



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:33 pm BST

PDB ID : 3DAH  
Title : 2.3 Å crystal structure of ribose-phosphate pyrophosphokinase from  
Burkholderia pseudomallei  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2008-05-29  
Resolution : 2.30 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

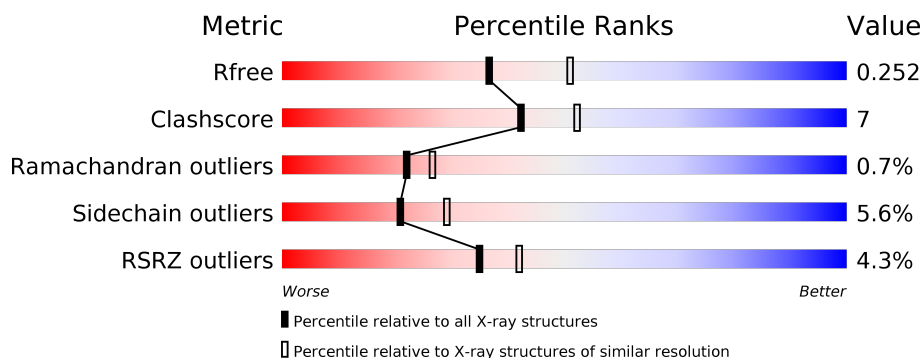
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	319	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>••</div> <div>9%</div> </div> </div>
1	B	319	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	319	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>•</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6879 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.

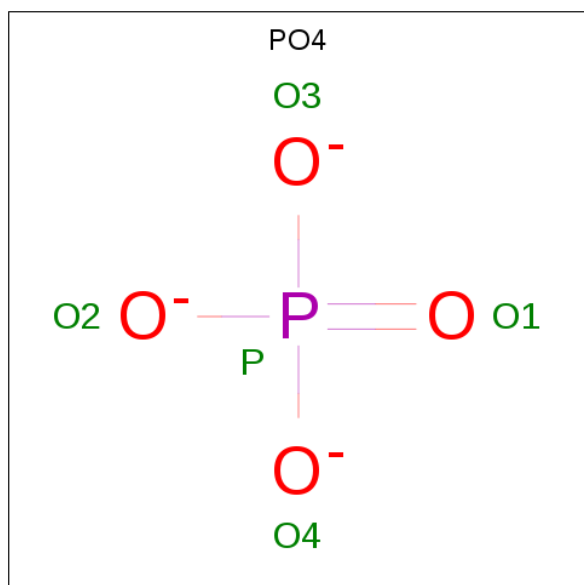
- Molecule 1 is a protein called Ribose-phosphate pyrophosphokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2174	1364	385	410	15			
1	B	294	Total	C	N	O	S	0	0	0
			2205	1385	389	416	15			
1	C	300	Total	C	N	O	S	0	0	0
			2258	1417	403	422	16			

There are 3 discrepancies between the modelled and reference sequences:

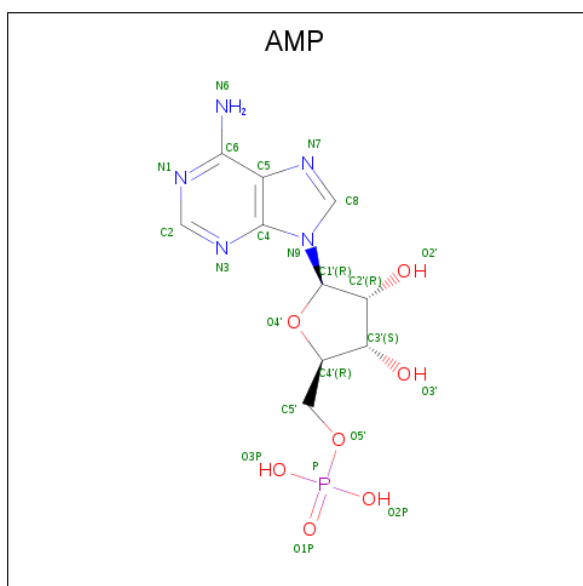
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q3JW86
B	0	SER	-	EXPRESSION TAG	UNP Q3JW86
C	0	SER	-	EXPRESSION TAG	UNP Q3JW86

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

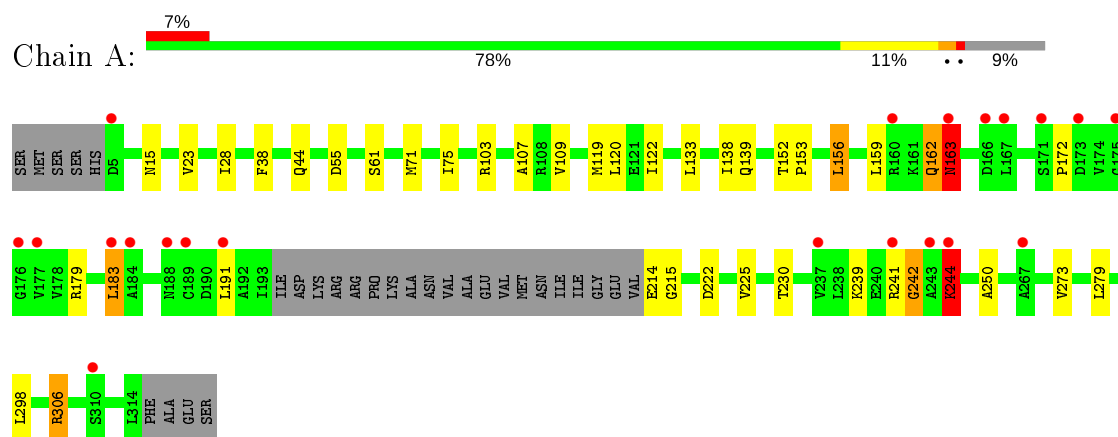
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	45	Total 45	O 45	0	0
4	C	43	Total 43	O 43	0	0

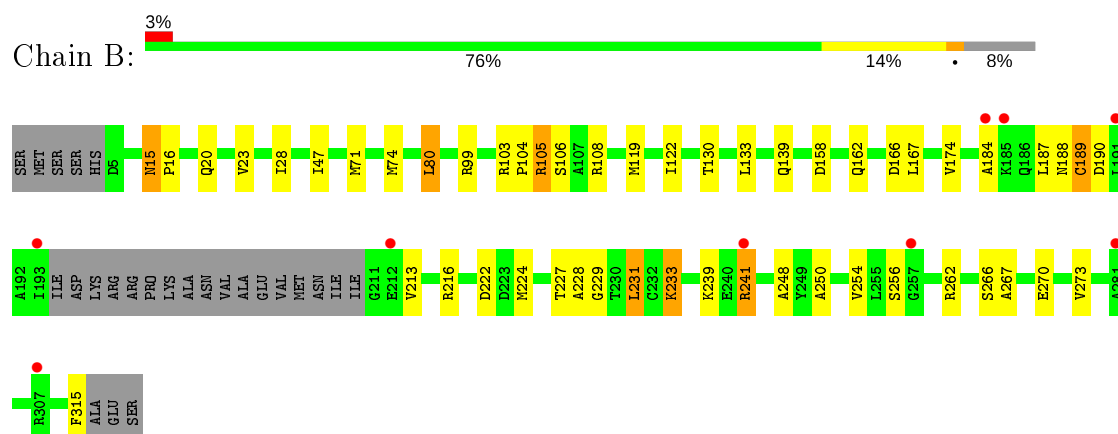
### 3 Residue-property plots [i](#)

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.

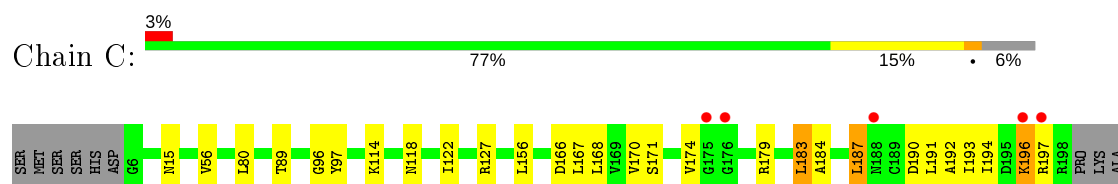
- Molecule 1: Ribose-phosphate pyrophosphokinase

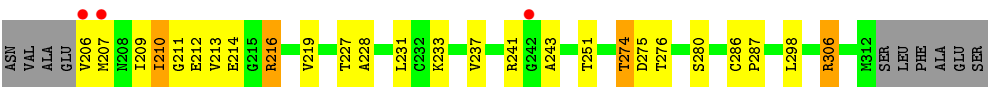


- Molecule 1: Ribose-phosphate pyrophosphokinase



- Molecule 1: Ribose-phosphate pyrophosphokinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.97Å 123.24Å 197.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 2.30 40.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.93-2.30) 97.9 (40.22-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.206 , 0.255 0.205 , 0.252	Depositor DCC
$R_{free}$ test set	2110 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: AMP, PO4

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	0.48	0/2199	0.64	1/2977 (0.0%)
1	B	0.59	1/2231 (0.0%)	0.67	0/3020
1	C	0.55	0/2283	0.63	1/3088 (0.0%)
All	All	0.54	1/6713 (0.0%)	0.65	2/9085 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	CYS	CB-SG	-5.84	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	LEU	N-CA-C	-7.21	91.53	111.00
1	A	242	GLY	N-CA-C	5.04	125.71	113.10

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	2174	0	2243	20	0
1	B	2205	0	2270	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2258	0	2341	33	1
2	A	10	0	0	1	0
2	B	20	0	0	1	0
2	C	5	0	0	0	0
3	A	23	0	12	0	0
3	B	46	0	24	0	0
4	A	50	0	0	0	0
4	B	45	0	0	0	0
4	C	43	0	0	0	0
All	All	6879	0	6890	94	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (94) 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:184:ALA:O	1:C:187:LEU:O	1.60	1.19
1:C:210:ILE:HD12	1:C:211:GLY:N	1.61	1.13
1:C:210:ILE:HD12	1:C:211:GLY:H	1.35	0.91
1:B:229:GLY:HA2	1:B:262:ARG:CZ	2.00	0.90
1:C:274:THR:HG22	1:C:276:THR:H	1.47	0.78
1:B:227:THR:O	1:B:228:ALA:HB3	1.84	0.76
1:B:224:MET:HE3	1:B:254:VAL:HG21	1.66	0.75
1:C:196:LYS:HB3	1:C:206:VAL:HA	1.69	0.74
1:B:229:GLY:HA2	1:B:262:ARG:NH1	2.02	0.73
1:C:210:ILE:HD12	1:C:210:ILE:C	2.06	0.71
1:B:104:PRO:O	1:B:106:SER:N	2.29	0.66
1:C:251:THR:O	1:C:274:THR:HB	1.96	0.65
1:A:179:ARG:HH21	1:B:105:ARG:HD2	1.61	0.64
1:C:274:THR:HG21	1:C:276:THR:HG23	1.79	0.64
1:C:156:LEU:HD21	1:C:183:LEU:HD21	1.80	0.63
1:A:239:LYS:NZ	1:A:244:LYS:O	2.32	0.62
1:B:122:ILE:HD13	1:C:122:ILE:HD12	1.83	0.61
1:B:71:MET:CE	1:B:119:MET:HE1	2.32	0.60
1:B:227:THR:O	1:B:228:ALA:CB	2.50	0.59
1:B:104:PRO:O	1:B:105:ARG:C	2.39	0.58
1:C:274:THR:CG2	1:C:276:THR:HG23	2.33	0.58
1:B:71:MET:HE1	1:B:74:MET:HG3	1.86	0.58
1:C:206:VAL:N	1:C:233:LYS:HZ1	2.02	0.57
1:A:133:LEU:HD21	1:A:138:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:VAL:CG1	1:B:213:VAL:O	2.52	0.57
1:B:187:LEU:O	1:B:188:ASN:HB3	2.04	0.57
1:B:227:THR:HA	1:B:256:SER:O	2.06	0.56
1:A:103:ARG:HH11	1:B:139:GLN:HE22	1.52	0.56
1:A:23:VAL:HG13	1:A:28:ILE:O	2.05	0.56
1:C:168:LEU:HD13	1:C:216:ARG:HD3	1.88	0.56
1:C:210:ILE:CD1	1:C:211:GLY:N	2.52	0.55
1:B:250:ALA:O	1:B:273:VAL:HA	2.06	0.55
1:A:179:ARG:NH2	1:B:105:ARG:HD2	2.22	0.55
1:B:104:PRO:C	1:B:106:SER:N	2.59	0.54
1:B:167:LEU:O	1:B:189:CYS:HB2	2.08	0.54
1:A:152:THR:OG1	1:A:153:PRO:HD3	2.08	0.53
1:A:156:LEU:HD11	1:A:183:LEU:HD21	1.89	0.53
1:B:229:GLY:CA	1:B:262:ARG:NH1	2.70	0.53
1:C:274:THR:CG2	1:C:275:ASP:N	2.72	0.52
1:A:162:GLN:O	1:A:163:ASN:C	2.48	0.52
1:A:15:ASN:ND2	1:A:61:SER:H	2.09	0.51
1:A:55:ASP:OD2	1:A:306:ARG:NH1	2.42	0.51
1:B:231:LEU:HD11	1:B:248:ALA:CB	2.41	0.51
1:C:274:THR:HG22	1:C:276:THR:N	2.23	0.51
1:B:187:LEU:O	1:B:188:ASN:CB	2.57	0.51
1:B:71:MET:HE1	1:B:119:MET:CE	2.40	0.50
1:C:306:ARG:O	1:C:306:ARG:HD2	2.10	0.50
1:B:187:LEU:O	1:B:188:ASN:C	2.46	0.50
1:B:184:ALA:O	1:B:188:ASN:N	2.45	0.49
1:C:213:VAL:CG1	1:C:243:ALA:HB2	2.42	0.49
1:B:224:MET:CE	1:B:254:VAL:HG21	2.37	0.49
1:B:71:MET:CE	1:B:119:MET:CE	2.91	0.49
1:C:170:VAL:HG22	1:C:192:ALA:HB3	1.94	0.48
1:B:158:ASP:O	1:B:162:GLN:HG2	2.13	0.48
1:C:168:LEU:HD12	1:C:190:ASP:HB2	1.96	0.48
1:B:239:LYS:HD2	1:B:267:ALA:HB1	1.96	0.48
1:C:227:THR:O	1:C:228:ALA:HB3	2.14	0.48
1:B:104:PRO:C	1:B:106:SER:H	2.18	0.47
1:A:119:MET:O	1:A:122:ILE:HG22	2.15	0.47
1:C:209:ILE:HD12	1:C:241:ARG:HG3	1.96	0.47
1:C:209:ILE:HD11	1:C:237:VAL:HG12	1.98	0.46
1:C:114:LYS:NZ	1:C:118:ASN:HD21	2.14	0.46
1:A:139:GLN:HE22	1:B:103:ARG:HH11	1.62	0.46
1:C:194:ILE:HG12	1:C:209:ILE:HG12	1.97	0.46
1:C:96:GLY:O	1:C:97:TYR:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLY:HA2	1:B:262:ARG:NH2	2.32	0.44
1:B:99:ARG:CZ	1:B:224:MET:HE1	2.48	0.43
1:C:171:SER:HB3	1:C:193:ILE:HG23	2.00	0.43
1:A:38:PHE:CZ	1:A:44:GLN:HG3	2.53	0.43
1:B:241:ARG:HA	1:B:241:ARG:HD2	1.73	0.43
1:B:15:ASN:N	1:B:16:PRO:HD3	2.33	0.43
1:B:23:VAL:HB	1:B:28:ILE:O	2.19	0.43
1:B:229:GLY:O	1:B:233:LYS:HE3	2.18	0.42
1:C:286:CYS:HA	1:C:287:PRO:HD2	1.93	0.42
1:A:71:MET:O	1:A:75:ILE:HG12	2.18	0.42
1:B:166:ASP:HB3	1:B:216:ARG:HG2	2.01	0.42
1:B:190:ASP:OD2	1:B:216:ARG:NH1	2.52	0.42
1:B:47:ILE:HG13	1:B:80:LEU:HD13	2.02	0.42
1:B:71:MET:HE3	1:B:119:MET:HE1	2.02	0.41
1:C:168:LEU:HD12	1:C:190:ASP:CB	2.51	0.41
1:A:15:ASN:HD21	1:A:61:SER:H	1.68	0.41
1:A:250:ALA:O	1:A:273:VAL:HA	2.20	0.41
1:A:214:GLU:HG2	1:A:242:GLY:HA3	2.03	0.41
2:A:319:PO4:P	1:B:108:ARG:HH11	2.44	0.41
1:B:99:ARG:CZ	1:B:224:MET:CE	2.99	0.41
1:B:262:ARG:CZ	2:B:322:PO4:O3	2.69	0.41
1:C:167:LEU:HD11	1:C:219:VAL:HG21	2.02	0.41
1:A:225:VAL:HG23	1:A:250:ALA:CB	2.50	0.41
1:B:130:THR:HG21	1:B:133:LEU:HD13	2.03	0.41
1:B:262:ARG:O	1:B:266:SER:HB3	2.21	0.41
1:C:237:VAL:O	1:C:241:ARG:HG2	2.21	0.41
1:A:107:ALA:HB1	1:A:109:VAL:HG13	2.04	0.40
1:C:89:THR:HG23	1:C:127:ARG:HG3	2.03	0.40
1:C:56:VAL:HG11	1:C:80:LEU:HD13	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:CD1	1:C:197:ARG:NH2[2_555]	2.02	0.18

## 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	286/319 (90%)	268 (94%)	14 (5%)	4 (1%)	11	11
1	B	290/319 (91%)	270 (93%)	19 (7%)	1 (0%)	41	50
1	C	296/319 (93%)	283 (96%)	12 (4%)	1 (0%)	41	50
All	All	872/957 (91%)	821 (94%)	45 (5%)	6 (1%)	22	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	ARG
1	C	174	VAL
1	A	163	ASN
1	A	172	PRO
1	A	244	LYS
1	A	215	GLY

### 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	232/257 (90%)	218 (94%)	14 (6%)	19	26
1	B	235/257 (91%)	225 (96%)	10 (4%)	29	40
1	C	241/257 (94%)	225 (93%)	16 (7%)	16	22
All	All	708/771 (92%)	668 (94%)	40 (6%)	21	29

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LEU
1	A	156	LEU
1	A	159	LEU
1	A	162	GLN
1	A	163	ASN
1	A	183	LEU
1	A	191	LEU
1	A	222	ASP
1	A	230	THR
1	A	241	ARG
1	A	244	LYS
1	A	279	LEU
1	A	298	LEU
1	A	306	ARG
1	B	15	ASN
1	B	20	GLN
1	B	80	LEU
1	B	174	VAL
1	B	222	ASP
1	B	231	LEU
1	B	233	LYS
1	B	241	ARG
1	B	270	GLU
1	B	315	PHE
1	C	15	ASN
1	C	166	ASP
1	C	179	ARG
1	C	183	LEU
1	C	191	LEU
1	C	196	LYS
1	C	207	MET
1	C	210	ILE
1	C	212	GLU
1	C	214	GLU
1	C	216	ARG
1	C	231	LEU
1	C	274	THR
1	C	280	SER
1	C	298	LEU
1	C	306	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	15	ASN
1	A	20	GLN
1	A	139	GLN
1	A	162	GLN
1	B	13	ASN
1	B	67	ASN
1	B	100	GLN
1	B	139	GLN
1	B	236	GLN
1	C	13	ASN
1	C	67	ASN
1	C	118	ASN
1	C	139	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	B	321	-	4,4,4	0.86	0	6,6,6	0.47	0
3	AMP	B	402	-	22,25,25	1.02	2 (9%)	25,38,38	1.36	4 (16%)
2	PO4	A	319	-	4,4,4	1.11	0	6,6,6	0.91	0
2	PO4	B	319	-	4,4,4	1.04	0	6,6,6	0.51	0
2	PO4	B	322	-	4,4,4	0.98	0	6,6,6	0.70	0
3	AMP	B	401	-	22,25,25	1.04	2 (9%)	25,38,38	1.34	3 (12%)
2	PO4	A	320	-	4,4,4	1.01	0	6,6,6	0.36	0
2	PO4	B	320	-	4,4,4	0.98	0	6,6,6	0.38	0
2	PO4	C	319	-	4,4,4	0.92	0	6,6,6	0.54	0
3	AMP	A	401	-	22,25,25	1.03	2 (9%)	25,38,38	1.35	3 (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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	B	401	-	-	0/6/26/26	0/3/3/3
3	AMP	B	402	-	-	2/6/26/26	0/3/3/3
3	AMP	A	401	-	-	3/6/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	AMP	C5-C4	2.64	1.47	1.40
3	A	401	AMP	C5-C4	2.58	1.47	1.40
3	B	402	AMP	C5-C4	2.55	1.47	1.40
3	A	401	AMP	O4'-C1'	2.12	1.44	1.41
3	B	401	AMP	C2-N3	2.08	1.35	1.32
3	B	402	AMP	O4'-C1'	2.07	1.44	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	AMP	N3-C2-N1	-3.45	123.29	128.68
3	A	401	AMP	N3-C2-N1	-3.38	123.39	128.68
3	B	402	AMP	N3-C2-N1	-3.37	123.41	128.68
3	B	401	AMP	C3'-C2'-C1'	2.93	105.40	100.98
3	B	402	AMP	C4-C5-N7	-2.65	106.64	109.40
3	A	401	AMP	C4-C5-N7	-2.36	106.94	109.40
3	B	402	AMP	C3'-C2'-C1'	2.26	104.38	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	AMP	C4-C5-N7	-2.21	107.09	109.40
3	A	401	AMP	C3'-C2'-C1'	2.09	104.12	100.98
3	B	402	AMP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	AMP	O4'-C4'-C5'-O5'
3	A	401	AMP	C3'-C4'-C5'-O5'
3	A	401	AMP	C5'-O5'-P-O1P
3	B	402	AMP	C5'-O5'-P-O1P
3	B	402	AMP	C3'-C4'-C5'-O5'

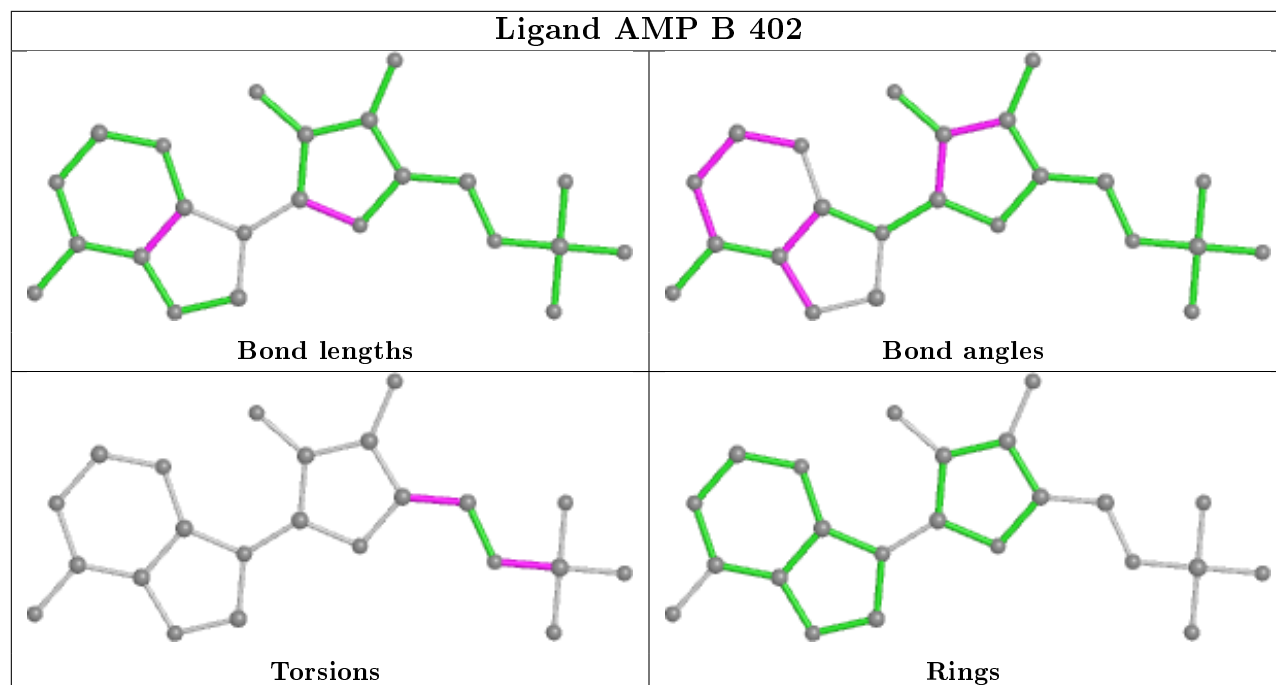
There are no ring outliers.

2 monomers are involved in 2 short contacts:

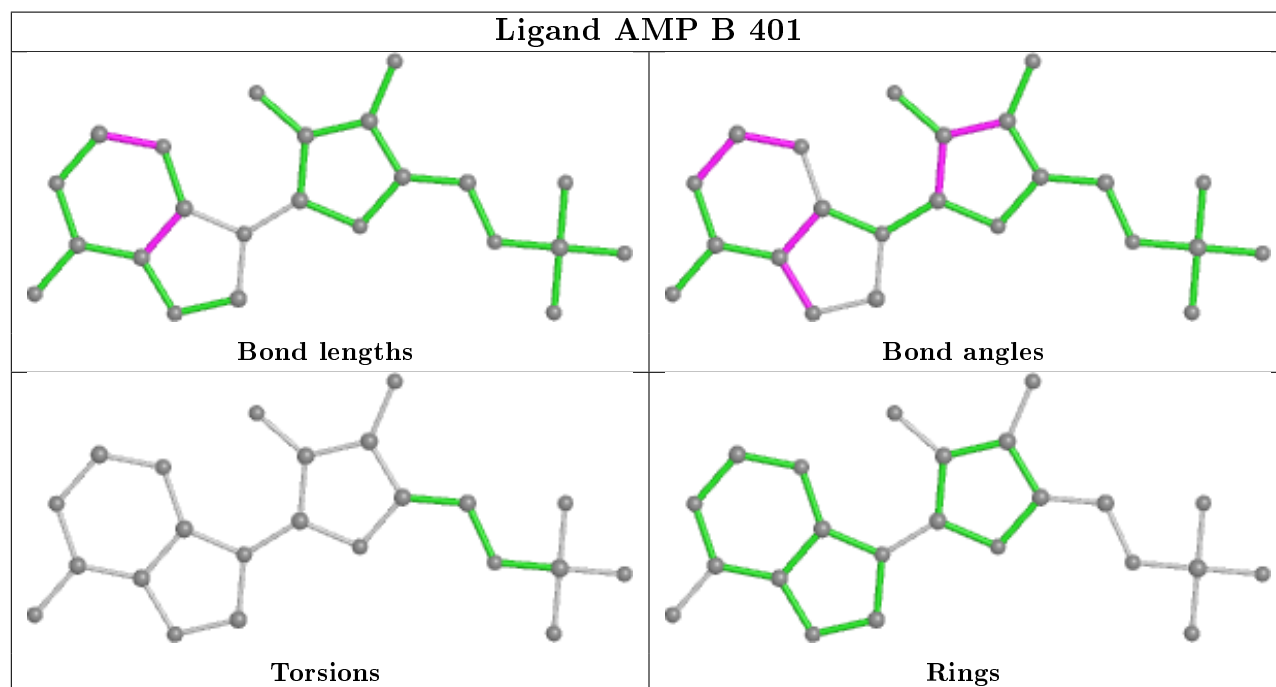
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	319	PO4	1	0
2	B	322	PO4	1	0

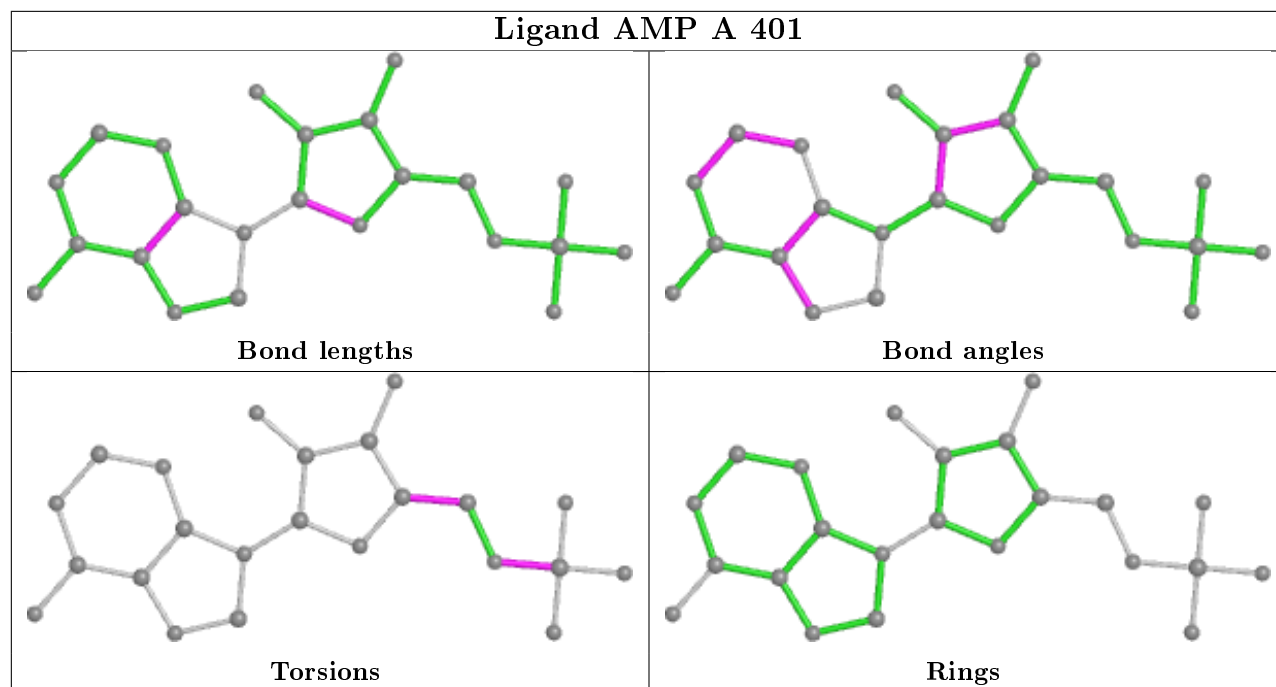
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand AMP B 402



## Ligand AMP B 401





## 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	290/319 (90%)	0.28	21 (7%) 15 20	31, 42, 84, 93	0
1	B	294/319 (92%)	0.05	9 (3%) 49 56	31, 44, 76, 86	0
1	C	300/319 (94%)	0.08	8 (2%) 54 62	31, 45, 77, 96	0
All	All	884/957 (92%)	0.14	38 (4%) 35 42	31, 44, 81, 96	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	GLY	5.3
1	C	197	ARG	4.8
1	A	177	VAL	4.6
1	B	212	GLU	4.6
1	A	188	ASN	4.4
1	B	191	LEU	4.3
1	A	175	GLY	4.1
1	A	5	ASP	3.8
1	A	173	ASP	3.7
1	A	191	LEU	3.7
1	C	206	VAL	3.5
1	A	167	LEU	3.3
1	B	193	ILE	2.9
1	A	184	ALA	2.8
1	C	207	MET	2.8
1	C	196	LYS	2.7
1	A	237	VAL	2.6
1	C	188	ASN	2.6
1	A	244	LYS	2.6
1	B	241	ARG	2.5
1	B	185	LYS	2.5
1	A	166	ASP	2.5
1	A	241	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	242	GLY	2.4
1	A	267	ALA	2.4
1	A	171	SER	2.4
1	A	243	ALA	2.3
1	B	307	ARG	2.3
1	C	175	GLY	2.3
1	B	257	GLY	2.2
1	A	163	ASN	2.2
1	A	160	ARG	2.2
1	A	189	CYS	2.2
1	A	310	SER	2.1
1	B	184	ALA	2.1
1	C	176	GLY	2.1
1	B	281	ALA	2.1
1	A	183	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.

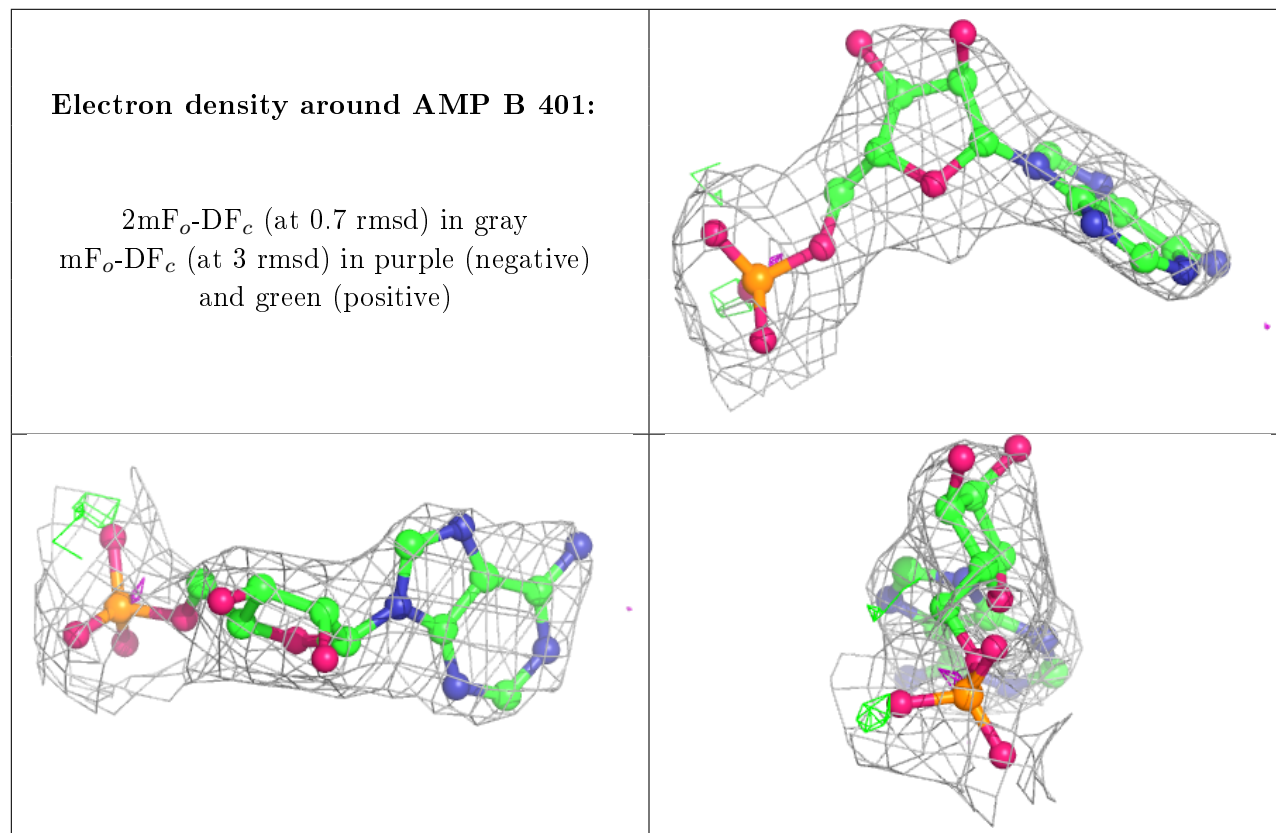
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AMP	B	401	23/23	0.79	0.17	84,85,94,95	0
3	AMP	A	401	23/23	0.86	0.14	60,62,77,77	0
3	AMP	B	402	23/23	0.87	0.13	58,59,73,74	0
2	PO4	A	320	5/5	0.89	0.13	70,71,71,72	0
2	PO4	B	322	5/5	0.92	0.13	68,68,69,69	0
2	PO4	B	320	5/5	0.95	0.10	74,74,75,76	0
2	PO4	C	319	5/5	0.95	0.10	63,64,65,65	0
2	PO4	B	321	5/5	0.95	0.09	70,71,72,72	0

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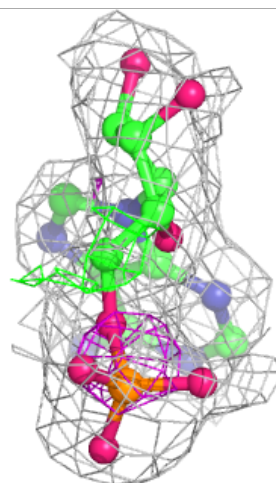
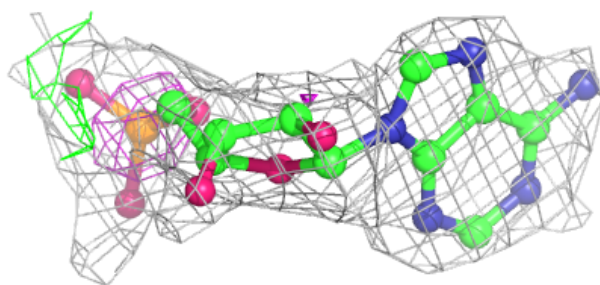
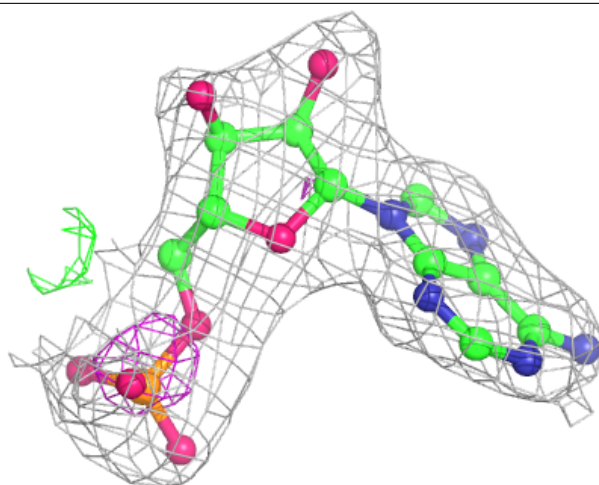
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	A	319	5/5	0.98	0.11	52,52,53,54	0
2	PO4	B	319	5/5	0.99	0.13	46,46,48,48	0

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.



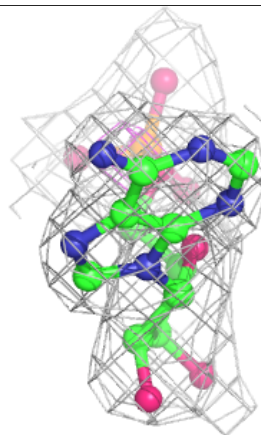
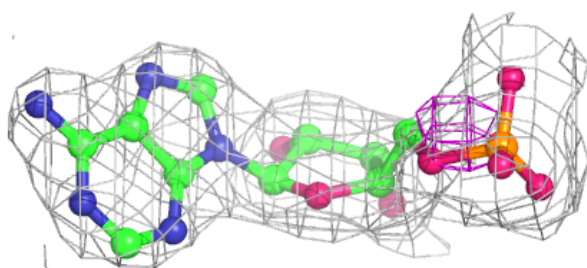
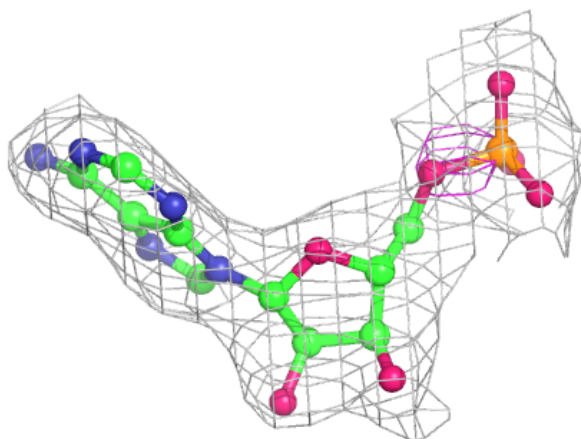
**Electron density around AMP A 401:**

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



**Electron density around AMP B 402:**

$2mF_o-DF_c$  (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.