



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 01:24 AM EST

PDB ID : 2AQX  
Title : Crystal Structure of the Catalytic and CaM-Binding domains of Inositol 1,4,5-Trisphosphate 3-Kinase B  
Authors : Chamberlain, P.P.; Sandberg, M.L.; Sauer, K.; Cooke, M.P.; Lesley, S.A.; Spraggon, G.  
Deposited on : 2005-08-18  
Resolution : 2.50 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.

The types of validation reports are described at

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

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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 : 2.36  
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) : 2.36

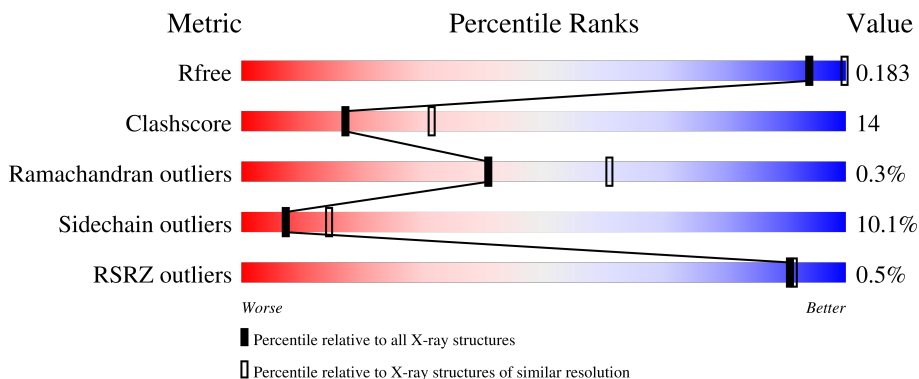
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	289	
1	B	289	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4837 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.

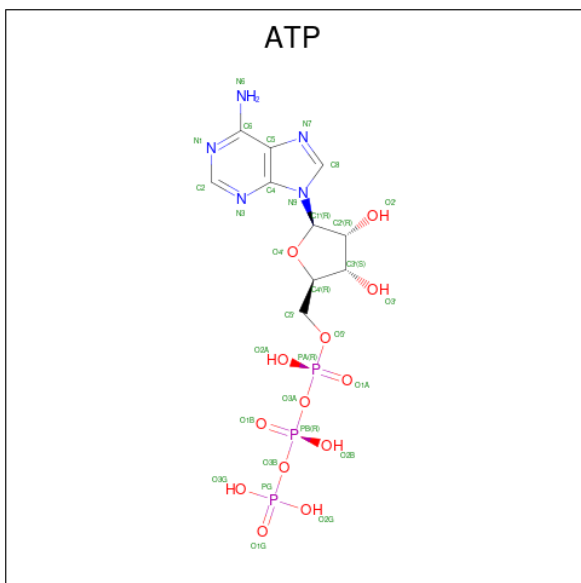
- Molecule 1 is a protein called PREDICTED: inositol 1,4,5-trisphosphate 3-kinase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	Total 2342	C 1479	N 411	O 436	S 16	0	0	0
1	B	287	Total 2330	C 1472	N 409	O 434	S 15	5	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

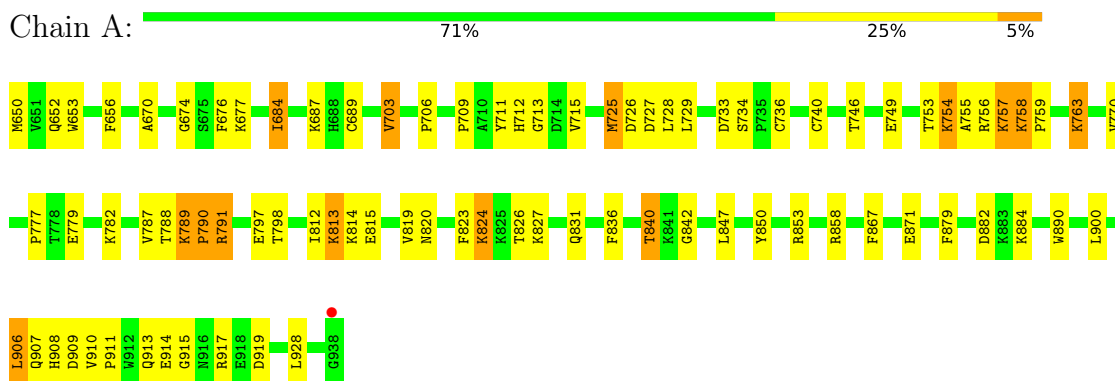
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	51	Total	O	0	0
			51	51		

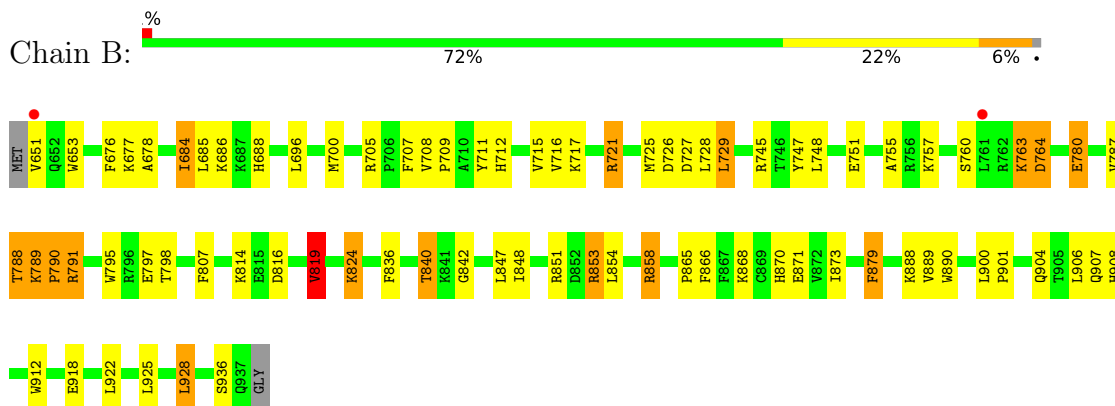
### 3 Residue-property plots [i](#)

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: PREDICTED: inositol 1,4,5-trisphosphate 3-kinase B



- Molecule 1: PREDICTED: inositol 1,4,5-trisphosphate 3-kinase B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.20Å 60.66Å 56.85Å 59.90° 72.74° 88.18°	Depositor
Resolution (Å)	50.00 – 2.50 46.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.50) 95.4 (46.52-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.184 , 0.268 0.190 , 0.183	Depositor DCC
$R_{free}$ test set	973 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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: MG, 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	0.69	2/2391 (0.1%)	0.77	1/3215 (0.0%)
1	B	0.67	2/2379 (0.1%)	0.73	1/3200 (0.0%)
All	All	0.68	4/4770 (0.1%)	0.75	2/6415 (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	1
1	B	1	1
All	All	1	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	780	GLU	CD-OE1	7.82	1.34	1.25
1	A	740	CYS	CB-SG	-6.36	1.71	1.82
1	A	689	CYS	CB-SG	-5.91	1.72	1.81
1	B	780	GLU	CD-OE2	5.09	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	819	VAL	CB-CA-C	-5.94	100.12	111.40
1	A	909	ASP	CB-CG-OD2	5.38	123.15	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	651	VAL	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	789	LYS	Peptide
1	B	789	LYS	Peptide

## 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	2342	0	2334	66	0
1	B	2330	0	2322	70	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	12	5	0
3	B	31	0	12	3	0
4	A	48	0	0	2	0
4	B	51	0	0	0	0
All	All	4837	0	4680	131	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 14.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:MET:CE	3:A:1462:ATP:HN61	1.83	0.91
1:A:763:LYS:HD3	1:A:763:LYS:H	1.33	0.90
1:B:707:PHE:HD2	1:B:853:ARG:NH1	1.69	0.90
1:B:788:THR:CG2	1:B:790:PRO:HB2	2.03	0.89
1:A:725:MET:HE2	3:A:1462:ATP:HN61	1.40	0.87
1:B:789:LYS:N	1:B:790:PRO:HD2	1.90	0.86
1:B:788:THR:HG23	1:B:790:PRO:HB2	1.58	0.83
1:B:789:LYS:H	1:B:790:PRO:HD2	1.46	0.81
1:A:840:THR:HG22	1:A:842:GLY:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:ARG:HE	1:B:922:LEU:HD22	1.47	0.79
1:A:763:LYS:H	1:A:763:LYS:CD	1.98	0.76
1:B:853:ARG:HH21	1:B:888:LYS:HE3	1.49	0.76
1:B:707:PHE:HD2	1:B:853:ARG:HH11	1.36	0.74
1:B:788:THR:HG22	1:B:791:ARG:H	1.53	0.73
1:B:763:LYS:HD3	1:B:763:LYS:H	1.56	0.70
1:B:788:THR:CG2	1:B:791:ARG:H	2.04	0.70
1:A:836:PHE:O	1:A:840:THR:HB	1.93	0.68
1:B:853:ARG:NH2	1:B:888:LYS:HE3	2.09	0.67
1:A:814:LYS:NZ	1:A:820:ASN:HD21	1.95	0.65
1:A:908:HIS:HD2	1:A:919:ASP:OD1	1.82	0.63
1:B:709:PRO:HG3	1:B:728:LEU:HD11	1.79	0.63
1:A:789:LYS:HB3	1:A:790:PRO:HD2	1.82	0.62
1:A:725:MET:HE1	3:A:1462:ATP:HN61	1.64	0.62
1:B:684:ILE:HD13	1:B:727:ASP:HB2	1.82	0.61
1:B:707:PHE:CD2	1:B:853:ARG:NH1	2.60	0.61
1:A:757:LYS:O	1:A:759:PRO:HD3	2.01	0.61
1:B:709:PRO:HB2	1:B:725:MET:HE2	1.82	0.61
1:A:753:THR:O	1:A:757:LYS:HE2	2.02	0.60
1:B:696:LEU:O	1:B:700:MET:HG2	2.01	0.59
1:B:788:THR:HG23	1:B:790:PRO:CB	2.31	0.58
1:B:712:HIS:HE1	1:B:726:ASP:OD1	1.87	0.58
1:A:712:HIS:HE1	1:A:726:ASP:OD1	1.85	0.58
1:B:789:LYS:N	1:B:790:PRO:CD	2.67	0.58
1:A:819:VAL:HG21	1:B:653:TRP:CG	2.40	0.57
1:A:703:VAL:O	1:A:706:PRO:HD2	2.04	0.56
1:A:725:MET:HE2	3:A:1462:ATP:N6	2.16	0.56
1:B:858:ARG:HH21	1:B:922:LEU:HD13	1.70	0.56
1:A:812:ILE:HD12	1:A:823:PHE:CZ	2.41	0.56
1:B:795:TRP:O	1:B:798:THR:HG22	2.06	0.56
1:B:788:THR:HG22	1:B:791:ARG:HB3	1.86	0.56
1:A:813:LYS:HB2	1:A:819:VAL:HG22	1.86	0.56
1:B:789:LYS:HB3	1:B:790:PRO:CD	2.36	0.56
1:A:840:THR:HG22	1:A:842:GLY:N	2.19	0.55
1:B:907:GLN:O	1:B:908:HIS:HB2	2.05	0.55
1:A:867:PHE:O	1:A:908:HIS:HE1	1.89	0.55
1:B:688:HIS:HB3	1:B:721:ARG:HB3	1.89	0.55
1:B:788:THR:HG21	1:B:790:PRO:HB2	1.88	0.55
1:A:907:GLN:O	1:A:908:HIS:HB2	2.07	0.54
1:B:684:ILE:CD1	1:B:727:ASP:HB2	2.37	0.54
1:A:736:CYS:SG	1:A:815:GLU:HG2	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:LYS:HZ3	1:A:820:ASN:HD21	1.56	0.54
1:B:789:LYS:CB	1:B:790:PRO:CD	2.86	0.54
1:B:836:PHE:O	1:B:840:THR:HB	2.07	0.53
1:A:709:PRO:HG2	1:A:725:MET:HE2	1.91	0.53
1:B:715:VAL:HG22	1:B:716:VAL:N	2.23	0.53
1:B:763:LYS:H	1:B:763:LYS:CD	2.22	0.53
1:A:913:GLN:O	1:A:914:GLU:C	2.46	0.52
1:A:787:VAL:HG12	1:A:788:THR:N	2.25	0.52
1:A:826:THR:HG23	1:A:831:GLN:HB3	1.91	0.52
1:B:700:MET:HA	1:B:705:ARG:HG3	1.92	0.52
1:A:824:LYS:HA	4:A:98:HOH:O	2.09	0.51
1:B:763:LYS:HG2	1:B:764:ASP:H	1.74	0.51
1:A:746:THR:N	1:A:797:GLU:OE1	2.33	0.51
1:A:827:LYS:NZ	1:A:827:LYS:HB3	2.25	0.51
1:A:900:LEU:HD11	1:A:906:LEU:HD22	1.92	0.51
1:A:910:VAL:HB	1:A:911:PRO:HD2	1.93	0.51
1:A:758:LYS:CG	1:A:758:LYS:O	2.58	0.50
1:B:745:ARG:NH1	1:B:918:GLU:O	2.43	0.50
1:B:900:LEU:HD11	1:B:906:LEU:HG	1.94	0.49
1:A:733:ASP:O	1:A:882:ASP:HB2	2.11	0.49
1:B:727:ASP:OD1	1:B:729:LEU:HB2	2.12	0.49
1:B:854:LEU:HD21	1:B:889:VAL:HG11	1.94	0.49
1:B:755:ALA:HB1	1:B:789:LYS:HG2	1.93	0.48
1:A:725:MET:HE1	3:A:1462:ATP:N7	2.28	0.48
1:B:745:ARG:NH1	1:B:912:TRP:CD1	2.81	0.48
1:B:901:PRO:HD2	1:B:904:GLN:HE21	1.78	0.48
1:A:653:TRP:CD1	1:B:819:VAL:HG22	2.48	0.48
1:A:674:GLY:O	1:A:687:LYS:HD3	2.14	0.48
1:B:748:LEU:HB2	1:B:751:GLU:HG3	1.96	0.48
1:A:787:VAL:CG1	1:A:791:ARG:HD2	2.43	0.48
1:A:709:PRO:HG3	1:A:728:LEU:HD11	1.95	0.47
1:B:865:PRO:HA	1:B:868:LYS:HE2	1.96	0.47
1:B:906:LEU:HD22	1:B:918:GLU:CD	2.34	0.47
1:A:840:THR:CG2	1:A:842:GLY:H	2.23	0.47
1:B:807:PHE:CE2	1:B:928:LEU:HD13	2.50	0.47
1:B:866:PHE:CE1	1:B:870:HIS:CE1	3.03	0.46
1:B:840:THR:HG22	1:B:842:GLY:H	1.80	0.46
1:A:670:ALA:HB1	4:A:6:HOH:O	2.15	0.46
1:B:676:PHE:HA	1:B:685:LEU:O	2.16	0.45
1:B:871:GLU:HG2	1:B:873:ILE:HG12	1.98	0.45
1:A:787:VAL:HG11	1:A:791:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ALA:HB1	1:A:790:PRO:CD	2.46	0.45
1:B:814:LYS:HB2	1:B:814:LYS:HE2	1.65	0.45
1:A:656:PHE:CD1	1:B:678:ALA:HB2	2.52	0.45
1:A:840:THR:CG2	1:A:842:GLY:N	2.79	0.45
1:A:777:PRO:HG2	1:A:782:LYS:HE3	1.97	0.45
1:B:858:ARG:HB2	1:B:925:LEU:HD21	1.99	0.44
1:B:685:LEU:HD22	1:B:715:VAL:HG11	2.00	0.44
1:B:789:LYS:HB3	1:B:790:PRO:HD3	1.98	0.44
1:A:711:TYR:CZ	1:A:713:GLY:HA2	2.53	0.43
1:B:824:LYS:HE3	1:B:824:LYS:HB2	1.58	0.43
1:A:879:PHE:CD2	1:A:879:PHE:N	2.86	0.43
1:B:676:PHE:CE1	3:B:2462:ATP:H5'1	2.53	0.43
1:A:728:LEU:HD22	1:A:890:TRP:CE2	2.53	0.43
1:A:755:ALA:HB1	1:A:790:PRO:HD2	1.99	0.43
1:B:879:PHE:N	1:B:879:PHE:CD2	2.86	0.43
1:B:676:PHE:CZ	1:B:686:LYS:HD2	2.53	0.43
1:B:728:LEU:HD22	1:B:890:TRP:CE2	2.54	0.43
1:A:684:ILE:HG22	1:A:725:MET:HG2	2.00	0.43
1:B:745:ARG:HD2	1:B:747:TYR:CE1	2.54	0.42
1:A:867:PHE:O	1:A:908:HIS:CE1	2.72	0.42
1:A:676:PHE:O	1:A:677:LYS:HD2	2.18	0.42
1:B:848:ILE:HG13	1:B:936:SER:HB2	2.01	0.42
1:A:756:ARG:NH2	1:A:914:GLU:OE1	2.53	0.42
1:B:696:LEU:HB3	1:B:711:TYR:CG	2.54	0.42
1:A:684:ILE:HD13	1:A:727:ASP:HB2	2.02	0.42
1:A:910:VAL:HA	1:A:911:PRO:HD3	1.85	0.42
1:A:653:TRP:HD1	1:B:819:VAL:HG22	1.85	0.42
1:A:819:VAL:HG21	1:B:653:TRP:CD1	2.55	0.42
1:B:712:HIS:CE1	1:B:726:ASP:OD1	2.72	0.42
1:A:754:LYS:O	1:A:757:LYS:HB2	2.20	0.41
1:B:686:LYS:NZ	3:B:2462:ATP:O1A	2.40	0.41
1:A:749:GLU:OE2	1:A:915:GLY:N	2.54	0.41
1:A:871:GLU:OE1	1:A:917:ARG:NE	2.48	0.41
1:A:712:HIS:CE1	1:A:726:ASP:OD1	2.71	0.41
1:A:727:ASP:OD1	1:A:729:LEU:HB2	2.21	0.41
1:A:814:LYS:HE2	1:A:814:LYS:HB2	1.54	0.41
1:A:755:ALA:CB	1:A:790:PRO:HD3	2.51	0.40
1:A:814:LYS:HZ2	1:A:820:ASN:HD21	1.69	0.40
1:B:676:PHE:HE1	3:B:2462:ATP:H5'1	1.84	0.40
1:B:858:ARG:O	1:B:858:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	287/289 (99%)	271 (94%)	15 (5%)	1 (0%)	41	61
1	B	285/289 (99%)	269 (94%)	15 (5%)	1 (0%)	34	54
All	All	572/578 (99%)	540 (94%)	30 (5%)	2 (0%)	41	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	790	PRO
1	B	790	PRO

### 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	254/254 (100%)	229 (90%)	25 (10%)	8	15
1	B	253/254 (100%)	227 (90%)	26 (10%)	7	14
All	All	507/508 (100%)	456 (90%)	51 (10%)	7	14

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	650	MET
1	A	652	GLN
1	A	684	ILE
1	A	703	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	715	VAL
1	A	725	MET
1	A	734	SER
1	A	754	LYS
1	A	757	LYS
1	A	758	LYS
1	A	763	LYS
1	A	770	VAL
1	A	779	GLU
1	A	791	ARG
1	A	798	THR
1	A	813	LYS
1	A	824	LYS
1	A	840	THR
1	A	847	LEU
1	A	850	TYR
1	A	853	ARG
1	A	858	ARG
1	A	884	LYS
1	A	906	LEU
1	A	928	LEU
1	B	651	VAL
1	B	677	LYS
1	B	684	ILE
1	B	708	VAL
1	B	717	LYS
1	B	721	ARG
1	B	729	LEU
1	B	757	LYS
1	B	760	SER
1	B	763	LYS
1	B	764	ASP
1	B	780	GLU
1	B	787	VAL
1	B	788	THR
1	B	791	ARG
1	B	797	GLU
1	B	816	ASP
1	B	819	VAL
1	B	824	LYS
1	B	840	THR
1	B	847	LEU

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Mol	Chain	Res	Type
1	B	851	ARG
1	B	853	ARG
1	B	858	ARG
1	B	879	PHE
1	B	928	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	712	HIS
1	A	784	GLN
1	A	820	ASN
1	A	908	HIS
1	B	693	GLN
1	B	712	HIS
1	B	784	GLN
1	B	820	ASN
1	B	886	GLN
1	B	904	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
3	ATP	A	1462	2	26,33,33	0.92	1 (3%)	31,52,52	1.56	6 (19%)
3	ATP	B	2462	2	26,33,33	1.12	2 (7%)	31,52,52	1.44	4 (12%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1462	2	-	1/18/38/38	0/3/3/3
3	ATP	B	2462	2	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2462	ATP	C5-C4	2.84	1.48	1.40
3	A	1462	ATP	C5-C4	2.33	1.47	1.40
3	B	2462	ATP	C2'-C1'	-2.12	1.50	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1462	ATP	N3-C2-N1	-4.12	122.24	128.68
3	B	2462	ATP	PB-O3B-PG	-2.98	122.59	132.83
3	B	2462	ATP	C4-C5-N7	-2.66	106.62	109.40
3	B	2462	ATP	PA-O3A-PB	-2.32	124.86	132.83
3	A	1462	ATP	O3'-C3'-C4'	-2.24	104.56	111.05
3	B	2462	ATP	C3'-C2'-C1'	2.19	104.28	100.98
3	A	1462	ATP	O3G-PG-O2G	2.15	115.86	107.64
3	A	1462	ATP	O2G-PG-O3B	-2.14	97.47	104.64
3	A	1462	ATP	C2-N1-C6	2.09	122.33	118.75
3	A	1462	ATP	C3'-C2'-C1'	2.06	104.08	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2462	ATP	C5'-O5'-PA-O3A
3	B	2462	ATP	C5'-O5'-PA-O1A
3	B	2462	ATP	C5'-O5'-PA-O2A
3	A	1462	ATP	PG-O3B-PB-O1B

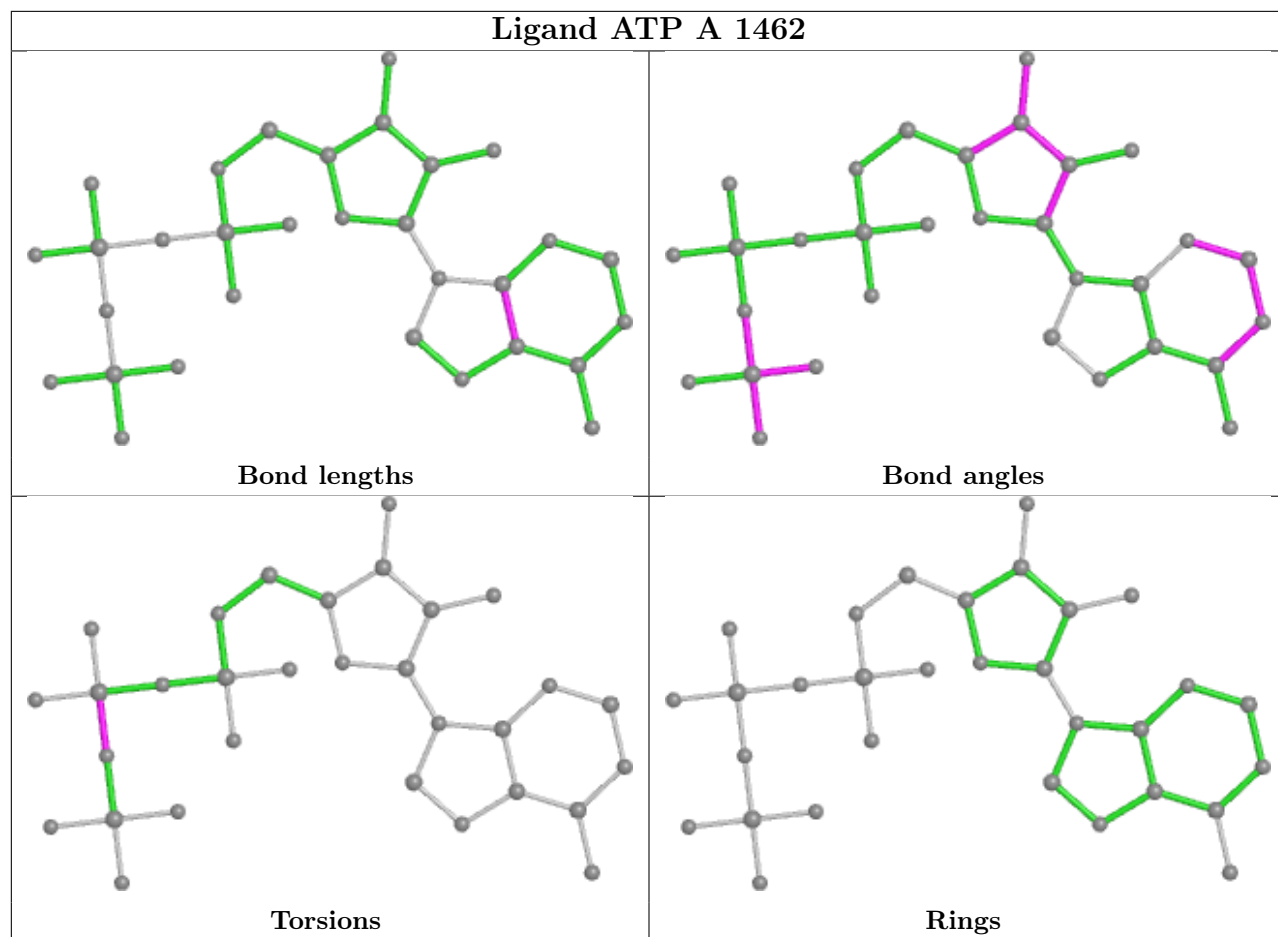
There are no ring outliers.

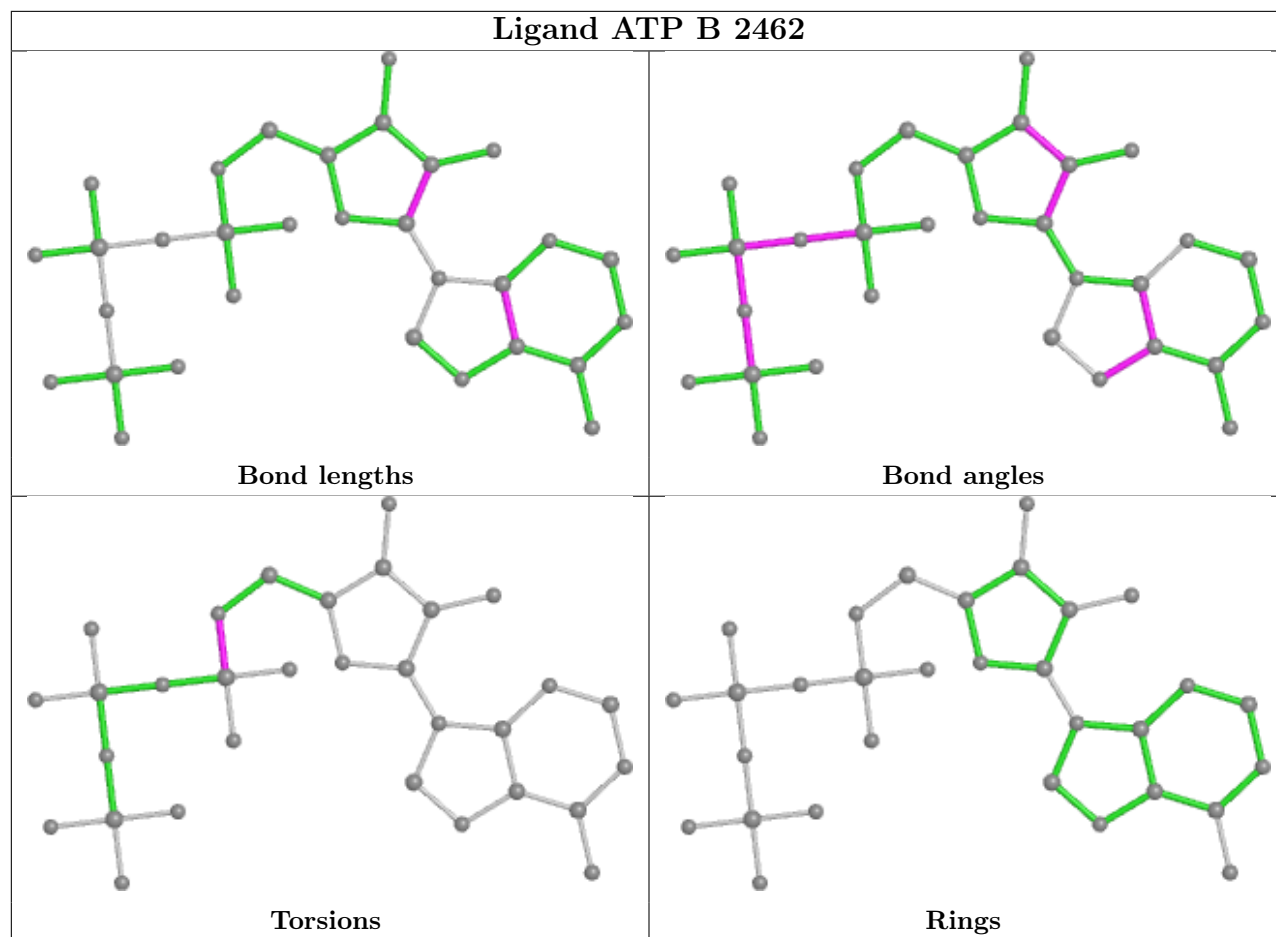
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1462	ATP	5	0
3	B	2462	ATP	3	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	289/289 (100%)	-0.43	1 (0%) 94   94	19, 32, 53, 57	0
1	B	287/289 (99%)	-0.30	2 (0%) 87   89	18, 36, 52, 57	1 (0%)
All	All	576/578 (99%)	-0.37	3 (0%) 91   91	18, 34, 53, 57	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	651	VAL	4.3
1	A	938	GLY	3.8
1	B	761	LEU	2.1

### 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 monosaccharides 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.

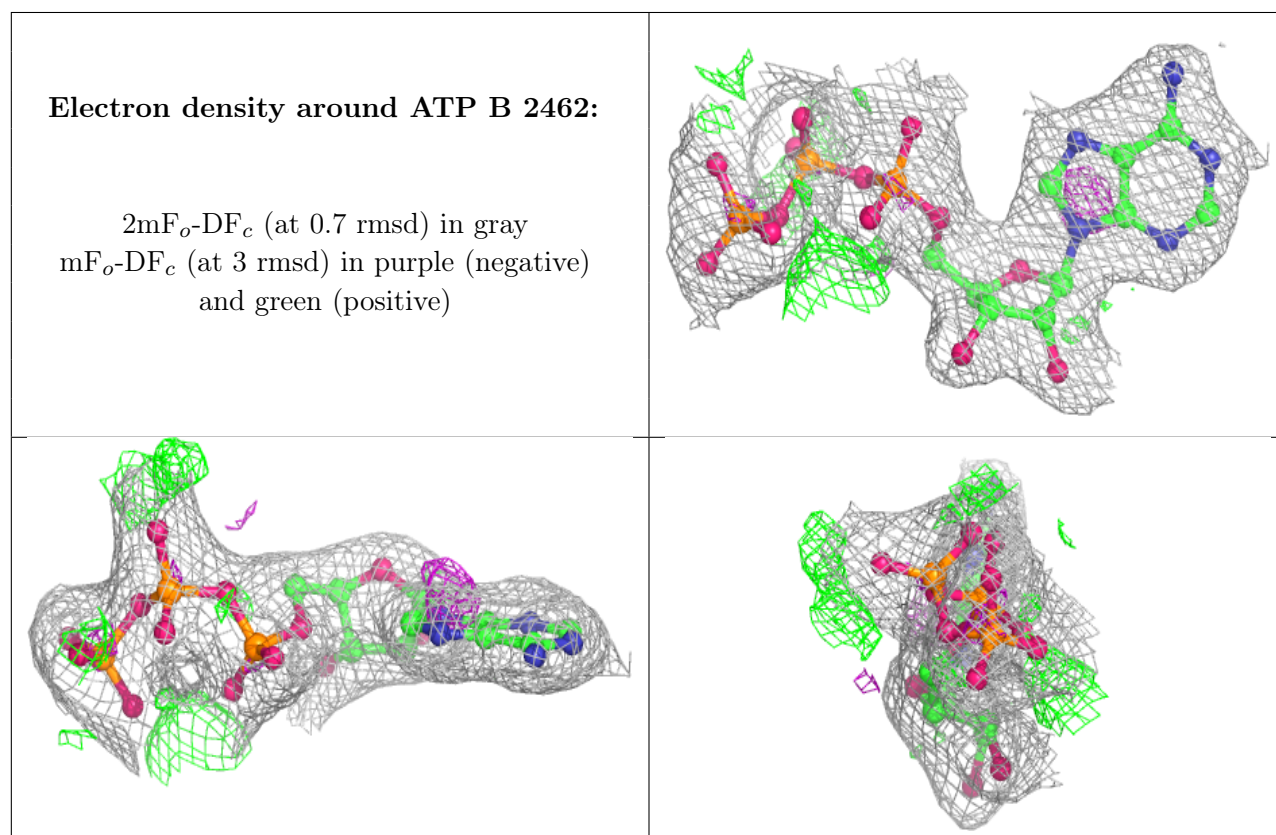
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	1600	1/1	0.94	0.13	33,33,33,33	0
2	MG	B	1601	1/1	0.94	0.10	20,20,20,20	0

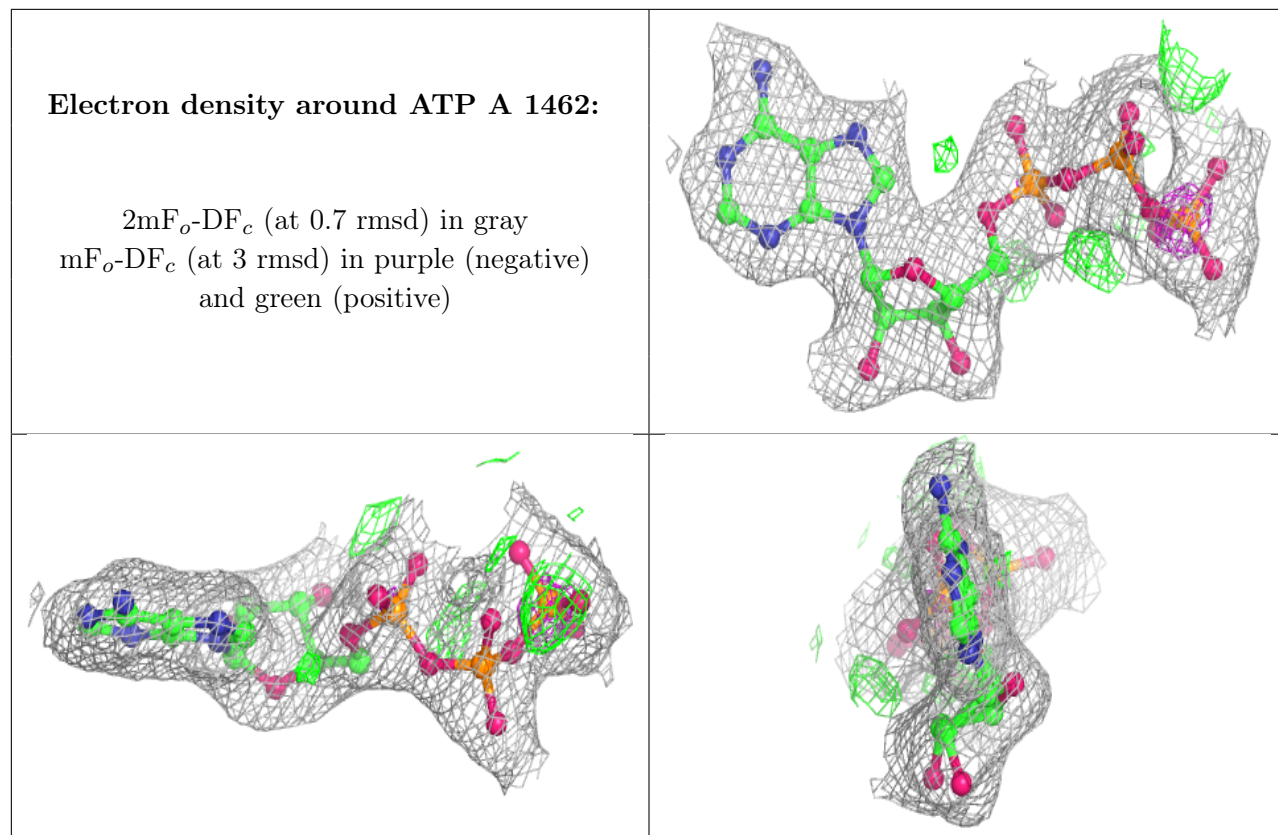
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	601	1/1	0.96	0.23	26,26,26,26	0
2	MG	A	600	1/1	0.98	0.14	17,17,17,17	0
3	ATP	B	2462	31/31	0.98	0.08	15,17,21,22	0
3	ATP	A	1462	31/31	0.99	0.07	10,20,23,23	0

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.