.8
1	A	12	PHE	8.4
1	A	66	THR	8.3
1	A	121	THR	8.1
1	A	36	ASN	8.0
1	A	118	THR	7.6
1	A	502	PRO	7.3
1	A	64	ASP	7.2
1	A	152	GLN	6.8
1	A	148	LEU	6.7
1	A	1	MET	6.7
1	A	622	TYR	6.5
1	A	62	GLY	6.2
1	A	204	VAL	6.1
1	A	83	ASP	6.1
1	A	493	ASP	6.1
1	A	747	GLU	6.1
1	A	38	VAL	6.0
1	A	68	HIS	6.0
1	A	396	VAL	6.0
1	A	544	VAL	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	241	PHE	5.9
1	A	88	LYS	5.9
1	A	164	GLY	5.9
1	A	742	MET	5.9
1	A	507	GLY	5.7
1	A	542	ILE	5.7
1	A	19	VAL	5.7
1	A	4	TRP	5.7
1	A	740	ARG	5.6
1	A	694	VAL	5.6
1	A	272	GLY	5.6
1	A	540	HIS	5.6
1	A	696	SER	5.5
1	A	403	ALA	5.5
1	A	452	PHE	5.5
1	A	506	SER	5.5
1	A	203	PHE	5.5
1	A	505	ASP	5.4
1	A	702	LYS	5.3
1	A	748	LYS	5.3
1	A	171	LEU	5.2
1	A	496	LYS	5.2
1	A	697	ASP	5.2
1	A	147	ILE	5.2
1	A	151	TYR	5.1
1	A	750	GLY	5.0
1	A	122	VAL	5.0
1	A	457	LEU	4.9
1	A	144	ASP	4.9
1	A	142	ASP	4.8
1	A	491	ASP	4.8
1	A	454	THR	4.8
1	A	739	PRO	4.6
1	A	11	GLN	4.6
1	A	713	LEU	4.6
1	A	508	SER	4.5
1	A	58	ASP	4.5
1	A	495	GLU	4.5
1	A	59	GLU	4.4
1	A	501	ARG	4.4
1	A	279	VAL	4.4
1	A	624	PRO	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	587	VAL	4.4
1	A	170	GLY	4.3
1	A	433	PRO	4.3
1	A	621	ASN	4.3
1	A	404	PHE	4.3
1	A	347	ALA	4.3
1	A	384	GLU	4.3
1	A	453	ARG	4.2
1	A	65	ARG	4.2
1	A	116	ASP	4.2
1	A	699	VAL	4.2
1	A	79	LYS	4.2
1	A	240[A]	PHE	4.1
1	A	143	ASP	4.1
1	A	620	MET	4.1
1	A	684	LEU	4.0
1	A	695	PHE	4.0
1	A	554	GLN	4.0
1	A	760	ARG	4.0
1	A	69	VAL	4.0
1	A	141	GLY	4.0
1	A	123	SER	4.0
1	A	759	GLU	4.0
1	A	601	GLY	4.0
1	A	383	GLU	3.9
1	A	675	THR	3.9
1	A	172	ASN	3.9
1	A	136	SER	3.9
1	A	741	TRP	3.9
1	A	78	ASP	3.8
1	A	726	ALA	3.8
1	A	432	LEU	3.8
1	A	483	THR	3.8
1	A	416	ILE	3.7
1	A	698	LEU	3.7
1	A	535	ALA	3.7
1	A	110	GLY	3.7
1	A	385	VAL	3.7
1	A	397	VAL	3.7
1	A	348	LEU	3.7
1	A	399	LYS	3.7
1	A	761	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	623	THR	3.6
1	A	85	ALA	3.6
1	A	557	ILE	3.6
1	A	39	THR	3.6
1	A	35	GLY	3.6
1	A	598	LEU	3.6
1	A	680	THR	3.6
1	A	746	GLN	3.6
1	A	541	GLY	3.6
1	A	352	THR	3.5
1	A	459	LEU	3.5
1	A	602	SER	3.5
1	A	663	SER	3.5
1	A	722	PHE	3.5
1	A	92	GLU	3.5
1	A	503	ALA	3.5
1	A	520	LEU	3.5
1	A	169	ALA	3.5
1	A	494	PRO	3.5
1	A	246	VAL	3.4
1	A	527	ALA	3.4
1	A	430	LYS	3.4
1	A	580	PHE	3.4
1	A	139	LEU	3.4
1	A	271	GLU	3.4
1	A	80	LYS	3.3
1	A	473	GLN	3.3
1	A	201	LEU	3.3
1	A	678	LEU	3.3
1	A	400	ARG	3.3
1	A	590	ILE	3.3
1	A	758	ASP	3.3
1	A	117	THR	3.3
1	A	652	SER	3.3
1	A	161	VAL	3.3
1	A	86	TRP	3.3
1	A	472	ALA	3.3
1	A	756	LEU	3.2
1	A	464	GLU	3.2
1	A	410	VAL	3.2
1	A	463	ARG	3.2
1	A	523	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	633	GLY	3.2
1	A	516	ILE	3.2
1	A	425	GLY	3.2
1	A	685	ILE	3.1
1	A	436	ASN	3.1
1	A	387	ARG	3.1
1	A	754	THR	3.1
1	A	604	MET	3.1
1	A	402	ILE	3.1
1	A	131	ARG	3.1
1	A	206	GLY	3.0
1	A	311	PHE	3.0
1	A	70	VAL	3.0
1	A	567	MET	3.0
1	A	448	LEU	3.0
1	A	619	LEU	3.0
1	A	693	PHE	3.0
1	A	468	PRO	2.9
1	A	751	LEU	2.9
1	A	611	PHE	2.9
1	A	735	CYS	2.9
1	A	109	VAL	2.9
1	A	563	LYS	2.9
1	A	650	LEU	2.9
1	A	205	PHE	2.9
1	A	617	SER	2.9
1	A	469	ILE	2.9
1	A	586	VAL	2.9
1	A	140	GLN	2.9
1	A	676	GLY	2.9
1	A	594	LEU	2.9
1	A	635	ILE	2.8
1	A	613	ASP	2.8
1	A	146	GLU	2.8
1	A	239	HIS	2.8
1	A	200	VAL	2.8
1	A	434	PRO	2.8
1	A	14	TYR	2.8
1	A	451	GLY	2.8
1	A	597	ALA	2.8
1	A	281	ARG	2.8
1	A	585	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	16	VAL	2.7
1	A	97	VAL	2.7
1	A	23	LEU	2.7
1	A	683	ALA	2.7
1	A	57	GLY	2.7
1	A	706	PHE	2.7
1	A	278	ALA	2.7
1	A	538	PRO	2.7
1	A	339	ALA	2.7
1	A	677	ARG	2.7
1	A	498	TRP	2.7
1	A	40	GLN	2.7
1	A	614	GLY	2.6
1	A	194	ILE	2.6
1	A	202	PHE	2.6
1	A	393	LEU	2.6
1	A	692	ALA	2.6
1	A	462	LYS	2.6
1	A	138	PRO	2.6
1	A	662	MET	2.6
1	A	753	GLU	2.6
1	A	149	LYS	2.6
1	A	344	ARG	2.6
1	A	345	VAL	2.6
1	A	612	VAL	2.6
1	A	615	HIS	2.6
1	A	346	ASP	2.5
1	A	477	MET	2.5
1	A	270	ALA	2.5
1	A	389	PHE	2.5
1	A	533	LEU	2.5
1	A	392	ARG	2.5
1	A	125	MET	2.5
1	A	492	ASN	2.5
1	A	509	LYS	2.5
1	A	37	HIS	2.5
1	A	335	ALA	2.4
1	A	189	ALA	2.4
1	A	422	LEU	2.4
1	A	631	MET	2.4
1	A	539	PRO	2.4
1	A	530	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	LEU	2.4
1	A	168	LEU	2.4
1	A	616	GLY	2.3
1	A	284	MET	2.3
1	A	743	LYS	2.3
1	A	655	VAL	2.3
1	A	258	GLY	2.3
1	A	296	ILE	2.3
1	A	610	MET	2.3
1	A	235	PHE	2.3
1	A	223	ALA	2.3
1	A	382	ARG	2.3
1	A	534	ARG	2.3
1	A	426	GLY	2.3
1	A	423	SER	2.3
1	A	412	MET	2.3
1	A	700	MET	2.3
1	A	9	VAL	2.3
1	A	199	VAL	2.3
1	A	660	ARG	2.3
1	A	625	GLN	2.2
1	A	579	MET	2.2
1	A	545	PHE	2.2
1	A	757	PRO	2.2
1	A	18	GLY	2.2
1	A	701	MET	2.2
1	A	249	ILE	2.2
1	A	185	ASP	2.2
1	A	465	ASP	2.2
1	A	744	ARG	2.2
1	A	238	VAL	2.2
1	A	245	VAL	2.2
1	A	242	ALA	2.2
1	A	24	CYS	2.2
1	A	424	LEU	2.2
1	A	282	THR	2.1
1	A	7	ARG	2.1
1	A	583	PHE	2.1
1	A	628	MET	2.1
1	A	61	TYR	2.1
1	A	324	MET	2.1
1	A	537	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	175	ALA	2.1
1	A	551	ALA	2.1
1	A	248	LEU	2.1
1	A	166	ILE	2.1
1	A	725	PRO	2.1
1	A	3	ALA	2.1
1	A	526	ALA	2.1
1	A	409	LEU	2.1
1	A	703	TYR	2.1
1	A	176	SER	2.1
1	A	421	GLN	2.0
1	A	90	VAL	2.0
1	A	188	ARG	2.0
1	A	260	PHE	2.0
1	A	627	LEU	2.0
1	A	661	GLY	2.0
1	A	398	MET	2.0
1	A	550	PRO	2.0
1	A	132	HIS	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 oligosaccharides 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, 95th 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.

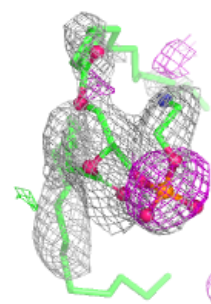
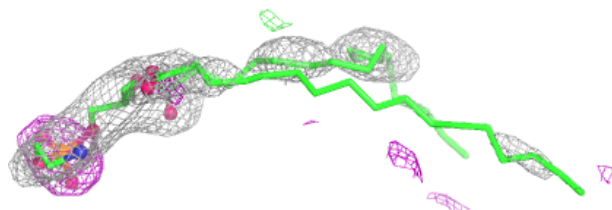
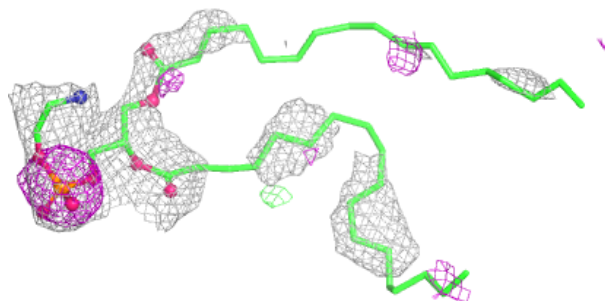
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	L9Q	A	801	50/51	0.78	0.28	81,104,129,139	0
3	LMT	A	802	35/35	0.88	0.19	73,101,128,132	0

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.

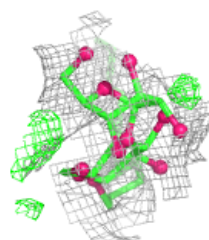
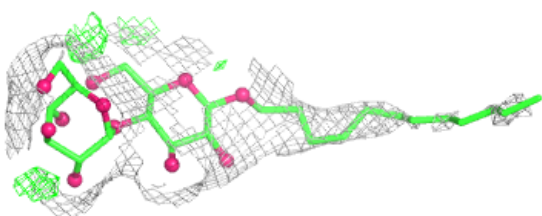
Electron density around L9Q A 801:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.