



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:05 AM UTC

PDB ID : 4GXR / pdb_00004gxr
Title : Structure of ATP bound RpMatB-BxBclM chimera B3
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

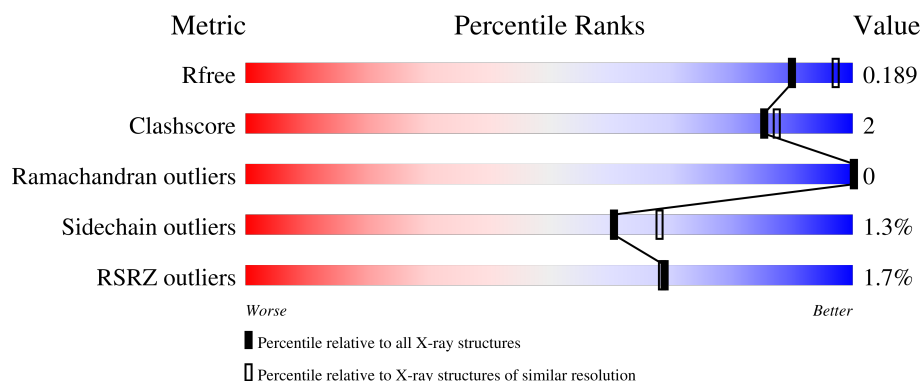
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

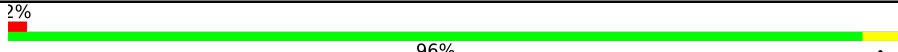
The reported resolution of this entry is 2.00 Å.

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	503	

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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CO3	A	608	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4556 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.

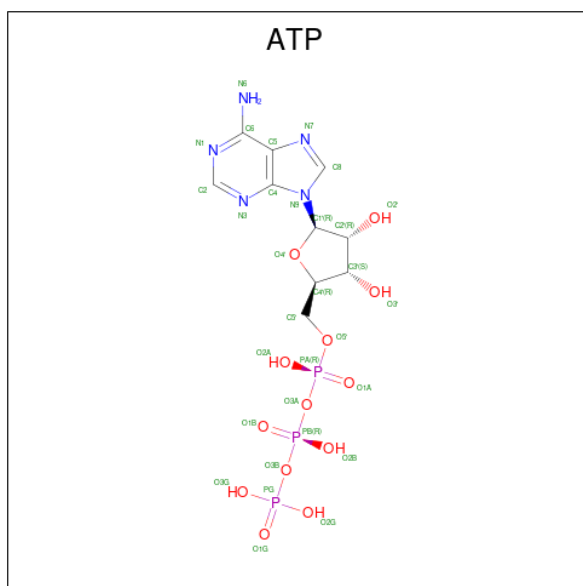
- Molecule 1 is a protein called Malonyl CoA synthetase, Benzoate-CoA ligase Chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	503	3958	2536	677	731	14	0	10	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	488	ALA	LYS	engineered mutation	UNP Q6ND88

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



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



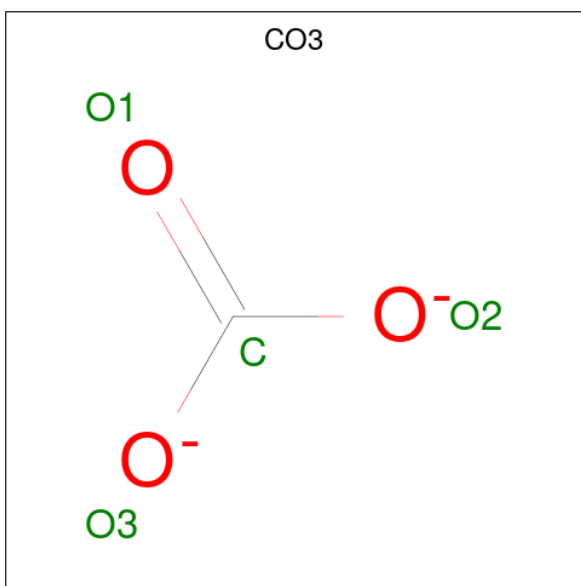
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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

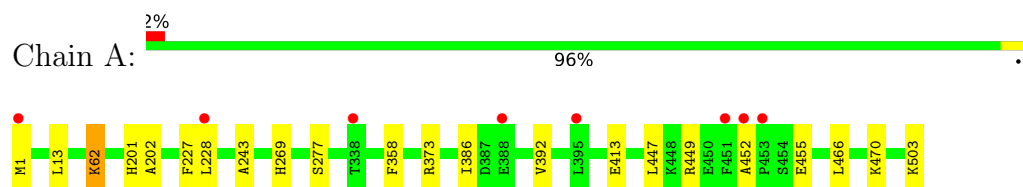
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	533	Total 533	O 533	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	173.16Å 173.16Å 47.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.00) 99.6 (25.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.148 , 0.178 0.159 , 0.189	Depositor DCC
R_{free} test set	2840 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4556	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, MG, GOL, SO4, 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	0.42	0/3757	0.64	0/5128

There are no bond length outliers.

There are no bond angle outliers.

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	3958	0	4017	17	0
2	A	31	0	12	0	0
3	A	1	0	0	0	0
4	A	24	0	32	0	0
5	A	5	0	0	0	0
6	A	4	0	0	2	0
7	A	533	0	0	3	0
All	All	4556	0	4061	18	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.

All (18) 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)
6:A:608:CO3:O1	7:A:842:HOH:O	2.04	0.75
1:A:62:MLY:HH13	1:A:227:PHE:CG	2.33	0.63
1:A:62:MLY:HH12	1:A:201:HIS:ND1	2.14	0.62
1:A:62:MLY:CH2	1:A:228:LEU:O	2.51	0.58
1:A:62:MLY:NZ	1:A:228:LEU:O	2.39	0.55
1:A:243:ALA:O	1:A:269[A]:HIS:HD2	1.91	0.54
1:A:62:MLY:HH21	1:A:202:ALA:HA	1.90	0.53
1:A:62:MLY:HH11	1:A:201:HIS:O	2.10	0.52
1:A:413:GLU:OE2	1:A:470:MLY:NZ	2.44	0.51
1:A:62:MLY:HH21	1:A:228:LEU:O	2.12	0.49
1:A:447:LEU:HD13	1:A:452:ALA:HB1	1.95	0.49
1:A:373[A]:ARG:NH2	7:A:1186:HOH:O	2.28	0.47
1:A:62:MLY:HH13	1:A:227:PHE:CD1	2.50	0.46
1:A:386:ILE:HG12	1:A:392:VAL:HG22	1.96	0.46
1:A:1:MET:N	7:A:811:HOH:O	2.49	0.45
1:A:277:SER:OG	6:A:608:CO3:O3	2.34	0.43
1:A:62:MLY:HH13	1:A:227:PHE:CD2	2.55	0.41
1:A:62:MLY:HH12	1:A:201:HIS:CG	2.56	0.41

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	484/503 (96%)	477 (99%)	7 (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	385/375 (103%)	380 (99%)	5 (1%)	61	68

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	358	PHE
1	A	449	ARG
1	A	455	GLU
1	A	466	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	492	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 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	369	1	9,10,11	0.44	0	6,11,13	0.61	0
1	MLY	A	102	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	A	230	1	9,10,11	0.49	0	6,11,13	0.73	0
1	MLY	A	120	1	9,10,11	0.44	0	6,11,13	0.67	0
1	MLY	A	503	1	10,11,11	0.84	1 (10%)	10,13,13	1.04	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	470	1	9,10,11	0.47	0	6,11,13	0.52	0
1	MLY	A	491	1	9,10,11	0.53	0	6,11,13	0.40	0
1	MLY	A	171	1	9,10,11	0.44	0	6,11,13	0.56	0
1	MLY	A	474	1	9,10,11	0.53	0	6,11,13	0.71	0
1	MLY	A	473	1	9,10,11	0.43	0	6,11,13	0.62	0
1	MLY	A	235	1	9,10,11	0.51	0	6,11,13	0.37	0
1	MLY	A	448	1	9,10,11	0.47	0	6,11,13	0.64	0
1	MLY	A	340	1	9,10,11	0.49	0	6,11,13	0.63	0
1	MLY	A	385	1	9,10,11	0.56	0	6,11,13	0.57	0
1	MLY	A	359	1	9,10,11	0.56	0	6,11,13	0.39	0
1	MLY	A	264	1	9,10,11	0.56	0	6,11,13	0.34	0
1	MLY	A	28	1	9,10,11	0.47	0	6,11,13	0.63	0
1	MLY	A	291	1	9,10,11	0.54	0	6,11,13	0.36	0
1	MLY	A	499	1	9,10,11	0.45	0	6,11,13	0.70	0
1	MLY	A	18	1	9,10,11	0.52	0	6,11,13	0.40	0
1	MLY	A	399	1	9,10,11	0.47	0	6,11,13	0.66	0
1	MLY	A	62	1	9,10,11	0.69	0	6,11,13	1.67	2 (33%)
1	MLY	A	12	1	9,10,11	0.52	0	6,11,13	0.51	0
1	MLY	A	412	1	9,10,11	0.52	0	6,11,13	0.50	0
1	MLY	A	468	1	9,10,11	0.46	0	6,11,13	0.70	0
1	MLY	A	110	1	9,10,11	0.50	0	6,11,13	0.39	0
1	MLY	A	353	1	9,10,11	0.55	0	6,11,13	0.60	0
1	MLY	A	367	1	9,10,11	0.52	0	6,11,13	0.38	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	369	1	-	5/8/9/11	-
1	MLY	A	102	1	-	0/8/9/11	-
1	MLY	A	230	1	-	6/8/9/11	-
1	MLY	A	120	1	-	0/8/9/11	-
1	MLY	A	503	1	-	6/11/11/11	-
1	MLY	A	470	1	-	0/8/9/11	-
1	MLY	A	491	1	-	1/8/9/11	-
1	MLY	A	171	1	-	1/8/9/11	-
1	MLY	A	474	1	-	4/8/9/11	-
1	MLY	A	473	1	-	2/8/9/11	-
1	MLY	A	235	1	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	448	1	-	2/8/9/11	-
1	MLY	A	340	1	-	3/8/9/11	-
1	MLY	A	385	1	-	1/8/9/11	-
1	MLY	A	359	1	-	2/8/9/11	-
1	MLY	A	264	1	-	1/8/9/11	-
1	MLY	A	28	1	-	1/8/9/11	-
1	MLY	A	291	1	-	2/8/9/11	-
1	MLY	A	499	1	-	0/8/9/11	-
1	MLY	A	18	1	-	2/8/9/11	-
1	MLY	A	399	1	-	1/8/9/11	-
1	MLY	A	62	1	-	1/8/9/11	-
1	MLY	A	12	1	-	0/8/9/11	-
1	MLY	A	412	1	-	0/8/9/11	-
1	MLY	A	468	1	-	4/8/9/11	-
1	MLY	A	110	1	-	2/8/9/11	-
1	MLY	A	353	1	-	0/8/9/11	-
1	MLY	A	367	1	-	1/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	503	MLY	OXT-C	-2.33	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	MLY	OXT-C-O	-2.89	117.51	124.08
1	A	62	MLY	CD-CE-NZ	-2.87	106.29	113.71
1	A	62	MLY	CD-CG-CB	-2.00	106.07	113.62

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	18	MLY	O-C-CA-CB
1	A	230	MLY	N-CA-CB-CG
1	A	230	MLY	C-CA-CB-CG
1	A	369	MLY	C-CA-CB-CG
1	A	468	MLY	N-CA-CB-CG
1	A	474	MLY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	503	MLY	N-CA-CB-CG
1	A	340	MLY	CD-CE-NZ-CH1
1	A	340	MLY	CD-CE-NZ-CH2
1	A	62	MLY	CG-CD-CE-NZ
1	A	399	MLY	CG-CD-CE-NZ
1	A	369	MLY	CD-CE-NZ-CH1
1	A	369	MLY	CD-CE-NZ-CH2
1	A	291	MLY	CG-CD-CE-NZ
1	A	474	MLY	CG-CD-CE-NZ
1	A	503	MLY	CG-CD-CE-NZ
1	A	474	MLY	CD-CE-NZ-CH2
1	A	367	MLY	CG-CD-CE-NZ
1	A	18	MLY	CA-CB-CG-CD
1	A	110	MLY	CG-CD-CE-NZ
1	A	468	MLY	CA-CB-CG-CD
1	A	503	MLY	CD-CE-NZ-CH1
1	A	369	MLY	CE-CD-CG-CB
1	A	385	MLY	CG-CD-CE-NZ
1	A	503	MLY	CD-CE-NZ-CH2
1	A	171	MLY	CE-CD-CG-CB
1	A	448	MLY	CG-CD-CE-NZ
1	A	340	MLY	CG-CD-CE-NZ
1	A	473	MLY	CD-CE-NZ-CH1
1	A	235	MLY	CD-CE-NZ-CH1
1	A	503	MLY	CA-CB-CG-CD
1	A	359	MLY	CA-CB-CG-CD
1	A	503	MLY	C-CA-CB-CG
1	A	230	MLY	CA-CB-CG-CD
1	A	28	MLY	C-CA-CB-CG
1	A	468	MLY	C-CA-CB-CG
1	A	491	MLY	C-CA-CB-CG
1	A	473	MLY	CD-CE-NZ-CH2
1	A	474	MLY	N-CA-CB-CG
1	A	230	MLY	CD-CE-NZ-CH2
1	A	230	MLY	CG-CD-CE-NZ
1	A	359	MLY	CD-CE-NZ-CH2
1	A	230	MLY	CD-CE-NZ-CH1
1	A	264	MLY	CD-CE-NZ-CH1
1	A	291	MLY	CA-CB-CG-CD
1	A	468	MLY	CD-CE-NZ-CH1
1	A	448	MLY	CE-CD-CG-CB
1	A	110	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	A	369	MLY	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	470	MLY	1	0
1	A	62	MLY	10	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	GOL	A	605	-	5,5,5	0.27	0	5,5,5	0.27	0
4	GOL	A	603	-	5,5,5	0.29	0	5,5,5	0.26	0
5	SO4	A	604	-	4,4,4	0.52	0	6,6,6	0.18	0
4	GOL	A	606	-	5,5,5	0.36	0	5,5,5	0.52	0
6	CO3	A	608	-	3,3,3	1.81	0	2,3,3	0.55	0
2	ATP	A	601	3	32,33,33	1.46	8 (25%)	48,52,52	1.67	10 (20%)
4	GOL	A	607	-	5,5,5	0.28	0	5,5,5	0.50	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
4	GOL	A	605	-	-	3/4/4/4	-
4	GOL	A	603	-	-	2/4/4/4	-
4	GOL	A	606	-	-	2/4/4/4	-
2	ATP	A	601	3	-	5/22/38/38	0/3/3/3
4	GOL	A	607	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ATP	C5-C4	4.36	1.46	1.39
2	A	601	ATP	C5-N7	-2.73	1.34	1.39
2	A	601	ATP	PB-O3A	2.61	1.62	1.59
2	A	601	ATP	C5-C6	2.44	1.47	1.41
2	A	601	ATP	C4-N9	-2.35	1.32	1.37
2	A	601	ATP	PB-O3B	2.24	1.61	1.59
2	A	601	ATP	C8-N7	2.15	1.35	1.31
2	A	601	ATP	PA-O3A	2.02	1.61	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ATP	C5-C4-N3	-5.24	119.50	126.72
2	A	601	ATP	N3-C4-N9	4.29	134.47	127.17
2	A	601	ATP	N3-C2-N1	-3.64	123.08	128.58
2	A	601	ATP	C2-N3-C4	3.48	120.34	111.83
2	A	601	ATP	C4-C5-N7	-3.18	106.94	110.58
2	A	601	ATP	C4-N9-C8	3.07	108.96	105.74
2	A	601	ATP	C5-N7-C8	2.56	107.47	103.45
2	A	601	ATP	N9-C8-N7	-2.35	110.60	113.94
2	A	601	ATP	C2-N1-C6	2.26	122.45	118.73
2	A	601	ATP	C6-C5-N7	2.04	136.01	132.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	PB-O3A-PA-O5'
2	A	601	ATP	C5'-O5'-PA-O1A
2	A	601	ATP	C5'-O5'-PA-O3A
4	A	603	GOL	O1-C1-C2-C3
4	A	606	GOL	O1-C1-C2-C3

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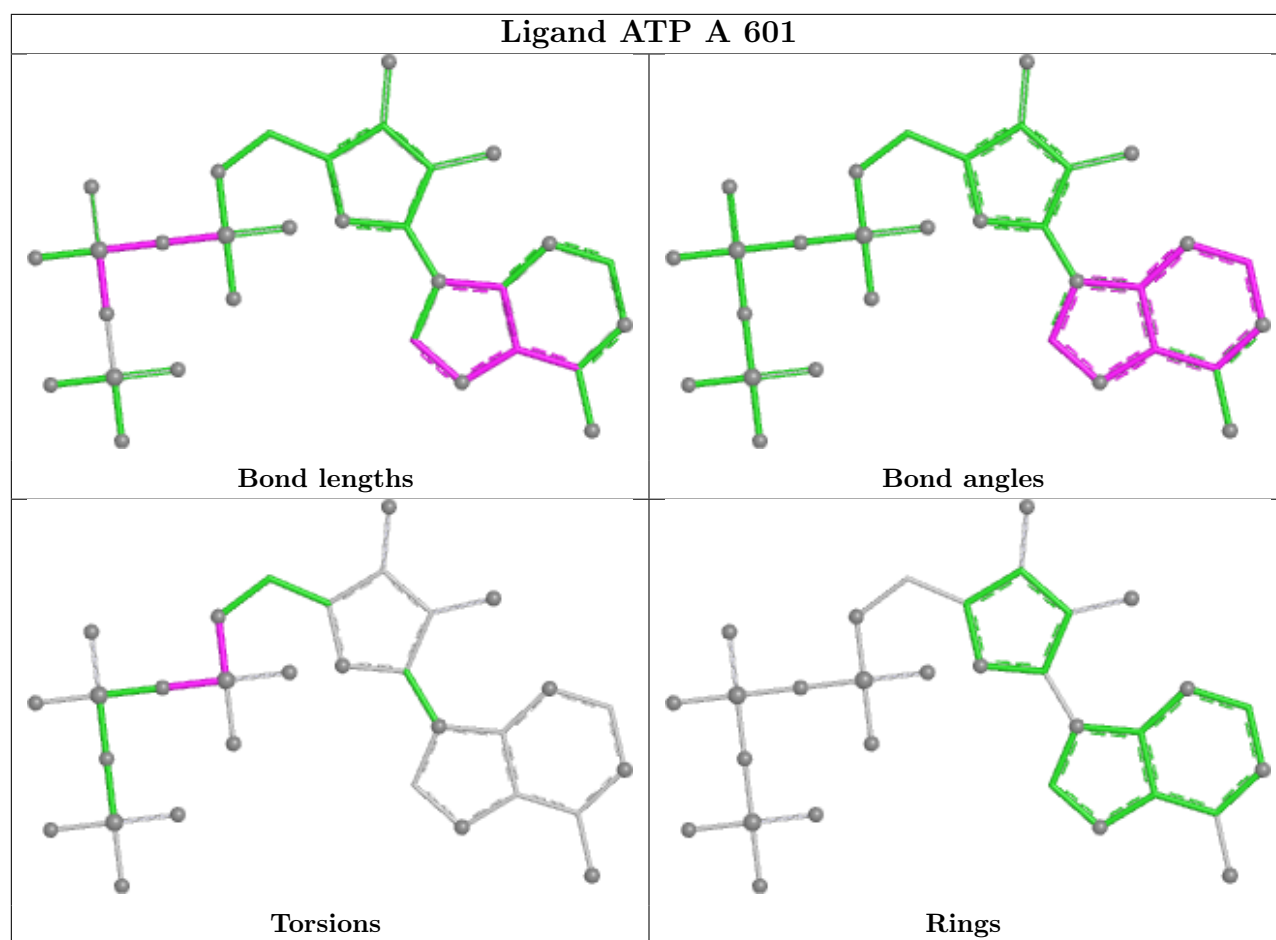
Mol	Chain	Res	Type	Atoms
4	A	607	GOL	C1-C2-C3-O3
4	A	607	GOL	O2-C2-C3-O3
4	A	603	GOL	O1-C1-C2-O2
4	A	606	GOL	O1-C1-C2-O2
4	A	605	GOL	O2-C2-C3-O3
2	A	601	ATP	C5'-O5'-PA-O2A
4	A	605	GOL	C1-C2-C3-O3
4	A	605	GOL	O1-C1-C2-O2
2	A	601	ATP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	608	CO3	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	475/503 (94%)	-0.33	8 (1%) 69 68	14, 27, 52, 123	10 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	PHE	8.0
1	A	338	THR	3.8
1	A	1	MET	2.7
1	A	228	LEU	2.6
1	A	452	ALA	2.5
1	A	395	LEU	2.1
1	A	388	GLU	2.1
1	A	453	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MLY	A	468	11/12	0.85	0.18	43,61,104,106	0
1	MLY	A	359	11/12	0.86	0.16	25,39,57,58	0
1	MLY	A	503	12/12	0.86	0.15	48,69,96,97	0
1	MLY	A	367	11/12	0.87	0.24	36,49,122,130	0
1	MLY	A	399	11/12	0.87	0.17	30,39,91,96	0
1	MLY	A	230	11/12	0.88	0.16	32,44,70,73	0
1	MLY	A	448	11/12	0.88	0.16	42,52,87,93	0
1	MLY	A	470	11/12	0.89	0.12	38,43,66,67	0
1	MLY	A	474	11/12	0.89	0.14	32,44,58,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	A	369	11/12	0.89	0.17	33,49,87,89	0
1	MLY	A	171	11/12	0.91	0.15	24,31,68,75	0
1	MLY	A	120	11/12	0.91	0.11	37,43,69,73	0
1	MLY	A	291	11/12	0.91	0.18	28,35,84,86	0
1	MLY	A	110	11/12	0.92	0.12	29,35,57,60	0
1	MLY	A	473	11/12	0.92	0.13	32,39,68,76	0
1	MLY	A	18	11/12	0.93	0.17	22,33,71,76	0
1	MLY	A	412	11/12	0.93	0.09	32,35,45,45	0
1	MLY	A	12	11/12	0.93	0.15	33,43,87,87	0
1	MLY	A	340	11/12	0.93	0.13	35,55,96,103	0
1	MLY	A	235	11/12	0.94	0.13	26,37,84,85	0
1	MLY	A	385	11/12	0.94	0.12	24,30,66,70	0
1	MLY	A	62	11/12	0.95	0.12	25,29,49,75	0
1	MLY	A	102	11/12	0.95	0.10	21,23,44,52	0
1	MLY	A	491	11/12	0.95	0.08	27,29,34,35	0
1	MLY	A	499	11/12	0.95	0.10	33,38,74,77	0
1	MLY	A	28	11/12	0.95	0.09	27,37,55,59	0
1	MLY	A	264	11/12	0.96	0.06	25,28,29,31	0
1	MLY	A	353	11/12	0.96	0.09	22,25,51,53	0

6.3 Carbohydrates [i](#)

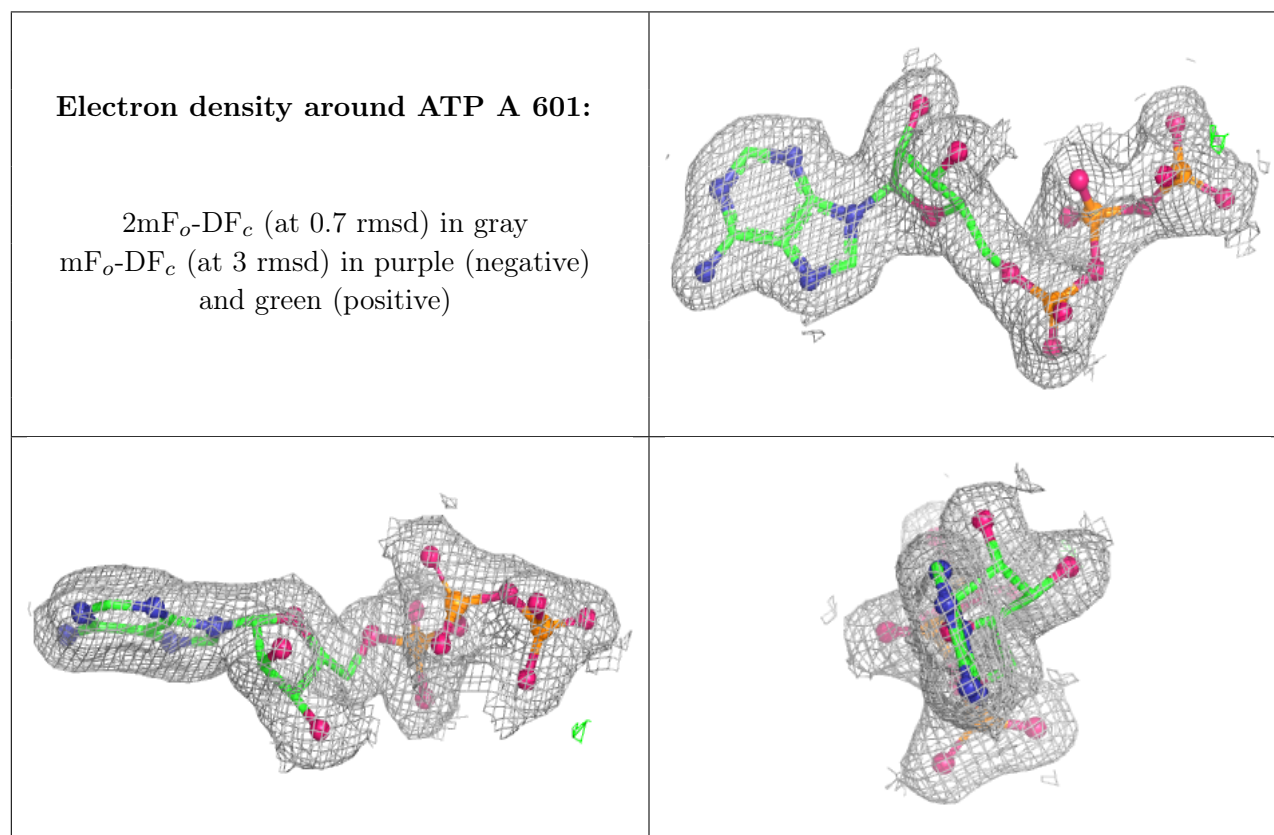
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	A	604	5/5	0.48	0.20	54,70,89,97	0
4	GOL	A	606	6/6	0.68	0.25	60,65,78,80	0
4	GOL	A	607	6/6	0.86	0.17	43,59,63,80	0
4	GOL	A	605	6/6	0.87	0.13	56,68,68,72	0
4	GOL	A	603	6/6	0.89	0.15	48,62,69,75	0
6	CO3	A	608	4/4	0.92	0.25	13,31,43,44	0
2	ATP	A	601	31/31	0.99	0.04	20,22,26,27	0
3	MG	A	602	1/1	0.99	0.03	22,22,22,22	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.