



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:08 am BST

PDB ID : 5F49  
Title : Crystal structure of an aminoglycoside acetyltransferase meta-AAC0020 from an uncultured soil metagenomic sample in complex with malonyl-coenzyme A  
Authors : Xu, Z.; Skarina, T.; Stogios, P.J.; Yim, V.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2015-12-03  
Resolution : 2.15 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

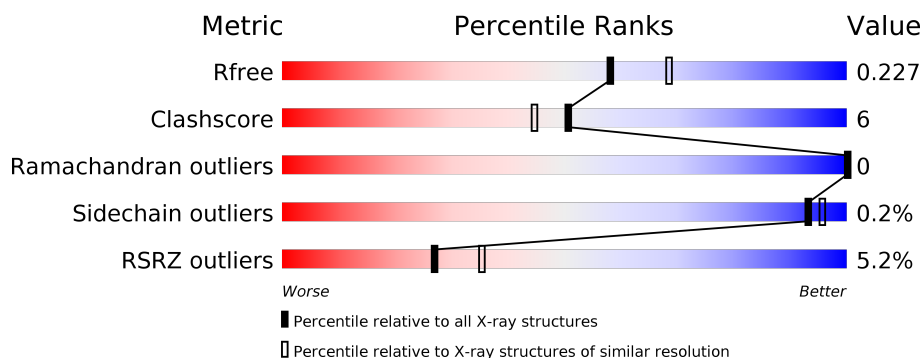
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	157	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>•</div> </div> </div>
1	B	157	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>•</div> </div> </div>
1	C	157	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>•</div> <div>6%</div> </div> </div>
1	D	157	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

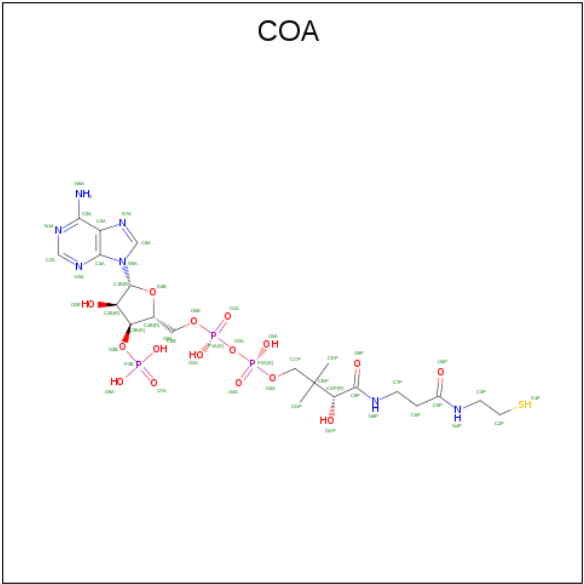
There are 5 unique types of molecules in this entry. The entry contains 5639 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 aminoglycoside acetyltransferase meta-AAC0020.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1257	822	197	237	1			
1	B	150	Total	C	N	O	S	0	1	0
			1261	825	197	238	1			
1	C	148	Total	C	N	O	S	0	0	0
			1241	814	194	232	1			
1	D	148	Total	C	N	O	S	0	0	0
			1241	814	194	232	1			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).

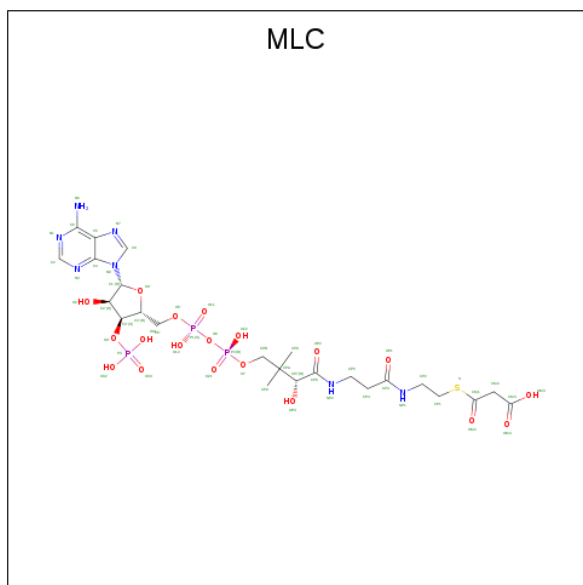


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	A	3	Total Mg 3 3	0	0
3	D	2	Total Mg 2 2	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is MALONYL-COENZYME A (three-letter code: MLC) (formula:  $C_{24}H_{38}N_7O_{19}P_3S$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	138	Total O 142 142	0	4
5	B	135	Total O 139 139	0	4
5	C	76	Total O 76 76	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	61	Total	O	0	3
			64	64		



- Molecule 1: aminoglycoside acetyltransferase meta-AAC0020



- | MET  |
|------|
| GLY  |
| GIN  |
| ASN  |
| MET  |
| GIU  |
| IIE  |
| D8   |
| N9   |
| F10  |
| L11  |
| R15  |
| F35  |
| L64  |
| V69  |
| A87  |
| D95  |
| T96  |
| N97  |
| Q98  |
| K99  |
| K106 |
| V123 |
| Y133 |
| K157 |

- | MET  |
|------|
| GLY  |
| GIN  |
| ASN  |
| MET  |
| GLU  |
| IIE  |
| ASP  |
| ASN  |
| F10  |
| L11  |
| K12  |
| I13  |
| N19  |
| L27  |
| N53  |
| Q54  |
| N55  |
| N56  |
| L64  |
| E65  |
| N66  |
| K67  |
| G70  |
| G71  |
| L72  |
| A87  |
| R100 |
| K105 |
| F114 |
| K118 |
| V123 |
| D128 |
| K129 |
| V130 |
| T133 |
| F137 |
| T141 |
| F147 |

- [illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.16Å 54.05Å 84.85Å 72.30° 74.57° 88.07°	Depositor
Resolution (Å)	23.49 – 2.15 23.49 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.4 (23.49-2.15) 89.1 (23.49-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.15Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.192 , 0.227 0.194 , 0.227	Depositor DCC
$R_{free}$ test set	1958 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for h,-k,h-l 0.025 for -h,k,k-l 0.019 for -h,-k,-h-k+l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.64% 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: COA, MLC, MG

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	0.30	0/1287	0.46	0/1741
1	B	0.31	0/1294	0.49	0/1751
1	C	0.35	0/1271	0.57	2/1719 (0.1%)
1	D	0.28	0/1271	0.46	0/1719
All	All	0.31	0/5123	0.50	2/6930 (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	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	67	LYS	CD-CE-NZ	6.82	127.39	111.70
1	C	10	PHE	CB-CA-C	-5.62	99.16	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	10	PHE	Mainchain



## 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	1257	0	1230	9	0
1	B	1261	0	1237	11	0
1	C	1241	0	1220	18	0
1	D	1241	0	1220	15	0
2	A	48	0	31	2	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	B	54	0	32	6	0
4	C	54	0	33	5	0
4	D	54	0	33	6	0
5	A	142	0	0	1	0
5	B	139	0	0	3	0
5	C	76	0	0	2	0
5	D	64	0	0	3	0
All	All	5639	0	5036	58	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 (58) 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:C:65:GLU:HG2	1:C:66:ASN:H	1.24	1.01
1:B:8:ASP:OD1	1:B:9:ASN:N	2.05	0.90
1:A:100:ARG:NH1	2:A:201:COA:O7A	2.07	0.87
1:C:65:GLU:CG	1:C:66:ASN:H	1.96	0.76
4:B:201:MLC:H3'	4:B:201:MLC:H8	1.68	0.76
1:C:12:LYS:NZ	1:C:13:ILE:O	2.18	0.73
1:D:132:ASP:OD1	5:D:301:HOH:O	2.08	0.72
4:D:201:MLC:HP2	4:D:201:MLC:HP81	1.53	0.71
1:B:133:TYR:HB3	4:B:201:MLC:H2	1.73	0.71
1:C:56:ASN:ND2	5:C:301:HOH:O	2.20	0.68
1:C:12:LYS:HD2	1:C:13:ILE:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:201:MLC:H3'	4:B:201:MLC:C8	2.30	0.62
1:B:11:LEU:HD23	1:B:106:LYS:HD2	1.81	0.61
1:C:100:ARG:NH1	4:C:201:MLC:H3'	2.16	0.60
1:C:100:ARG:NH1	4:C:201:MLC:O32	2.35	0.59
1:B:133:TYR:CB	4:B:201:MLC:H2	2.33	0.58
1:C:100:ARG:HH12	4:C:201:MLC:P3	2.26	0.58
1:C:137:PHE:HD1	4:C:201:MLC:H5'1	1.67	0.58
1:C:65:GLU:HG2	1:C:66:ASN:N	2.08	0.58
4:B:201:MLC:C3'	4:B:201:MLC:C8	2.83	0.57
1:D:50:LYS:NZ	5:D:303:HOH:O	2.37	0.56
1:B:35:PHE:CE1	4:B:201:MLC:HM22	2.42	0.55
1:D:100:ARG:N	4:D:201:MLC:O21	2.29	0.53
1:A:54:GLN:NE2	5:B:304:HOH:O	2.42	0.52
1:A:114:PHE:CZ	1:A:118:LYS:HD2	2.46	0.51
1:B:8:ASP:CG	1:B:9:ASN:H	2.14	0.51
1:C:54:GLN:HB3	1:C:56:ASN:OD1	2.11	0.50
1:D:79:GLN:NE2	1:D:84:LYS:O	2.43	0.50
4:D:201:MLC:O7	4:D:201:MLC:OP3	2.25	0.49
1:C:128:ASP:HA	1:D:149:VAL:HG12	1.94	0.49
1:C:12:LYS:C	1:C:12:LYS:HD2	2.31	0.49
1:C:87:ALA:HB3	1:C:123:VAL:HG22	1.95	0.49
1:D:131:ASP:OD1	5:D:302[A]:HOH:O	2.20	0.49
1:D:99:GLN:NE2	4:D:201:MLC:OP2	2.46	0.49
1:A:87:ALA:HB3	1:A:123:VAL:HG22	1.94	0.48
1:B:64:LEU:HD12	1:B:69:VAL:HG11	1.94	0.48
1:A:64:LEU:O	1:A:65:GLU:HG3	2.14	0.47
1:C:65:GLU:CG	1:C:66:ASN:N	2.70	0.47
1:A:15:ARG:NH1	5:A:311:HOH:O	2.47	0.46
1:C:114:PHE:CZ	1:C:118:LYS:HD2	2.49	0.46
1:B:97:ASN:ND2	5:B:309:HOH:O	2.49	0.44
1:D:95:ASP:OD2	1:D:97:ASN:HB2	2.18	0.44
1:A:105:LYS:HG3	2:A:201:COA:H52A	2.00	0.43
1:A:84:LYS:HA	1:A:85:PRO:HD3	1.82	0.43
1:A:11:LEU:HD11	1:A:62:ALA:HB1	2.00	0.43
1:D:91:ASP:OD1	4:D:201:MLC:HM22	2.19	0.43
1:C:105:LYS:HZ2	1:C:141:THR:HA	1.83	0.43
1:D:84:LYS:HA	1:D:85:PRO:HD3	1.88	0.43
1:B:87:ALA:HB3	1:B:123:VAL:HG22	2.01	0.42
4:C:201:MLC:H2'	4:C:201:MLC:O31	2.20	0.42
1:D:87:ALA:HB3	1:D:123:VAL:HG22	2.01	0.42
1:D:26:GLN:HB3	1:D:68:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLY:N	4:D:201:MLC:O11	2.35	0.41
1:D:11:LEU:HD11	1:D:62:ALA:HB1	2.01	0.41
1:C:53:ASN:O	5:C:302:HOH:O	2.22	0.41
1:B:15:ARG:NH1	5:B:306:HOH:O	2.45	0.41
1:D:138:TYR:O	1:D:143:PRO:HD3	2.21	0.40
1:B:95:ASP:O	1:B:99:GLN:HG3	2.21	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	148/157 (94%)	147 (99%)	1 (1%)	0	100	100
1	B	149/157 (95%)	148 (99%)	1 (1%)	0	100	100
1	C	146/157 (93%)	143 (98%)	3 (2%)	0	100	100
1	D	146/157 (93%)	143 (98%)	3 (2%)	0	100	100
All	All	589/628 (94%)	581 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	136/142 (96%)	136 (100%)	0	100	100
1	B	137/142 (96%)	137 (100%)	0	100	100
1	C	134/142 (94%)	133 (99%)	1 (1%)	84	89
1	D	134/142 (94%)	134 (100%)	0	100	100
All	All	541/568 (95%)	540 (100%)	1 (0%)	93	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	100	ARG

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	66	ASN
1	C	49	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 ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z  > 2$
4	MLC	B	201	-	44,56,56	2.37	13 (29%)	56,83,83	3.94	19 (33%)
2	COA	A	201	3	41,50,50	2.27	9 (21%)	52,75,75	3.27	13 (25%)
4	MLC	D	201	-	44,56,56	1.62	6 (13%)	56,83,83	3.77	10 (17%)
4	MLC	C	201	3	44,56,56	2.04	9 (20%)	56,83,83	3.80	19 (33%)

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
4	MLC	B	201	-	-	13/48/71/71	0/3/3/3
2	COA	A	201	3	-	4/44/64/64	0/3/3/3
4	MLC	D	201	-	-	12/48/71/71	0/3/3/3
4	MLC	C	201	3	-	14/48/71/71	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	201	MLC	O4'-C1'	7.89	1.52	1.41
4	C	201	MLC	O4'-C1'	7.17	1.51	1.41
2	A	201	COA	O9P-C9P	6.33	1.36	1.23
4	B	201	MLC	C2'-C3'	6.04	1.66	1.52
2	A	201	COA	C3B-C4B	-5.98	1.36	1.52
4	D	201	MLC	C2-N3	5.41	1.40	1.32
2	A	201	COA	C2B-C3B	5.35	1.64	1.52
4	D	201	MLC	O4'-C1'	5.32	1.48	1.41
4	C	201	MLC	C2-N3	5.27	1.40	1.32
4	B	201	MLC	O4'-C4'	5.02	1.56	1.45
2	A	201	COA	C2A-N3A	4.91	1.40	1.32
4	C	201	MLC	P3-O3'	4.86	1.68	1.59
4	B	201	MLC	C2-N3	4.63	1.39	1.32
4	B	201	MLC	C2'-C1'	-4.17	1.47	1.53
4	B	201	MLC	C3'-C4'	-4.12	1.41	1.52
2	A	201	COA	O4B-C1B	3.46	1.45	1.41
4	C	201	MLC	CM1-S	3.33	1.84	1.76
2	A	201	COA	C2A-N1A	3.30	1.40	1.33
4	D	201	MLC	C2-N1	3.30	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	MLC	C2-N1	3.24	1.39	1.33
4	B	201	MLC	C2-N1	3.21	1.39	1.33
4	C	201	MLC	C3'-C4'	2.96	1.60	1.52
2	A	201	COA	P3B-O3B	-2.82	1.54	1.59
4	B	201	MLC	C6-C5	-2.74	1.33	1.43
2	A	201	COA	C6A-C5A	-2.64	1.33	1.43
4	D	201	MLC	C6-C5	-2.64	1.33	1.43
4	B	201	MLC	C5-C4	-2.57	1.34	1.40
4	C	201	MLC	C6-C5	-2.53	1.33	1.43
4	D	201	MLC	C5-C4	-2.42	1.34	1.40
4	B	201	MLC	P1-O5'	2.37	1.68	1.59
4	B	201	MLC	C5'-C4'	2.34	1.58	1.51
4	C	201	MLC	C5-C4	-2.33	1.34	1.40
2	A	201	COA	C5A-C4A	-2.28	1.34	1.40
4	D	201	MLC	CM1-S	-2.28	1.70	1.76
4	C	201	MLC	C2'-C3'	-2.11	1.48	1.52
4	B	201	MLC	C5-N7	-2.10	1.32	1.39
4	B	201	MLC	P3-O32	-2.02	1.47	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	201	MLC	C1'-N9-C4	-16.92	96.90	126.64
4	D	201	MLC	O4'-C4'-C3'	-14.57	73.66	104.87
4	B	201	MLC	O4'-C1'-C2'	-14.36	85.94	106.93
2	A	201	COA	O4B-C1B-C2B	-14.31	86.02	106.93
4	C	201	MLC	O4'-C1'-C2'	-14.21	86.16	106.93
4	D	201	MLC	O4'-C1'-C2'	-14.12	86.29	106.93
4	D	201	MLC	C1'-N9-C4	13.55	150.44	126.64
4	C	201	MLC	O4'-C4'-C3'	-12.17	78.79	104.87
4	C	201	MLC	C1'-N9-C4	9.63	143.56	126.64
4	C	201	MLC	C2'-C3'-C4'	-8.81	87.61	103.22
4	B	201	MLC	C2'-C3'-C4'	-8.70	87.80	103.22
2	A	201	COA	C2B-C3B-C4B	-8.35	88.42	103.22
4	D	201	MLC	C2'-C3'-C4'	-6.97	90.86	103.22
4	B	201	MLC	C3'-C2'-C1'	6.88	115.13	99.89
2	A	201	COA	C5B-C4B-C3B	6.83	137.03	114.40
4	C	201	MLC	CP5-CP4-CP3	6.82	123.71	112.36
4	D	201	MLC	N3-C2-N1	-6.47	118.57	128.68
4	C	201	MLC	N3-C2-N1	-6.36	118.74	128.68
4	B	201	MLC	O5'-P1-O11	-6.29	84.50	109.07
2	A	201	COA	N3A-C2A-N1A	-6.26	118.89	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	COA	O3B-C3B-C4B	-6.06	88.18	110.08
4	B	201	MLC	C5'-C4'-C3'	5.76	133.49	114.40
4	B	201	MLC	N3-C2-N1	-5.51	120.06	128.68
2	A	201	COA	O3B-C3B-C2B	-5.50	91.75	111.68
4	B	201	MLC	O5'-C5'-C4'	5.28	127.16	108.99
4	C	201	MLC	O3'-C3'-C2'	-5.26	92.61	111.68
4	D	201	MLC	CP1-CP2-NP1	-5.24	101.40	112.42
4	C	201	MLC	CP2-NP1-CP3	-4.87	113.80	122.84
4	C	201	MLC	O5'-C5'-C4'	4.65	124.99	108.99
2	A	201	COA	O5B-C5B-C4B	-4.43	93.74	108.99
2	A	201	COA	C3B-C2B-C1B	4.32	109.45	99.89
2	A	201	COA	O6A-CCP-CBP	4.25	117.38	110.55
4	C	201	MLC	CP1-S-CM1	-3.95	89.57	101.87
4	C	201	MLC	C3'-C2'-C1'	3.94	108.61	99.89
4	B	201	MLC	O7-CPB-CPA	3.82	116.69	110.55
4	D	201	MLC	O7-CPB-CPA	-3.76	104.51	110.55
2	A	201	COA	O3B-P3B-O7A	-3.51	95.86	109.39
4	C	201	MLC	CP1-CP2-NP1	3.27	119.28	112.42
4	B	201	MLC	P2-O6-P1	-3.26	121.64	132.83
4	B	201	MLC	C5-C6-N6	-3.15	115.57	120.35
4	C	201	MLC	O7-CPB-CPA	2.96	115.30	110.55
4	D	201	MLC	C5-C6-N6	-2.94	115.88	120.35
4	B	201	MLC	O12-P1-O5'	-2.94	94.08	107.75
4	D	201	MLC	C5'-C4'-C3'	-2.89	104.81	114.40
2	A	201	COA	C1B-N9A-C4A	2.80	131.57	126.64
4	C	201	MLC	CP4-CP5-NP2	2.79	117.52	111.90
4	B	201	MLC	CP2-NP1-CP3	2.77	127.97	122.84
4	C	201	MLC	CP4-CP3-NP1	2.73	121.01	116.42
4	B	201	MLC	O3'-C3'-C4'	-2.72	100.25	110.08
4	C	201	MLC	OP1-CP3-CP4	-2.56	117.33	122.02
4	B	201	MLC	OM2-CM1-S	2.54	125.91	122.61
2	A	201	COA	C5A-C6A-N6A	-2.52	116.52	120.35
2	A	201	COA	O9A-P3B-O8A	2.48	117.11	107.64
4	C	201	MLC	C5-C6-N6	-2.47	116.60	120.35
4	B	201	MLC	O3'-C3'-C2'	-2.35	103.15	111.68
4	C	201	MLC	CM2-CM1-S	2.33	116.60	113.69
4	B	201	MLC	O12-P1-O11	2.27	123.45	112.24
4	D	201	MLC	CP8-CPA-CP7	2.25	112.73	108.82
4	C	201	MLC	O3'-C3'-C4'	2.24	118.18	110.08
4	B	201	MLC	O32-P3-O31	2.24	116.19	107.64
4	B	201	MLC	CP1-CP2-NP1	2.02	116.66	112.42

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	201	MLC	C3'-O3'-P3-O31
4	B	201	MLC	C5'-O5'-P1-O11
4	B	201	MLC	C5'-O5'-P1-O12
4	B	201	MLC	CP2-CP1-S-CM1
4	B	201	MLC	CM2-CM1-S-CP1
4	B	201	MLC	OM2-CM1-S-CP1
4	D	201	MLC	C3'-O3'-P3-O33
4	D	201	MLC	CPB-O7-P2-O22
4	D	201	MLC	OP2-CP6-CP7-CPA
4	D	201	MLC	NP2-CP6-CP7-CPA
4	D	201	MLC	CP2-CP1-S-CM1
4	C	201	MLC	O4'-C4'-C5'-O5'
4	C	201	MLC	C5'-O5'-P1-O12
4	C	201	MLC	C5'-O5'-P1-O6
4	C	201	MLC	OM2-CM1-S-CP1
4	B	201	MLC	O4'-C4'-C5'-O5'
4	D	201	MLC	O4'-C4'-C5'-O5'
4	D	201	MLC	C2'-C3'-O3'-P3
2	A	201	COA	C6P-C7P-N8P-C9P
4	C	201	MLC	C4'-C3'-O3'-P3
4	B	201	MLC	P1-O6-P2-O21
4	C	201	MLC	P1-O6-P2-O21
4	B	201	MLC	C3'-O3'-P3-O33
4	C	201	MLC	NP2-CP6-CP7-OP3
4	C	201	MLC	CM2-CM1-S-CP1
4	B	201	MLC	C5'-O5'-P1-O6
4	D	201	MLC	CPB-O7-P2-O6
4	D	201	MLC	P1-O6-P2-O22
4	B	201	MLC	CPA-CPB-O7-P2
4	D	201	MLC	CPB-O7-P2-O21
4	C	201	MLC	C5'-O5'-P1-O11
4	C	201	MLC	P1-O6-P2-O22
4	C	201	MLC	CP1-CP2-NP1-CP3
2	A	201	COA	P1A-O3A-P2A-O5A
4	B	201	MLC	OP2-CP6-CP7-OP3
4	C	201	MLC	OP2-CP6-CP7-OP3
4	C	201	MLC	CP4-CP5-NP2-CP6
4	D	201	MLC	C3'-O3'-P3-O32
4	B	201	MLC	P1-O6-P2-O22
4	D	201	MLC	P1-O6-P2-O21
2	A	201	COA	P1A-O3A-P2A-O4A
4	C	201	MLC	CPA-CPB-O7-P2

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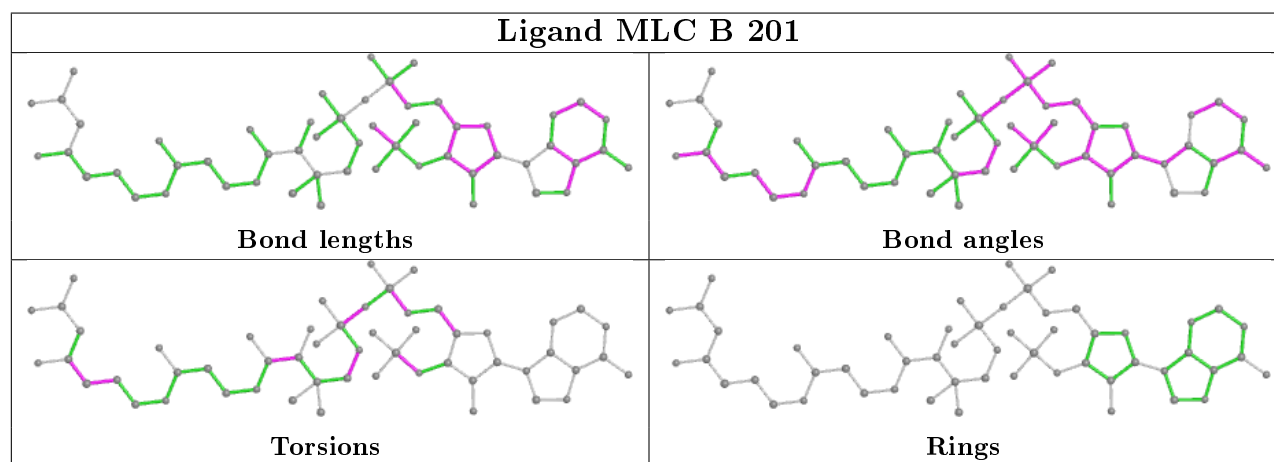
Mol	Chain	Res	Type	Atoms
2	A	201	COA	C5B-O5B-P1A-O2A

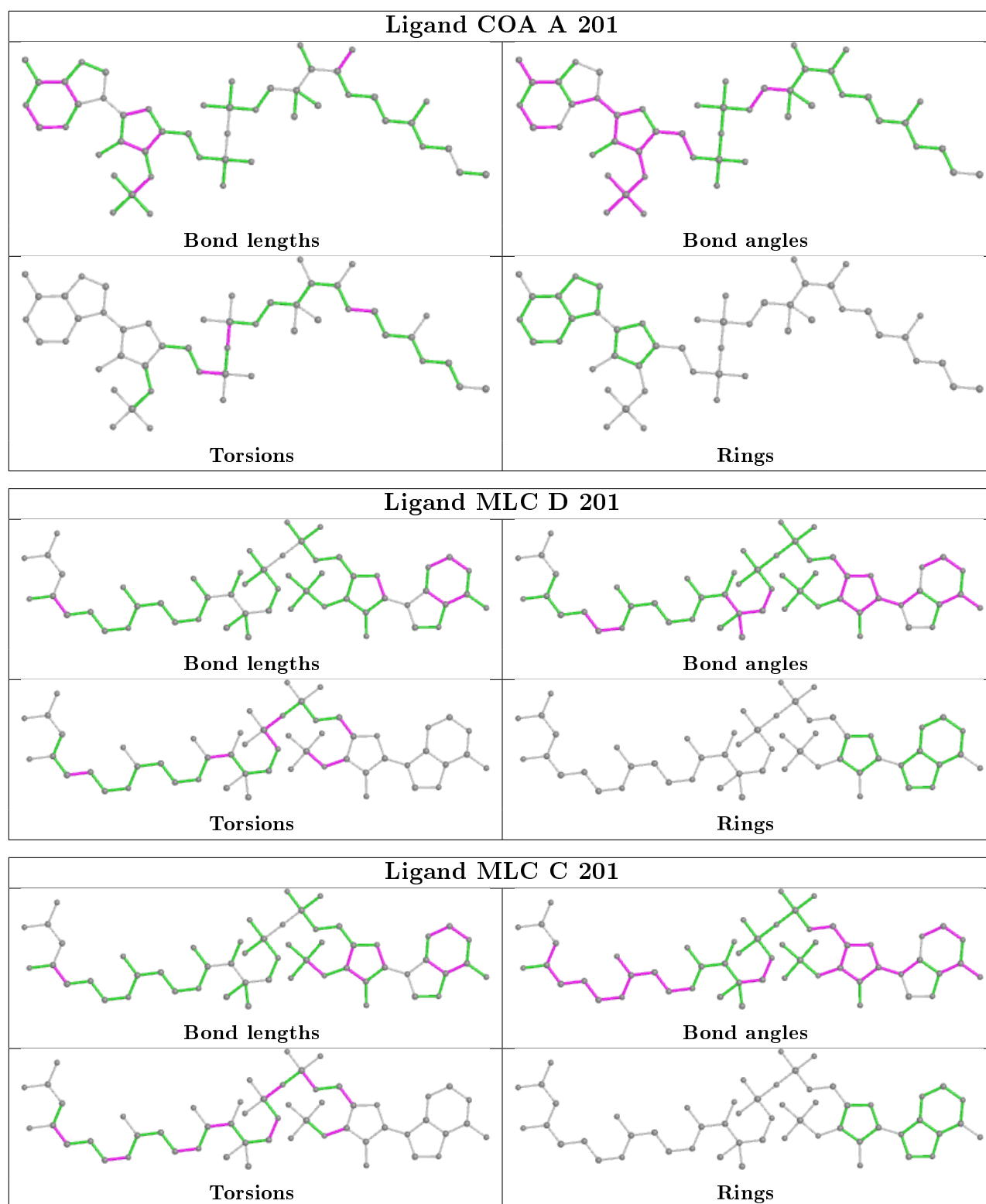
There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	MLC	6	0
2	A	201	COA	2	0
4	D	201	MLC	6	0
4	C	201	MLC	5	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 ⓘ

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	150/157 (95%)	-0.01	3 (2%) 65 72	18, 29, 49, 80	0
1	B	150/157 (95%)	-0.09	4 (2%) 54 63	18, 27, 48, 96	0
1	C	148/157 (94%)	0.41	11 (7%) 14 20	29, 44, 72, 103	0
1	D	148/157 (94%)	0.34	13 (8%) 10 14	26, 43, 78, 104	0
All	All	596/628 (94%)	0.16	31 (5%) 27 35	18, 36, 71, 104	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	PHE	7.1
1	C	10	PHE	5.9
1	C	66	ASN	4.4
1	C	11	LEU	4.2
1	D	133	TYR	3.9
1	D	132	ASP	3.8
1	C	133	TYR	3.6
1	B	10	PHE	3.5
1	B	8	ASP	3.3
1	D	98	TRP	3.2
1	C	19	ASN	3.2
1	D	130	VAL	3.1
1	C	72	LEU	3.0
1	C	71	GLY	2.9
1	C	130	VAL	2.8
1	A	72	LEU	2.6
1	D	101	GLN	2.6
1	A	133	TYR	2.6
1	D	64	LEU	2.6
1	B	157	LYS	2.5
1	C	64	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	9	ASN	2.5
1	C	27	LEU	2.3
1	D	27	LEU	2.3
1	C	70	GLY	2.3
1	D	66	ASN	2.3
1	D	67	LYS	2.2
1	A	66	ASN	2.2
1	D	92	LEU	2.2
1	D	65	GLU	2.1
1	D	72	LEU	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](#)

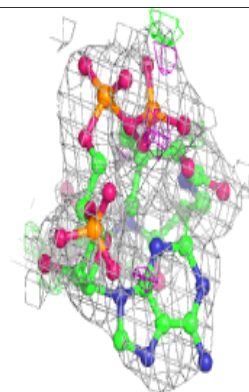
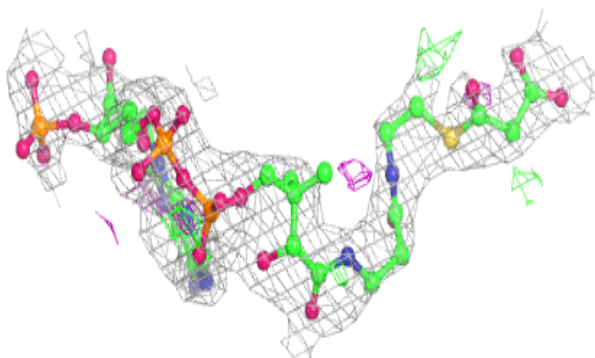
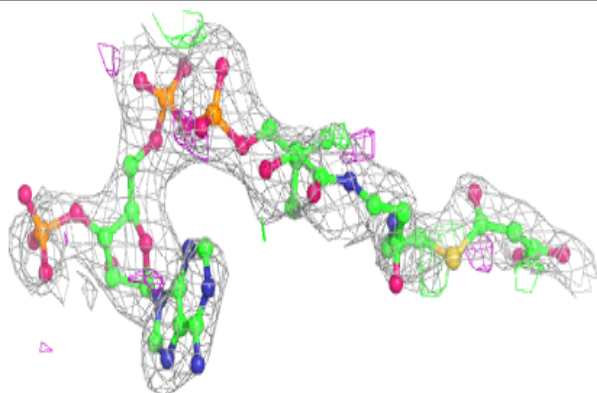
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	203	1/1	0.84	0.06	46,46,46,46	0
3	MG	C	202	1/1	0.85	0.07	46,46,46,46	0
4	MLC	D	201	54/54	0.86	0.20	49,87,130,158	0
4	MLC	C	201	54/54	0.88	0.19	32,75,104,109	0
2	COA	A	201	48/48	0.92	0.16	24,50,87,172	0
4	MLC	B	201	54/54	0.93	0.15	18,43,95,111	0
3	MG	A	204	1/1	0.96	0.07	33,33,33,33	0
3	MG	A	202	1/1	0.96	0.09	33,33,33,33	0
3	MG	D	203	1/1	0.98	0.05	23,23,23,23	0
3	MG	B	203	1/1	0.98	0.04	20,20,20,20	0
3	MG	B	202	1/1	0.99	0.10	16,16,16,16	0
3	MG	D	202	1/1	0.99	0.06	24,24,24,24	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.

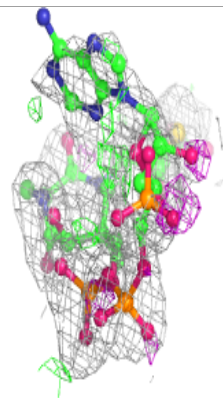
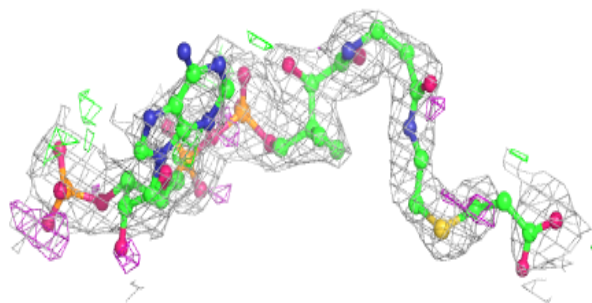
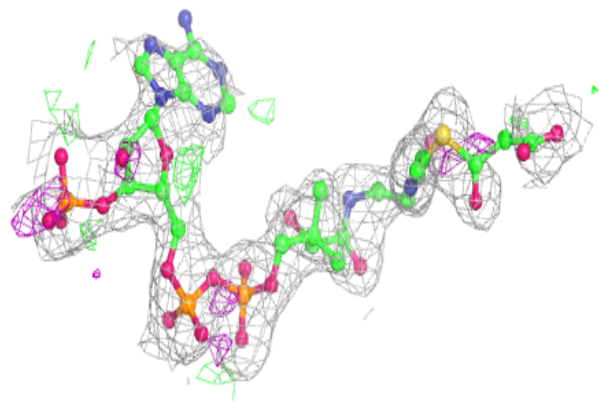
**Electron density around MLC D 201:**

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)

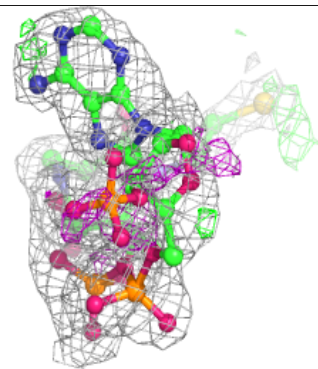
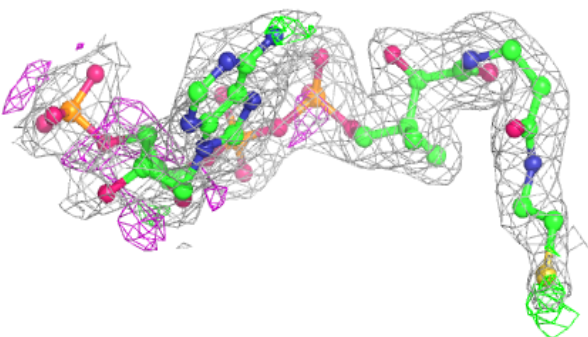
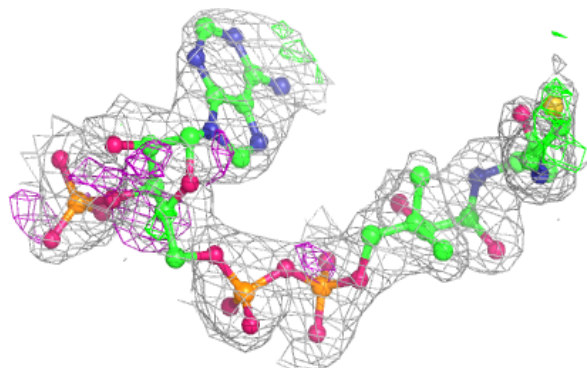


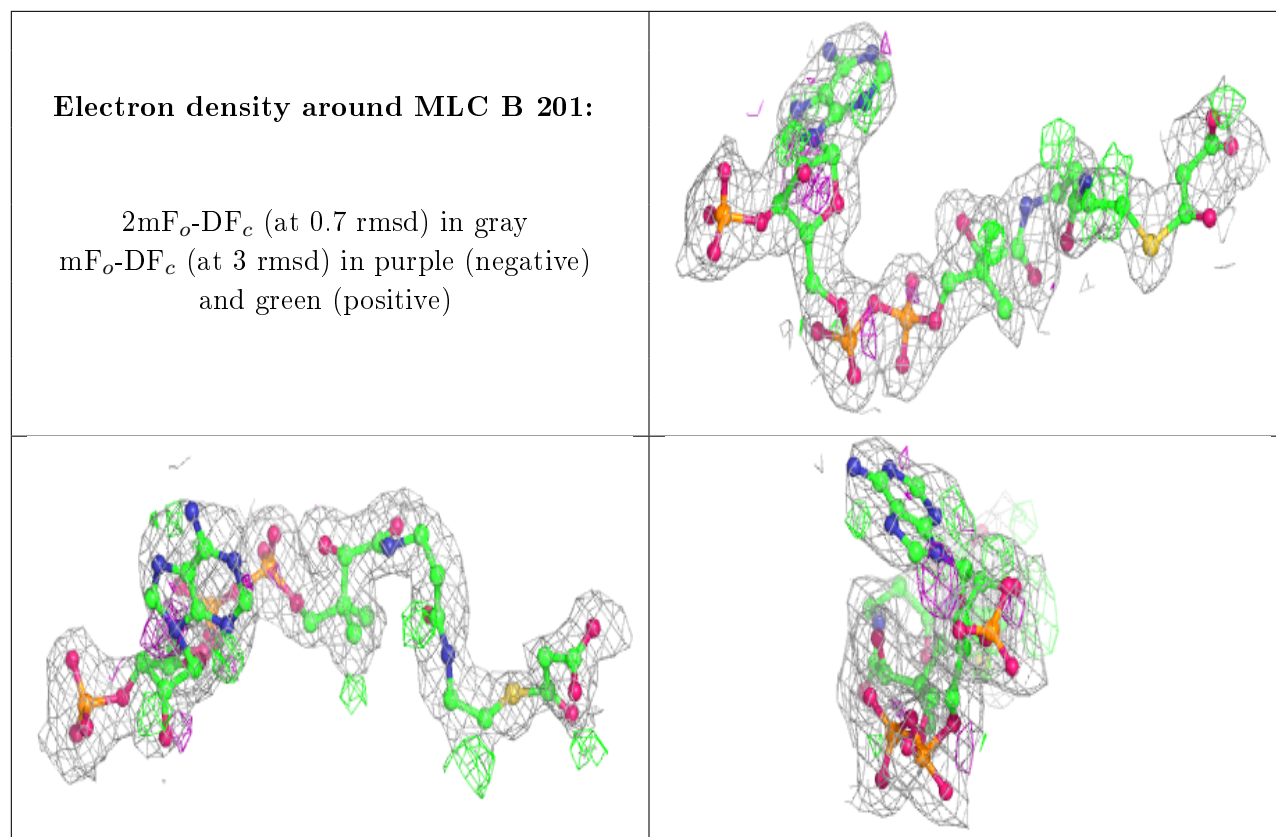
**Electron density around MLC C 201:**

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

**Electron density around COA A 201:**

$2mF_o-DF_c$  (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.