



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:18 am BST

PDB ID : 5AGE  
Title : CRYSTAL STRUCTURE OF LEISHMANIA MAJOR N-MYRISTOYLTRANSFERASE (NMT) WITH BOUND MYRISTOYL-COA AND A BENZOMORPHOLINONE LIGAND  
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Deposited on : 2015-01-29  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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

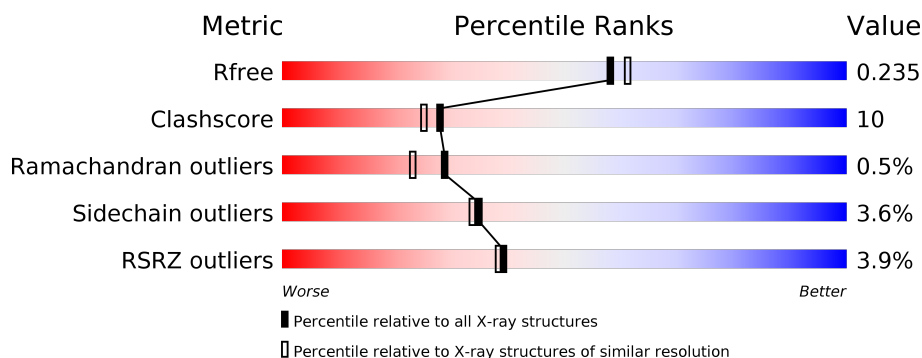
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	438	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3621 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.

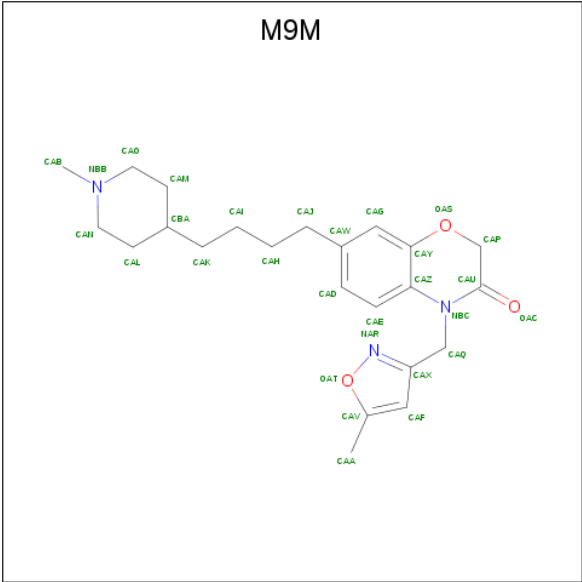
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3344	2163	560	606	15			

There are 21 discrepancies between the modelled and reference sequences:

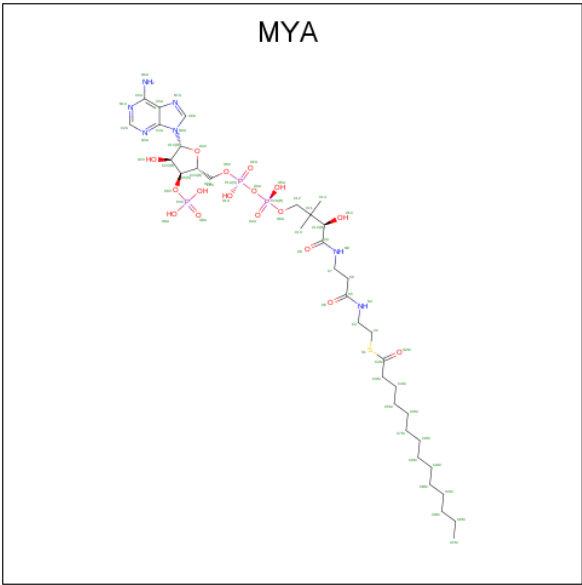
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP Q4Q5S8
A	-15	GLY	-	expression tag	UNP Q4Q5S8
A	-14	SER	-	expression tag	UNP Q4Q5S8
A	-13	SER	-	expression tag	UNP Q4Q5S8
A	-12	HIS	-	expression tag	UNP Q4Q5S8
A	-11	HIS	-	expression tag	UNP Q4Q5S8
A	-10	HIS	-	expression tag	UNP Q4Q5S8
A	-9	HIS	-	expression tag	UNP Q4Q5S8
A	-8	HIS	-	expression tag	UNP Q4Q5S8
A	-7	HIS	-	expression tag	UNP Q4Q5S8
A	-6	SER	-	expression tag	UNP Q4Q5S8
A	-5	SER	-	expression tag	UNP Q4Q5S8
A	-4	GLY	-	expression tag	UNP Q4Q5S8
A	-3	ARG	-	expression tag	UNP Q4Q5S8
A	-2	GLU	-	expression tag	UNP Q4Q5S8
A	-1	ASN	-	expression tag	UNP Q4Q5S8
A	0	LEU	-	expression tag	UNP Q4Q5S8
A	1	TYR	-	expression tag	UNP Q4Q5S8
A	2	PHE	-	expression tag	UNP Q4Q5S8
A	3	GLN	-	expression tag	UNP Q4Q5S8
A	4	GLY	-	expression tag	UNP Q4Q5S8

- Molecule 2 is 4-[(5-methyl-1,2-oxazol-3-yl)methyl]-7-[4-(1-methylpiperidin-4-yl)butyl]-2H-1,4-benzoxazin-3(4H)-one (three-letter code: M9M) (formula: C<sub>23</sub>H<sub>31</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	23	3	3		

- Molecule 3 is TETRADECANOYL-COA (three-letter code: MYA) (formula:  $C_{35}H_{62}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total 185	O 185	0	0



• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.02Å 90.17Å 52.97Å 90.00° 113.78° 90.00°	Depositor
Resolution (Å)	19.75 – 2.00 19.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (19.75-2.00) 92.0 (19.72-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.174 , 0.235 0.176 , 0.235	Depositor DCC
$R_{free}$ test set	1319 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 47.6	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	0.96	EDS
Total number of atoms	3621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MYA, M9M

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	1.14	6/3443 (0.2%)	0.98	11/4688 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	GLU	CG-CD	5.68	1.60	1.51
1	A	48	GLU	CB-CG	5.64	1.62	1.52
1	A	375	CYS	CB-SG	5.60	1.91	1.82
1	A	84	ASP	CB-CG	5.47	1.63	1.51
1	A	153	GLU	CG-CD	5.40	1.60	1.51
1	A	201	VAL	CB-CG1	5.28	1.64	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASP	CB-CG-OD2	-12.66	106.90	118.30
1	A	89	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	A	134	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	134	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	85	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	89	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	304	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	400	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	191	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	333	ILE	CB-CA-C	-5.22	101.16	111.60
1	A	84	ASP	CB-CG-OD1	5.11	122.90	118.30

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	3344	0	3255	67	0
2	A	29	0	31	2	0
3	A	63	0	58	0	0
4	A	185	0	0	31	0
All	All	3621	0	3344	67	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 (67) 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:41:THR:HB	4:A:2020:HOH:O	1.18	1.29
1:A:285:SER:HB3	4:A:2137:HOH:O	1.32	1.28
1:A:101:LEU:HD12	4:A:2059:HOH:O	1.11	1.24
1:A:231:ARG:HG2	4:A:2122:HOH:O	1.57	1.03
1:A:121:LYS:HE3	4:A:2067:HOH:O	1.68	0.94
1:A:358:GLN:HB2	4:A:2165:HOH:O	1.69	0.92
1:A:276:ARG:HH21	1:A:294:ASP:H	1.24	0.82
1:A:342:ASN:HB2	4:A:2155:HOH:O	1.79	0.81
1:A:244:ASN:HB2	4:A:2126:HOH:O	1.82	0.79
1:A:335:ASN:HD21	1:A:337:ASN:HB2	1.51	0.76
1:A:29:LYS:HB2	4:A:2010:HOH:O	1.87	0.74
1:A:102:CYS:HB2	4:A:2036:HOH:O	1.88	0.73
1:A:28:GLU:HA	4:A:2011:HOH:O	1.91	0.71
1:A:342:ASN:CB	4:A:2155:HOH:O	2.37	0.69
1:A:126:ILE:HD12	1:A:169:LEU:HD13	1.77	0.66
1:A:276:ARG:HD2	4:A:2134:HOH:O	1.95	0.66
1:A:77:ARG:O	1:A:89:ARG:HD2	1.98	0.64
1:A:102:CYS:CB	4:A:2036:HOH:O	2.43	0.64
1:A:98:GLN:HG3	4:A:2036:HOH:O	1.97	0.63
1:A:398:HIS:HD2	4:A:2176:HOH:O	1.81	0.63
1:A:236:PRO:HB2	4:A:2124:HOH:O	1.99	0.62
1:A:162:HIS:HE1	4:A:2094:HOH:O	1.82	0.61
1:A:234:GLY:O	1:A:236:PRO:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:HG22	1:A:42:VAL:N	2.16	0.59
1:A:276:ARG:NH2	1:A:294:ASP:H	1.98	0.59
1:A:117:LYS:HD2	4:A:2029:HOH:O	2.02	0.58
1:A:44:ASP:CG	4:A:2020:HOH:O	2.42	0.57
1:A:238:GLN:HB2	4:A:2124:HOH:O	2.04	0.57
1:A:236:PRO:O	1:A:239:TYR:N	2.32	0.55
1:A:41:THR:HG22	1:A:43:ALA:H	1.73	0.54
1:A:235:ILE:HD12	1:A:240:GLN:HE22	1.73	0.53
1:A:335:ASN:ND2	1:A:337:ASN:HB2	2.23	0.52
1:A:40:LYS:HE2	4:A:2018:HOH:O	2.09	0.52
1:A:72:ILE:HD13	1:A:122:LEU:HD21	1.92	0.51
1:A:274:GLN:HE21	1:A:318:LYS:HE3	1.76	0.51
1:A:236:PRO:CB	4:A:2124:HOH:O	2.57	0.51
1:A:347:HIS:HE1	4:A:2158:HOH:O	1.93	0.50
1:A:280:MET:HE2	1:A:283:LEU:HD12	1.93	0.50
1:A:21:PRO:CB	1:A:27:THR:HG22	2.42	0.50
1:A:280:MET:CE	1:A:283:LEU:HD12	2.42	0.50
1:A:314:GLU:CG	1:A:317:LYS:HA	2.43	0.49
1:A:236:PRO:O	1:A:238:GLN:N	2.47	0.48
1:A:117:LYS:CD	4:A:2029:HOH:O	2.62	0.48
1:A:283:LEU:HD22	1:A:417:ALA:HB1	1.96	0.47
1:A:333:ILE:O	1:A:333:ILE:CG2	2.60	0.47
1:A:101:LEU:CG	4:A:2059:HOH:O	2.50	0.47
1:A:117:LYS:HE2	4:A:2031:HOH:O	2.14	0.47
1:A:52:ILE:HG22	1:A:183:ILE:HG21	1.97	0.47
1:A:41:THR:CG2	1:A:42:VAL:N	2.77	0.47
1:A:124:ALA:HB1	1:A:184:LEU:HD11	1.96	0.47
1:A:276:ARG:NE	1:A:294:ASP:OD1	2.48	0.46
1:A:52:ILE:HD12	4:A:2027:HOH:O	2.16	0.46
1:A:29:LYS:HG2	1:A:29:LYS:O	2.16	0.46
1:A:205:GLY:HA3	2:A:1422:M9M:HAH1	1.98	0.44
1:A:101:LEU:CD1	4:A:2059:HOH:O	1.98	0.44
1:A:21:PRO:HB2	1:A:27:THR:HG22	1.99	0.44
1:A:235:ILE:HD12	1:A:240:GLN:NE2	2.33	0.44
1:A:50:TYR:OH	1:A:186:LYS:HE3	2.17	0.43
1:A:314:GLU:HG3	1:A:317:LYS:HA	2.01	0.43
1:A:274:GLN:NE2	1:A:319:VAL:H	2.16	0.42
1:A:276:ARG:CD	4:A:2134:HOH:O	2.58	0.42
1:A:116:ARG:HD2	1:A:119:ASP:OD1	2.18	0.42
1:A:172:HIS:CE1	1:A:174:GLN:HG3	2.54	0.42
1:A:237:ALA:HA	1:A:240:GLN:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:OG1	2:A:1422:M9M:HAB3	2.20	0.41
1:A:342:ASN:CG	4:A:2155:HOH:O	2.59	0.40
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.91	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	409/438 (93%)	388 (95%)	19 (5%)	2 (0%)	29 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	LYS
1	A	237	ALA

### 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	357/385 (93%)	344 (96%)	13 (4%)	35 34

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	48	GLU
1	A	115	ARG
1	A	175	LEU
1	A	182	PRO
1	A	195	THR
1	A	220	ARG
1	A	228	VAL
1	A	231	ARG
1	A	233	SER
1	A	238	GLN
1	A	284	ASP
1	A	298	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	146	GLN
1	A	162	HIS
1	A	274	GLN
1	A	335	ASN
1	A	339	ASN
1	A	347	HIS
1	A	398	HIS

### 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

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
3	MYA	A	1423	-	54,65,65	0.90	1 (1%)	67,91,91	1.73	11 (16%)
2	M9M	A	1422	-	30,32,32	2.31	6 (20%)	39,44,44	1.97	9 (23%)

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	MYA	A	1423	-	-	3/59/80/80	0/3/3/3
2	M9M	A	1422	-	-	1/10/34/34	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1422	M9M	CAP-CAU	-7.74	1.41	1.51
2	A	1422	M9M	CAA-CAV	6.13	1.55	1.48
2	A	1422	M9M	CAF-CAV	-3.97	1.34	1.39
3	A	1423	MYA	P3X-O9A	3.64	1.62	1.50
2	A	1422	M9M	CAF-CAX	-2.88	1.35	1.39
2	A	1422	M9M	CAU-NBC	2.77	1.40	1.36
2	A	1422	M9M	CAO-NBB	2.36	1.51	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1423	MYA	O2M-C2M-C3M	6.63	120.82	109.02
3	A	1423	MYA	N3A-C2A-N1A	-5.14	120.64	128.68
2	A	1422	M9M	CAX-CAQ-NBC	-5.08	104.53	112.76
2	A	1422	M9M	CAO-NBB-CAN	4.56	115.91	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1422	M9M	CAB-NBB-CAO	4.55	117.46	110.66
2	A	1422	M9M	CAQ-CAX-CAF	-4.43	123.07	129.51
3	A	1423	MYA	O4X-C1X-C2X	-4.39	100.51	106.93
2	A	1422	M9M	CAN-CAL-CBA	-3.84	102.27	111.99
3	A	1423	MYA	C7-N8-C9	3.63	129.06	122.59
3	A	1423	MYA	C5A-C6A-N6A	2.99	124.90	120.35
3	A	1423	MYA	C2-S1-C2M	2.99	105.83	100.16
2	A	1422	M9M	CAM-CAO-NBB	2.68	114.81	111.22
3	A	1423	MYA	C4A-C5A-N7A	-2.66	106.63	109.40
3	A	1423	MYA	O8A-P3X-O7A	2.44	116.96	107.64
2	A	1422	M9M	CAQ-NBC-CAU	2.39	120.35	117.36
3	A	1423	MYA	P2A-O3A-P1A	-2.31	124.89	132.83
3	A	1423	MYA	C4M-C3M-C2M	-2.31	107.44	113.80
2	A	1422	M9M	OAS-CAY-CAG	2.21	120.44	117.05
2	A	1422	M9M	OAC-CAU-NBC	-2.20	119.76	122.57
3	A	1423	MYA	O3X-C3X-C4X	-2.02	102.76	110.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1423	MYA	S1-C2M-C3M-C4M
2	A	1422	M9M	CAI-CAK-CBA-CAM
3	A	1423	MYA	C8M-C9M-CAM-CBM
3	A	1423	MYA	C6-C7-N8-C9

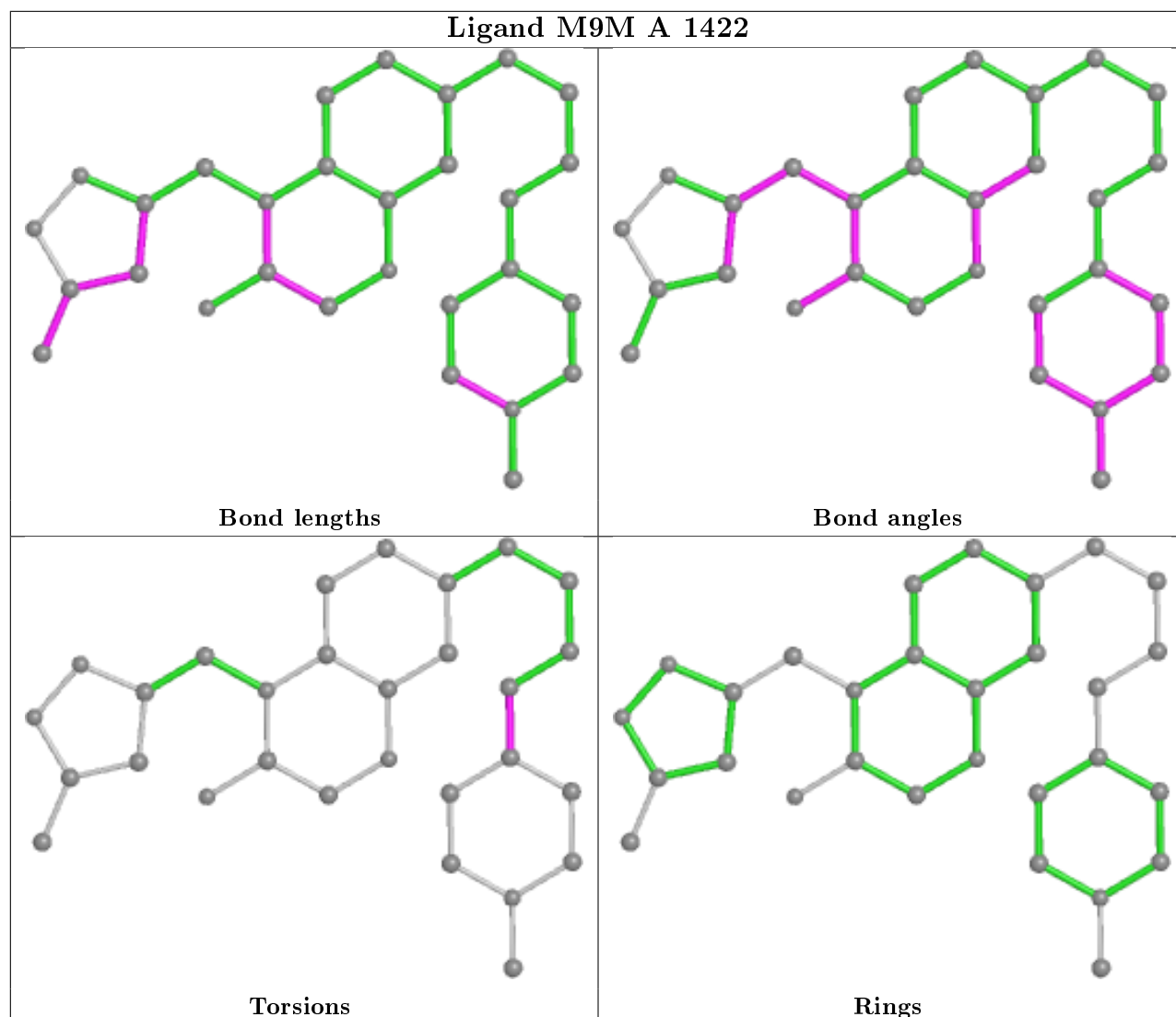
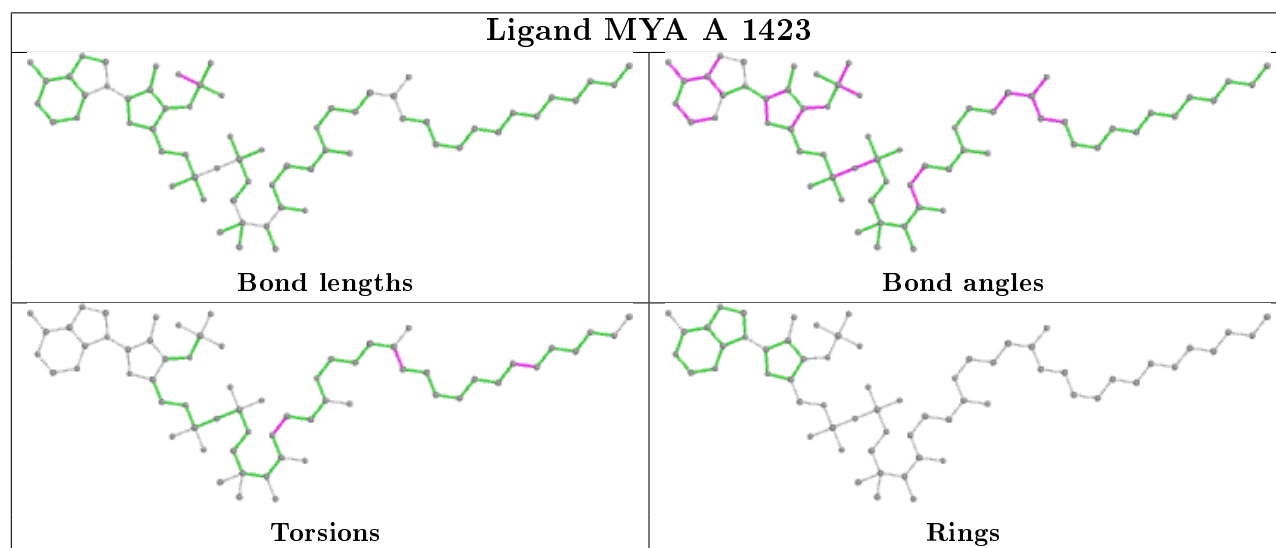
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1422	M9M	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	411/438 (93%)	-0.29	16 (3%) 39 38	20, 27, 50, 73	3 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	GLY	4.7
1	A	237	ALA	4.6
1	A	72	ILE	3.7
1	A	315	ASN	3.6
1	A	11	ALA	3.3
1	A	25	ASP	3.2
1	A	29	LYS	3.1
1	A	337	ASN	2.9
1	A	242	PHE	2.9
1	A	316	ASP	2.9
1	A	235	ILE	2.7
1	A	243	GLN	2.6
1	A	231	ARG	2.4
1	A	262	SER	2.3
1	A	322	PHE	2.3
1	A	28	GLU	2.3

### 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](#)

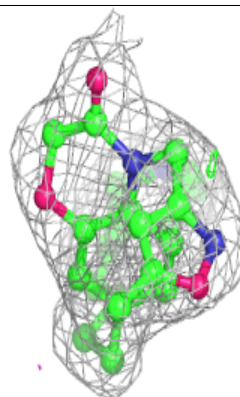
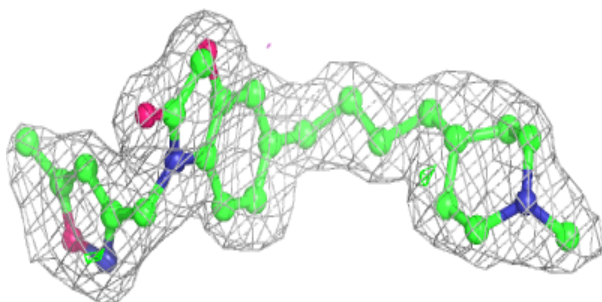
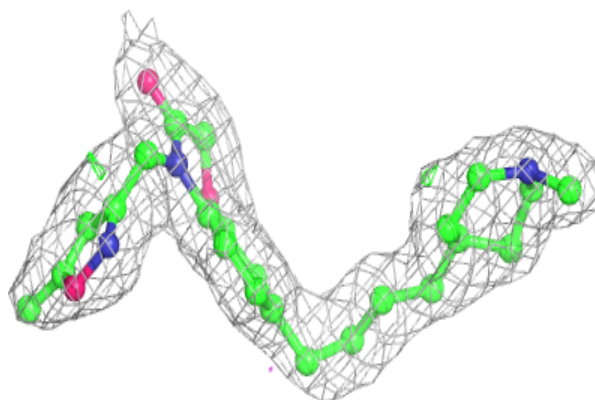
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	M9M	A	1422	29/29	0.93	0.10	26,32,44,46	0
3	MYA	A	1423	63/63	0.98	0.07	16,25,30,32	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.

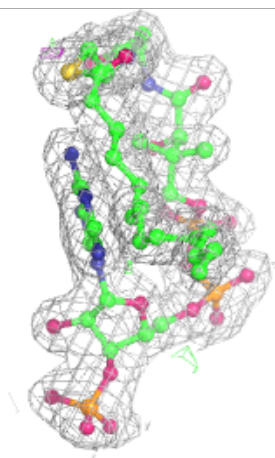
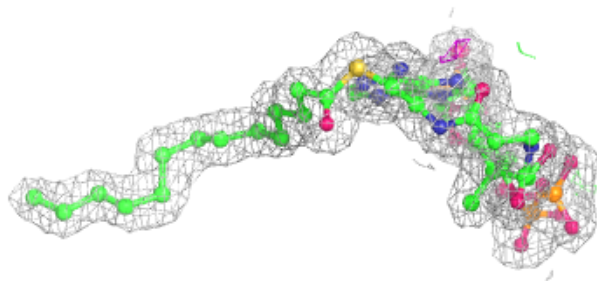
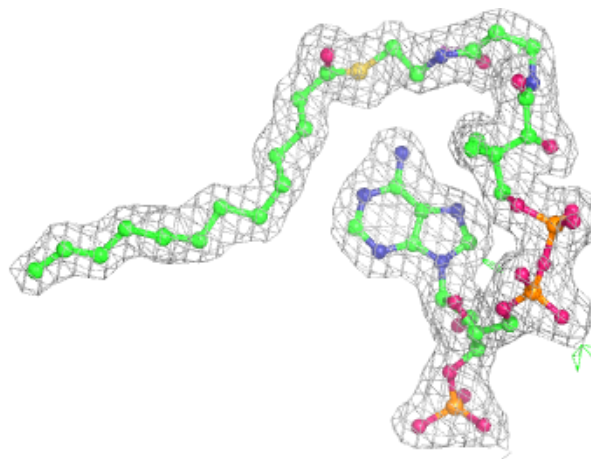
### Electron density around M9M A 1422:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MYA A 1423:**

$2mF_o-DF_c$  (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.