



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:48 am BST

PDB ID : 4GXQ  
Title : Crystal Structure of ATP bound RpMatB-BxBclM chimera B1  
Authors : Rank, K.C.; Crosby, H.A.; Escalante-Semerena, J.C.; Rayment, I.  
Deposited on : 2012-09-04  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

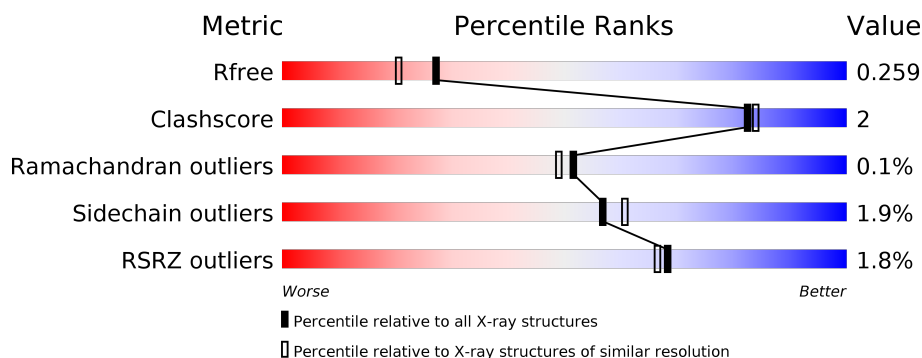
# 1 Overall quality at a glance

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	506	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	506	<div> <div></div> <div>94%</div> <div>5%</div> </div>
1	C	506	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>6%</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
1	MLY	A	62	-	-	X	-
1	MLY	C	62	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13557 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.

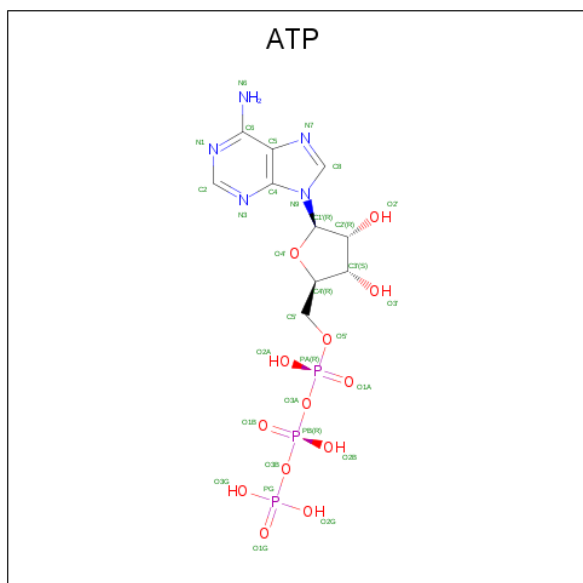
- Molecule 1 is a protein called Malonyl CoA synthetase, Benzoate-CoA ligase Chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	1	0
			3944	2532	669	729	14			
1	B	506	Total	C	N	O	S	0	6	0
			3972	2550	673	735	14			
1	C	506	Total	C	N	O	S	0	2	0
			3947	2534	669	730	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	491	ALA	LYS	ENGINEERED MUTATION	UNP Q6ND88
B	491	ALA	LYS	ENGINEERED MUTATION	UNP Q6ND88
C	491	ALA	LYS	ENGINEERED MUTATION	UNP Q6ND88

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

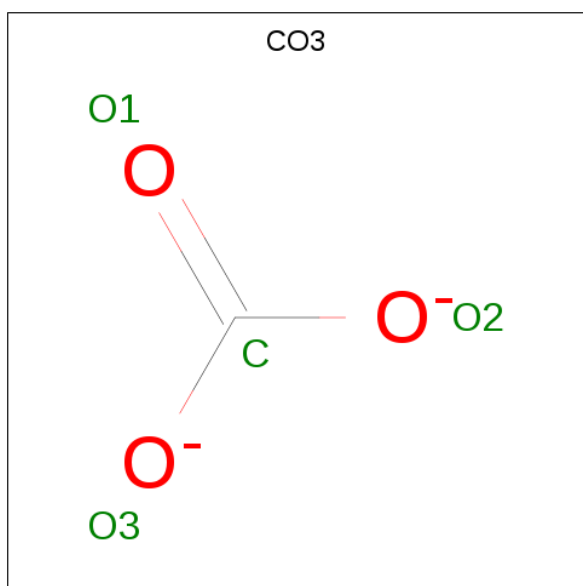


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		
4	C	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	476	Total 476	O 476	0	0
5	B	668	Total 668	O 668	0	0
5	C	442	Total 442	O 442	0	0

### 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.

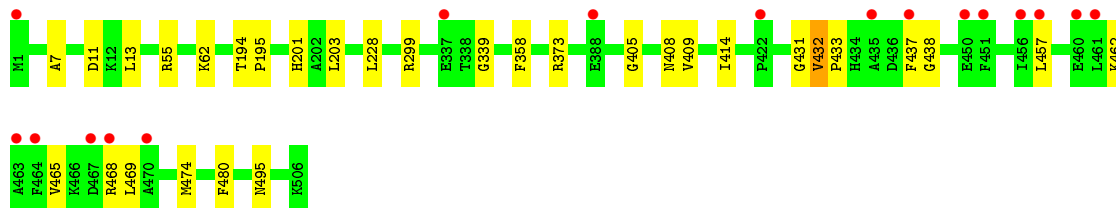
- Molecule 1: Malonyl CoA synthetase, Benzoate-CoA ligase Chimeric protein



- Molecule 1: Malonyl CoA synthetase, Benzoate-CoA ligase Chimeric protein



- Molecule 1: Malonyl CoA synthetase, Benzoate-CoA ligase Chimeric protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	299.31Å 299.31Å 47.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.95 – 2.00 24.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.95-2.00) 99.6 (24.94-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.219 , 0.254 0.225 , 0.259	Depositor DCC
$R_{free}$ test set	8364 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2680e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: MG, MLY, CO3, ATP

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	0.39	0/3696	0.59	0/5048
1	B	0.49	0/3739	0.66	1/5105 (0.0%)
1	C	0.39	0/3702	0.59	0/5056
All	All	0.43	0/11137	0.61	1/15209 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	498	ARG	NE-CZ-NH1	5.13	122.87	120.30

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	3944	0	3994	17	0
1	B	3972	0	4032	18	0
1	C	3947	0	4000	24	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
5	A	476	0	0	1	0
5	B	668	0	0	3	0
5	C	442	0	0	3	0
All	All	13557	0	12062	59	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 2.

The worst 5 of 59 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:438:GLY:HA2	5:C:1112:HOH:O	1.75	0.85
1:A:62:MLY:HH23	1:A:203:LEU:O	1.83	0.78
1:A:461:LEU:O	1:A:465:VAL:HG23	1.84	0.78
1:C:495:ASN:HB2	5:C:1046:HOH:O	1.86	0.74
1:A:465:VAL:CG1	1:A:469:LEU:HD12	2.18	0.73

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	476/506 (94%)	472 (99%)	3 (1%)	1 (0%)	47	44
1	B	481/506 (95%)	478 (99%)	2 (0%)	1 (0%)	47	44
1	C	477/506 (94%)	473 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1434/1518 (94%)	1423 (99%)	9 (1%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	VAL
1	B	450	GLU

### 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	378/377 (100%)	368 (97%)	10 (3%)	46	48
1	B	383/377 (102%)	376 (98%)	7 (2%)	59	63
1	C	379/377 (100%)	374 (99%)	5 (1%)	69	74
All	All	1140/1131 (101%)	1118 (98%)	22 (2%)	57	61

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	483	ASP
1	B	299	ARG
1	C	358	PHE
1	B	55	ARG
1	B	70	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	ASN
1	C	216	ASN
1	C	408	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

90 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	MLY	A	264	1	9,10,11	0.67	0	6,11,13	0.50	0
1	MLY	B	494	1	9,10,11	0.64	0	6,11,13	0.61	0
1	MLY	C	385	1	9,10,11	0.47	0	6,11,13	0.76	0
1	MLY	B	171	1	9,10,11	0.54	0	6,11,13	0.48	0
1	MLY	C	476	1	9,10,11	0.56	0	6,11,13	0.50	0
1	MLY	B	62	1	9,10,11	1.12	1 (11%)	6,11,13	1.70	2 (33%)
1	MLY	B	18	1	9,10,11	0.53	0	6,11,13	0.46	0
1	MLY	A	369	1	9,10,11	0.51	0	6,11,13	0.35	0
1	MLY	A	476	1	9,10,11	0.53	0	6,11,13	0.54	0
1	MLY	B	412	1	9,10,11	0.56	0	6,11,13	0.52	0
1	MLY	C	473	1	9,10,11	0.49	0	6,11,13	0.90	0
1	MLY	C	171	1	9,10,11	0.57	0	6,11,13	0.64	0
1	MLY	C	471	1	9,10,11	0.53	0	6,11,13	0.29	0
1	MLY	B	102	1	9,10,11	0.68	0	6,11,13	0.73	0
1	MLY	B	28	1	9,10,11	0.65	0	6,11,13	0.75	0
1	MLY	B	471	1	9,10,11	0.50	0	6,11,13	0.43	0
1	MLY	B	120	1	9,10,11	0.49	0	6,11,13	0.53	0
1	MLY	C	412	1	9,10,11	0.58	0	6,11,13	0.44	0
1	MLY	C	353	1	9,10,11	0.63	0	6,11,13	0.60	0
1	MLY	B	385	1	9,10,11	0.63	0	6,11,13	0.34	0
1	MLY	A	120	1	9,10,11	0.46	0	6,11,13	0.59	0
1	MLY	C	12	1	9,10,11	0.53	0	6,11,13	0.44	0
1	MLY	A	399	1	9,10,11	0.46	0	6,11,13	0.52	0
1	MLY	C	359	1	9,10,11	0.57	0	6,11,13	0.45	0
1	MLY	B	448	1	9,10,11	0.55	0	6,11,13	0.73	0
1	MLY	A	448	1	9,10,11	0.59	0	6,11,13	0.64	0
1	MLY	C	466	1	9,10,11	0.48	0	6,11,13	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	B	466	1	9,10,11	0.47	0	6,11,13	0.60	0
1	MLY	C	506	1	7,11,11	0.40	0	7,13,13	0.61	0
1	MLY	C	291	1	9,10,11	0.58	0	6,11,13	0.41	0
1	MLY	B	235	1	9,10,11	0.51	0	6,11,13	0.53	0
1	MLY	C	28	1	9,10,11	0.65	0	6,11,13	0.53	0
1	MLY	B	399	1	9,10,11	0.54	0	6,11,13	0.35	0
1	MLY	C	340	1	9,10,11	0.55	0	6,11,13	0.85	0
1	MLY	A	171	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	C	369	1	9,10,11	0.42	0	6,11,13	0.67	0
1	MLY	C	62	1	9,10,11	0.54	0	6,11,13	0.85	0
1	MLY	C	102	1	9,10,11	0.63	0	6,11,13	0.43	0
1	MLY	B	462	1	9,10,11	0.48	0	6,11,13	0.65	0
1	MLY	B	476	1	9,10,11	0.49	0	6,11,13	0.53	0
1	MLY	B	110	1	9,10,11	0.78	0	6,11,13	0.46	0
1	MLY	B	340	1	9,10,11	0.52	0	6,11,13	0.64	0
1	MLY	A	235	1	9,10,11	0.42	0	6,11,13	0.45	0
1	MLY	A	340	1	9,10,11	0.62	0	6,11,13	0.71	0
1	MLY	A	502	1	9,10,11	0.47	0	6,11,13	0.94	0
1	MLY	B	473	1	9,10,11	0.49	0	6,11,13	0.69	0
1	MLY	B	291	1	9,10,11	0.58	0	6,11,13	0.46	0
1	MLY	B	230	1	9,10,11	0.47	0	6,11,13	0.46	0
1	MLY	A	412	1	9,10,11	0.42	0	6,11,13	0.58	0
1	MLY	B	353	1	9,10,11	0.58	0	6,11,13	0.66	0
1	MLY	B	359	1	9,10,11	0.51	0	6,11,13	0.49	0
1	MLY	A	494	1	9,10,11	0.62	0	6,11,13	0.61	0
1	MLY	C	367	1	9,10,11	0.59	0	6,11,13	0.53	0
1	MLY	A	353	1	9,10,11	0.56	0	6,11,13	0.59	0
1	MLY	B	264	1	9,10,11	0.63	0	6,11,13	0.60	0
1	MLY	A	385	1	9,10,11	0.56	0	6,11,13	0.52	0
1	MLY	B	477	1	9,10,11	0.58	0	6,11,13	0.63	0
1	MLY	A	102	1	9,10,11	0.55	0	6,11,13	0.46	0
1	MLY	A	367	1	9,10,11	0.56	0	6,11,13	0.37	0
1	MLY	C	502	1	9,10,11	0.37	0	6,11,13	0.81	0
1	MLY	B	369	1	9,10,11	0.46	0	6,11,13	0.65	0
1	MLY	B	12	1	9,10,11	0.56	0	6,11,13	0.54	0
1	MLY	A	12	1	9,10,11	0.53	0	6,11,13	0.70	0
1	MLY	A	506	1	7,11,11	0.48	0	7,13,13	0.53	0
1	MLY	C	120	1	9,10,11	0.43	0	6,11,13	0.85	0
1	MLY	A	466	1	9,10,11	0.57	0	6,11,13	0.71	0
1	MLY	C	230	1	9,10,11	0.48	0	6,11,13	0.61	0
1	MLY	C	494	1	9,10,11	0.54	0	6,11,13	0.55	0
1	MLY	A	471	1	9,10,11	0.52	0	6,11,13	0.41	0
1	MLY	A	230	1	9,10,11	0.48	0	6,11,13	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	B	367	1	9,10,11	0.59	0	6,11,13	0.43	0
1	MLY	C	448	1	9,10,11	0.52	0	6,11,13	0.34	0
1	MLY	A	110	1	9,10,11	0.50	0	6,11,13	0.54	0
1	MLY	C	477	1	9,10,11	0.57	0	6,11,13	0.57	0
1	MLY	A	291	1	9,10,11	0.57	0	6,11,13	0.55	0
1	MLY	A	28	1	9,10,11	0.59	0	6,11,13	0.67	0
1	MLY	C	462	1	9,10,11	0.51	0	6,11,13	0.72	0
1	MLY	C	235	1	9,10,11	0.48	0	6,11,13	0.45	0
1	MLY	C	399	1	9,10,11	0.42	0	6,11,13	0.58	0
1	MLY	A	62	1	9,10,11	1.00	1 (11%)	6,11,13	1.26	1 (16%)
1	MLY	A	477	1	9,10,11	0.47	0	6,11,13	0.57	0
1	MLY	A	462	1	9,10,11	0.46	0	6,11,13	0.66	0
1	MLY	C	110	1	9,10,11	0.49	0	6,11,13	0.48	0
1	MLY	B	506	1	7,11,11	0.48	0	7,13,13	0.57	0
1	MLY	B	502	1	9,10,11	0.46	0	6,11,13	0.44	0
1	MLY	A	18	1	9,10,11	0.58	0	6,11,13	0.56	0
1	MLY	C	18	1	9,10,11	0.51	0	6,11,13	0.54	0
1	MLY	A	359	1	9,10,11	0.49	0	6,11,13	0.39	0
1	MLY	A	473	1	9,10,11	0.52	0	6,11,13	0.73	0
1	MLY	C	264	1	9,10,11	0.55	0	6,11,13	0.63	0

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
1	MLY	A	264	1	-	1/8/9/11	-
1	MLY	B	494	1	-	2/8/9/11	-
1	MLY	C	385	1	-	1/8/9/11	-
1	MLY	B	171	1	-	0/8/9/11	-
1	MLY	C	476	1	-	2/8/9/11	-
1	MLY	B	62	1	-	5/8/9/11	-
1	MLY	B	18	1	-	4/8/9/11	-
1	MLY	A	369	1	-	4/8/9/11	-
1	MLY	A	476	1	-	1/8/9/11	-
1	MLY	B	412	1	-	0/8/9/11	-
1	MLY	C	473	1	-	4/8/9/11	-
1	MLY	C	171	1	-	3/8/9/11	-
1	MLY	C	471	1	-	3/8/9/11	-
1	MLY	B	102	1	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	28	1	-	2/8/9/11	-
1	MLY	B	471	1	-	3/8/9/11	-
1	MLY	B	120	1	-	0/8/9/11	-
1	MLY	C	412	1	-	0/8/9/11	-
1	MLY	C	353	1	-	0/8/9/11	-
1	MLY	B	385	1	-	1/8/9/11	-
1	MLY	A	120	1	-	0/8/9/11	-
1	MLY	C	12	1	-	3/8/9/11	-
1	MLY	A	399	1	-	2/8/9/11	-
1	MLY	C	359	1	-	2/8/9/11	-
1	MLY	B	448	1	-	5/8/9/11	-
1	MLY	A	448	1	-	1/8/9/11	-
1	MLY	C	466	1	-	1/8/9/11	-
1	MLY	B	466	1	-	5/8/9/11	-
1	MLY	C	506	1	-	4/7/11/11	-
1	MLY	C	291	1	-	2/8/9/11	-
1	MLY	B	235	1	-	0/8/9/11	-
1	MLY	C	28	1	-	0/8/9/11	-
1	MLY	B	399	1	-	1/8/9/11	-
1	MLY	C	340	1	-	2/8/9/11	-
1	MLY	A	171	1	-	1/8/9/11	-
1	MLY	C	369	1	-	1/8/9/11	-
1	MLY	C	62	1	-	3/8/9/11	-
1	MLY	C	102	1	-	3/8/9/11	-
1	MLY	B	462	1	-	3/8/9/11	-
1	MLY	B	476	1	-	0/8/9/11	-
1	MLY	B	110	1	-	0/8/9/11	-
1	MLY	B	340	1	-	2/8/9/11	-
1	MLY	A	235	1	-	0/8/9/11	-
1	MLY	A	340	1	-	1/8/9/11	-
1	MLY	A	502	1	-	0/8/9/11	-
1	MLY	B	473	1	-	0/8/9/11	-
1	MLY	B	291	1	-	3/8/9/11	-
1	MLY	B	230	1	-	0/8/9/11	-
1	MLY	A	412	1	-	0/8/9/11	-
1	MLY	B	353	1	-	0/8/9/11	-
1	MLY	B	359	1	-	1/8/9/11	-
1	MLY	A	494	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	C	367	1	-	0/8/9/11	-
1	MLY	A	353	1	-	1/8/9/11	-
1	MLY	B	264	1	-	1/8/9/11	-
1	MLY	A	385	1	-	1/8/9/11	-
1	MLY	B	477	1	-	0/8/9/11	-
1	MLY	A	102	1	-	3/8/9/11	-
1	MLY	A	367	1	-	0/8/9/11	-
1	MLY	C	502	1	-	0/8/9/11	-
1	MLY	B	369	1	-	5/8/9/11	-
1	MLY	B	12	1	-	3/8/9/11	-
1	MLY	A	12	1	-	3/8/9/11	-
1	MLY	A	506	1	-	2/7/11/11	-
1	MLY	C	120	1	-	4/8/9/11	-
1	MLY	A	466	1	-	1/8/9/11	-
1	MLY	C	230	1	-	1/8/9/11	-
1	MLY	C	494	1	-	2/8/9/11	-
1	MLY	A	471	1	-	3/8/9/11	-
1	MLY	A	230	1	-	2/8/9/11	-
1	MLY	B	367	1	-	1/8/9/11	-
1	MLY	C	448	1	-	2/8/9/11	-
1	MLY	A	110	1	-	0/8/9/11	-
1	MLY	C	477	1	-	1/8/9/11	-
1	MLY	A	291	1	-	2/8/9/11	-
1	MLY	A	28	1	-	1/8/9/11	-
1	MLY	C	462	1	-	2/8/9/11	-
1	MLY	C	235	1	-	2/8/9/11	-
1	MLY	C	399	1	-	2/8/9/11	-
1	MLY	A	62	1	-	3/8/9/11	-
1	MLY	A	477	1	-	1/8/9/11	-
1	MLY	A	462	1	-	0/8/9/11	-
1	MLY	C	110	1	-	0/8/9/11	-
1	MLY	B	506	1	-	3/7/11/11	-
1	MLY	B	502	1	-	0/8/9/11	-
1	MLY	A	18	1	-	6/8/9/11	-
1	MLY	C	18	1	-	2/8/9/11	-
1	MLY	A	359	1	-	1/8/9/11	-
1	MLY	A	473	1	-	0/8/9/11	-
1	MLY	C	264	1	-	0/8/9/11	-



All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	MLY	CB-CA	-2.80	1.49	1.53
1	A	62	MLY	CB-CA	-2.48	1.50	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	MLY	CD-CG-CB	-2.57	104.53	113.62
1	A	62	MLY	CD-CG-CB	-2.38	105.22	113.62
1	B	62	MLY	CG-CD-CE	-2.08	103.61	113.21

There are no chirality outliers.

5 of 147 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	18	MLY	O-C-CA-CB
1	A	369	MLY	C-CA-CB-CG
1	C	171	MLY	O-C-CA-CB
1	B	102	MLY	O-C-CA-CB
1	B	466	MLY	N-CA-CB-CG

There are no ring outliers.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	62	MLY	6	0
1	B	471	MLY	1	0
1	C	62	MLY	7	0
1	A	466	MLY	1	0
1	A	471	MLY	1	0
1	B	367	MLY	1	0
1	C	462	MLY	1	0
1	A	62	MLY	8	0
1	A	462	MLY	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	CO3	A	603	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ATP	A	601	3	26,33,33	0.86	1 (3%)	31,52,52	1.34	5 (16%)
2	ATP	C	601	3	26,33,33	0.91	1 (3%)	31,52,52	1.29	3 (9%)
4	CO3	C	603	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	B	603	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ATP	B	601	3	26,33,33	1.06	2 (7%)	31,52,52	1.33	3 (9%)

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	ATP	A	601	3	-	7/18/38/38	0/3/3/3
2	ATP	C	601	3	-	6/18/38/38	0/3/3/3
2	ATP	B	601	3	-	6/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ATP	C5-C4	2.61	1.47	1.40
2	B	601	ATP	C5-C4	2.53	1.47	1.40
2	C	601	ATP	C5-C4	2.14	1.46	1.40
2	B	601	ATP	C2-N3	2.03	1.35	1.32

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ATP	N3-C2-N1	-3.66	122.96	128.68
2	A	601	ATP	N3-C2-N1	-3.62	123.02	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	ATP	N3-C2-N1	-3.61	123.03	128.68
2	C	601	ATP	PA-O3A-PB	-2.67	123.67	132.83
2	A	601	ATP	PA-O3A-PB	-2.60	123.90	132.83

There are no chirality outliers.

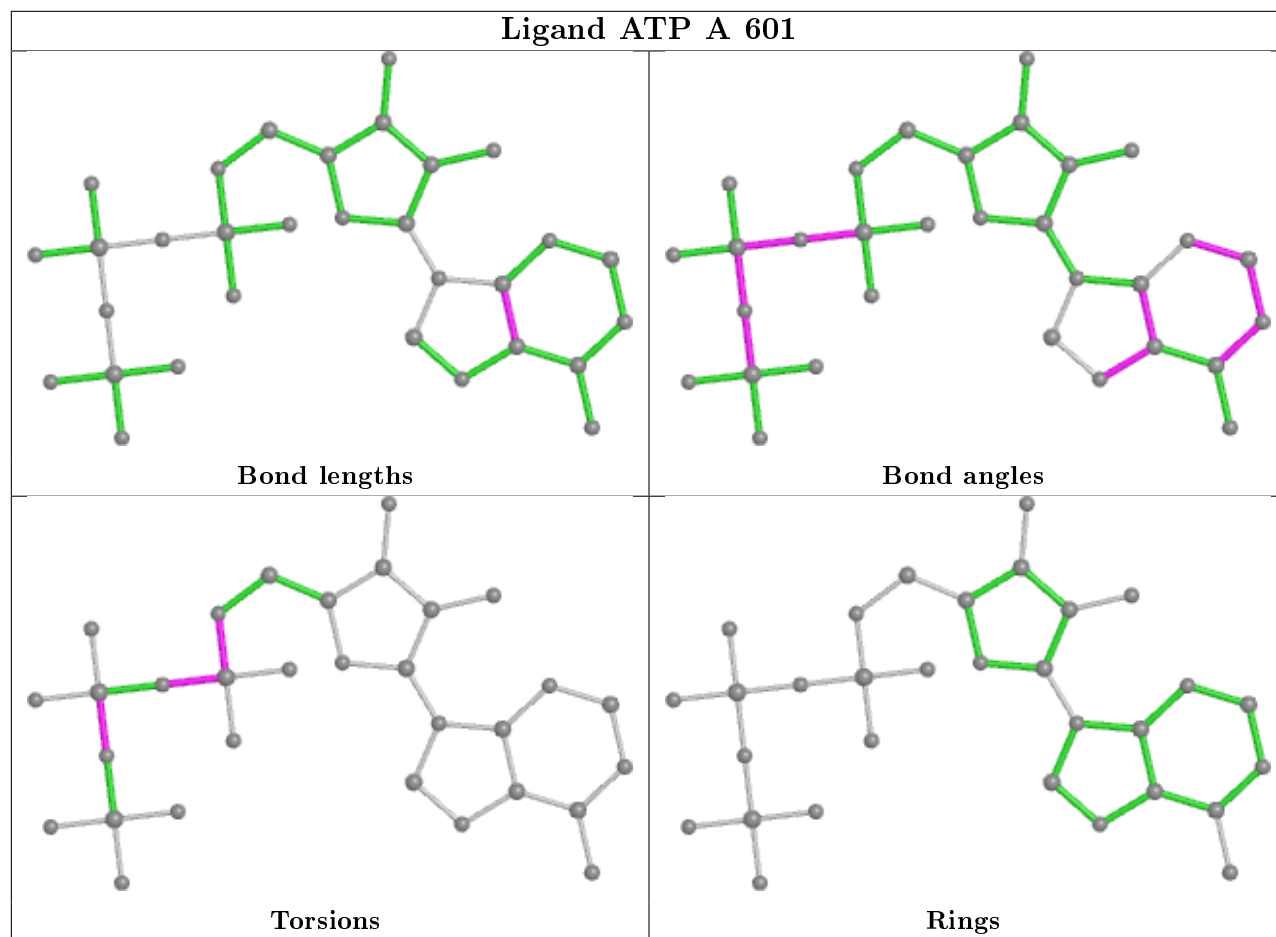
5 of 19 torsion outliers are listed below:

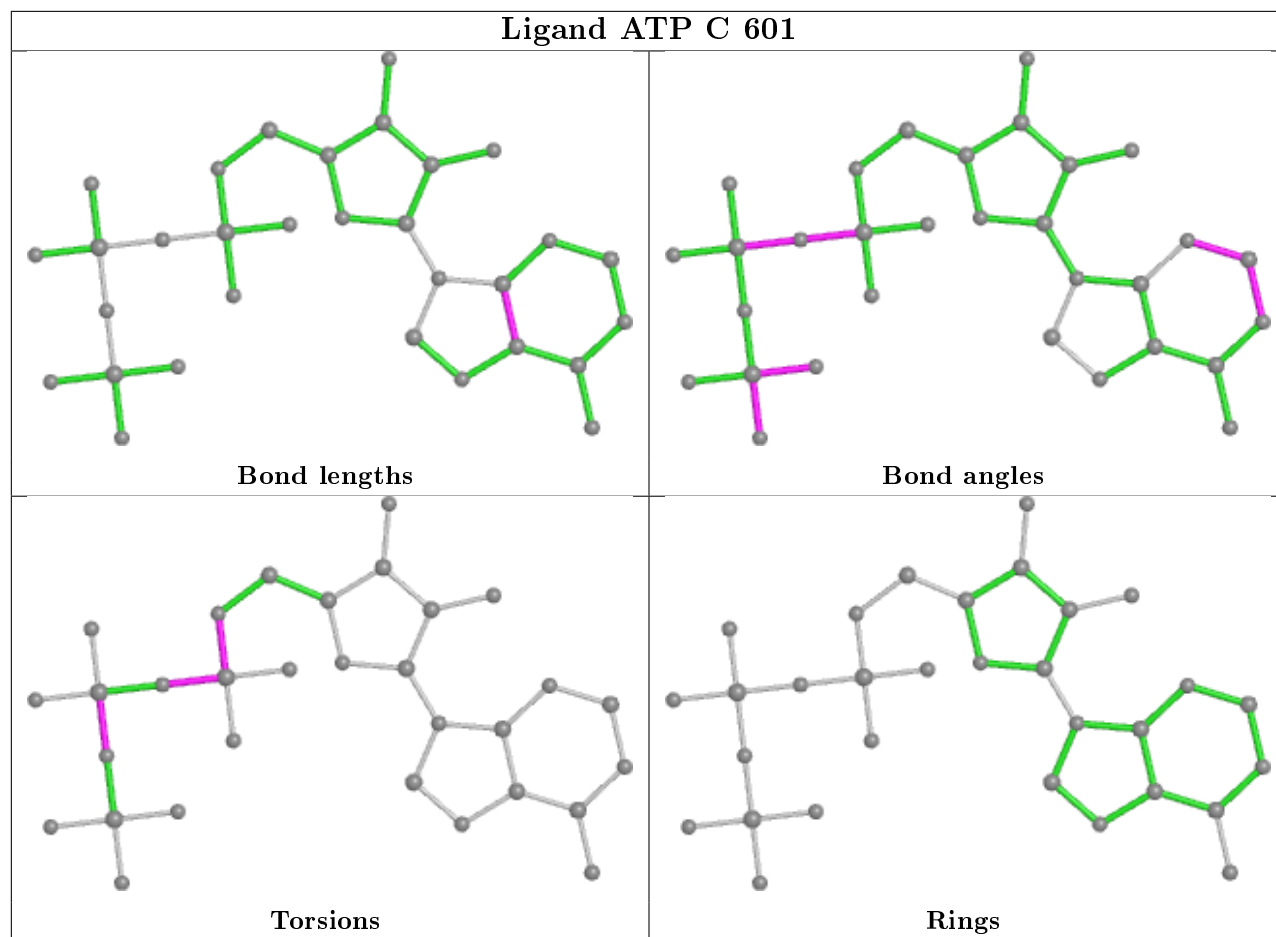
Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A
2	C	601	ATP	PB-O3A-PA-O5'
2	C	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	PB-O3A-PA-O5'
2	B	601	ATP	C5'-O5'-PA-O1A

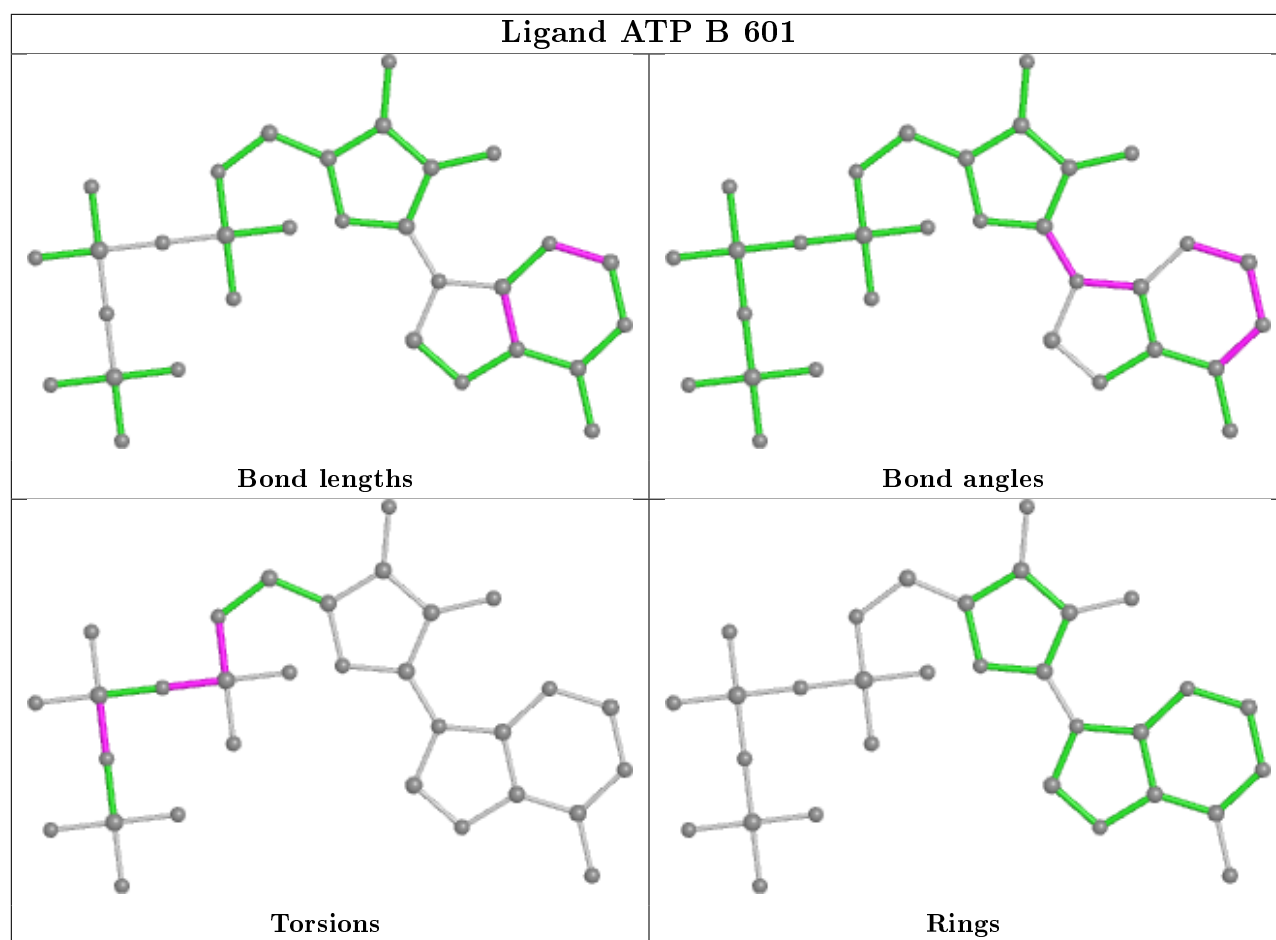
There are no ring outliers.

No monomer is involved in short contacts.

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	476/506 (94%)	-0.21	6 (1%) 77 76	21, 29, 49, 79	0
1	B	476/506 (94%)	-0.27	2 (0%) 92 92	13, 19, 43, 82	0
1	C	476/506 (94%)	0.03	17 (3%) 42 42	19, 30, 70, 107	0
All	All	1428/1518 (94%)	-0.15	25 (1%) 68 66	13, 27, 61, 107	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	456	ILE	4.4
1	C	450	GLU	4.2
1	C	422	PRO	3.8
1	B	1	MET	3.6
1	C	464	PHE	3.5

### 6.2 Non-standard residues in protein, DNA, RNA chains

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
1	MLY	C	473	11/12	0.80	0.20	61,65,82,89	0
1	MLY	C	476	11/12	0.81	0.20	55,68,84,94	0
1	MLY	C	477	11/12	0.82	0.17	51,54,77,90	0
1	MLY	C	506	12/12	0.84	0.30	72,85,104,107	0
1	MLY	A	466	11/12	0.85	0.22	38,55,90,98	0
1	MLY	C	494	11/12	0.86	0.16	52,56,63,63	0
1	MLY	C	359	11/12	0.86	0.17	28,40,64,69	0
1	MLY	C	448	11/12	0.87	0.24	53,61,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	C	412	11/12	0.88	0.17	53,59,70,74	0
1	MLY	A	473	11/12	0.88	0.14	29,33,42,44	0
1	MLY	A	506	12/12	0.89	0.24	29,56,90,91	0
1	MLY	C	466	11/12	0.89	0.41	61,84,139,141	0
1	MLY	C	291	11/12	0.89	0.20	38,44,99,103	0
1	MLY	B	462	11/12	0.89	0.13	37,45,53,59	0
1	MLY	B	473	11/12	0.89	0.16	29,31,50,61	0
1	MLY	A	12	11/12	0.89	0.29	37,47,91,100	0
1	MLY	A	62	11/12	0.90	0.13	30,32,50,52	0
1	MLY	A	359	11/12	0.90	0.15	29,43,68,70	0
1	MLY	C	462	11/12	0.90	0.15	71,81,93,106	0
1	MLY	C	471	11/12	0.91	0.34	65,99,124,128	0
1	MLY	A	471	11/12	0.91	0.23	33,65,103,113	0
1	MLY	B	506	12/12	0.91	0.27	33,53,74,81	0
1	MLY	A	340	11/12	0.91	0.23	35,55,84,94	0
1	MLY	C	62	11/12	0.91	0.16	26,31,63,93	0
1	MLY	B	12	11/12	0.92	0.28	33,46,112,123	0
1	MLY	C	171	11/12	0.92	0.15	31,37,54,72	0
1	MLY	A	462	11/12	0.92	0.12	32,37,42,48	0
1	MLY	B	466	11/12	0.92	0.33	42,54,88,89	0
1	MLY	A	18	11/12	0.92	0.17	23,32,64,69	0
1	MLY	B	359	11/12	0.92	0.13	18,34,53,55	0
1	MLY	A	291	11/12	0.92	0.16	29,41,82,84	0
1	MLY	C	264	11/12	0.92	0.11	27,30,35,41	0
1	MLY	B	494	11/12	0.93	0.13	19,21,31,32	0
1	MLY	C	399	11/12	0.93	0.23	38,62,100,102	0
1	MLY	B	230	11/12	0.93	0.15	26,38,80,90	0
1	MLY	C	230	11/12	0.93	0.18	32,43,72,77	0
1	MLY	C	110	11/12	0.93	0.14	31,40,56,59	0
1	MLY	A	448	11/12	0.93	0.18	32,40,92,95	0
1	MLY	C	367	11/12	0.93	0.16	36,42,69,75	0
1	MLY	C	502	11/12	0.93	0.23	54,58,92,96	0
1	MLY	A	235	11/12	0.93	0.24	29,41,120,122	0
1	MLY	A	369	11/12	0.93	0.31	40,59,93,101	0
1	MLY	B	340	11/12	0.94	0.17	28,41,74,78	0
1	MLY	B	102	11/12	0.94	0.14	16,18,36,44	0
1	MLY	B	471	11/12	0.94	0.19	37,59,89,94	0
1	MLY	A	230	11/12	0.94	0.21	33,49,96,102	0
1	MLY	B	367	11/12	0.94	0.14	25,30,60,73	0
1	MLY	C	385	11/12	0.94	0.14	35,40,64,67	0
1	MLY	A	110	11/12	0.94	0.16	33,38,53,55	0
1	MLY	B	385	11/12	0.94	0.11	17,20,48,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	C	12	11/12	0.94	0.26	36,56,93,99	0
1	MLY	A	494	11/12	0.94	0.10	25,27,32,32	0
1	MLY	B	235	11/12	0.94	0.20	18,30,86,96	0
1	MLY	B	291	11/12	0.94	0.15	21,30,69,74	0
1	MLY	B	264	11/12	0.94	0.11	18,19,23,24	0
1	MLY	A	385	11/12	0.94	0.11	29,35,60,66	0
1	MLY	B	399	11/12	0.94	0.17	22,32,81,82	0
1	MLY	C	340	11/12	0.94	0.26	39,63,93,97	0
1	MLY	C	369	11/12	0.94	0.28	39,57,105,112	0
1	MLY	A	399	11/12	0.94	0.24	31,54,117,123	0
1	MLY	A	264	11/12	0.94	0.11	25,35,39,39	0
1	MLY	B	476	11/12	0.95	0.12	23,28,48,59	0
1	MLY	A	102	11/12	0.95	0.13	27,33,55,57	0
1	MLY	B	18	11/12	0.95	0.14	19,26,58,62	0
1	MLY	B	369	11/12	0.95	0.21	24,35,98,109	0
1	MLY	A	28	11/12	0.95	0.13	27,38,54,54	0
1	MLY	B	171	11/12	0.95	0.11	16,19,33,35	0
1	MLY	C	235	11/12	0.95	0.22	27,42,89,97	0
1	MLY	B	448	11/12	0.95	0.15	28,35,77,82	0
1	MLY	C	353	11/12	0.95	0.11	25,28,56,58	0
1	MLY	C	120	11/12	0.95	0.23	35,47,82,83	0
1	MLY	A	171	11/12	0.95	0.12	30,32,48,51	0
1	MLY	A	353	11/12	0.95	0.09	25,30,58,60	0
1	MLY	B	502	11/12	0.95	0.16	21,29,58,61	0
1	MLY	A	120	11/12	0.95	0.26	38,56,75,79	0
1	MLY	C	18	11/12	0.95	0.17	20,29,66,74	0
1	MLY	C	102	11/12	0.95	0.14	26,30,57,64	0
1	MLY	A	476	11/12	0.95	0.12	20,24,55,70	0
1	MLY	B	412	11/12	0.95	0.10	21,24,30,32	0
1	MLY	A	367	11/12	0.96	0.19	34,39,54,57	0
1	MLY	B	120	11/12	0.96	0.12	29,35,50,53	0
1	MLY	A	477	11/12	0.96	0.15	20,23,31,31	0
1	MLY	B	28	11/12	0.96	0.11	23,29,55,64	0
1	MLY	B	477	11/12	0.96	0.15	20,22,32,33	0
1	MLY	B	62	11/12	0.96	0.14	17,19,33,49	0
1	MLY	A	502	11/12	0.97	0.16	24,32,72,72	0
1	MLY	B	110	11/12	0.97	0.08	19,22,35,43	0
1	MLY	C	28	11/12	0.97	0.12	27,35,48,54	0
1	MLY	A	412	11/12	0.97	0.09	22,27,43,45	0
1	MLY	B	353	11/12	0.97	0.09	16,18,40,45	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

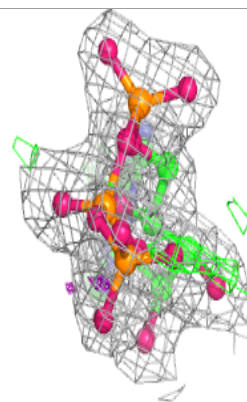
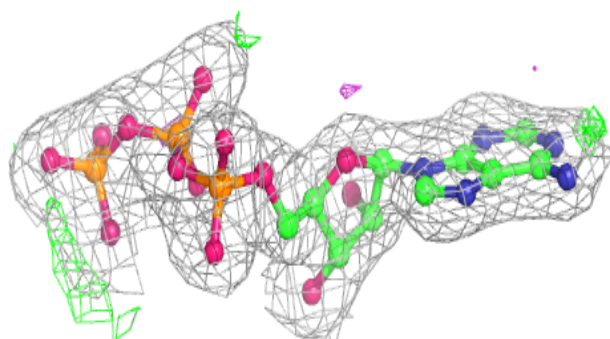
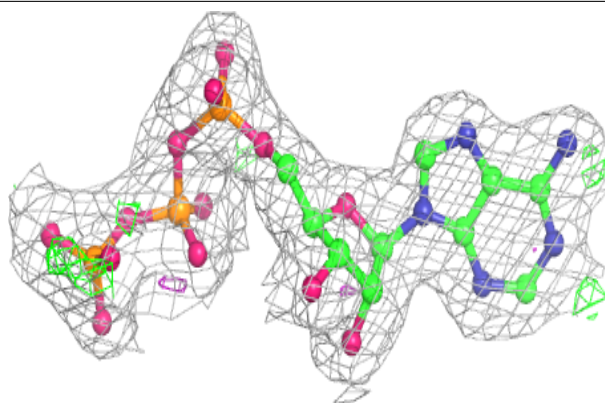
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	CO3	B	603	4/4	0.93	0.15	9,28,32,43	0
3	MG	C	602	1/1	0.94	0.06	27,27,27,27	0
4	CO3	A	603	4/4	0.95	0.15	21,38,45,48	0
3	MG	B	602	1/1	0.96	0.11	16,16,16,16	0
4	CO3	C	603	4/4	0.96	0.10	23,39,45,50	0
2	ATP	C	601	31/31	0.97	0.10	22,30,37,43	0
3	MG	A	602	1/1	0.97	0.10	29,29,29,29	0
2	ATP	A	601	31/31	0.98	0.08	22,27,32,36	0
2	ATP	B	601	31/31	0.98	0.10	10,16,23,27	0

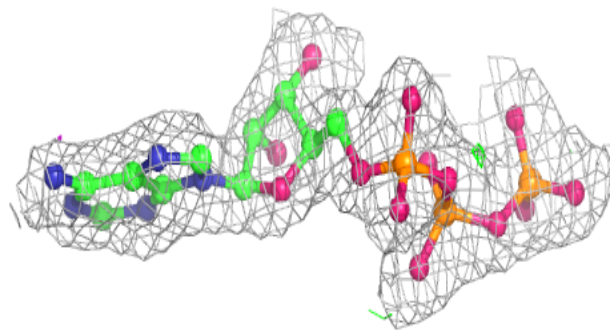
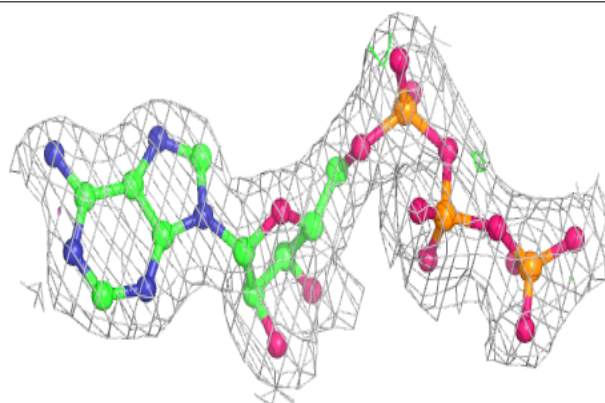
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

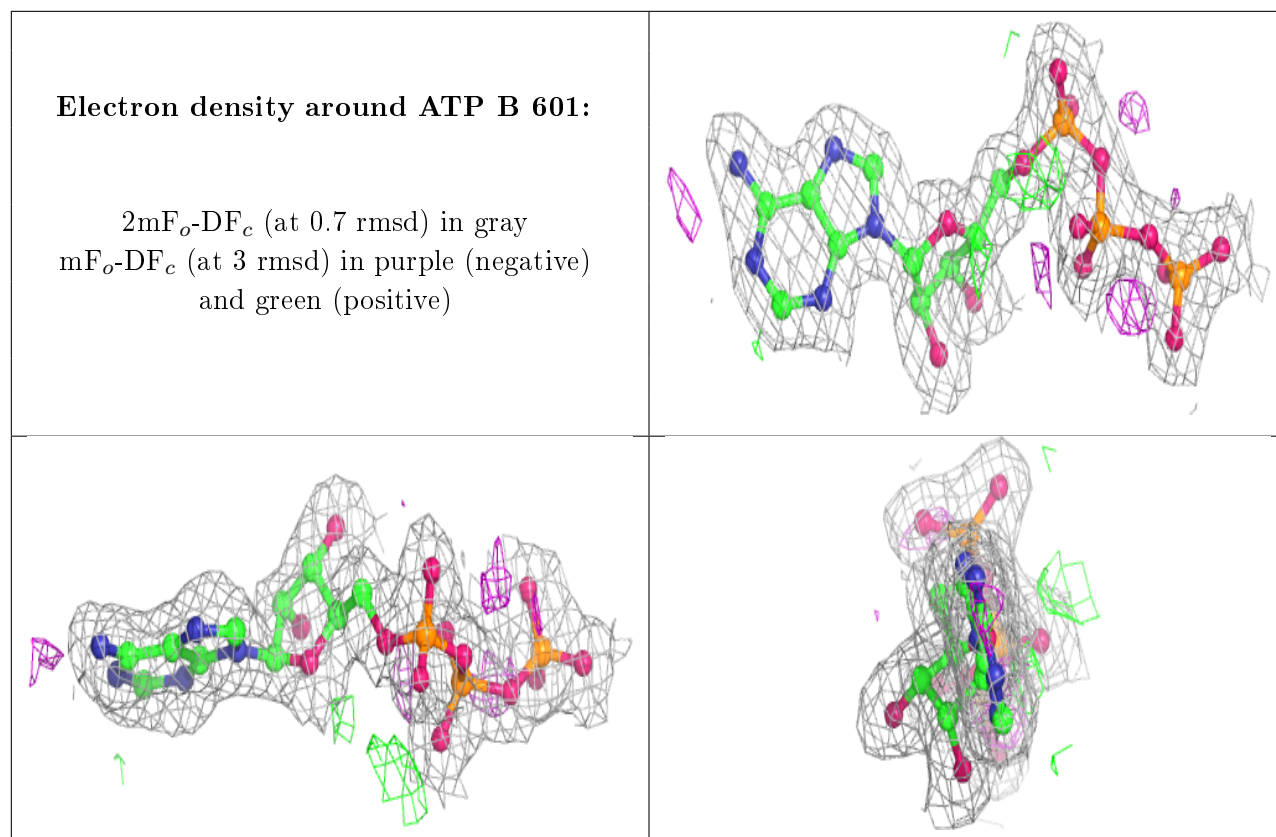
**Electron density around ATP C 601:**

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

**Electron density around ATP A 601:**

$2mF_o-DF_c$  (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.