



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:10 pm BST

PDB ID : 2E1T  
Title : Crystal structure of Dendranthema morifolium DmAT complexed with malonyl-CoA  
Authors : Unno, H.; Ichimaida, F.; Kusunoki, M.; Nakayama, T.  
Deposited on : 2006-10-28  
Resolution : 2.10 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

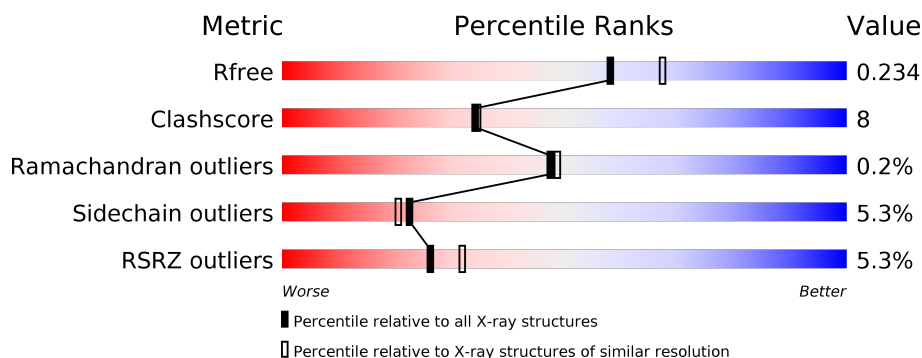
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	454	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>...</div> </div> </div>
1	B	454	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>...</div> </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
2	MLC	A	1001	X	-	-	-
2	MLC	B	1002	X	-	-	-

## 2 Entry composition [i](#)

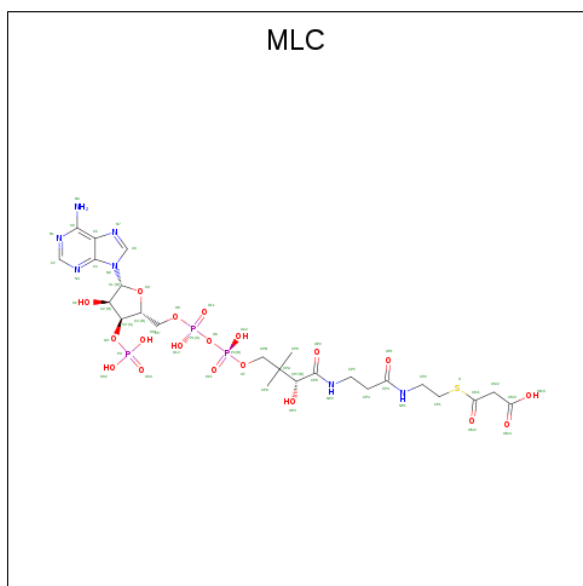
There are 3 unique types of molecules in this entry. The entry contains 7503 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 acyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3466	2229	573	646	18			
1	B	440	Total	C	N	O	S	0	0	0
			3466	2229	573	646	18			

- Molecule 2 is MALONYL-COENZYME A (three-letter code: MLC) (formula:  $C_{24}H_{38}N_7O_{19}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			54	24	7	19	3 1		
2	B	1	Total	C	N	O	P S	0	0
			54	24	7	19	3 1		

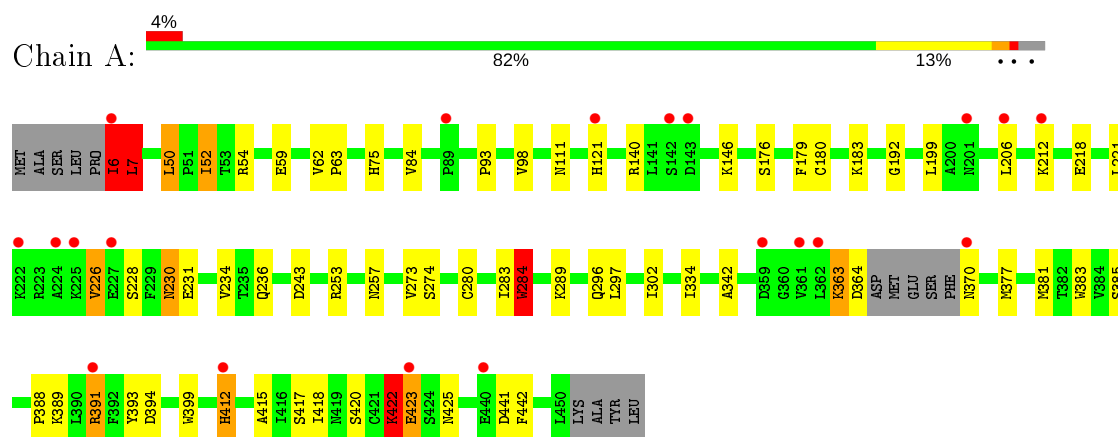
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	228	Total 228	O 228	0	0
3	B	235	Total 235	O 235	0	0

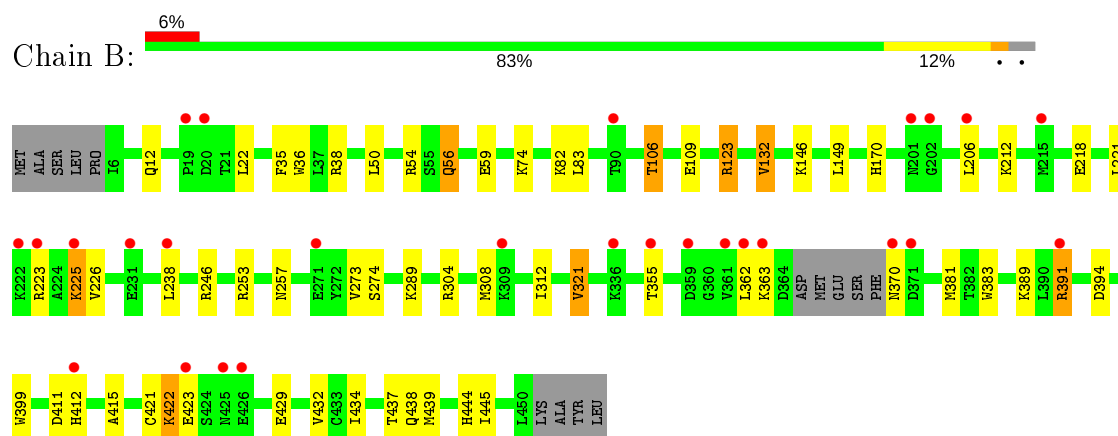
### 3 Residue-property plots

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: acyl transferase



#### • Molecule 1: acyl transferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.65Å 122.92Å 69.85Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	35.49 – 2.10 35.49 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (35.49-2.10) 95.8 (35.49-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.64 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.196 , 0.234 0.196 , 0.234	Depositor DCC
$R_{free}$ test set	2520 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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: MLC

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	0.55	0/3549	0.65	4/4821 (0.1%)
1	B	0.55	0/3549	0.63	0/4821
All	All	0.55	0/7098	0.64	4/9642 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	7	LEU	N-CA-C	7.15	130.30	111.00
1	A	284	TRP	CA-CB-CG	5.75	124.62	113.70
1	A	422	LYS	N-CA-C	5.33	125.41	111.00
1	A	6	ILE	C-N-CA	5.31	134.97	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	422	LYS	Peptide
1	A	6	ILE	Peptide



## 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	3466	0	3457	70	1
1	B	3466	0	3457	48	1
2	A	54	0	33	6	0
2	B	54	0	33	8	0
3	A	228	0	0	20	0
3	B	235	0	0	17	0
All	All	7503	0	6980	118	1

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 8.

All (118) 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:B:421:CYS:O	1:B:422:LYS:HB2	1.56	1.04
1:A:180:CYS:HB2	3:A:1222:HOH:O	1.61	1.00
1:B:421:CYS:O	1:B:422:LYS:CB	2.15	0.95
1:B:54:ARG:HB3	3:B:1200:HOH:O	1.69	0.92
1:A:391:ARG:NH1	3:A:1033:HOH:O	2.04	0.90
1:A:54:ARG:HB3	3:A:1206:HOH:O	1.72	0.88
1:A:393:TYR:HB3	1:A:422:LYS:CB	2.03	0.88
1:A:284:TRP:NE1	3:A:1220:HOH:O	2.06	0.82
1:B:56:GLN:HG3	3:B:1029:HOH:O	1.80	0.82
1:A:364:ASP:O	3:A:1101:HOH:O	1.97	0.81
1:A:176:SER:HB3	3:A:1225:HOH:O	1.80	0.79
1:A:393:TYR:HB3	1:A:422:LYS:HB2	1.66	0.78
1:A:393:TYR:CB	1:A:422:LYS:HB2	2.15	0.76
1:A:284:TRP:HZ3	1:A:296:GLN:OE1	1.70	0.75
1:A:289:LYS:HG2	1:A:334:ILE:HG23	1.67	0.74
1:B:389:LYS:NZ	2:B:1002:MLC:H5'2	2.02	0.74
1:A:297:LEU:HD13	1:A:381:MET:CE	2.18	0.73
1:B:212:LYS:HE2	3:B:1199:HOH:O	1.87	0.72
1:A:253:ARG:CZ	1:A:257:ASN:HD21	2.02	0.72
1:A:393:TYR:HB3	1:A:422:LYS:HB3	1.73	0.70
1:B:438:GLN:NE2	3:B:1111:HOH:O	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:CYS:HA	1:A:183:LYS:HE3	1.72	0.69
1:A:226:VAL:HG11	3:A:1066:HOH:O	1.96	0.64
1:A:391:ARG:HB2	1:A:391:ARG:CZ	2.26	0.64
1:B:123:ARG:NH2	3:B:1119:HOH:O	2.30	0.63
1:B:38:ARG:NH2	1:B:225:LYS:O	2.30	0.62
1:B:289:LYS:HD3	1:B:445:ILE:HG12	1.82	0.62
1:A:422:LYS:HZ3	1:A:425:ASN:HD22	1.45	0.61
1:A:284:TRP:CZ2	3:A:1220:HOH:O	2.53	0.61
1:B:12:GLN:OE1	1:B:106:THR:HB	2.01	0.61
1:A:391:ARG:HG2	1:A:422:LYS:NZ	2.15	0.61
1:B:321:VAL:HG13	3:B:1117:HOH:O	2.01	0.60
1:B:253:ARG:HH21	1:B:257:ASN:ND2	1.99	0.60
1:A:230:ASN:H	1:A:230:ASN:ND2	2.00	0.60
1:A:420:SER:OG	1:A:422:LYS:NZ	2.35	0.59
1:A:422:LYS:HE3	1:A:422:LYS:CA	2.32	0.58
1:B:439:MET:HE1	3:B:1225:HOH:O	2.04	0.58
1:A:284:TRP:CE2	3:A:1220:HOH:O	2.52	0.58
1:A:412:HIS:CD2	3:A:1074:HOH:O	2.56	0.57
1:A:280:CYS:O	1:A:284:TRP:HB2	2.06	0.56
1:B:238:LEU:CD2	3:B:1198:HOH:O	2.54	0.56
1:A:363:LYS:HD3	1:A:363:LYS:H	1.70	0.55
1:B:253:ARG:HE	1:B:257:ASN:HD21	1.55	0.55
1:A:391:ARG:HG2	1:A:422:LYS:HZ2	1.70	0.55
1:A:236:GLN:NE2	1:A:412:HIS:HE1	2.04	0.54
1:A:50:LEU:O	1:A:52:ILE:HG22	2.08	0.53
1:B:246:ARG:NH2	1:B:411:ASP:OD1	2.41	0.53
1:A:377:MET:HE3	1:B:381:MET:HB3	1.90	0.53
1:A:284:TRP:HH2	1:A:296:GLN:CB	2.22	0.53
1:A:422:LYS:N	1:A:422:LYS:HE3	2.23	0.53
1:A:183:LYS:HD2	3:A:1132:HOH:O	2.08	0.52
1:A:394:ASP:OD1	1:A:422:LYS:HG2	2.10	0.52
1:B:238:LEU:HD21	3:B:1198:HOH:O	2.10	0.52
1:B:439:MET:CE	3:B:1225:HOH:O	2.58	0.51
1:A:274:SER:HB2	2:A:1001:MLC:H3'	1.91	0.51
1:B:321:VAL:HG23	3:B:1014:HOH:O	2.11	0.51
1:A:234:VAL:HB	3:A:1209:HOH:O	2.10	0.51
1:B:54:ARG:HG2	1:B:109:GLU:OE2	2.11	0.51
1:B:132:VAL:HB	3:B:1226:HOH:O	2.11	0.51
1:B:273:VAL:H	2:B:1002:MLC:H2	1.75	0.50
1:A:273:VAL:H	2:A:1001:MLC:H2	1.76	0.50
1:A:297:LEU:HB3	1:A:381:MET:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:NH2	3:A:1059:HOH:O	2.45	0.50
1:A:273:VAL:H	2:A:1001:MLC:C2	2.25	0.50
1:B:253:ARG:HH21	1:B:257:ASN:HD22	1.59	0.50
1:B:274:SER:HB3	2:B:1002:MLC:H2'	1.94	0.49
1:A:284:TRP:CH2	1:A:296:GLN:CB	2.95	0.49
1:A:212:LYS:HE3	3:A:1221:HOH:O	2.14	0.48
1:B:391:ARG:NH2	1:B:394:ASP:OD2	2.46	0.48
1:B:106:THR:CG2	3:B:1004:HOH:O	2.61	0.48
1:B:308:MET:HG3	1:B:312:ILE:HG12	1.95	0.48
1:A:179:PHE:CD2	1:A:183:LYS:HE2	2.49	0.48
1:A:93:PRO:HD2	1:A:221:LEU:HD11	1.96	0.48
1:B:106:THR:HG22	3:B:1004:HOH:O	2.14	0.48
1:A:111:ASN:HB2	3:A:1020:HOH:O	2.14	0.48
1:B:434:ILE:HG12	3:B:1225:HOH:O	2.13	0.48
1:A:283:ILE:HD11	1:A:442:PHE:HZ	1.79	0.47
1:B:444:HIS:HB3	3:B:1129:HOH:O	2.14	0.47
1:A:284:TRP:CH2	1:A:296:GLN:HB3	2.50	0.47
1:A:284:TRP:HH2	1:A:296:GLN:HB2	1.79	0.46
1:A:284:TRP:CH2	1:A:296:GLN:HB2	2.49	0.46
1:A:228:SER:O	1:A:231:GLU:HG2	2.16	0.46
2:A:1001:MLC:HM21	3:A:1039:HOH:O	2.16	0.46
1:B:83:LEU:HB2	1:B:149:LEU:HD21	1.98	0.46
1:A:389:LYS:NZ	2:A:1001:MLC:H5'1	2.30	0.46
1:A:192:GLY:HA2	3:A:1154:HOH:O	2.16	0.46
1:A:84:VAL:HG22	1:A:146:LYS:HG2	1.97	0.46
1:A:297:LEU:HD13	1:A:381:MET:HE2	1.95	0.45
1:A:388:PRO:HG3	1:A:418:ILE:HG22	1.98	0.44
1:A:383:TRP:O	1:A:415:ALA:HA	2.17	0.44
1:A:75:HIS:CE1	1:A:199:LEU:HD21	2.53	0.44
1:B:36:TRP:HB3	1:B:170:HIS:HB3	1.99	0.43
1:B:389:LYS:HZ1	2:B:1002:MLC:H5'2	1.78	0.43
1:B:432:VAL:HG12	3:B:1225:HOH:O	2.17	0.43
1:B:321:VAL:HG11	2:B:1002:MLC:CP1	2.48	0.43
1:A:236:GLN:HG3	3:A:1057:HOH:O	2.18	0.43
1:B:82:LYS:HD2	1:B:146:LYS:HE2	2.01	0.42
1:B:253:ARG:NH2	1:B:257:ASN:ND2	2.65	0.42
1:A:253:ARG:NH1	1:A:257:ASN:ND2	2.67	0.42
1:A:284:TRP:CD1	1:A:342:ALA:HB1	2.54	0.42
1:A:62:VAL:HB	1:A:63:PRO:HD3	2.01	0.42
1:B:304:ARG:HH22	1:B:362:LEU:HA	1.85	0.42
1:B:383:TRP:O	1:B:415:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:HZ2	2:B:1002:MLC:H5'2	1.84	0.42
1:A:121:HIS:HD2	3:A:1156:HOH:O	2.03	0.42
1:A:441:ASP:HB2	3:A:1143:HOH:O	2.19	0.42
1:A:253:ARG:NH2	1:A:257:ASN:HD21	2.18	0.42
1:A:385:SER:O	1:A:417:SER:HA	2.20	0.42
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.81	0.41
1:B:273:VAL:H	2:B:1002:MLC:C2	2.32	0.41
1:A:393:TYR:HB2	1:A:422:LYS:HB2	1.98	0.41
1:B:391:ARG:NH2	1:B:394:ASP:OD1	2.53	0.41
1:B:321:VAL:HG11	2:B:1002:MLC:HP12	2.03	0.41
1:B:421:CYS:SG	1:B:429:GLU:HG3	2.60	0.41
1:A:180:CYS:HA	1:A:183:LYS:CE	2.45	0.41
1:B:35:PHE:HE1	1:B:223:ARG:HH22	1.69	0.40
1:B:253:ARG:NH2	1:B:257:ASN:HD22	2.20	0.40
1:A:302:ILE:HG12	2:A:1001:MLC:HP81	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLU:O	1:B:253:ARG:NH2[1_556]	2.18	0.02

## 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	436/454 (96%)	423 (97%)	12 (3%)	1 (0%)	47	49
1	B	436/454 (96%)	423 (97%)	12 (3%)	1 (0%)	47	49
All	All	872/908 (96%)	846 (97%)	24 (3%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	B	422	LYS

### 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	388/400 (97%)	369 (95%)	19 (5%)	25	23
1	B	388/400 (97%)	366 (94%)	22 (6%)	20	18
All	All	776/800 (97%)	735 (95%)	41 (5%)	22	20

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	7	LEU
1	A	50	LEU
1	A	52	ILE
1	A	59	GLU
1	A	98	VAL
1	A	206	LEU
1	A	218	GLU
1	A	226	VAL
1	A	230	ASN
1	A	243	ASP
1	A	284	TRP
1	A	363	LYS
1	A	370	ASN
1	A	391	ARG
1	A	399	TRP
1	A	412	HIS
1	A	422	LYS
1	A	423	GLU
1	B	22	LEU
1	B	50	LEU
1	B	56	GLN

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Mol	Chain	Res	Type
1	B	59	GLU
1	B	74	LYS
1	B	106	THR
1	B	123	ARG
1	B	132	VAL
1	B	206	LEU
1	B	218	GLU
1	B	221	LEU
1	B	225	LYS
1	B	226	VAL
1	B	321	VAL
1	B	355	THR
1	B	363	LYS
1	B	370	ASN
1	B	391	ARG
1	B	399	TRP
1	B	412	HIS
1	B	423	GLU
1	B	437	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	230	ASN
1	A	236	GLN
1	A	257	ASN
1	A	266	GLN
1	A	349	ASN
1	A	412	HIS
1	A	425	ASN
1	B	28	GLN
1	B	43	ASN
1	B	159	ASN
1	B	236	GLN
1	B	257	ASN
1	B	266	GLN
1	B	370	ASN
1	B	425	ASN

### 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
2	MLC	B	1002	-	44,56,56	1.04	4 (9%)	56,83,83	1.50	8 (14%)
2	MLC	A	1001	-	44,56,56	1.00	2 (4%)	56,83,83	1.80	11 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLC	B	1002	-	4/4/13/15	20/48/71/71	0/3/3/3
2	MLC	A	1001	-	4/4/13/15	24/48/71/71	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	MLC	CM1-S	-3.36	1.67	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	MLC	CM1-S	-2.89	1.69	1.76
2	B	1002	MLC	O4'-C1'	2.53	1.44	1.41
2	B	1002	MLC	C5-C4	2.51	1.47	1.40
2	A	1001	MLC	C5-C4	2.38	1.47	1.40
2	B	1002	MLC	OM2-CM1	2.27	1.24	1.21

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	MLC	CM2-CM1-S	6.38	121.64	113.69
2	A	1001	MLC	CP9-CPA-CP7	4.38	116.42	108.82
2	A	1001	MLC	N3-C2-N1	-4.20	122.11	128.68
2	B	1002	MLC	CM2-CM1-S	4.17	118.89	113.69
2	B	1002	MLC	CP9-CPA-CP7	4.17	116.05	108.82
2	B	1002	MLC	N3-C2-N1	-3.62	123.02	128.68
2	A	1001	MLC	CP7-CP6-NP2	3.39	123.34	116.58
2	A	1001	MLC	CP1-S-CM1	3.39	112.42	101.87
2	B	1002	MLC	O4'-C1'-C2'	-3.32	102.07	106.93
2	B	1002	MLC	CP8-CPA-CP7	-2.74	104.07	108.82
2	B	1002	MLC	CP7-CP6-NP2	2.70	121.96	116.58
2	A	1001	MLC	O4'-C1'-C2'	-2.70	102.98	106.93
2	A	1001	MLC	OM2-CM1-S	-2.64	119.18	122.61
2	A	1001	MLC	OM2-CM1-CM2	-2.42	119.16	123.35
2	B	1002	MLC	C4-C5-N7	-2.35	106.95	109.40
2	A	1001	MLC	CP8-CPA-CP7	-2.22	104.97	108.82
2	B	1002	MLC	OM2-CM1-S	-2.21	119.75	122.61
2	A	1001	MLC	C2-N1-C6	2.18	122.48	118.75
2	A	1001	MLC	O3'-P3-O33	-2.15	101.08	109.39

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1002	MLC	C4'
2	B	1002	MLC	C2'
2	B	1002	MLC	C3'
2	B	1002	MLC	CP7
2	A	1001	MLC	C4'
2	A	1001	MLC	C2'
2	A	1001	MLC	C3'
2	A	1001	MLC	CP7

All (44) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	B	1002	MLC	C5'-O5'-P1-O12
2	B	1002	MLC	C5'-O5'-P1-O6
2	B	1002	MLC	OP3-CP7-CPA-CPB
2	B	1002	MLC	CP6-CP7-CPA-CPB
2	B	1002	MLC	OP3-CP7-CPA-CP9
2	B	1002	MLC	CP6-CP7-CPA-CP9
2	B	1002	MLC	OP3-CP7-CPA-CP8
2	B	1002	MLC	CP6-CP7-CPA-CP8
2	B	1002	MLC	OP2-CP6-CP7-CPA
2	B	1002	MLC	NP2-CP6-CP7-CPA
2	B	1002	MLC	OP2-CP6-CP7-OP3
2	B	1002	MLC	NP2-CP6-CP7-OP3
2	B	1002	MLC	CM2-CM1-S-CP1
2	B	1002	MLC	OM2-CM1-S-CP1
2	A	1001	MLC	C3'-C4'-C5'-O5'
2	A	1001	MLC	O4'-C4'-C5'-O5'
2	A	1001	MLC	C5'-O5'-P1-O11
2	A	1001	MLC	OP3-CP7-CPA-CPB
2	A	1001	MLC	CP6-CP7-CPA-CPB
2	A	1001	MLC	OP3-CP7-CPA-CP9
2	A	1001	MLC	CP6-CP7-CPA-CP9
2	A	1001	MLC	OP3-CP7-CPA-CP8
2	A	1001	MLC	CP6-CP7-CPA-CP8
2	A	1001	MLC	OP2-CP6-CP7-CPA
2	A	1001	MLC	NP2-CP6-CP7-CPA
2	A	1001	MLC	OP2-CP6-CP7-OP3
2	A	1001	MLC	NP2-CP6-CP7-OP3
2	A	1001	MLC	CP4-CP3-NP1-CP2
2	A	1001	MLC	OP1-CP3-NP1-CP2
2	A	1001	MLC	S-CP1-CP2-NP1
2	A	1001	MLC	CP2-CP1-S-CM1
2	A	1001	MLC	CM2-CM1-S-CP1
2	A	1001	MLC	OM2-CM1-S-CP1
2	B	1002	MLC	O4'-C4'-C5'-O5'
2	B	1002	MLC	C3'-O3'-P3-O33
2	A	1001	MLC	C5'-O5'-P1-O6
2	B	1002	MLC	C5'-O5'-P1-O11
2	B	1002	MLC	C3'-C4'-C5'-O5'
2	B	1002	MLC	OM2-CM1-CM2-CM3
2	B	1002	MLC	P1-O6-P2-O22
2	A	1001	MLC	C3'-O3'-P3-O33
2	A	1001	MLC	C3'-O3'-P3-O32
2	A	1001	MLC	P1-O6-P2-O21

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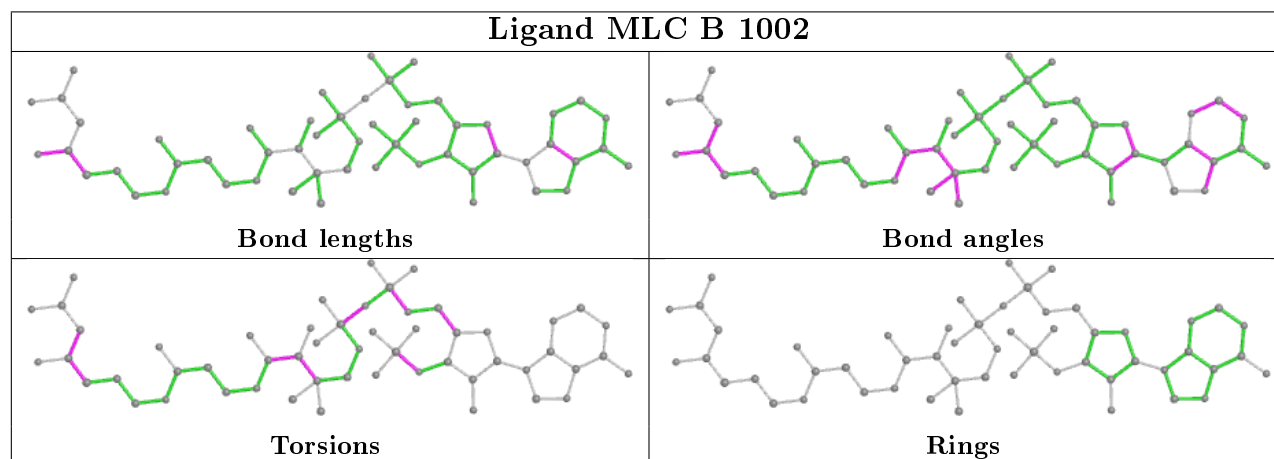
Mol	Chain	Res	Type	Atoms
2	A	1001	MLC	C4'-C3'-O3'-P3

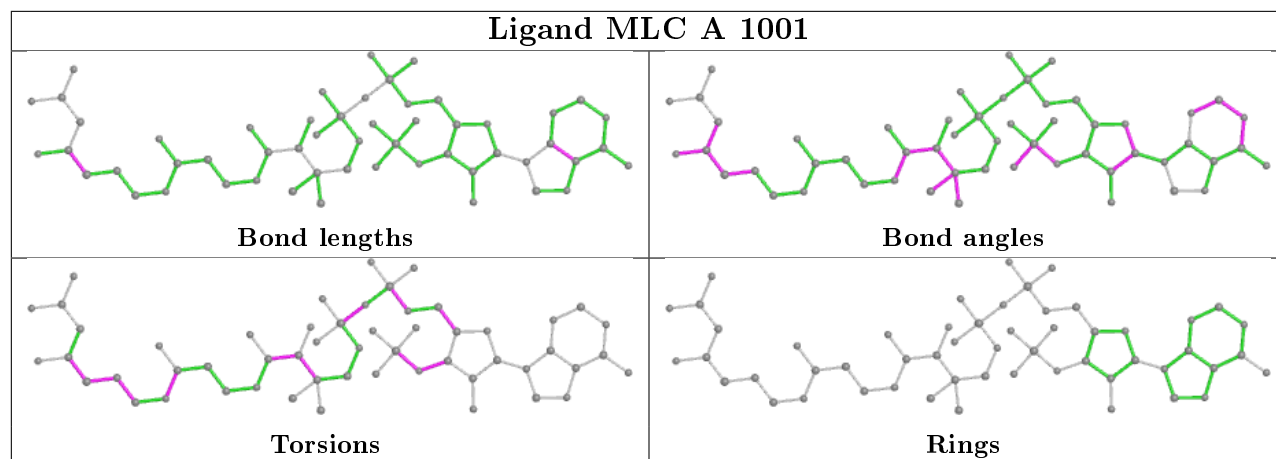
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	MLC	8	0
2	A	1001	MLC	6	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	440/454 (96%)	0.22	20 (4%) 33 38	17, 28, 46, 76	0
1	B	440/454 (96%)	0.25	27 (6%) 21 26	18, 28, 46, 78	0
All	All	880/908 (96%)	0.24	47 (5%) 26 32	17, 28, 46, 78	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	PRO	5.8
1	B	361	VAL	5.7
1	A	361	VAL	5.1
1	B	370	ASN	4.4
1	B	363	LYS	4.4
1	A	370	ASN	4.3
1	A	222	LYS	4.3
1	B	359	ASP	3.9
1	A	224	ALA	3.9
1	B	423	GLU	3.8
1	B	20	ASP	3.6
1	A	423	GLU	3.5
1	A	391	ARG	3.3
1	A	412	HIS	3.3
1	B	362	LEU	3.3
1	A	359	ASP	3.2
1	B	215	MET	3.1
1	B	225	LYS	2.8
1	A	206	LEU	2.8
1	B	238	LEU	2.7
1	B	19	PRO	2.6
1	B	206	LEU	2.6
1	B	371	ASP	2.6
1	B	202	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	90	THR	2.6
1	B	231	GLU	2.5
1	B	223	ARG	2.5
1	B	412	HIS	2.5
1	B	201	ASN	2.5
1	A	6	ILE	2.5
1	A	362	LEU	2.4
1	B	222	LYS	2.4
1	B	355	THR	2.4
1	A	121	HIS	2.3
1	A	225	LYS	2.2
1	A	142	SER	2.2
1	A	201	ASN	2.2
1	B	425	ASN	2.2
1	B	271	GLU	2.2
1	B	426	GLU	2.2
1	A	143	ASP	2.1
1	B	309	LYS	2.1
1	A	227	GLU	2.1
1	A	440	GLU	2.0
1	A	212	LYS	2.0
1	B	336	LYS	2.0
1	B	391	ARG	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, 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.

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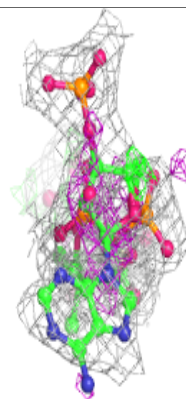
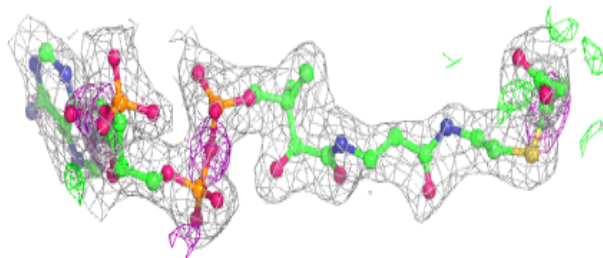
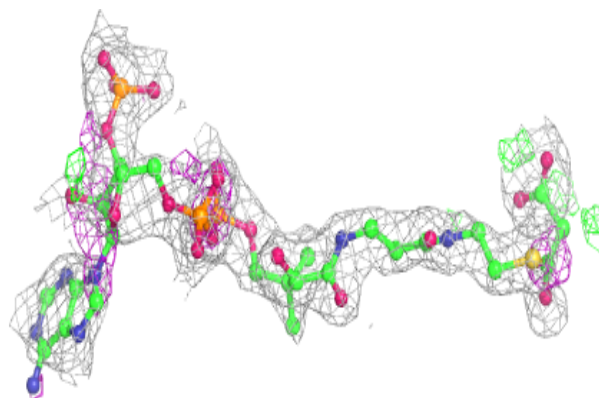
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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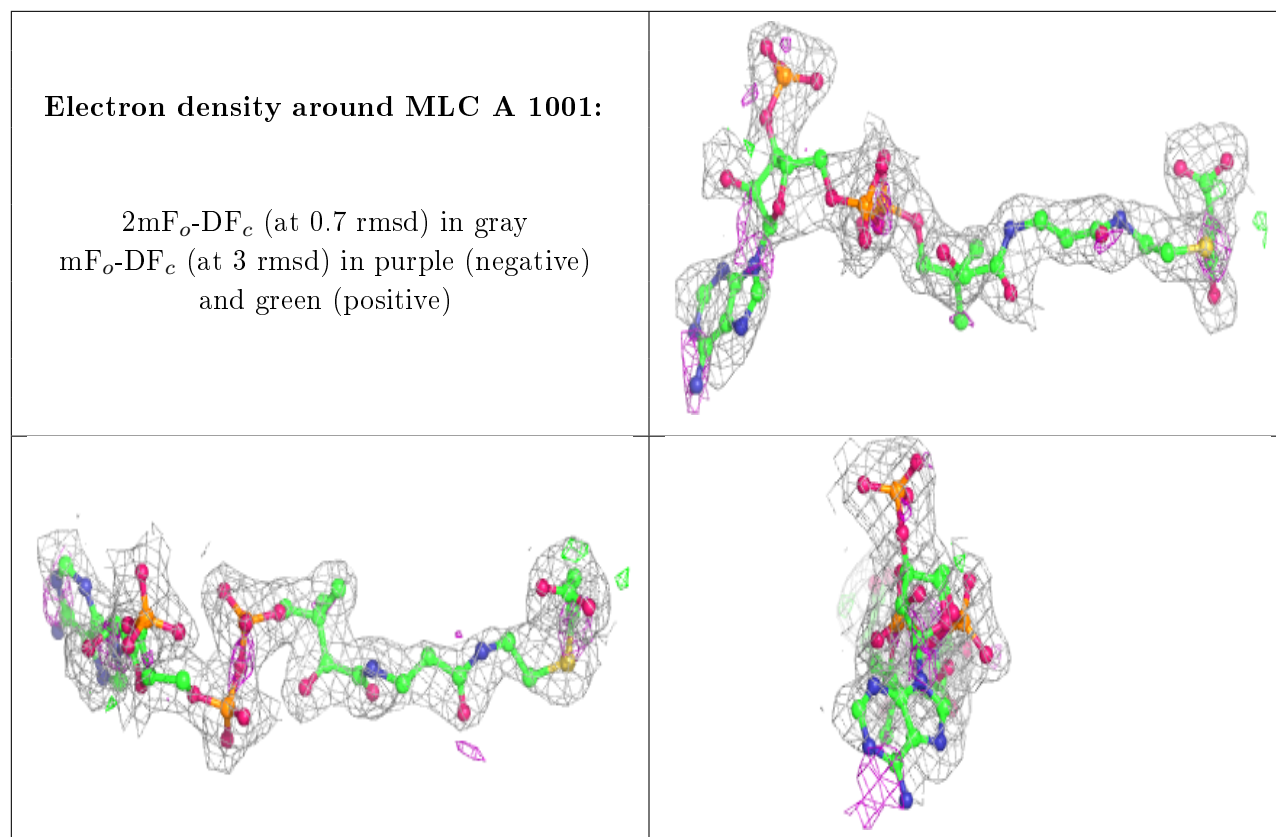
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MLC	B	1002	54/54	0.86	0.19	26,41,52,53	0
2	MLC	A	1001	54/54	0.87	0.18	26,40,55,55	0

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 MLC B 1002:**

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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.