



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:43 pm BST

PDB ID : 6AJG
Title : Crystal structure of mycolic acid transporter MmpL3 from Mycobacterium smegmatis complexed with SQ109
Authors : Zhang, B.; Li, J.; Yang, X.L.; Wu, L.J.; Yang, H.T.; Rao, Z.H.
Deposited on : 2018-08-27
Resolution : 2.60 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 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 : 2.11
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) : 2.11

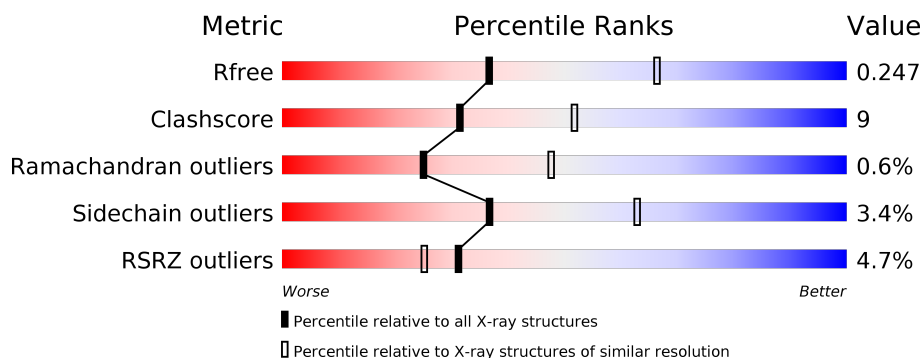
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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 ≥ 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	943	<div> <div>4%</div> <div>80%</div> <div>13%</div> <div>5%</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
3	LMT	A	1006	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7281 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 Drug exporters of the RND superfamily-like protein, Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	900	Total	C	N	O	S	0	0	0
			6952	4482	1182	1256	32			

There are 37 discrepancies between the modelled and reference sequences:

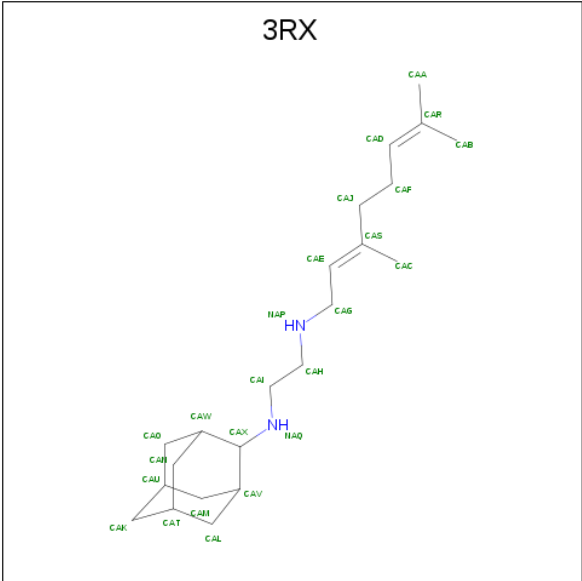
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP I7G2R2
A	-11	PRO	-	expression tag	UNP I7G2R2
A	-10	GLU	-	expression tag	UNP I7G2R2
A	-9	VAL	-	expression tag	UNP I7G2R2
A	-8	VAL	-	expression tag	UNP I7G2R2
A	-7	GLY	-	expression tag	UNP I7G2R2
A	-6	SER	-	expression tag	UNP I7G2R2
A	-5	TYR	-	expression tag	UNP I7G2R2
A	-4	PHE	-	expression tag	UNP I7G2R2
A	-3	GLN	-	expression tag	UNP I7G2R2
A	-2	SER	-	expression tag	UNP I7G2R2
A	-1	ASN	-	expression tag	UNP I7G2R2
A	0	ALA	-	expression tag	UNP I7G2R2
A	749	GLU	-	linker	UNP I7G2R2
A	750	PHE	-	linker	UNP I7G2R2
A	803	THR	CYS	engineered mutation	UNP D9IEF7
A	846	ALA	CYS	engineered mutation	UNP D9IEF7
A	911	GLU	-	expression tag	UNP D9IEF7
A	912	PHE	-	expression tag	UNP D9IEF7
A	913	HIS	-	expression tag	UNP D9IEF7
A	914	LEU	-	expression tag	UNP D9IEF7
A	915	GLY	-	expression tag	UNP D9IEF7
A	916	GLY	-	expression tag	UNP D9IEF7
A	917	ILE	-	expression tag	UNP D9IEF7
A	918	LYS	-	expression tag	UNP D9IEF7
A	919	ALA	-	expression tag	UNP D9IEF7
A	920	PHE	-	expression tag	UNP D9IEF7

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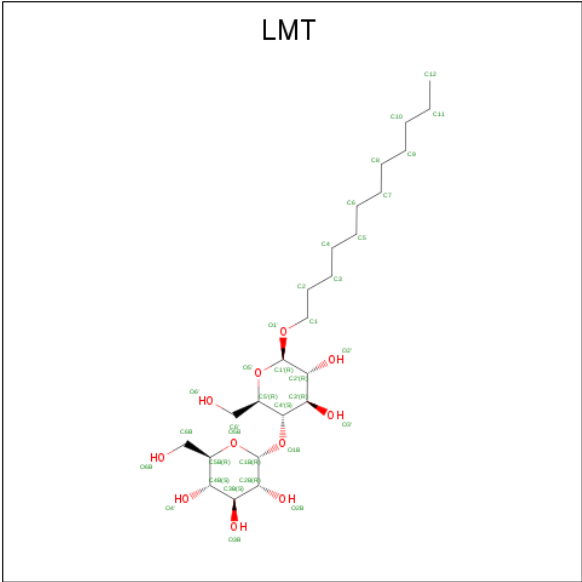
Chain	Residue	Modelled	Actual	Comment	Reference
A	921	HIS	-	expression tag	UNP D9IEF7
A	922	HIS	-	expression tag	UNP D9IEF7
A	923	HIS	-	expression tag	UNP D9IEF7
A	924	HIS	-	expression tag	UNP D9IEF7
A	925	HIS	-	expression tag	UNP D9IEF7
A	926	HIS	-	expression tag	UNP D9IEF7
A	927	HIS	-	expression tag	UNP D9IEF7
A	928	HIS	-	expression tag	UNP D9IEF7
A	929	HIS	-	expression tag	UNP D9IEF7
A	930	HIS	-	expression tag	UNP D9IEF7

- Molecule 2 is N-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]-N'-[(1R,3S,5R,7R)-tricyclo[3.3.1.1 3,7]dec-2-yl]ethane-1,2-diamine (three-letter code: 3RX) (formula: C₂₂H₃₈N₂).



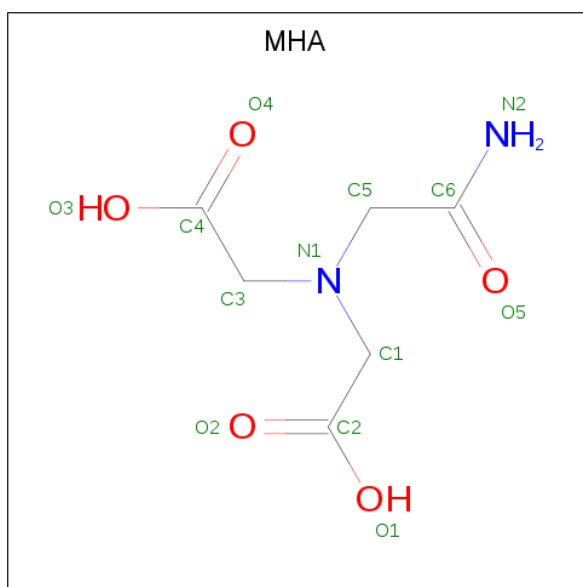
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			24	22	2		

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			28	17	11		
3	A	1	Total	C	O	0	0
			27	16	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			14	13	1		

- Molecule 4 is (CARBAMOYLMETHYL-CARBOXYMETHYL-AMINO)-ACETIC ACID (three-letter code: MHA) (formula: C₆H₁₀N₂O₅).

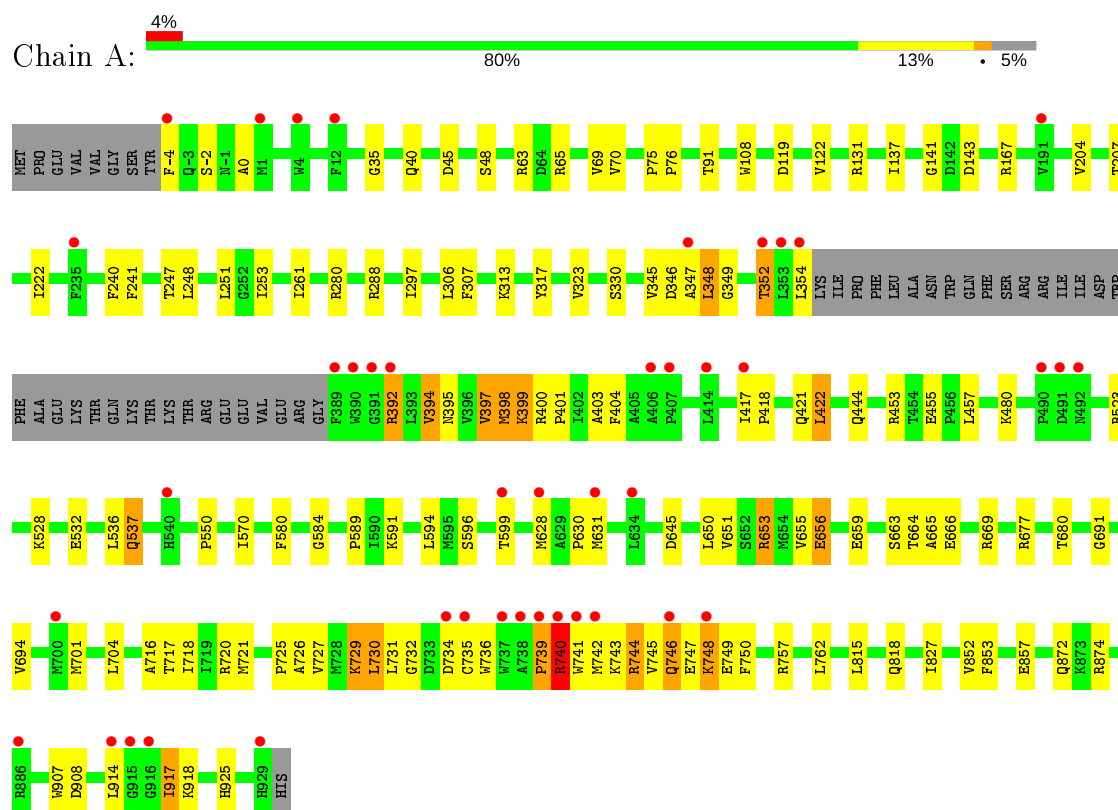


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	6	2	5		
4	A	1	Total	C	N	O	0	0
			13	6	2	5		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Drug exporters of the RND superfamily-like protein, Endolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.01Å 143.54Å 143.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.38 – 2.60 29.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.38-2.60) 98.3 (29.38-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9 _1692	Depositor
R, R_{free}	0.216 , 0.248 0.220 , 0.247	Depositor DCC
R_{free} test set	2644 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7281	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: 3RX, LMT, MHA

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	0.26	0/7097	0.44	1/9642 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	746	GLN	N-CA-C	-5.30	96.69	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	6952	0	7111	129	0
2	A	24	0	38	2	0
3	A	279	0	357	18	0
4	A	26	0	16	0	0
All	All	7281	0	7522	133	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 9.

All (133) 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:398:MET:SD	1:A:729:LYS:HE2	1.63	1.38
1:A:731:LEU:CD2	1:A:734:ASP:HB3	1.62	1.28
1:A:731:LEU:HD22	1:A:734:ASP:CB	1.67	1.25
1:A:398:MET:SD	1:A:729:LYS:CE	2.46	1.03
1:A:398:MET:HE1	1:A:665:ALA:O	1.66	0.93
1:A:628:MET:HG2	1:A:630:PRO:HD2	1.51	0.92
1:A:731:LEU:HD22	1:A:734:ASP:HB3	0.89	0.89
1:A:746:GLN:HG2	1:A:747:GLU:N	1.89	0.86
1:A:397:VAL:HB	1:A:404:PHE:CD2	2.12	0.84
1:A:914:LEU:O	1:A:914:LEU:HD12	1.81	0.80
1:A:653:ARG:HH22	3:A:1007:LMT:H6'2	1.43	0.79
1:A:747:GLU:O	1:A:748:LYS:C	2.20	0.79
1:A:584:GLY:O	1:A:742:MET:HE3	1.84	0.78
1:A:207:THR:HG23	1:A:348:LEU:O	1.84	0.78
1:A:655:VAL:HG22	1:A:736:TRP:HZ3	1.49	0.78
1:A:348:LEU:HD23	1:A:348:LEU:N	1.99	0.77
1:A:397:VAL:HB	1:A:404:PHE:HD2	1.49	0.76
1:A:584:GLY:O	1:A:742:MET:CE	2.35	0.75
1:A:731:LEU:HD13	1:A:734:ASP:H	1.54	0.71
1:A:746:GLN:HG2	1:A:747:GLU:H	1.53	0.71
1:A:347:ALA:C	1:A:348:LEU:HD23	2.11	0.71
1:A:537:GLN:HG3	1:A:537:GLN:O	1.91	0.70
1:A:731:LEU:HD11	1:A:735:CYS:H	1.55	0.70
1:A:528:LYS:H	1:A:528:LYS:HD2	1.57	0.69
1:A:656:GLU:OE2	1:A:656:GLU:HA	1.93	0.67
1:A:395:ASN:HA	1:A:398:MET:HB2	1.77	0.67
1:A:731:LEU:O	1:A:731:LEU:HD12	1.94	0.66
1:A:746:GLN:O	1:A:747:GLU:CB	2.43	0.66
1:A:716:ALA:O	1:A:720:ARG:NH2	2.29	0.66
1:A:731:LEU:HD11	1:A:735:CYS:N	2.10	0.65
1:A:739:PRO:C	1:A:741:TRP:H	1.99	0.65
1:A:740:ARG:HA	1:A:740:ARG:NH1	2.11	0.65
1:A:399:LYS:O	1:A:401:PRO:HD3	1.97	0.65
1:A:398:MET:CE	1:A:665:ALA:O	2.42	0.64
1:A:729:LYS:O	1:A:730:LEU:C	2.37	0.63
1:A:680:THR:HG21	3:A:1008:LMT:H5B	1.80	0.62
1:A:664:THR:HG21	1:A:732:GLY:HA2	1.79	0.62
1:A:306:LEU:HD11	1:A:570:ILE:HD12	1.82	0.62
1:A:653:ARG:NH2	3:A:1007:LMT:H6'2	2.15	0.61
1:A:204:VAL:O	1:A:677:ARG:NH2	2.33	0.61
1:A:207:THR:HG21	1:A:346:ASP:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:NH1	1:A:444:GLN:OE1	2.34	0.61
1:A:725:PRO:O	1:A:729:LYS:HG2	2.02	0.59
1:A:655:VAL:HA	1:A:736:TRP:CZ3	2.38	0.58
1:A:399:LYS:C	1:A:401:PRO:HD3	2.24	0.58
1:A:664:THR:OG1	1:A:732:GLY:O	2.13	0.58
1:A:653:ARG:HH22	3:A:1007:LMT:C6B	2.14	0.58
1:A:288:ARG:HH11	3:A:1007:LMT:H1B	1.68	0.57
1:A:119:ASP:OD2	3:A:1002:LMT:O4'	2.22	0.57
1:A:731:LEU:CD1	1:A:735:CYS:H	2.18	0.57
1:A:721:MET:SD	3:A:1008:LMT:O4'	2.60	0.57
1:A:35:GLY:HA3	3:A:1006:LMT:H6E	1.86	0.57
3:A:1009:LMT:H6D	3:A:1010:LMT:H12	1.85	0.57
1:A:580:PHE:CD1	1:A:589:PRO:HG2	2.39	0.57
1:A:523:ARG:NH2	1:A:550:PRO:HG3	2.19	0.56
1:A:744:ARG:O	1:A:745:VAL:C	2.44	0.56
1:A:746:GLN:O	1:A:747:GLU:HB2	2.05	0.56
1:A:422:LEU:HD13	1:A:422:LEU:O	2.08	0.54
1:A:241:PHE:HD1	3:A:1003:LMT:H122	1.71	0.54
1:A:400:ARG:HB3	1:A:403:ALA:HB3	1.90	0.54
1:A:914:LEU:C	1:A:914:LEU:HD12	2.28	0.54
1:A:523:ARG:HH22	1:A:550:PRO:HG3	1.73	0.53
1:A:248:LEU:HD22	1:A:701:MET:HE1	1.91	0.53
3:A:1006:LMT:H1B	3:A:1006:LMT:H6D	1.91	0.53
1:A:65:ARG:NH1	1:A:141:GLY:O	2.41	0.53
1:A:397:VAL:HG23	1:A:726:ALA:HB2	1.91	0.52
1:A:455:GLU:OE1	1:A:523:ARG:NH1	2.42	0.52
1:A:731:LEU:HD13	1:A:734:ASP:N	2.23	0.52
1:A:731:LEU:C	1:A:731:LEU:HD12	2.31	0.51
1:A:307:PHE:O	1:A:313:LYS:NZ	2.43	0.51
1:A:398:MET:SD	1:A:729:LYS:CD	2.99	0.51
1:A:857:GLU:OE2	1:A:925:HIS:NE2	2.40	0.51
1:A:596:SER:HA	1:A:599:THR:HG22	1.92	0.51
1:A:-4:PHE:O	1:A:-2:SER:OG	2.26	0.50
1:A:680:THR:HG23	1:A:720:ARG:HH12	1.76	0.50
1:A:745:VAL:HG12	1:A:745:VAL:O	2.12	0.50
1:A:650:LEU:HD22	1:A:720:ARG:HG3	1.93	0.49
1:A:666:GLU:O	1:A:669:ARG:N	2.46	0.49
1:A:75:PRO:O	1:A:131:ARG:NH1	2.46	0.49
1:A:253:ILE:HD11	2:A:1001:3RX:HAJ	1.95	0.49
1:A:417:ILE:HG12	1:A:418:PRO:HD3	1.94	0.49
1:A:591:LYS:O	1:A:594:LEU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:O	1:A:395:ASN:HB2	2.13	0.48
1:A:872:GLN:OE1	1:A:874:ARG:NH1	2.40	0.48
1:A:392:ARG:HA	1:A:395:ASN:OD1	2.13	0.48
1:A:731:LEU:HD22	1:A:734:ASP:HB2	1.82	0.48
1:A:349:GLY:O	1:A:352:THR:HG23	2.14	0.47
1:A:645:ASP:OD2	2:A:1001:3RX:NAP	2.47	0.47
1:A:631:MET:HE1	1:A:704:LEU:HB2	1.96	0.47
1:A:747:GLU:O	1:A:749:GLU:N	2.48	0.47
1:A:453:ARG:HG3	3:A:1003:LMT:H6'1	1.97	0.47
1:A:731:LEU:HD21	1:A:734:ASP:HB3	1.77	0.47
1:A:398:MET:SD	1:A:729:LYS:HD3	2.55	0.47
1:A:63:ARG:HH22	1:A:143:ASP:HA	1.79	0.47
1:A:422:LEU:HD12	1:A:422:LEU:H	1.80	0.47
1:A:394:VAL:HG22	1:A:398:MET:HG3	1.95	0.46
1:A:739:PRO:C	1:A:741:TRP:N	2.67	0.46
1:A:584:GLY:O	1:A:742:MET:HE2	2.14	0.46
1:A:740:ARG:HA	1:A:740:ARG:HH11	1.80	0.46
3:A:1002:LMT:H121	3:A:1003:LMT:H22	1.98	0.45
1:A:317:TYR:OH	3:A:1009:LMT:H6E	2.15	0.45
1:A:222:ILE:HD11	1:A:251:LEU:HB2	1.98	0.45
1:A:91:THR:HG23	1:A:108:TRP:HZ2	1.82	0.45
1:A:45:ASP:HB3	1:A:48:SER:HB3	1.99	0.45
1:A:261:ILE:HD12	1:A:330:SER:HB2	1.99	0.44
1:A:69:VAL:HB	1:A:137:ILE:HB	1.99	0.44
1:A:651:VAL:O	1:A:655:VAL:HG23	2.18	0.44
1:A:528:LYS:O	1:A:532:GLU:HG3	2.16	0.44
1:A:207:THR:HG21	1:A:345:VAL:O	2.17	0.44
1:A:480:LYS:HB3	1:A:536:LEU:HD13	2.00	0.43
1:A:729:LYS:C	1:A:731:LEU:N	2.68	0.43
3:A:1005:LMT:H121	3:A:1005:LMT:H92	1.78	0.43
1:A:240:PHE:HB3	3:A:1003:LMT:H111	1.99	0.43
1:A:744:ARG:HA	1:A:744:ARG:HD2	1.60	0.43
1:A:757:ARG:HG3	1:A:762:LEU:HB2	2.01	0.43
1:A:280:ARG:NH1	1:A:908:ASP:OD1	2.52	0.42
1:A:297:ILE:HG21	1:A:323:VAL:HG21	2.01	0.42
1:A:815:LEU:HD12	1:A:818:GLN:HE21	1.84	0.42
1:A:655:VAL:HG22	1:A:736:TRP:CZ3	2.39	0.42
1:A:119:ASP:HB3	1:A:122:VAL:HB	2.01	0.42
1:A:717:THR:OG1	1:A:718:ILE:N	2.53	0.42
1:A:247:THR:O	1:A:251:LEU:HB3	2.20	0.42
1:A:827:ILE:HD11	1:A:852:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:HD21	1:A:550:PRO:HB2	2.03	0.41
1:A:392:ARG:HH22	1:A:669:ARG:HH11	1.69	0.41
1:A:40:GLN:HB2	3:A:1003:LMT:H51	2.03	0.41
1:A:288:ARG:NH1	3:A:1007:LMT:H4'	2.36	0.41
1:A:-2:SER:C	1:A:0:ALA:H	2.23	0.41
1:A:740:ARG:CA	1:A:740:ARG:HH11	2.34	0.41
1:A:691:GLY:O	1:A:694:VAL:HG22	2.21	0.40
1:A:729:LYS:O	1:A:731:LEU:N	2.54	0.40
1:A:392:ARG:O	1:A:395:ASN:N	2.54	0.40
1:A:750:PHE:HB3	1:A:907:TRP:CG	2.57	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	896/943 (95%)	862 (96%)	29 (3%)	5 (1%)	25	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	740	ARG
1	A	76	PRO
1	A	727	VAL
1	A	739	PRO
1	A	917	ILE

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	738/777 (95%)	713 (97%)	25 (3%)	37	63

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	348	LEU
1	A	352	THR
1	A	354	LEU
1	A	392	ARG
1	A	394	VAL
1	A	397	VAL
1	A	398	MET
1	A	399	LYS
1	A	421	GLN
1	A	422	LEU
1	A	537	GLN
1	A	653	ARG
1	A	656	GLU
1	A	659	GLU
1	A	663	SER
1	A	729	LYS
1	A	730	LEU
1	A	740	ARG
1	A	743	LYS
1	A	744	ARG
1	A	748	LYS
1	A	853	PHE
1	A	917	ILE
1	A	918	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	537	GLN
1	A	818	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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
3	LMT	A	1003	-	36,36,36	1.12	2 (5%)	47,47,47	1.03	3 (6%)
3	LMT	A	1004	-	36,36,36	1.16	2 (5%)	47,47,47	0.88	1 (2%)
3	LMT	A	1007	-	29,29,36	1.24	2 (6%)	40,40,47	1.04	4 (10%)
3	LMT	A	1010	-	13,13,36	0.76	0	12,12,47	0.83	0
4	MHA	A	1012	-	6,12,12	1.63	1 (16%)	9,15,15	1.77	4 (44%)
3	LMT	A	1009	-	36,36,36	1.15	3 (8%)	47,47,47	1.35	8 (17%)
3	LMT	A	1002	-	36,36,36	1.15	2 (5%)	47,47,47	1.03	2 (4%)
3	LMT	A	1006	-	36,36,36	1.13	3 (8%)	47,47,47	1.07	3 (6%)
4	MHA	A	1011	-	6,12,12	1.64	1 (16%)	9,15,15	1.82	4 (44%)
3	LMT	A	1008	-	28,28,36	1.27	2 (7%)	39,39,47	0.93	2 (5%)
2	3RX	A	1001	-	25,26,26	0.30	0	32,35,35	1.20	5 (15%)
3	LMT	A	1005	-	36,36,36	1.18	3 (8%)	47,47,47	0.92	2 (4%)

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	A	1003	-	-	10/21/61/61	0/2/2/2
3	LMT	A	1004	-	-	7/21/61/61	0/2/2/2
3	LMT	A	1007	-	-	3/14/54/61	0/2/2/2
3	LMT	A	1010	-	-	4/11/11/61	-
4	MHA	A	1012	-	-	2/8/12/12	-
3	LMT	A	1009	-	-	15/21/61/61	0/2/2/2
3	LMT	A	1002	-	-	6/21/61/61	0/2/2/2
3	LMT	A	1006	-	-	15/21/61/61	0/2/2/2
4	MHA	A	1011	-	-	3/8/12/12	-
3	LMT	A	1008	-	-	5/13/53/61	0/2/2/2
2	3RX	A	1001	-	-	3/15/43/43	0/4/3/3
3	LMT	A	1005	-	-	9/21/61/61	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1008	LMT	O5B-C1B	3.88	1.51	1.41
3	A	1005	LMT	O5B-C1B	3.81	1.51	1.41
3	A	1004	LMT	O5B-C1B	3.72	1.51	1.41
3	A	1002	LMT	O5B-C1B	3.67	1.51	1.41
3	A	1003	LMT	O5B-C1B	3.56	1.50	1.41
3	A	1007	LMT	O5B-C1B	3.56	1.50	1.41
3	A	1009	LMT	O5B-C1B	3.46	1.50	1.41
3	A	1009	LMT	O5'-C1'	3.34	1.50	1.41
3	A	1002	LMT	O5'-C1'	3.29	1.50	1.41
3	A	1006	LMT	O5B-C1B	3.26	1.50	1.41
3	A	1007	LMT	O5'-C1'	3.21	1.50	1.41
3	A	1006	LMT	O5'-C1'	3.18	1.49	1.41
3	A	1005	LMT	O5'-C1'	3.15	1.49	1.41
3	A	1004	LMT	O5'-C1'	3.14	1.49	1.41
3	A	1008	LMT	O5'-C1'	3.12	1.49	1.41
4	A	1011	MHA	C6-N2	3.08	1.42	1.32
4	A	1012	MHA	C6-N2	3.06	1.42	1.32
3	A	1003	LMT	O5'-C1'	3.00	1.49	1.41
3	A	1006	LMT	O5'-C5'	2.12	1.49	1.44
3	A	1009	LMT	O5'-C5'	2.10	1.49	1.44
3	A	1005	LMT	O5'-C5'	2.05	1.49	1.44

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1009	LMT	O1B-C4'-C3'	3.44	116.44	107.28
2	A	1001	3RX	CAI-NAQ-CAX	-3.14	109.98	114.16
3	A	1007	LMT	O5B-C5B-C4B	3.11	115.33	109.69
3	A	1002	LMT	C1B-O1B-C4'	-3.10	110.30	117.96
2	A	1001	3RX	CAC-CAS-CAJ	3.02	120.35	115.27
3	A	1003	LMT	C1B-O1B-C4'	-2.97	110.62	117.96
4	A	1011	MHA	C5-C6-N2	2.92	120.47	115.86
3	A	1006	LMT	C1B-O5B-C5B	-2.87	108.06	113.69
3	A	1009	LMT	C1B-O5B-C5B	-2.78	108.24	113.69
3	A	1004	LMT	C1B-O1B-C4'	-2.73	111.21	117.96
3	A	1009	LMT	O5'-C5'-C4'	2.70	115.45	109.75
3	A	1005	LMT	O5'-C5'-C4'	2.67	115.38	109.75
4	A	1012	MHA	C6-C5-N1	-2.60	109.87	114.38
4	A	1012	MHA	C5-C6-N2	2.53	119.85	115.86
3	A	1006	LMT	O5'-C5'-C4'	2.45	114.91	109.75
3	A	1009	LMT	O1B-C1B-O5B	-2.43	103.87	110.67
4	A	1011	MHA	C4-C3-N1	-2.43	110.02	113.48
4	A	1012	MHA	C2-C1-N1	-2.43	110.02	113.48
3	A	1005	LMT	C1B-O1B-C4'	-2.40	112.02	117.96
2	A	1001	3RX	CAG-NAP-CAH	-2.39	109.55	113.33
3	A	1002	LMT	C1B-C2B-C3B	2.36	114.91	110.00
3	A	1007	LMT	C3B-C4B-C5B	2.33	114.39	110.24
3	A	1007	LMT	C1B-O1B-C4'	-2.28	112.33	117.96
3	A	1007	LMT	C6B-C5B-C4B	-2.28	107.67	113.00
3	A	1009	LMT	O5'-C1'-C2'	2.24	115.09	110.35
4	A	1011	MHA	C6-C5-N1	-2.22	110.53	114.38
3	A	1009	LMT	O1B-C4'-C5'	-2.22	103.37	109.45
2	A	1001	3RX	CAB-CAR-CAA	2.20	119.47	114.60
3	A	1003	LMT	O5'-C5'-C4'	2.20	114.39	109.75
3	A	1003	LMT	C2'-C3'-C4'	2.20	114.70	109.68
4	A	1011	MHA	C2-C1-N1	-2.18	110.38	113.48
3	A	1008	LMT	C1B-O5B-C5B	2.14	117.89	113.69
3	A	1009	LMT	O5'-C5'-C6'	2.12	111.71	106.44
2	A	1001	3RX	CAH-CAI-NAQ	-2.10	107.63	111.06
4	A	1012	MHA	C4-C3-N1	-2.09	110.51	113.48
3	A	1008	LMT	O5B-C5B-C4B	2.07	113.45	109.69
3	A	1006	LMT	O1B-C1B-O5B	-2.02	105.02	110.67
3	A	1009	LMT	C1'-C2'-C3'	2.01	114.19	110.00

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	LMT	C2-C1-O1'-C1'
3	A	1009	LMT	O5'-C1'-O1'-C1
3	A	1009	LMT	C3'-C4'-O1B-C1B
3	A	1003	LMT	O5'-C5'-C6'-O6'
3	A	1009	LMT	O5B-C5B-C6B-O6B
3	A	1008	LMT	O5B-C5B-C6B-O6B
3	A	1009	LMT	O5B-C1B-O1B-C4'
3	A	1006	LMT	O5B-C5B-C6B-O6B
3	A	1003	LMT	C4'-C5'-C6'-O6'
3	A	1002	LMT	O5B-C5B-C6B-O6B
3	A	1008	LMT	O5'-C5'-C6'-O6'
3	A	1005	LMT	O5'-C5'-C6'-O6'
2	A	1001	3RX	CAD-CAF-CAJ-CAS
3	A	1006	LMT	C4B-C5B-C6B-O6B
3	A	1009	LMT	C4B-C5B-C6B-O6B
3	A	1005	LMT	C4'-C5'-C6'-O6'
3	A	1009	LMT	C2'-C1'-O1'-C1
3	A	1002	LMT	C4B-C5B-C6B-O6B
3	A	1007	LMT	O5'-C5'-C6'-O6'
3	A	1008	LMT	C4'-C5'-C6'-O6'
3	A	1009	LMT	C2B-C1B-O1B-C4'
3	A	1005	LMT	O5B-C5B-C6B-O6B
3	A	1007	LMT	C4'-C5'-C6'-O6'
3	A	1003	LMT	O1'-C1-C2-C3
2	A	1001	3RX	NAP-CAH-CAI-NAQ
3	A	1006	LMT	C4'-C5'-C6'-O6'
3	A	1006	LMT	O5'-C5'-C6'-O6'
3	A	1010	LMT	C4-C5-C6-C7
3	A	1006	LMT	C6-C7-C8-C9
3	A	1004	LMT	C11-C10-C9-C8
3	A	1004	LMT	C7-C8-C9-C10
3	A	1005	LMT	C4-C5-C6-C7
3	A	1009	LMT	C5-C6-C7-C8
3	A	1009	LMT	C4-C5-C6-C7
3	A	1008	LMT	C4B-C5B-C6B-O6B
3	A	1008	LMT	C2-C1-O1'-C1'
3	A	1009	LMT	C3-C4-C5-C6
3	A	1006	LMT	C1-C2-C3-C4
3	A	1010	LMT	C1-C2-C3-C4
3	A	1003	LMT	C11-C10-C9-C8
3	A	1005	LMT	C2-C3-C4-C5
3	A	1007	LMT	C2-C3-C4-C5
3	A	1006	LMT	C3-C4-C5-C6

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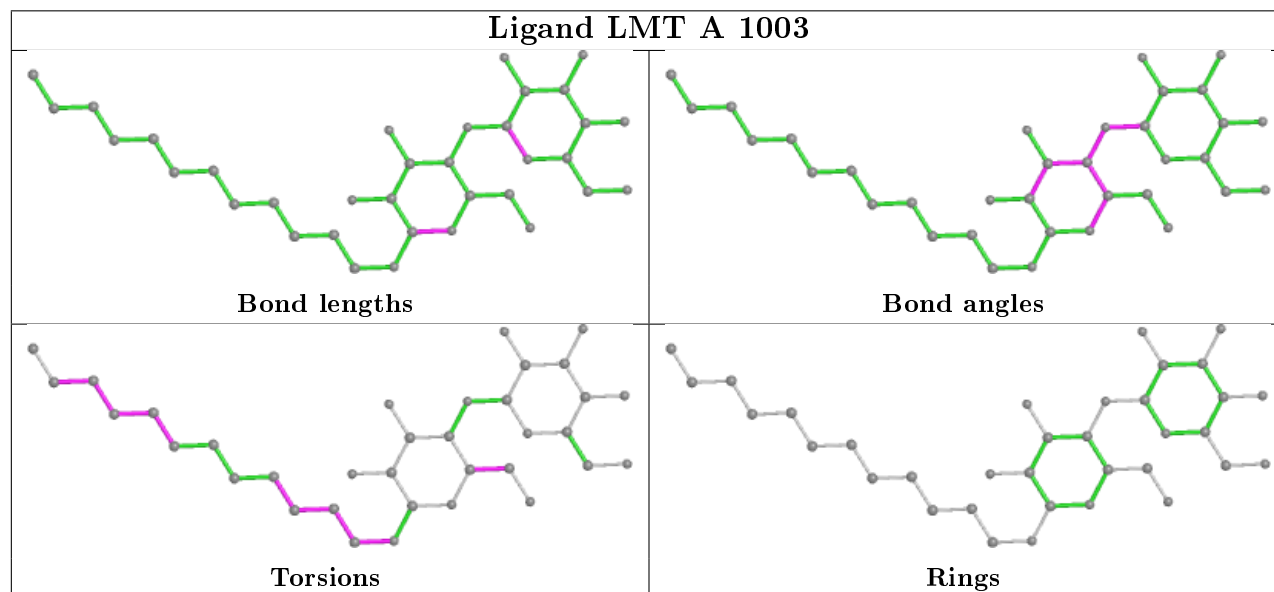
Mol	Chain	Res	Type	Atoms
3	A	1003	LMT	C6-C7-C8-C9
3	A	1010	LMT	O1'-C1-C2-C3
3	A	1006	LMT	C3'-C4'-O1B-C1B
3	A	1004	LMT	C5-C6-C7-C8
3	A	1003	LMT	C1-C2-C3-C4
2	A	1001	3RX	CAI-CAH-NAP-CAG
3	A	1004	LMT	C4-C5-C6-C7
3	A	1009	LMT	O5'-C5'-C6'-O6'
3	A	1006	LMT	C5'-C4'-O1B-C1B
3	A	1003	LMT	C9-C10-C11-C12
3	A	1010	LMT	C9-C10-C11-C12
4	A	1012	MHA	C2-C1-N1-C3
3	A	1009	LMT	C2-C1-O1'-C1'
3	A	1005	LMT	C2-C1-O1'-C1'
3	A	1009	LMT	C1-C2-C3-C4
3	A	1004	LMT	C1-C2-C3-C4
4	A	1011	MHA	C2-C1-N1-C5
3	A	1004	LMT	C4B-C5B-C6B-O6B
3	A	1003	LMT	C2-C3-C4-C5
3	A	1002	LMT	C1-C2-C3-C4
3	A	1006	LMT	C2-C1-O1'-C1'
3	A	1002	LMT	C5-C6-C7-C8
3	A	1006	LMT	C11-C10-C9-C8
3	A	1005	LMT	C4B-C5B-C6B-O6B
3	A	1003	LMT	C7-C8-C9-C10
3	A	1006	LMT	C2'-C1'-O1'-C1
4	A	1012	MHA	C2-C1-N1-C5
3	A	1006	LMT	C7-C8-C9-C10
3	A	1002	LMT	C2'-C1'-O1'-C1
3	A	1005	LMT	C5-C6-C7-C8
3	A	1006	LMT	O5'-C1'-O1'-C1
4	A	1011	MHA	C2-C1-N1-C3
4	A	1011	MHA	C4-C3-N1-C1
3	A	1009	LMT	C11-C10-C9-C8
3	A	1009	LMT	C6-C7-C8-C9
3	A	1004	LMT	O5B-C5B-C6B-O6B
3	A	1005	LMT	C1-C2-C3-C4
3	A	1006	LMT	C2-C3-C4-C5
3	A	1002	LMT	O5'-C1'-O1'-C1

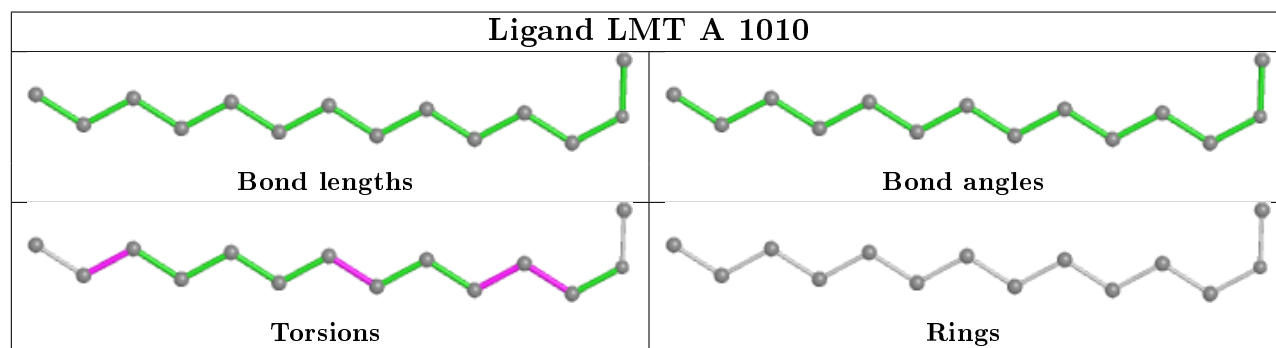
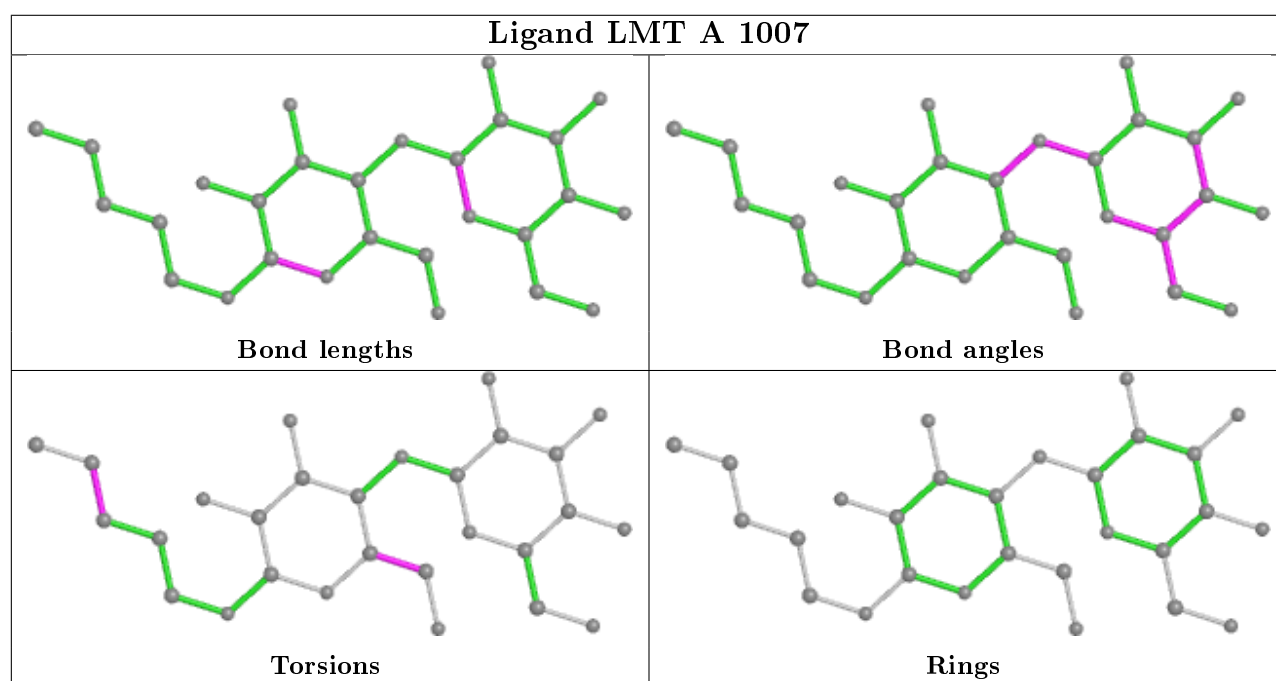
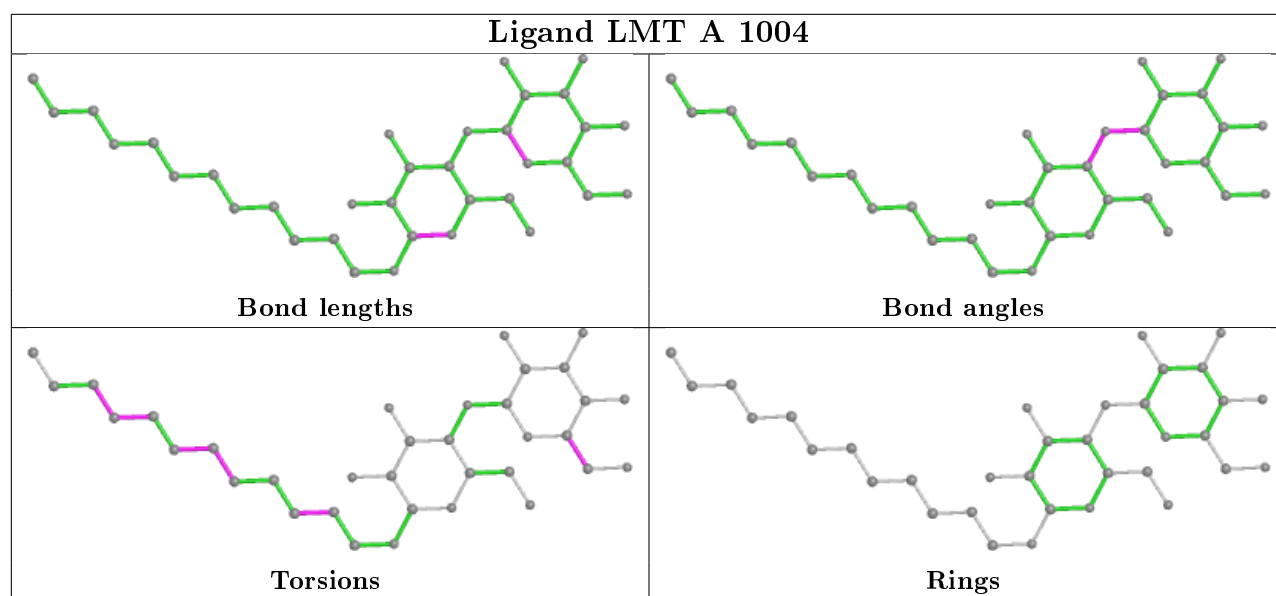
There are no ring outliers.

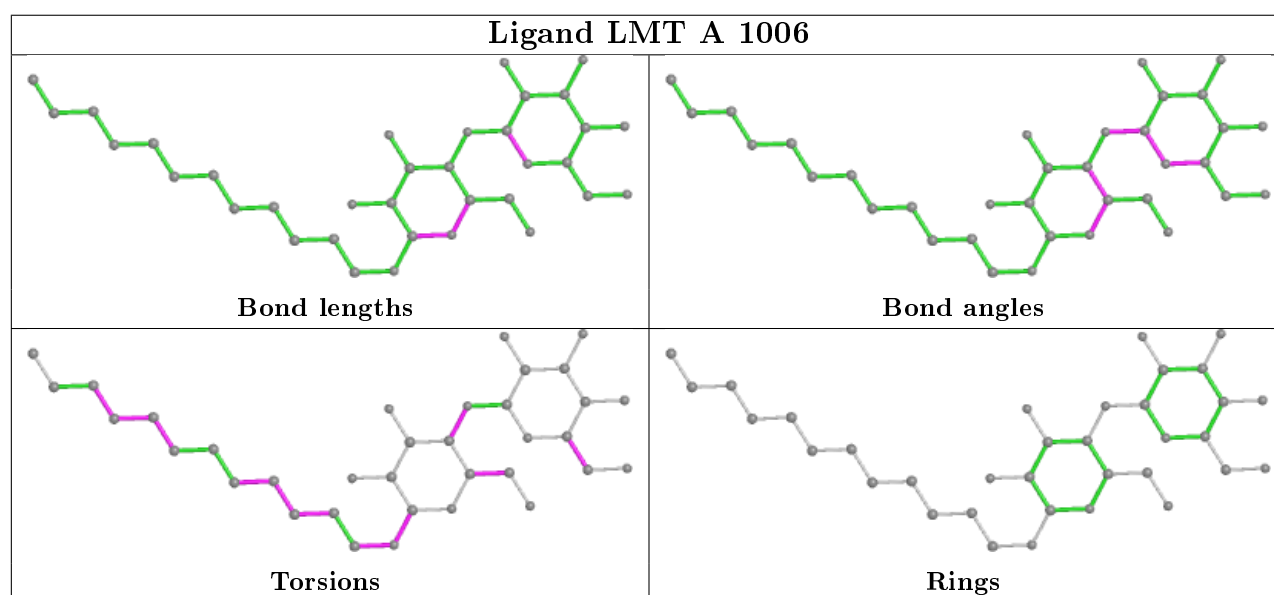
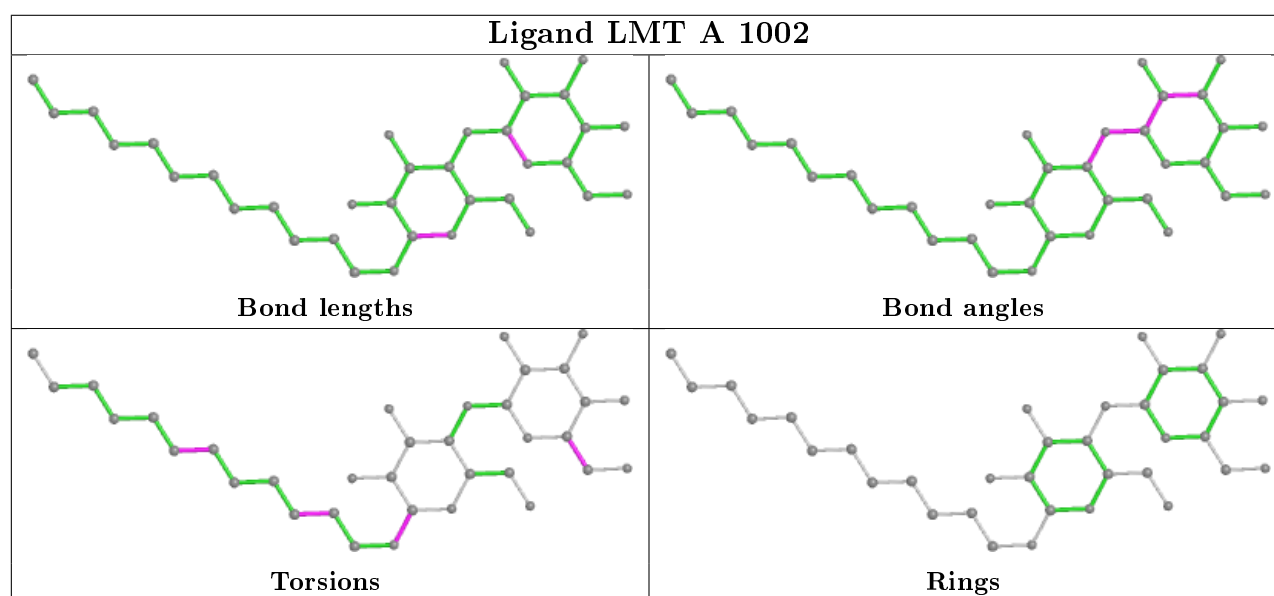
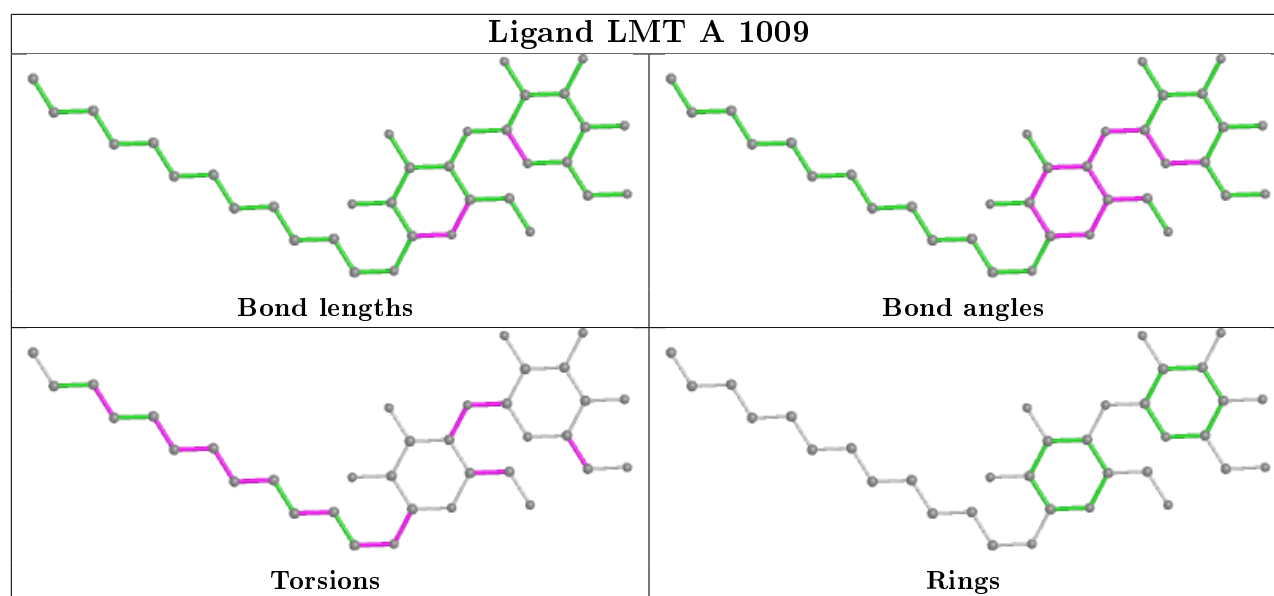
9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	LMT	5	0
3	A	1007	LMT	5	0
3	A	1010	LMT	1	0
3	A	1009	LMT	2	0
3	A	1002	LMT	2	0
3	A	1006	LMT	2	0
3	A	1008	LMT	2	0
2	A	1001	3RX	2	0
3	A	1005	LMT	1	0

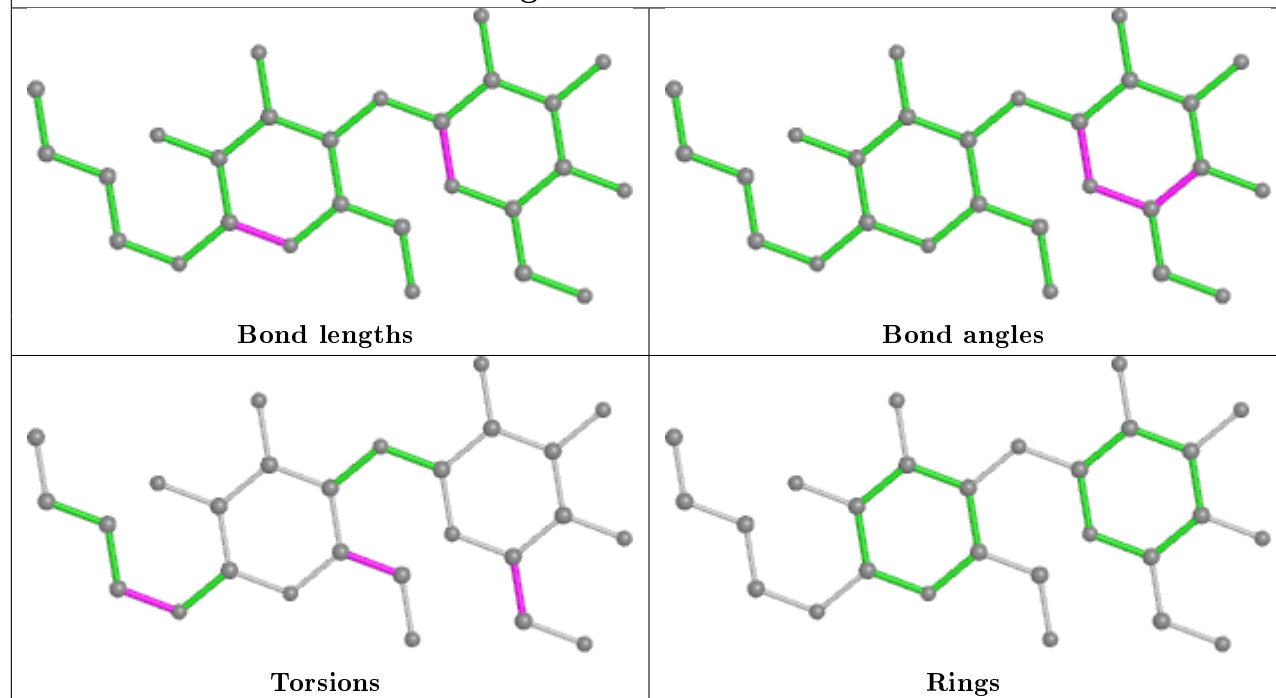
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



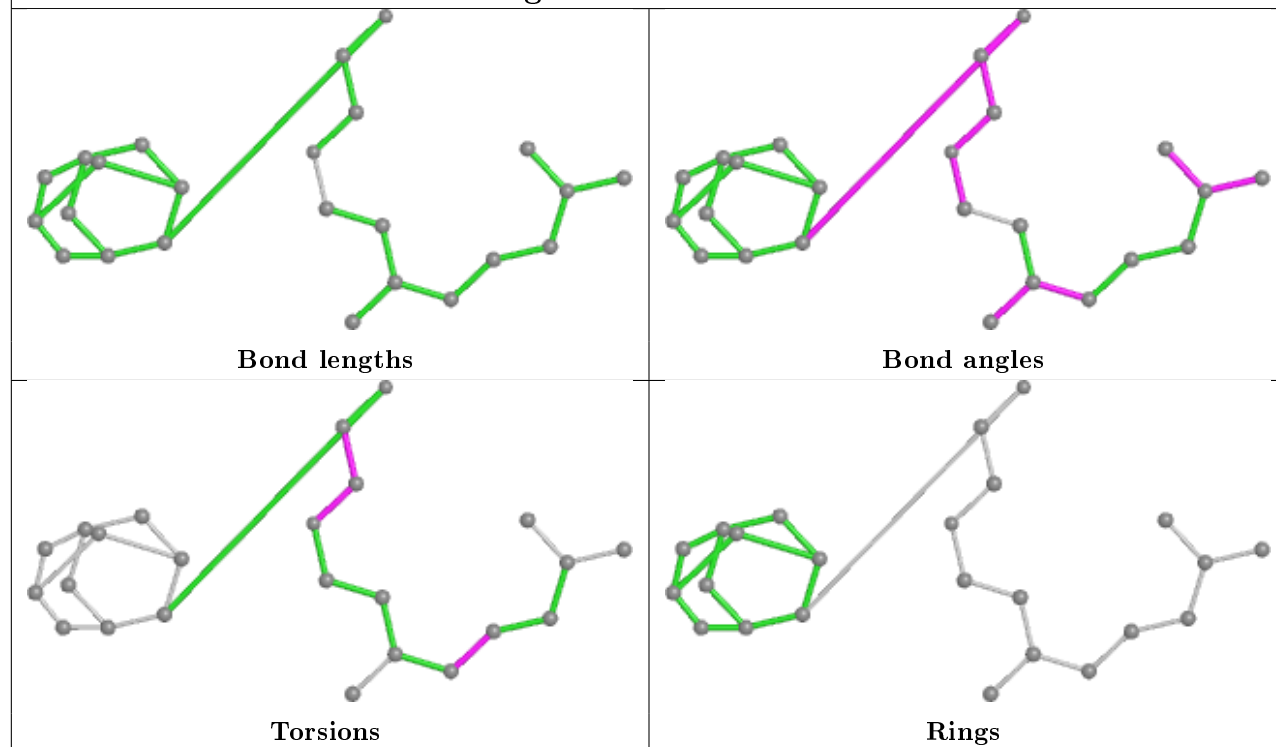


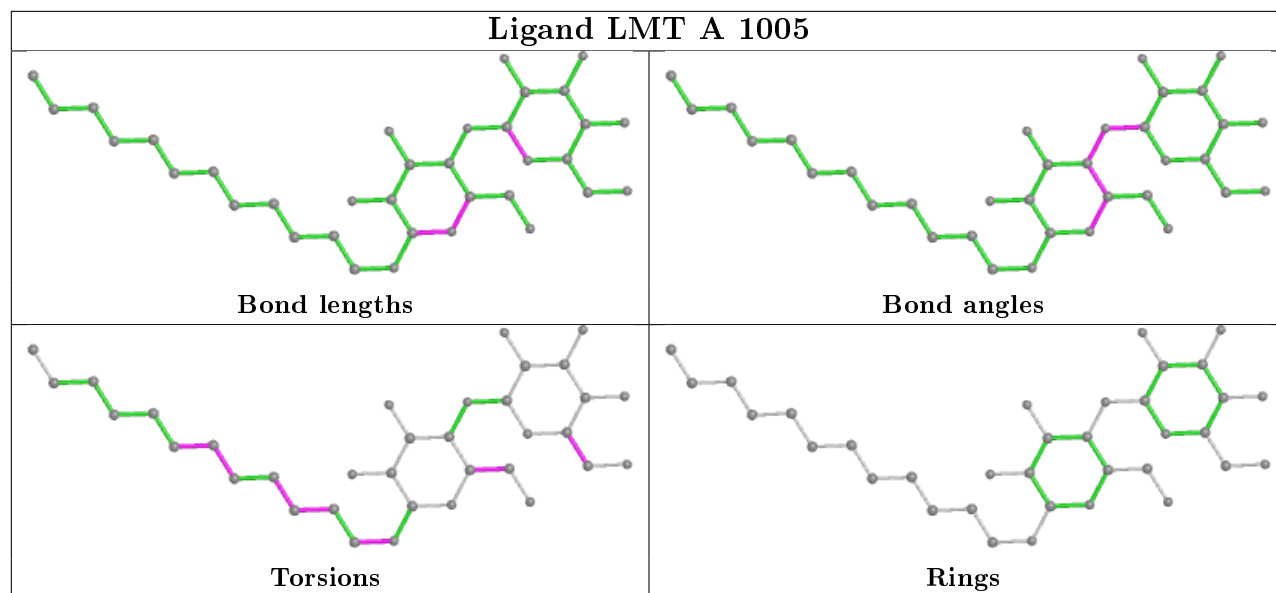


Ligand LMT A 1008



Ligand 3RX A 1001





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	900/943 (95%)	-0.02	42 (4%) 31 25	53, 79, 149, 205	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TRP	10.5
1	A	354	LEU	7.9
1	A	734	ASP	7.1
1	A	353	LEU	6.5
1	A	739	PRO	6.4
1	A	391	GLY	6.0
1	A	914	LEU	5.6
1	A	392	ARG	5.6
1	A	389	PHE	5.6
1	A	740	ARG	5.0
1	A	741	TRP	4.7
1	A	746	GLN	4.6
1	A	916	GLY	3.8
1	A	738	ALA	3.8
1	A	491	ASP	3.3
1	A	490	PRO	3.2
1	A	417	ILE	3.0
1	A	915	GLY	3.0
1	A	742	MET	3.0
1	A	-4	PHE	2.9
1	A	352	THR	2.8
1	A	540	HIS	2.8
1	A	700	MET	2.8
1	A	929	HIS	2.7
1	A	886	ARG	2.6
1	A	4	TRP	2.5
1	A	390	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	191	VAL	2.5
1	A	414	LEU	2.5
1	A	347	ALA	2.4
1	A	748	LYS	2.4
1	A	235	PHE	2.3
1	A	492	ASN	2.2
1	A	12	PHE	2.2
1	A	628	MET	2.2
1	A	599	THR	2.2
1	A	1	MET	2.2
1	A	407	PRO	2.1
1	A	631	MET	2.1
1	A	634	LEU	2.1
1	A	735	CYS	2.1
1	A	406	ALA	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 carbohydrates 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.

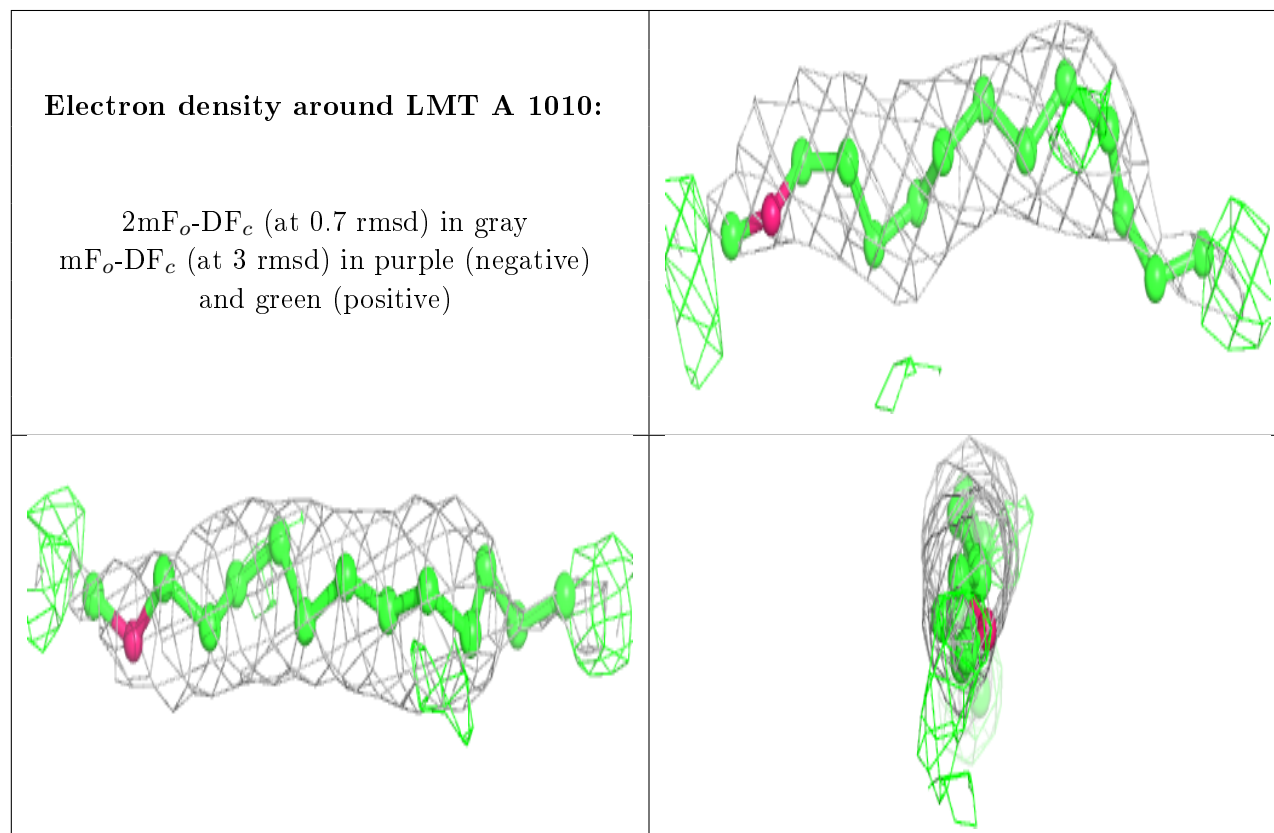
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	LMT	A	1010	14/35	0.72	0.29	68,89,121,130	0
3	LMT	A	1009	35/35	0.73	0.38	82,136,151,153	0
3	LMT	A	1008	27/35	0.74	0.28	83,115,141,144	0
3	LMT	A	1006	35/35	0.76	0.50	99,140,151,152	0
3	LMT	A	1005	35/35	0.76	0.39	71,132,142,143	0
3	LMT	A	1007	28/35	0.85	0.23	110,123,132,140	0
3	LMT	A	1003	35/35	0.85	0.28	77,130,138,144	0
3	LMT	A	1002	35/35	0.87	0.32	52,115,143,145	0

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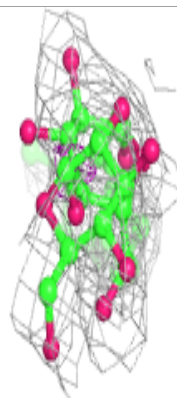
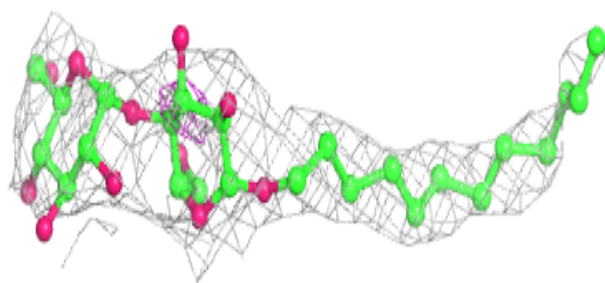
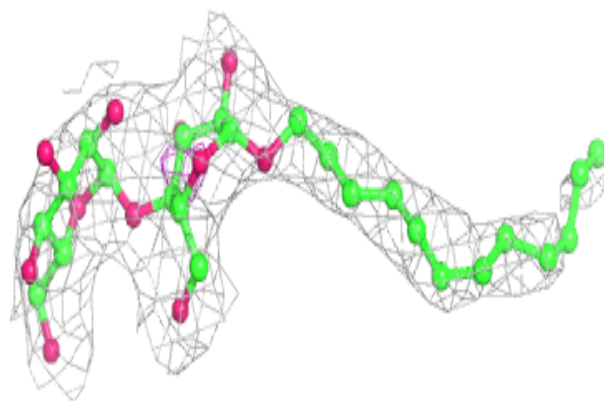
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MHA	A	1011	13/13	0.91	0.16	75,82,92,93	0
2	3RX	A	1001	24/24	0.94	0.31	81,90,96,98	0
4	MHA	A	1012	13/13	0.94	0.26	67,75,89,91	0
3	LMT	A	1004	35/35	0.96	0.21	71,86,108,113	0

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.

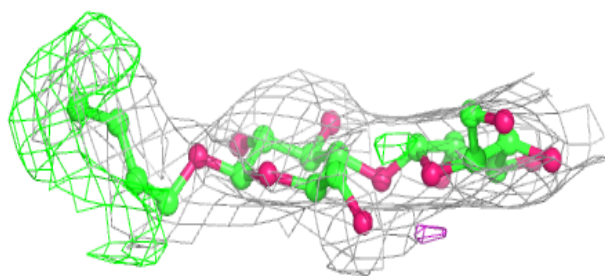
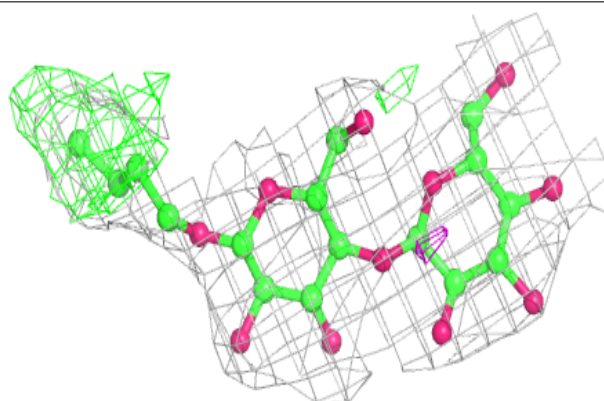


Electron density around LMT A 1009:

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

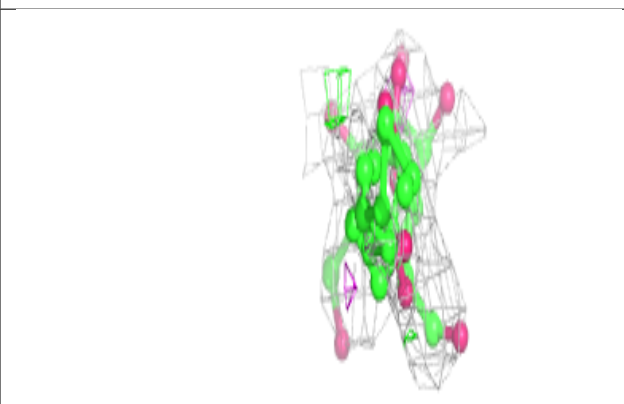
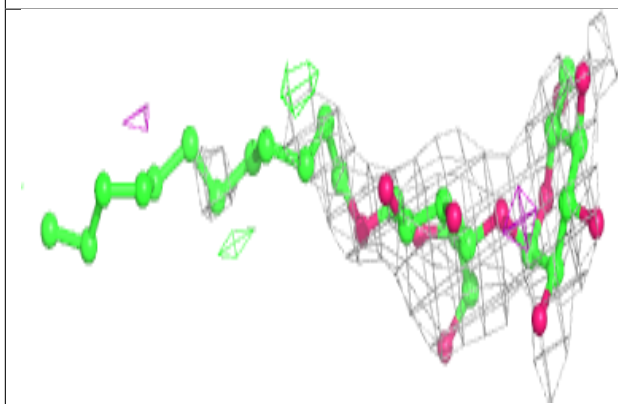
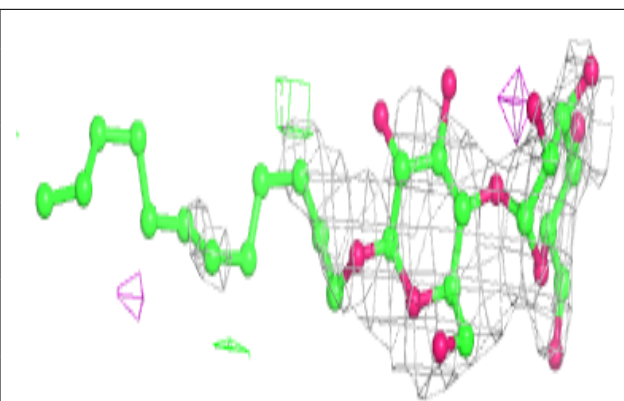
**Electron density around LMT A 1008:**

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

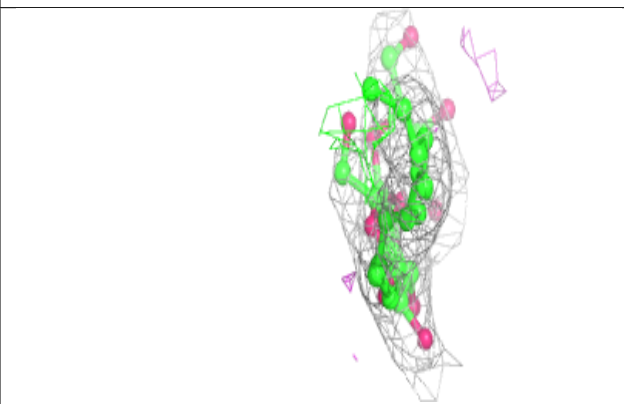
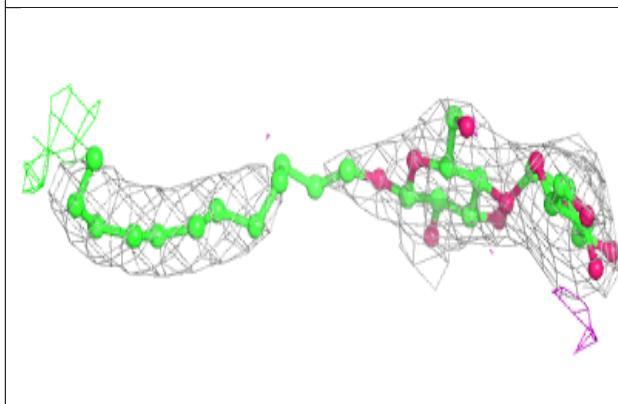
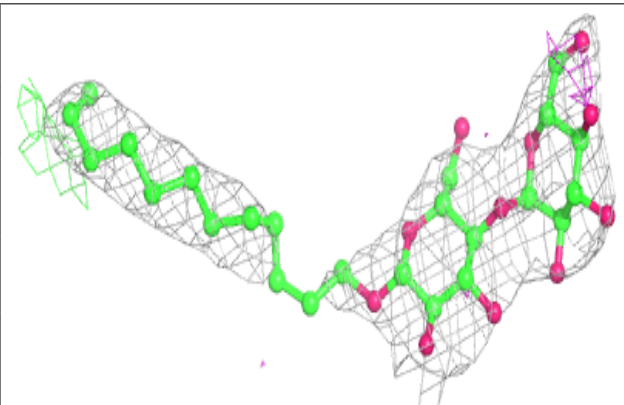


Electron density around LMT A 1006:

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

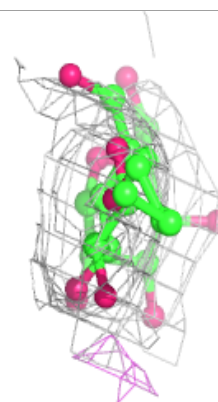
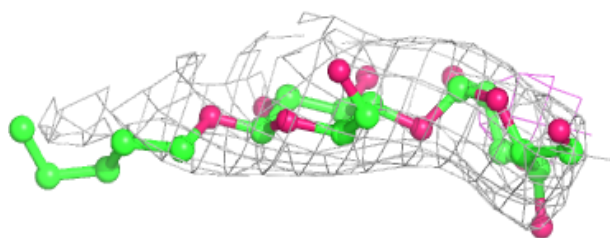
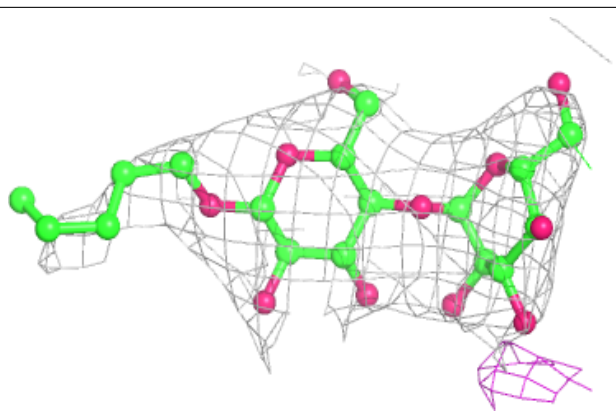
**Electron density around LMT A 1005:**

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

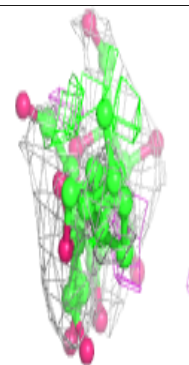
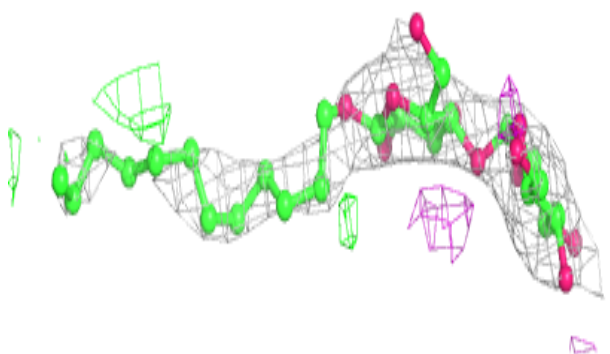
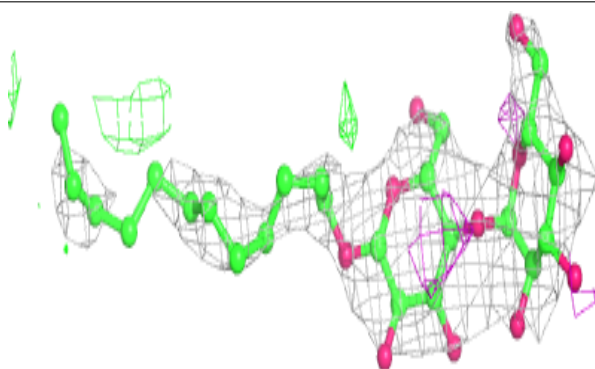


Electron density around LMT A 1007:

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

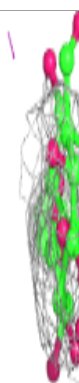
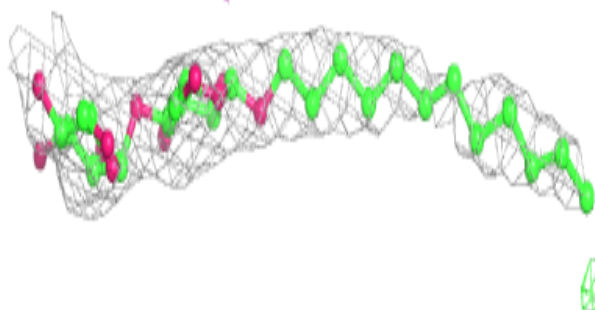
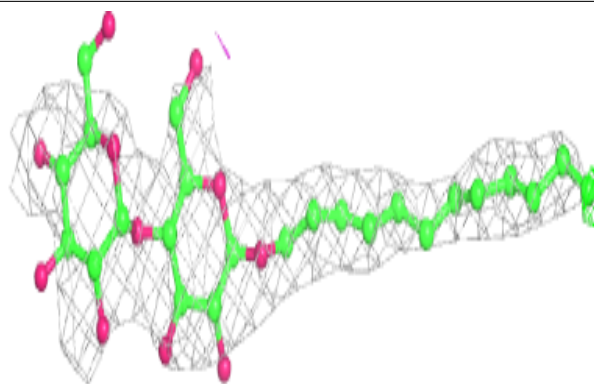
**Electron density around LMT A 1003:**

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

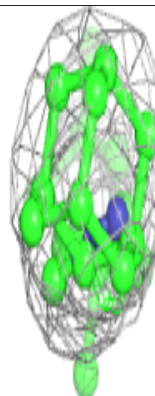
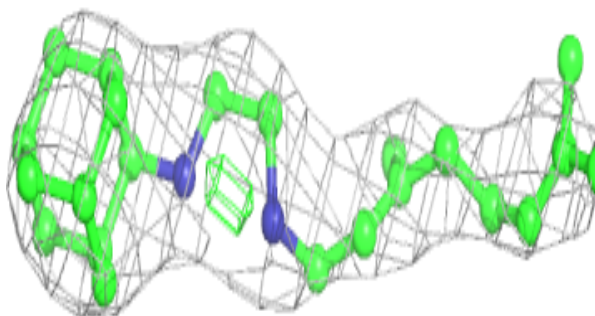
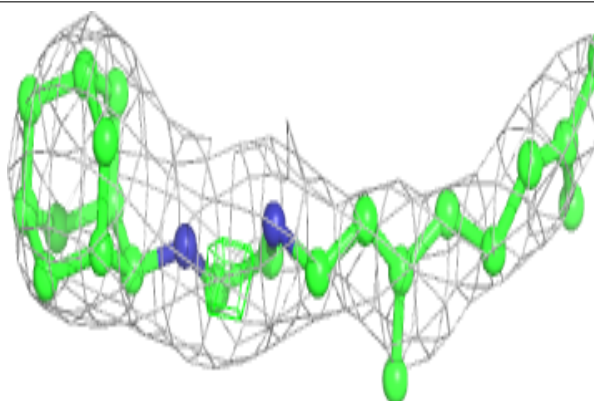


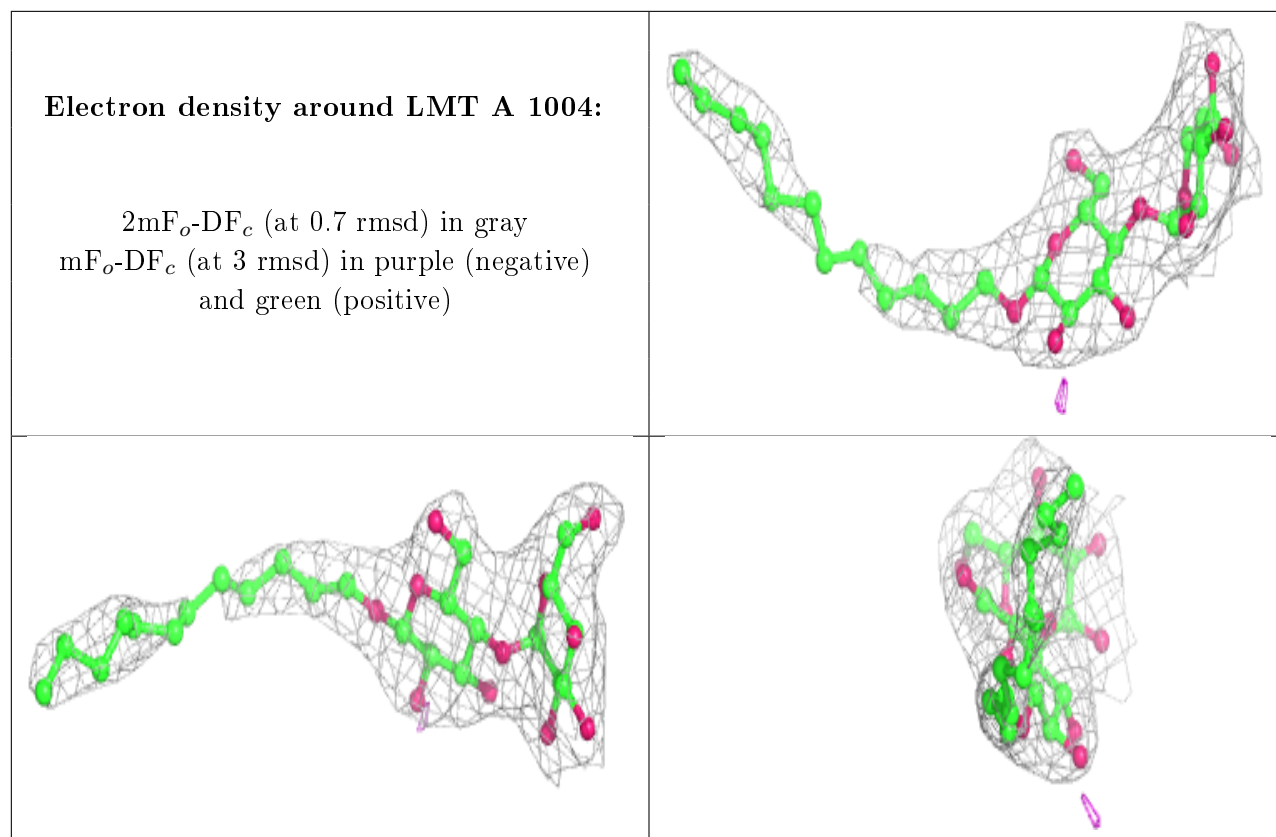
Electron density around LMT A 1002:

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

**Electron density around 3RX A 1001:**

$2mF_o-DF_c$ (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.