



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 07:47 PM EDT

PDB ID : 6BMS  
Title : Palmitoyltransferase structure  
Authors : Kumar, P.; Rajashankar, K.  
Deposited on : 2017-11-15  
Resolution : 2.44 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.

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

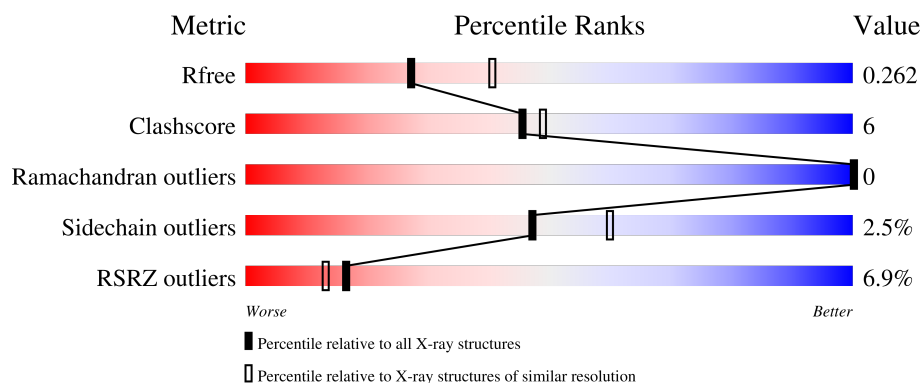
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	341	<div> <div>5%</div> <div>68%</div> <div>14%</div> <div>•</div> <div>18%</div> </div>
1	D	341	<div> <div>6%</div> <div>71%</div> <div>11%</div> <div>•</div> <div>17%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4863 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 Palmitoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2289	1526	371	373	19			
1	D	282	Total	C	N	O	S	0	0	0
			2295	1531	372	374	18			

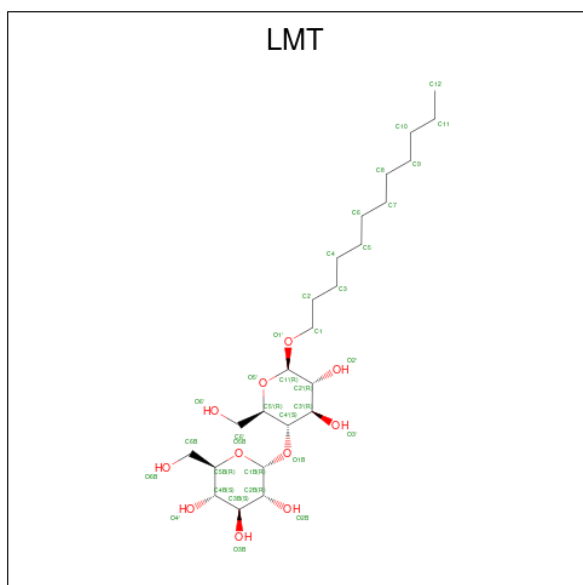
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	expression tag	UNP F1QXD3
A	-11	PRO	-	expression tag	UNP F1QXD3
A	-10	SER	-	expression tag	UNP F1QXD3
A	-9	ARG	-	expression tag	UNP F1QXD3
A	-8	ALA	-	expression tag	UNP F1QXD3
A	-7	THR	-	expression tag	UNP F1QXD3
A	143	SER	CYS	engineered mutation	UNP F1QXD3
A	323	SER	-	expression tag	UNP F1QXD3
A	324	ASN	-	expression tag	UNP F1QXD3
A	325	SER	-	expression tag	UNP F1QXD3
D	-11	GLY	-	expression tag	UNP F1QXD3
D	-10	PRO	-	expression tag	UNP F1QXD3
D	-9	SER	-	expression tag	UNP F1QXD3
D	-8	ARG	-	expression tag	UNP F1QXD3
D	-7	ALA	-	expression tag	UNP F1QXD3
D	-6	THR	-	expression tag	UNP F1QXD3
D	147	SER	CYS	engineered mutation	UNP F1QXD3
D	327	SER	-	expression tag	UNP F1QXD3
D	328	ASN	-	expression tag	UNP F1QXD3
D	329	SER	-	expression tag	UNP F1QXD3

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

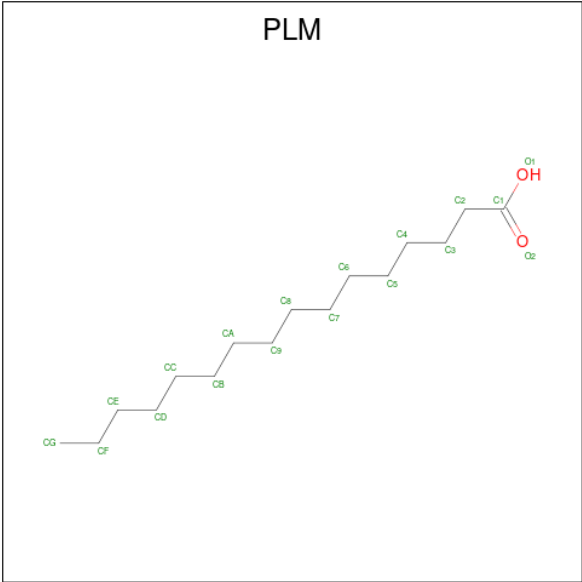
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

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



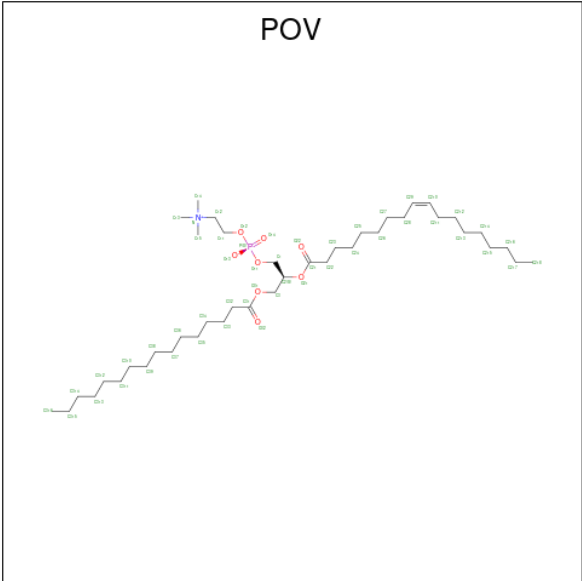
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			31	20	11		
3	A	1	Total	C	O	0	0
			28	17	11		
3	A	1	Total	C	O	0	0
			26	15	11		
3	D	1	Total	C	O	0	0
			29	18	11		
3	D	1	Total	C		0	0
			10	10			

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



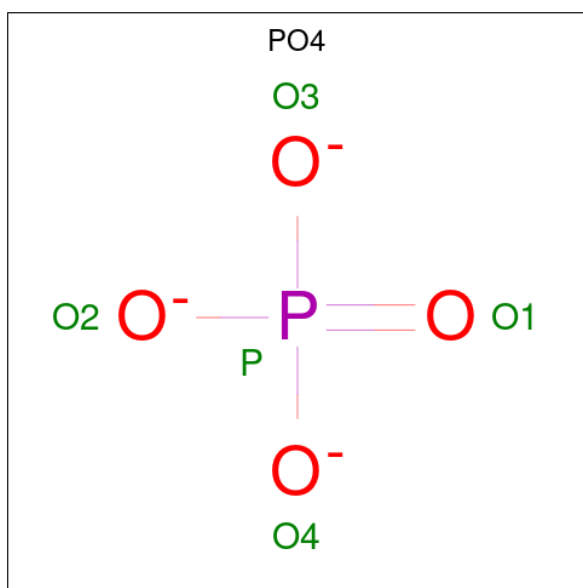
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			18	16	2		
4	D	1	Total	C	O	0	0
			18	16	2		

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		

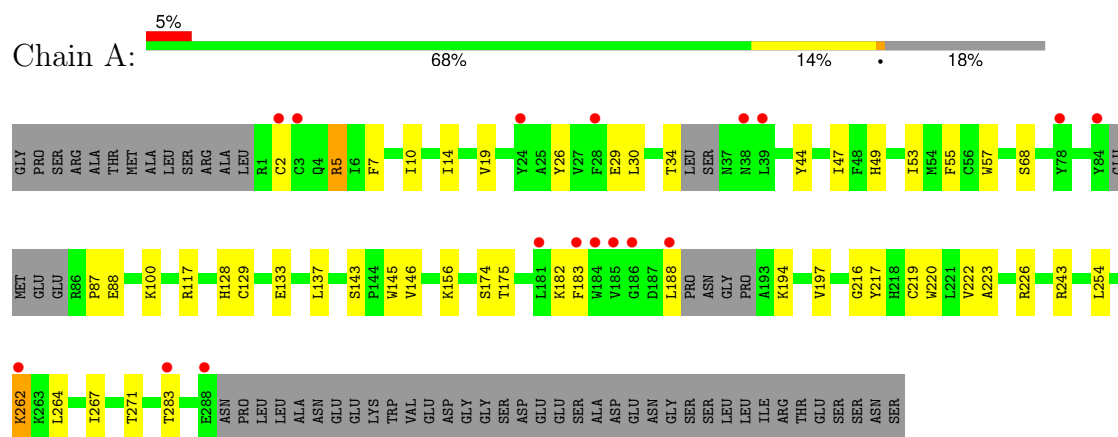
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	26	Total	O	0	0
			26	26		
7	D	22	Total	O	0	0
			22	22		

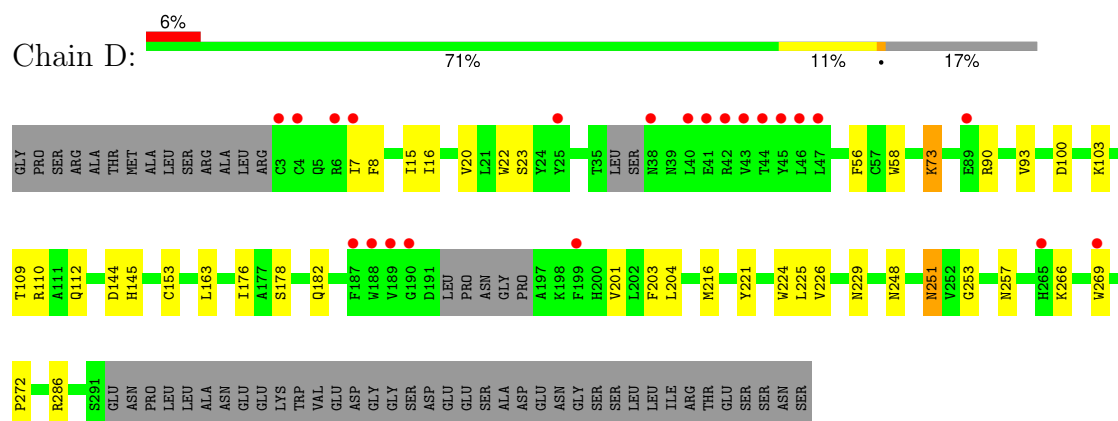
### 3 Residue-property plots [i](#)

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: Palmitoyltransferase



#### • Molecule 1: Palmitoyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.40Å 186.40Å 90.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.21 – 2.44 37.21 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.21-2.44) 99.1 (37.21-2.44)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.233 , 0.261 0.234 , 0.262	Depositor DCC
$R_{free}$ test set	2974 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, LMT, PO4, ZN, PLM

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	0.29	0/2367	0.42	0/3216
1	D	0.28	0/2374	0.41	0/3226
All	All	0.28	0/4741	0.42	0/6442

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

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	2289	0	2205	32	0
1	D	2295	0	2201	30	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
3	A	85	0	85	0	0
3	D	39	0	46	0	0
4	A	18	0	31	1	0
4	D	18	0	31	2	0
5	A	52	0	82	1	0
6	A	5	0	0	0	0
6	D	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	26	0	0	0	0
7	D	22	0	0	0	0
All	All	4863	0	4681	61	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 6.

All (61) 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)
1:A:29:GLU:HB3	1:A:194:LYS:HZ2	1.40	0.86
1:A:29:GLU:HB3	1:A:194:LYS:NZ	2.00	0.76
1:A:14:ILE:HG12	1:D:15:ILE:HG12	1.76	0.66
1:A:183:PHE:HA	1:A:188:LEU:HD23	1.77	0.66
1:A:29:GLU:CB	1:A:194:LYS:HZ2	2.13	0.61
1:A:34:THR:HG22	1:A:182:LYS:HE3	1.82	0.60
1:A:7:PHE:HA	1:A:10:ILE:HD12	1.81	0.60
1:A:44:TYR:HA	1:A:47:ILE:HD12	1.84	0.59
1:D:73:LYS:HD3	1:D:73:LYS:H	1.68	0.59
1:A:26:TYR:HA	1:A:30:LEU:HD12	1.85	0.59
1:D:7:ILE:HD12	1:D:8:PHE:CD1	2.39	0.58
1:A:262:LYS:HD2	1:A:262:LYS:H	1.68	0.57
1:A:264:LEU:HD22	1:A:267:ILE:HD11	1.87	0.56
1:D:178:SER:O	1:D:182:GLN:HG2	2.07	0.54
1:A:68:SER:HB3	1:A:137:LEU:HD12	1.90	0.54
1:D:7:ILE:HD12	1:D:8:PHE:HD1	1.73	0.53
1:A:49:HIS:O	1:A:53:ILE:HG13	2.08	0.53
1:D:109:THR:O	1:D:110:ARG:NH1	2.42	0.52
1:A:194:LYS:O	1:A:197:VAL:HG22	2.09	0.52
1:A:183:PHE:HA	1:A:188:LEU:CD2	2.39	0.52
1:D:73:LYS:H	1:D:73:LYS:CD	2.23	0.52
1:D:201:VAL:O	1:D:204:LEU:HB2	2.10	0.50
1:D:248:ASN:O	1:D:286:ARG:HD2	2.12	0.50
1:D:23:SER:HB2	1:D:176:ILE:HD13	1.94	0.49
1:A:223:ALA:HB2	5:A:1007:POV:H21C	1.95	0.48
1:D:7:ILE:CD1	1:D:8:PHE:CD1	2.96	0.48
1:A:217:TYR:O	1:A:220:TRP:HB3	2.12	0.48
1:D:266:LYS:HA	1:D:269:TRP:CD1	2.49	0.48
1:A:117:ARG:HH11	1:A:128:HIS:CD2	2.31	0.47
1:A:216:GLY:O	1:A:219:CYS:HB2	2.14	0.47
1:A:129:CYS:O	1:A:133:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ASN:HD22	1:D:251:ASN:C	2.19	0.46
1:D:22:TRP:HH2	1:D:203:PHE:HD2	1.64	0.46
1:D:73:LYS:HD3	1:D:73:LYS:N	2.29	0.46
1:D:145:HIS:NE2	4:D:1004:PLM:O2	2.49	0.46
1:D:221:TYR:CZ	1:D:225:LEU:HD11	2.51	0.45
1:A:19:VAL:HG21	1:A:55:PHE:CZ	2.51	0.45
1:D:144:ASP:OD2	1:D:145:HIS:ND1	2.41	0.45
1:A:145:TRP:HB2	4:A:1006:PLM:H21	2.00	0.44
1:A:222:VAL:HG12	1:A:254:LEU:HD23	1.99	0.44
1:D:16:ILE:HD12	4:D:1004:PLM:H81	1.99	0.44
1:D:90:ARG:HE	1:D:93:VAL:HG21	1.82	0.44
1:D:20:VAL:HG21	1:D:56:PHE:CE1	2.52	0.44
1:A:143:SER:HB3	1:A:146:VAL:HG22	1.98	0.44
1:A:2:CYS:HA	1:A:5:ARG:CZ	2.49	0.43
1:A:26:TYR:HD1	1:A:175:THR:HG21	1.82	0.43
1:A:26:TYR:CD1	1:A:175:THR:HG21	2.54	0.43
1:D:58:TRP:CE2	1:D:272:PRO:HG2	2.54	0.43
1:D:163:LEU:HD11	1:D:226:VAL:HG21	2.00	0.43
1:A:226:ARG:NH2	1:A:243:ARG:O	2.52	0.43
1:A:87:PRO:HG2	1:A:88:GLU:OE1	2.19	0.42
1:D:7:ILE:HD11	1:D:8:PHE:CE1	2.53	0.42
1:D:221:TYR:O	1:D:224:TRP:HB3	2.19	0.42
1:A:156:LYS:HD2	1:A:271:THR:HG22	2.01	0.41
1:D:251:ASN:ND2	1:D:253:GLY:H	2.18	0.41
1:A:156:LYS:NZ	1:A:264:LEU:O	2.50	0.41
1:D:204:LEU:HD23	1:D:204:LEU:HA	1.91	0.41
1:D:20:VAL:HG21	1:D:56:PHE:CZ	2.56	0.41
1:D:229:ASN:HB2	1:D:257:ASN:CG	2.42	0.41
1:D:103:LYS:HE3	1:D:103:LYS:HB2	1.91	0.40
1:A:29:GLU:CG	1:A:194:LYS:HZ2	2.35	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	273/341 (80%)	261 (96%)	12 (4%)	0	100	100
1	D	276/341 (81%)	272 (99%)	4 (1%)	0	100	100
All	All	549/682 (80%)	533 (97%)	16 (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	246/311 (79%)	240 (98%)	6 (2%)	49	61
1	D	243/311 (78%)	237 (98%)	6 (2%)	47	60
All	All	489/622 (79%)	477 (98%)	12 (2%)	47	60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	57	TRP
1	A	100	LYS
1	A	174	SER
1	A	262	LYS
1	A	283	THR
1	D	73	LYS
1	D	100	ASP
1	D	112	GLN
1	D	153	CYS
1	D	216	MET
1	D	251	ASN

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

Mol	Chain	Res	Type
1	A	273	GLN
1	D	146	HIS
1	D	251	ASN
1	D	277	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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z  > 2$
6	PO4	A	1008	-	4,4,4	0.96	0	6,6,6	0.47	0
3	LMT	D	1007	-	9,9,36	0.32	0	8,8,47	0.77	0
6	PO4	D	1005	-	4,4,4	0.97	0	6,6,6	0.45	0
6	PO4	D	1006	-	4,4,4	0.96	0	6,6,6	0.46	0
4	PLM	A	1006	-	17,17,17	0.90	1 (5%)	17,17,17	0.90	2 (11%)
3	LMT	A	1004	-	29,29,36	1.25	5 (17%)	40,40,47	1.01	1 (2%)
3	LMT	A	1005	-	26,26,36	1.26	5 (19%)	36,36,47	1.10	3 (8%)
3	LMT	D	1003	-	30,30,36	1.19	4 (13%)	41,41,47	0.94	2 (4%)
3	LMT	A	1003	-	32,32,36	1.14	3 (9%)	43,43,47	1.28	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	POV	A	1007	-	51,51,51	0.97	2 (3%)	57,59,59	0.98	3 (5%)
4	PLM	D	1004	-	17,17,17	0.88	1 (5%)	17,17,17	0.88	2 (11%)

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
3	LMT	D	1007	-	-	5/7/7/61	-
4	PLM	A	1006	-	-	2/15/15/15	-
3	LMT	A	1004	-	-	7/14/54/61	0/2/2/2
3	LMT	A	1005	-	-	2/8/48/61	0/2/2/2
3	LMT	D	1003	-	-	8/15/55/61	0/2/2/2
3	LMT	A	1003	-	-	9/17/57/61	0/2/2/2
5	POV	A	1007	-	-	12/55/55/55	-
4	PLM	D	1004	-	-	6/15/15/15	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	POV	O31-C31	4.29	1.45	1.33
5	A	1007	POV	O21-C21	4.22	1.46	1.34
4	A	1006	PLM	C2-C1	2.95	1.57	1.50
4	D	1004	PLM	C2-C1	2.81	1.57	1.50
3	D	1003	LMT	O3'-C3'	-2.57	1.36	1.43
3	A	1003	LMT	O3'-C3'	-2.49	1.36	1.43
3	A	1004	LMT	O3'-C3'	-2.47	1.36	1.43
3	A	1005	LMT	O3'-C3'	-2.46	1.36	1.43
3	A	1003	LMT	O2B-C2B	-2.34	1.37	1.43
3	A	1005	LMT	O2B-C2B	-2.26	1.37	1.43
3	D	1003	LMT	O2'-C2'	-2.20	1.37	1.43
3	A	1003	LMT	O3B-C3B	-2.18	1.37	1.43
3	D	1003	LMT	O2B-C2B	-2.18	1.37	1.43
3	A	1004	LMT	O2'-C2'	-2.18	1.37	1.43
3	D	1003	LMT	O3B-C3B	-2.17	1.37	1.43
3	A	1004	LMT	O3B-C3B	-2.14	1.37	1.43
3	A	1005	LMT	O4'-C4B	-2.13	1.37	1.43
3	A	1005	LMT	O2'-C2'	-2.13	1.37	1.43
3	A	1005	LMT	O3B-C3B	-2.12	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1004	LMT	O1'-C1'	-2.10	1.36	1.40
3	A	1004	LMT	O2B-C2B	-2.03	1.37	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	LMT	C3'-C4'-C5'	-4.24	101.53	110.93
5	A	1007	POV	O21-C21-C22	4.18	120.53	111.48
3	A	1004	LMT	C1'-O5'-C5'	-2.98	107.91	113.72
4	A	1006	PLM	O2-C1-C2	-2.76	114.35	123.09
5	A	1007	POV	O31-C31-C32	2.71	120.09	111.83
4	D	1004	PLM	O2-C1-C2	-2.69	114.56	123.09
3	A	1005	LMT	O5B-C5B-C4B	2.60	114.39	109.70
3	A	1005	LMT	C1'-O5'-C5'	-2.56	108.70	113.65
5	A	1007	POV	C2-O21-C21	-2.45	111.93	117.80
3	A	1005	LMT	C3'-C4'-C5'	-2.32	105.79	110.93
3	A	1003	LMT	O1B-C4'-C3'	2.31	113.11	107.23
4	A	1006	PLM	O1-C1-O2	2.11	128.76	123.33
4	D	1004	PLM	O1-C1-O2	2.09	128.72	123.33
3	D	1003	LMT	C1'-O5'-C5'	-2.09	109.65	113.72
3	D	1003	LMT	C3'-C4'-C5'	-2.06	106.37	110.93
3	A	1003	LMT	C1'-C2'-C3'	2.05	114.33	110.01

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	LMT	O5'-C1'-O1'-C1
3	D	1003	LMT	C2-C1-O1'-C1'
3	A	1004	LMT	C4'-C5'-C6'-O6'
3	A	1003	LMT	C3'-C4'-O1B-C1B
3	A	1004	LMT	O5'-C5'-C6'-O6'
3	A	1003	LMT	O5'-C5'-C6'-O6'
3	A	1003	LMT	C4'-C5'-C6'-O6'
3	A	1004	LMT	O1'-C1-C2-C3
3	A	1003	LMT	O1'-C1-C2-C3
3	A	1003	LMT	C4B-C5B-C6B-O6B
3	D	1003	LMT	C2'-C1'-O1'-C1
3	D	1003	LMT	O5'-C1'-O1'-C1
3	D	1003	LMT	O5B-C5B-C6B-O6B
5	A	1007	POV	C37-C38-C39-C310
3	D	1003	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	A	1007	POV	C35-C36-C37-C38
3	D	1003	LMT	O1'-C1-C2-C3
5	A	1007	POV	C32-C33-C34-C35
5	A	1007	POV	C26-C27-C28-C29
4	D	1004	PLM	C9-CA-CB-CC
3	A	1004	LMT	C1-C2-C3-C4
3	A	1003	LMT	O5B-C5B-C6B-O6B
4	D	1004	PLM	CB-CC-CD-CE
3	A	1004	LMT	O5B-C5B-C6B-O6B
3	A	1003	LMT	C5'-C4'-O1B-C1B
5	A	1007	POV	C215-C216-C217-C218
3	A	1003	LMT	C3-C4-C5-C6
3	D	1003	LMT	C3-C4-C5-C6
4	D	1004	PLM	CD-CE-CF-CG
5	A	1007	POV	C311-C310-C39-C38
3	D	1007	LMT	C7-C8-C9-C10
3	A	1005	LMT	C4B-C5B-C6B-O6B
3	D	1007	LMT	C2-C3-C4-C5
3	D	1003	LMT	C4'-C5'-C6'-O6'
3	D	1007	LMT	C6-C7-C8-C9
5	A	1007	POV	O12-C11-C12-N
5	A	1007	POV	C312-C313-C314-C315
3	D	1007	LMT	C5-C6-C7-C8
4	D	1004	PLM	C1-C2-C3-C4
3	A	1004	LMT	C2-C1-O1'-C1'
3	A	1005	LMT	C5'-C4'-O1B-C1B
4	A	1006	PLM	C9-CA-CB-CC
4	D	1004	PLM	O1-C1-C2-C3
4	A	1006	PLM	CD-CE-CF-CG
4	D	1004	PLM	O2-C1-C2-C3
3	D	1007	LMT	C4-C5-C6-C7
3	A	1004	LMT	C5'-C4'-O1B-C1B
5	A	1007	POV	C23-C24-C25-C26
5	A	1007	POV	C29-C210-C211-C212
5	A	1007	POV	C212-C213-C214-C215
5	A	1007	POV	C11-C12-N-C15

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1006	PLM	1	0

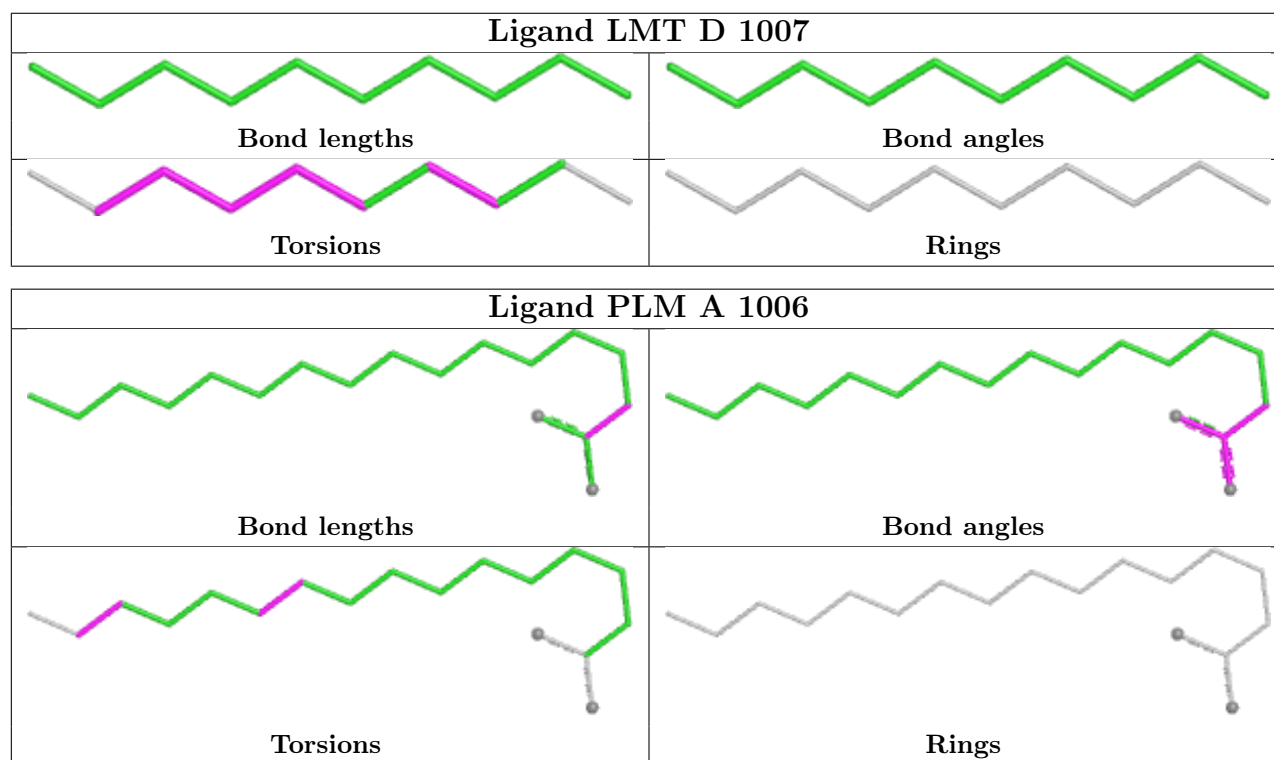
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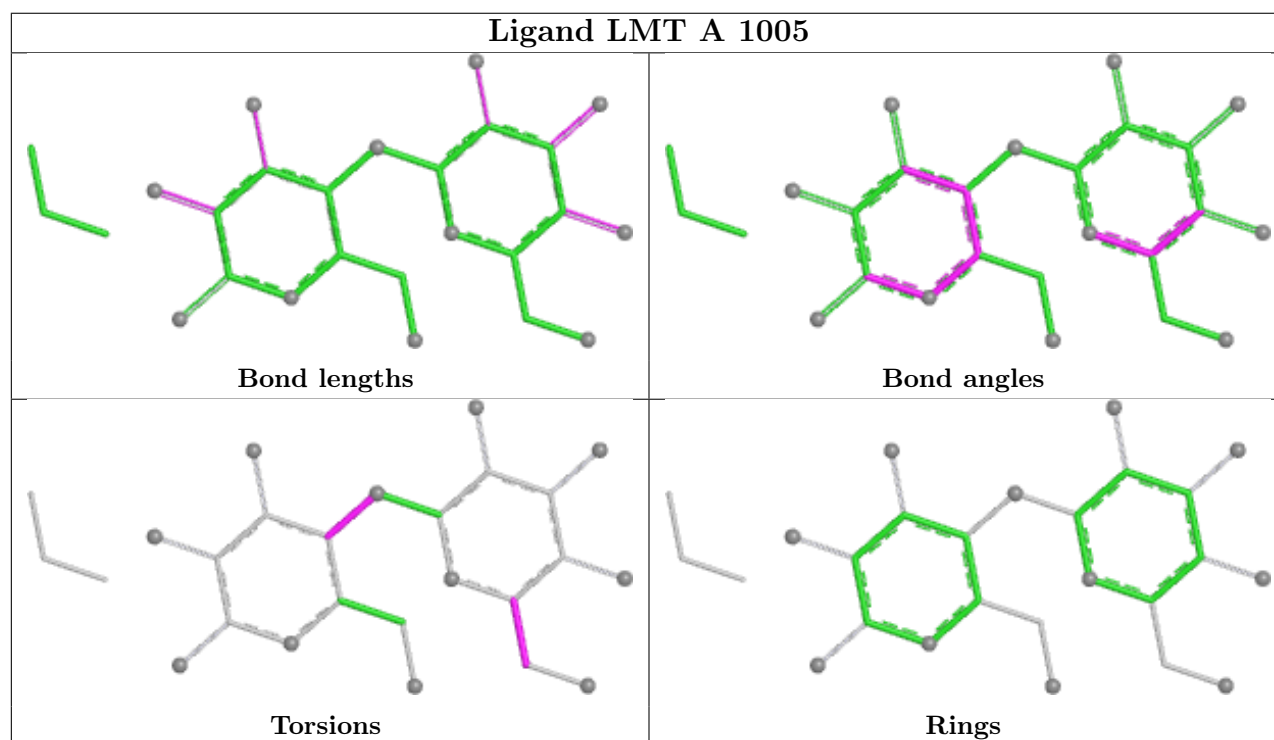
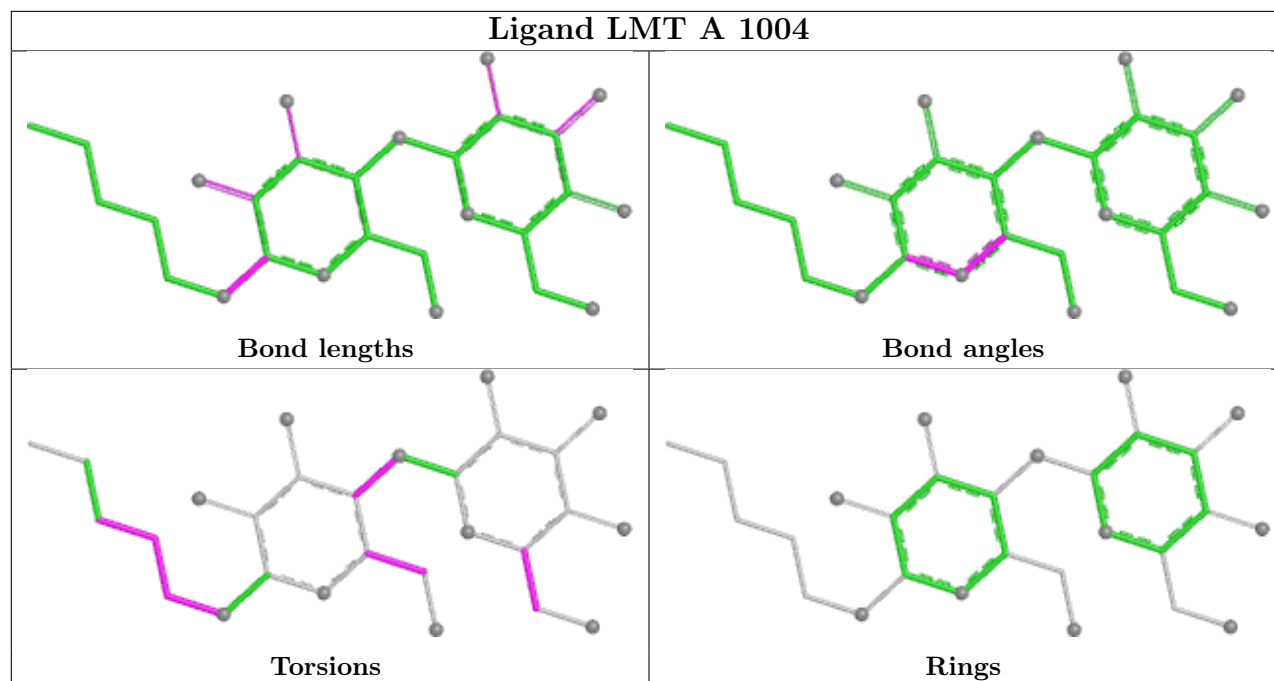


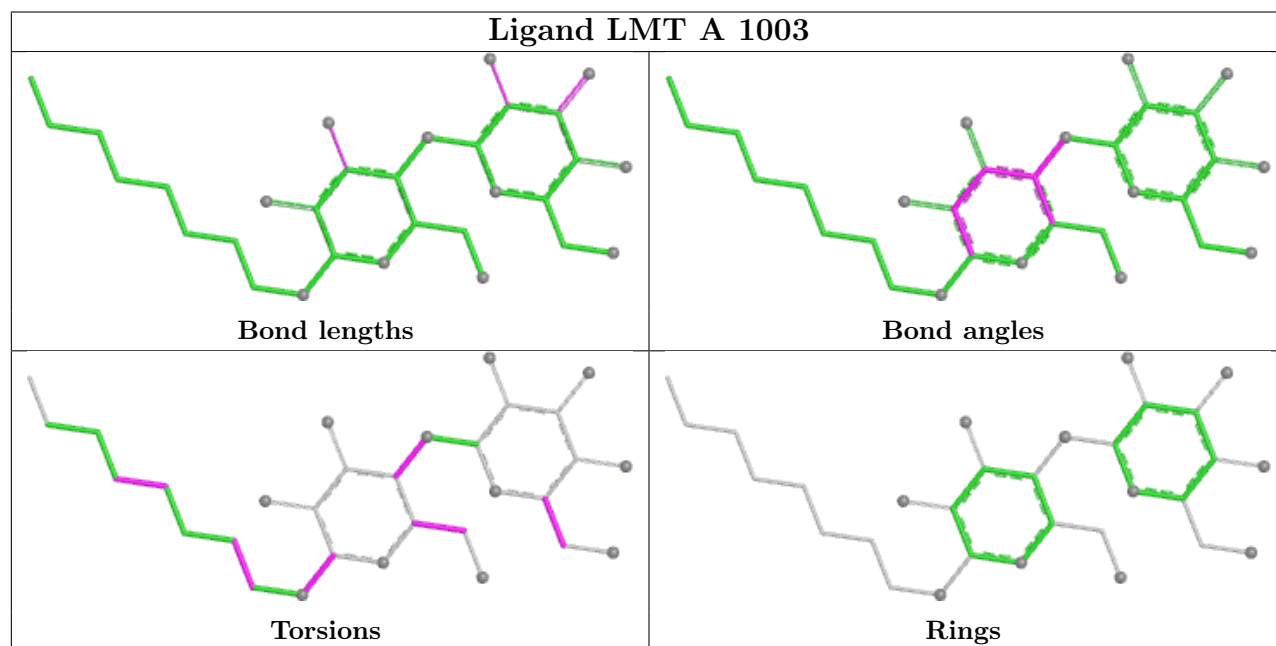
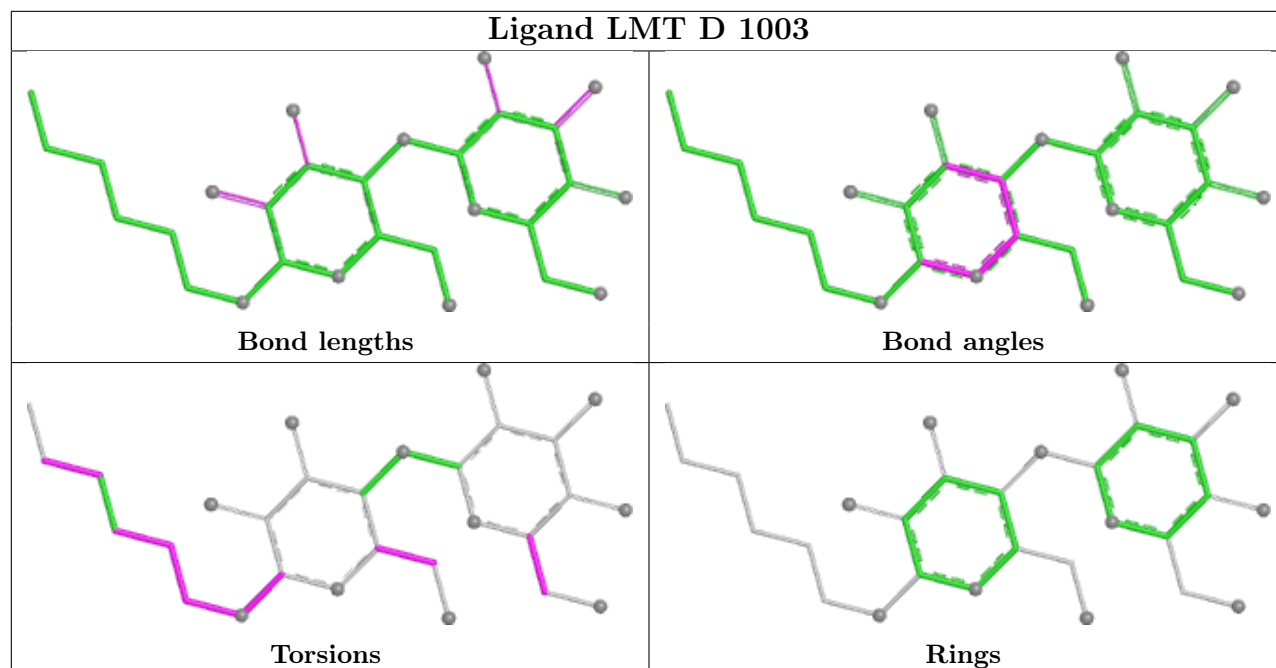
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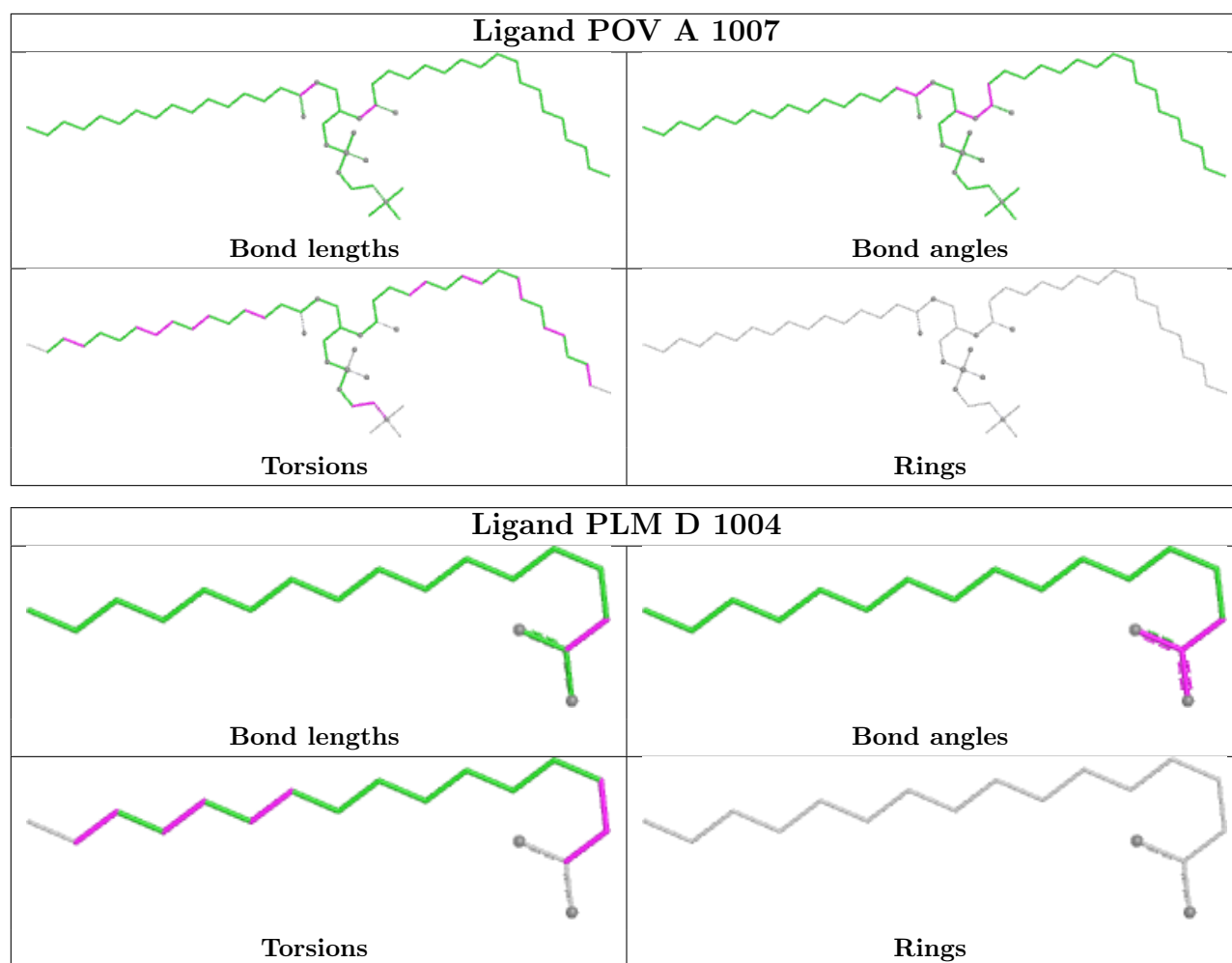
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1007	POV	1	0
4	D	1004	PLM	2	0

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.









## 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, 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	281/341 (82%)	0.13	17 (6%)	21 18	45, 68, 133, 163	0
1	D	282/341 (82%)	0.21	22 (7%)	13 10	48, 69, 110, 141	0
All	All	563/682 (82%)	0.17	39 (6%)	16 13	45, 69, 124, 163	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	GLY	4.1
1	D	43	VAL	4.0
1	A	38	ASN	4.0
1	D	188	TRP	3.7
1	A	184	TRP	3.6
1	D	38	ASN	3.5
1	D	40	LEU	3.5
1	A	39	LEU	3.3
1	D	187	PHE	3.3
1	A	2	CYS	3.3
1	D	42	ARG	3.3
1	D	45	TYR	3.1
1	A	181	LEU	3.0
1	D	3	CYS	2.9
1	D	265	HIS	2.9
1	D	41	GLU	2.7
1	A	188	LEU	2.7
1	D	6	ARG	2.6
1	A	183	PHE	2.6
1	A	185	VAL	2.5
1	D	89	GLU	2.5
1	D	46	LEU	2.5
1	A	288	GLU	2.5
1	D	189	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	28	PHE	2.3
1	A	24	TYR	2.3
1	D	269	TRP	2.3
1	D	25	TYR	2.2
1	D	190	GLY	2.2
1	A	283	THR	2.2
1	A	84	TYR	2.2
1	D	199	PHE	2.2
1	A	262	LYS	2.1
1	D	44	THR	2.1
1	D	7	ILE	2.1
1	D	47	LEU	2.1
1	D	4	CYS	2.1
1	A	3	CYS	2.1
1	A	78	TYR	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
5	POV	A	1007	52/52	0.59	0.34	86,126,154,158	0
3	LMT	D	1007	10/35	0.72	0.17	92,106,111,112	0
6	PO4	D	1006	5/5	0.77	0.27	144,153,158,158	0
6	PO4	A	1008	5/5	0.79	0.36	128,136,141,141	0
3	LMT	A	1005	26/35	0.80	0.27	83,119,130,135	0
3	LMT	A	1004	28/35	0.84	0.19	75,99,122,126	0
3	LMT	D	1003	29/35	0.85	0.19	57,91,123,125	0
4	PLM	D	1004	18/18	0.86	0.37	69,78,108,108	0

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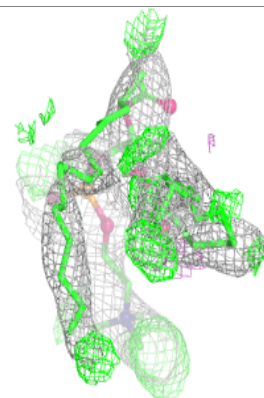
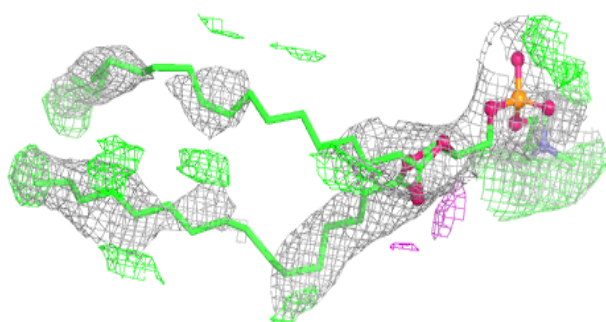
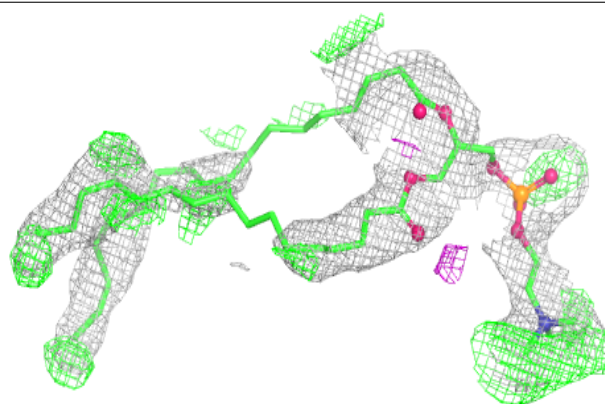
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LMT	A	1003	31/35	0.87	0.20	75,90,117,127	0
6	PO4	D	1005	5/5	0.88	0.21	144,145,146,151	0
4	PLM	A	1006	18/18	0.95	0.21	66,76,87,88	0
2	ZN	A	1002	1/1	0.98	0.11	61,61,61,61	0
2	ZN	D	1001	1/1	0.99	0.13	63,63,63,63	0
2	ZN	A	1001	1/1	0.99	0.12	58,58,58,58	0
2	ZN	D	1002	1/1	1.00	0.14	63,63,63,63	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.

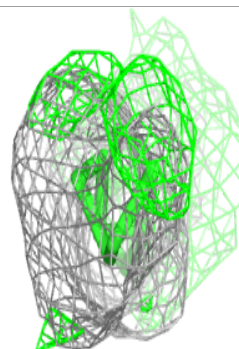
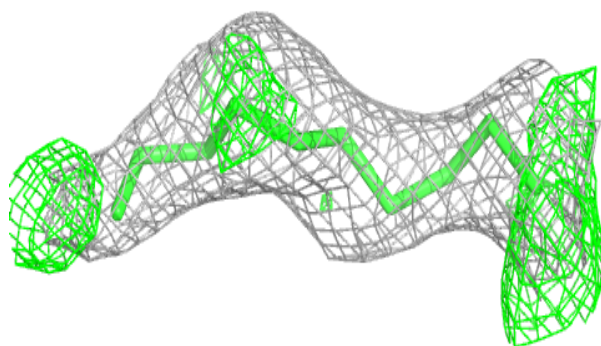
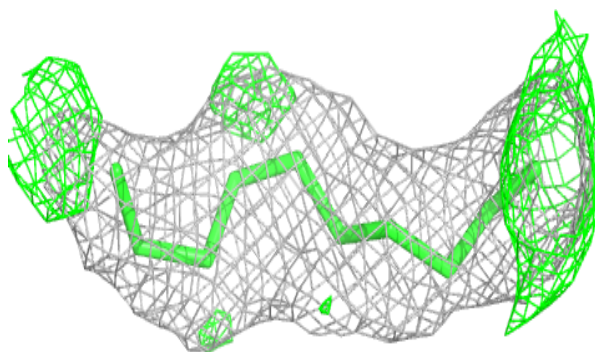
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mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

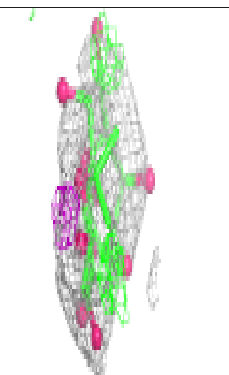
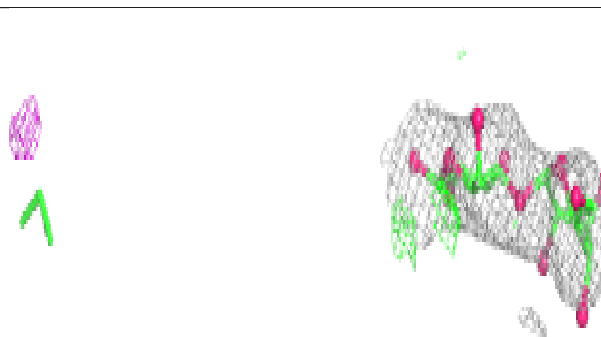
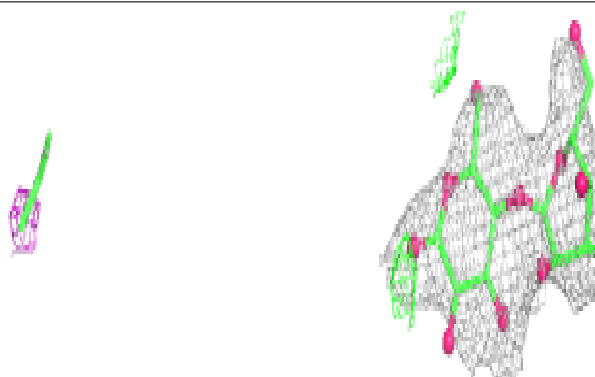


**Electron density around LMT D 1007:**

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

**Electron density around LMT A 1005:**

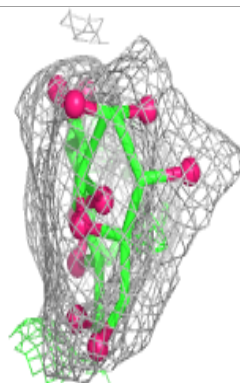
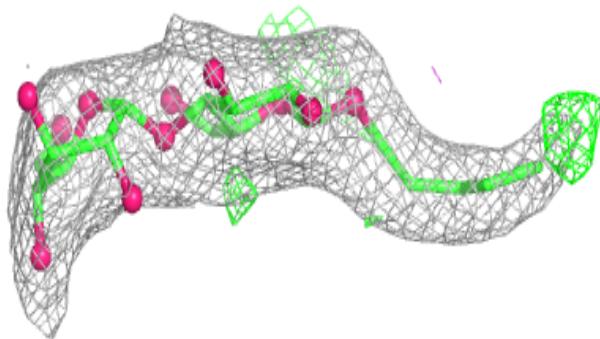
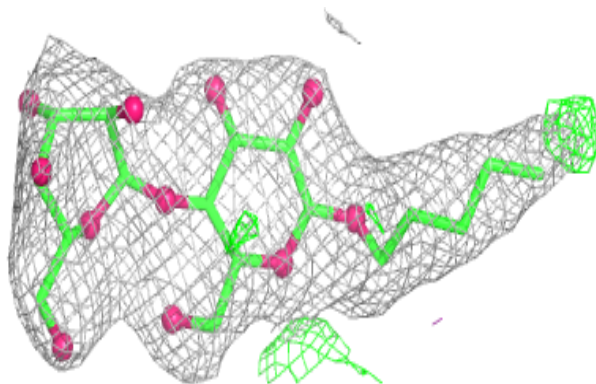
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



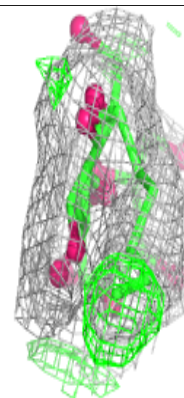
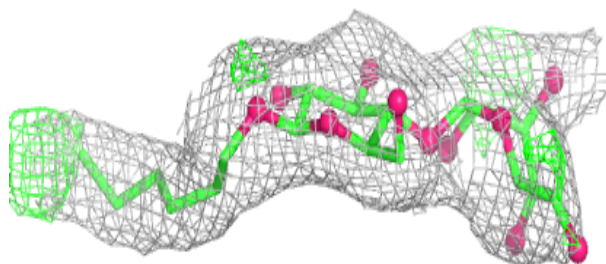
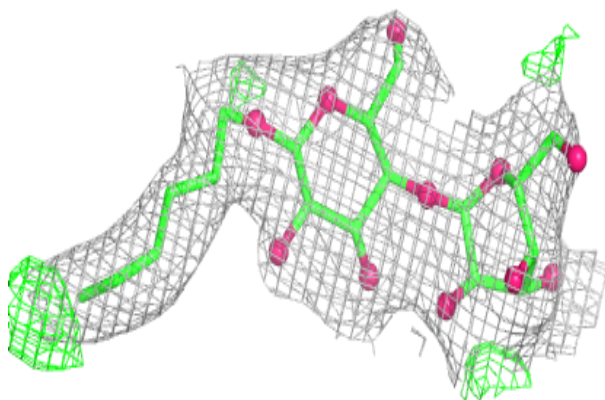


**Electron density around LMT A 1004:**

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and green (positive)

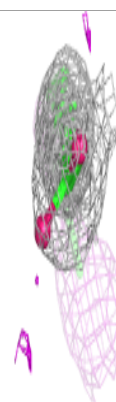
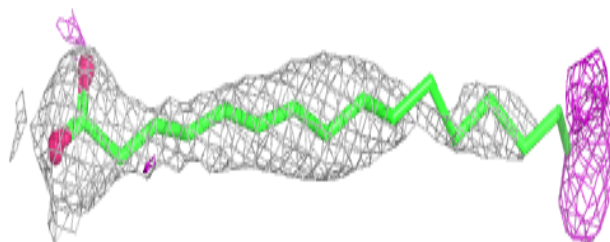
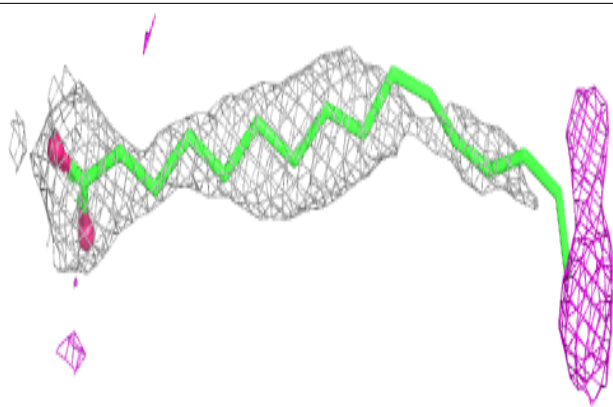
**Electron density around LMT D 1003:**

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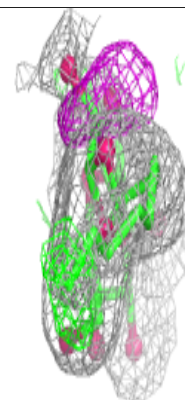
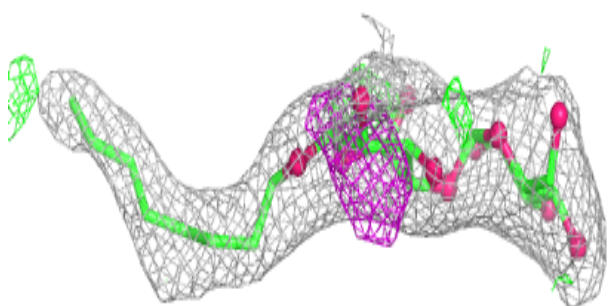
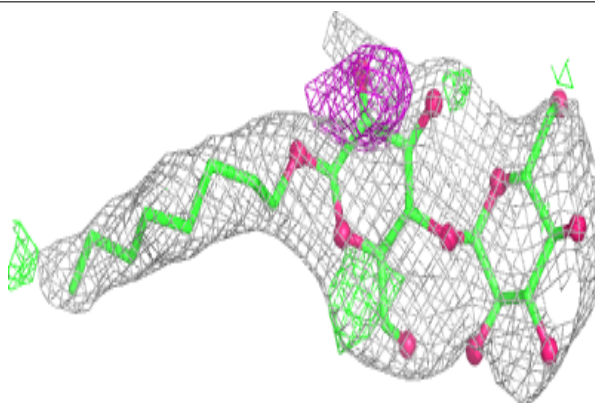


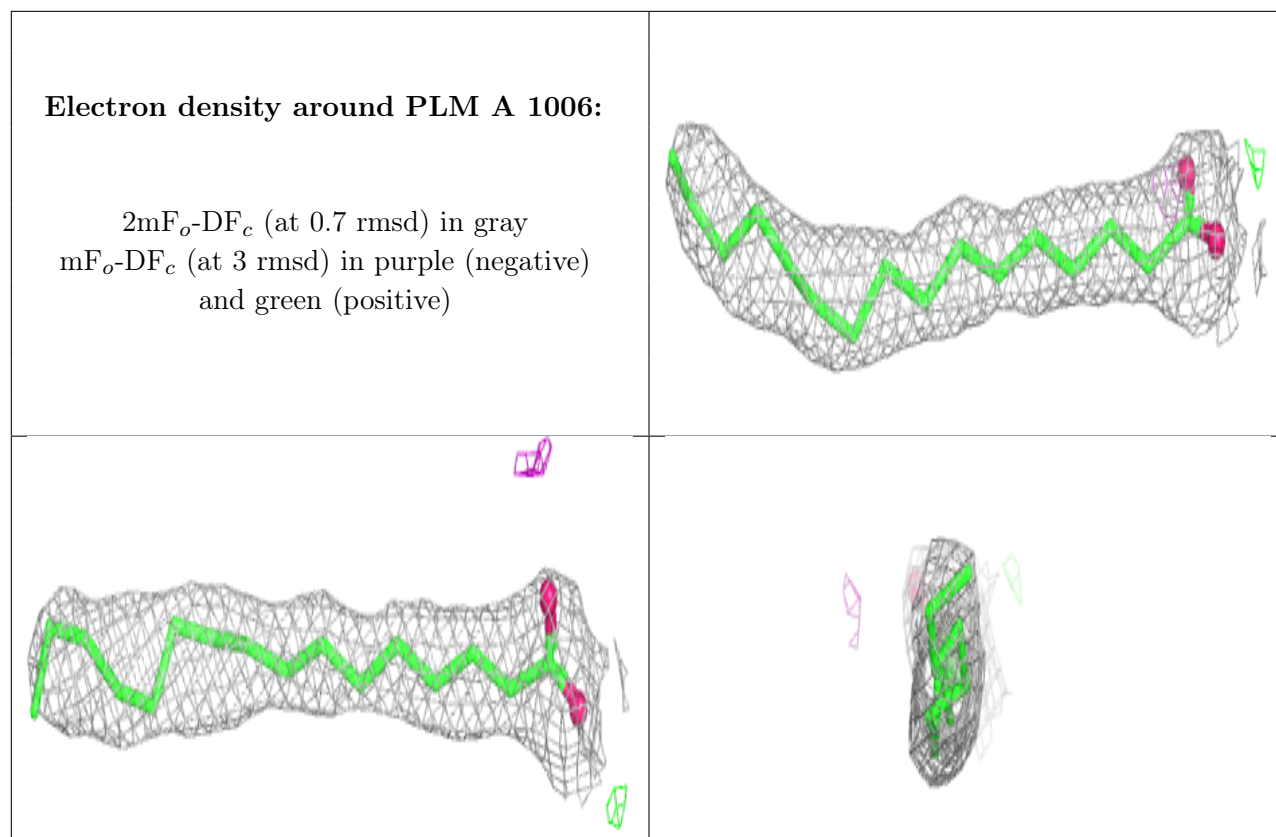
**Electron density around PLM D 1004:**

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and green (positive)

**Electron density around LMT A 1003:**

$2mF_o-DF_c$  (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.