



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:14 PM UTC

PDB ID : 9S4V / pdb_00009s4v
Title : AcuB from Bacillus subtilis with AMP and ADP
Authors : Janetzky, M.; Palm, G.J.; Lammers, M.
Deposited on : 2025-07-28
Resolution : 2.64 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	:	NOT EXECUTED
Xtriage (Phenix)	:	2.0
EDS	:	NOT EXECUTED
Buster-report	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

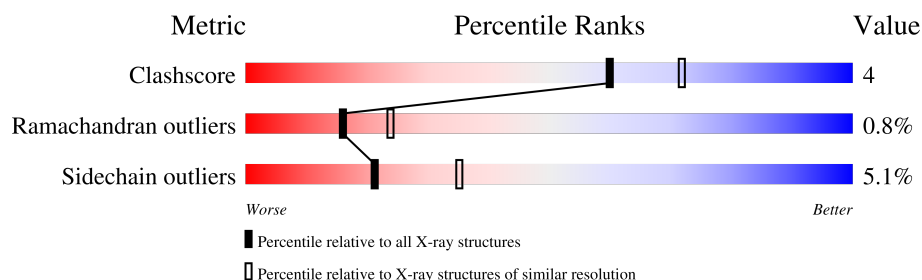
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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))
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	224	 79% 18% ..
1	B	224	 86% 11% ..
1	C	224	 77% 12% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10661 atoms, of which 5394 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 Acetoin utilization protein AcuB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	C	H	N	O	S	59	0	0
			3572	1118	1820	308	316	10			
1	B	220	Total	C	H	N	O	S	59	1	0
			3580	1119	1825	307	319	10			
1	C	202	Total	C	H	N	O	S	50	0	0
			3273	1024	1677	274	288	10			

There are 30 discrepancies between the modelled and reference sequences:

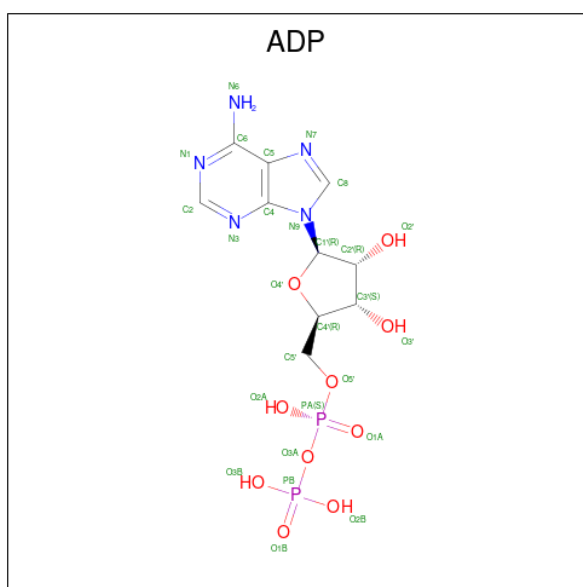
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P39066
A	215	GLY	-	expression tag	UNP P39066
A	216	SER	-	expression tag	UNP P39066
A	217	SER	-	expression tag	UNP P39066
A	218	HIS	-	expression tag	UNP P39066
A	219	HIS	-	expression tag	UNP P39066
A	220	HIS	-	expression tag	UNP P39066
A	221	HIS	-	expression tag	UNP P39066
A	222	HIS	-	expression tag	UNP P39066
A	223	HIS	-	expression tag	UNP P39066
B	0	GLY	-	expression tag	UNP P39066
B	215	GLY	-	expression tag	UNP P39066
B	216	SER	-	expression tag	UNP P39066
B	217	SER	-	expression tag	UNP P39066
B	218	HIS	-	expression tag	UNP P39066
B	219	HIS	-	expression tag	UNP P39066
B	220	HIS	-	expression tag	UNP P39066
B	221	HIS	-	expression tag	UNP P39066
B	222	HIS	-	expression tag	UNP P39066
B	223	HIS	-	expression tag	UNP P39066
C	0	GLY	-	expression tag	UNP P39066
C	215	GLY	-	expression tag	UNP P39066
C	216	SER	-	expression tag	UNP P39066

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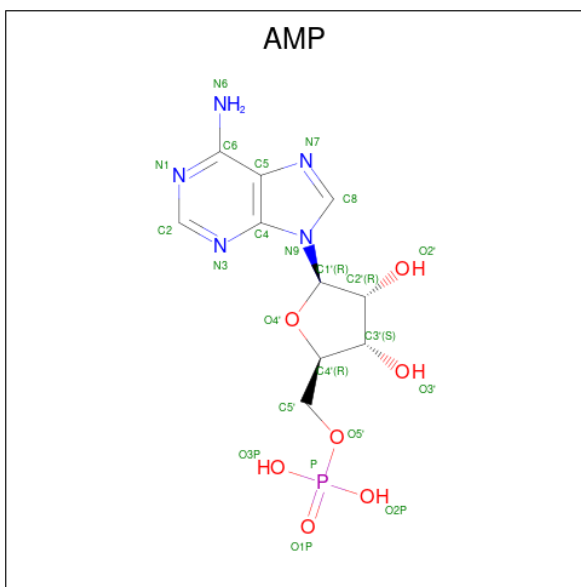
Chain	Residue	Modelled	Actual	Comment	Reference
C	217	SER	-	expression tag	UNP P39066
C	218	HIS	-	expression tag	UNP P39066
C	219	HIS	-	expression tag	UNP P39066
C	220	HIS	-	expression tag	UNP P39066
C	221	HIS	-	expression tag	UNP P39066
C	222	HIS	-	expression tag	UNP P39066
C	223	HIS	-	expression tag	UNP P39066

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	2	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	2	0
			39	10	12	5	10	2		
2	C	1	Total	C	H	N	O	P	2	0
			39	10	12	5	10	2		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	2	0
			35	10	12	5	7	1		
3	B	1	Total	C	H	N	O	P	2	0
			35	10	12	5	7	1		
3	C	1	Total	C	H	N	O	P	2	0
			35	10	12	5	7	1		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	5	Total	O	0	0
			5	5		
4	C	2	Total	O	0	0
			2	2		

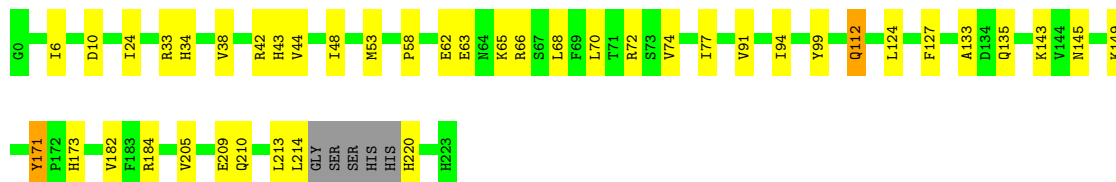
3 Residue-property plots

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. 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. 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.


Note EDS was not executed.

• Molecule 1: Acetoin utilization protein AcuB

Chain A:  79% 18% ..




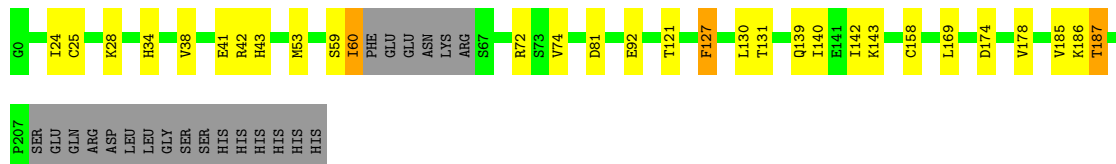
• Molecule 1: Acetoin utilization protein AcuB

Chain B:  86% 11% ..



• Molecule 1: Acetoin utilization protein AcuB

Chain C:  77% 12% • 10%



4 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value
Space group	P 21 2 21
Cell constants a, b, c, α , β , γ	67.31Å 79.78Å 153.79Å 90.00° 90.00° 90.00°
Resolution (Å)	48.79 – 2.64
% Data completeness (in resolution range)	97.4 (48.79-2.64)
R_{merge}	(Not available)
R_{sym}	0.14
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.65Å)
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105), REFMAC 5.8.0430 (refmacat 0.4.105)
R, R_{free}	0.207 , 0.266
Wilson B-factor (Å ²)	75.1
Anisotropy	0.520
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$
Estimated twinning fraction	No twinning to report.
Total number of atoms	10661
Average B, all atoms (Å ²)	101.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AMP

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	0.53	0/1786	1.07	4/2416 (0.2%)
1	B	0.51	0/1792	1.03	1/2425 (0.0%)
1	C	0.52	0/1625	1.03	2/2201 (0.1%)
All	All	0.52	0/5203	1.04	7/7042 (0.1%)

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	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	PHE	CB-CA-C	6.93	123.45	110.63
1	A	127	PHE	CA-CB-CG	6.68	120.48	113.80
1	A	10	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	62	GLU	N-CA-CB	-5.89	103.02	110.45
1	A	171	TYR	N-CA-CB	5.68	117.96	110.29
1	C	92	GLU	CB-CG-CD	5.26	121.54	112.60
1	B	118	LEU	N-CA-CB	-5.06	102.07	111.13

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	ARG	Sidechain
1	B	66	ARG	Sidechain

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	1752	1820	1805	19	0
1	B	1755	1825	1812	18	0
1	C	1596	1677	1666	13	0
2	A	27	12	12	1	0
2	B	27	12	12	1	0
2	C	27	12	12	1	0
3	A	23	12	12	1	0
3	B	23	12	12	1	0
3	C	23	12	12	1	0
4	A	7	0	0	1	0
4	B	5	0	0	0	0
4	C	2	0	0	0	0
All	All	5267	5394	5355	46	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 4.

All (46) 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:210:GLN:O	1:A:214:LEU:HG	1.82	0.79
1:A:214:LEU:HD22	1:B:5:GLN:HG2	1.67	0.76
1:B:121:THR:HB	2:B:301:ADP:O1B	1.87	0.73
1:C:139:GLN:C	1:C:140:ILE:HD12	2.20	0.66
1:B:139:GLN:C	1:B:140:ILE:HD12	2.20	0.66
1:C:127:PHE:HA	1:C:130:LEU:HD12	1.83	0.59
1:A:112:GLN:OE1	1:A:112:GLN:N	2.38	0.56
1:C:59:SER:O	1:C:60:ILE:C	2.48	0.56
1:A:34:HIS:ND1	2:A:301:ADP:O2A	2.34	0.55
1:B:121:THR:HG22	1:B:125:ARG:NH1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ILE:HD11	1:B:179:LYS:HG3	1.89	0.54
1:B:135:GLN:O	1:B:184:ARG:NH1	2.41	0.53
1:B:159:GLN:HE21	1:B:159:GLN:HA	1.73	0.52
1:B:147:ILE:H	1:B:147:ILE:HD12	1.75	0.52
1:C:121:THR:HB	2:C:301:ADP:O3'	2.11	0.51
1:A:135:GLN:O	1:A:184:ARG:NH1	2.44	0.51
1:A:173:HIS:NE2	1:A:213:LEU:HD22	2.27	0.49
1:A:58:PRO:HG3	1:A:65:LYS:HD2	1.94	0.49
1:B:140:ILE:HD13	1:B:185:VAL:HG22	1.94	0.49
1:C:185:VAL:HG23	1:C:187:THR:HG22	1.94	0.49
1:B:104:GLY:HA3	3:B:302:AMP:O2P	2.14	0.48
1:B:159:GLN:HA	1:B:159:GLN:NE2	2.28	0.47
1:C:24:ILE:HG13	1:C:53:MET:HE2	1.96	0.47
1:B:147:ILE:HD12	1:B:147:ILE:N	2.29	0.47
1:C:143:LYS:HE3	1:C:178:VAL:HG11	1.95	0.47
1:C:60:ILE:O	1:C:60:ILE:HD13	2.15	0.47
1:A:124:LEU:HB3	1:B:99:TYR:HB2	1.97	0.45
1:A:143:LYS:O	4:A:401:HOH:O	2.21	0.45
1:A:205:VAL:HG13	1:A:209:GLU:HB2	1.98	0.45
1:A:171:TYR:CZ	1:A:182:VAL:HG21	2.52	0.45
1:A:24:ILE:HG13	1:A:53:MET:HE2	1.98	0.45
1:A:99:TYR:HB3	1:B:121:THR:HG23	1.98	0.44
1:C:186:LYS:O	1:C:187:THR:HB	2.18	0.44
1:B:24:ILE:HG13	1:B:53:MET:HE2	1.98	0.44
1:B:159:GLN:HE21	1:B:159:GLN:CA	2.29	0.44
1:A:44:VAL:O	1:A:44:VAL:HG23	2.18	0.42
1:C:140:ILE:HG22	1:C:142:ILE:HD11	2.02	0.41
1:C:131:THR:HG22	1:C:169:LEU:HD11	2.01	0.41
1:C:38:VAL:HA	1:C:43:HIS:O	2.20	0.41
1:B:72:ARG:HH11	1:B:72:ARG:HG2	1.85	0.41
1:A:34:HIS:NE2	3:A:302:AMP:O3P	2.54	0.40
1:C:34:HIS:NE2	3:C:302:AMP:O1P	2.55	0.40
1:A:6:ILE:HD13	1:A:91:VAL:HG21	2.03	0.40
1:A:38:VAL:HA	1:A:43:HIS:O	2.21	0.40
1:A:77:ILE:CG2	1:B:61:PHE:HZ	2.34	0.40
1:A:68:LEU:HB3	1:A:70:LEU:HG	2.03	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	215/224 (96%)	208 (97%)	5 (2%)	2 (1%)	14	21
1	B	172/224 (77%)	164 (95%)	7 (4%)	1 (1%)	21	31
1	C	137/224 (61%)	132 (96%)	4 (3%)	1 (1%)	18	27
All	All	524/672 (78%)	504 (96%)	16 (3%)	4 (1%)	16	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	ALA
1	A	66	ARG
1	C	187	THR
1	B	66	ARG

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	203/207 (98%)	193 (95%)	10 (5%)	22	37
1	B	204/207 (99%)	194 (95%)	10 (5%)	22	37
1	C	186/207 (90%)	176 (95%)	10 (5%)	20	33
All	All	593/621 (96%)	563 (95%)	30 (5%)	21	35

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	48	ILE
1	A	63	GLU
1	A	72	ARG
1	A	74	VAL
1	A	94	ILE
1	A	112	GLN
1	A	145	ASN
1	A	149	LYS
1	A	220	HIS
1	B	60	ILE
1	B	62	GLU
1	B	63	GLU
1	B	65	LYS
1	B	72	ARG
1	B	74	VAL
1	B	81	ASP
1	B	159	GLN
1	B	204	VAL
1	B	211	ARG
1	C	25	CYS
1	C	28	LYS
1	C	41	GLU
1	C	42	ARG
1	C	60	ILE
1	C	72	ARG
1	C	74	VAL
1	C	81	ASP
1	C	158	CYS
1	C	174	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	135	GLN
1	A	198	GLN
1	A	203	HIS
1	B	43	HIS
1	B	55	GLN
1	B	101	HIS
1	B	112	GLN
1	B	135	GLN

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Mol	Chain	Res	Type
1	B	145	ASN
1	B	159	GLN
1	B	173	HIS
1	B	198	GLN
1	C	43	HIS
1	C	101	HIS
1	C	112	GLN
1	C	135	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](#)

Mogul was not executed - this section is therefore empty.

5.5 Carbohydrates [i](#)

Mogul was not executed - this section is therefore empty.

5.6 Ligand geometry [i](#)

Mogul was not executed - this section is therefore empty.

5.7 Other polymers [i](#)

Mogul was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

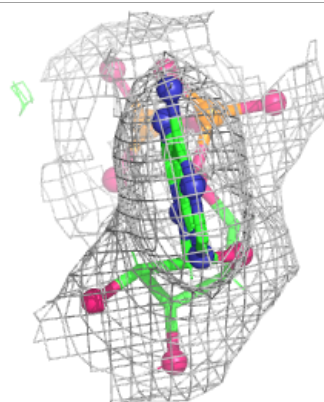
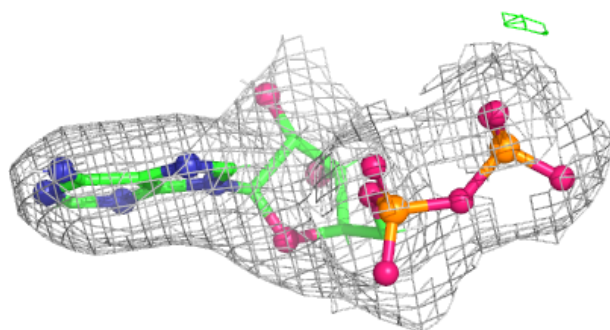
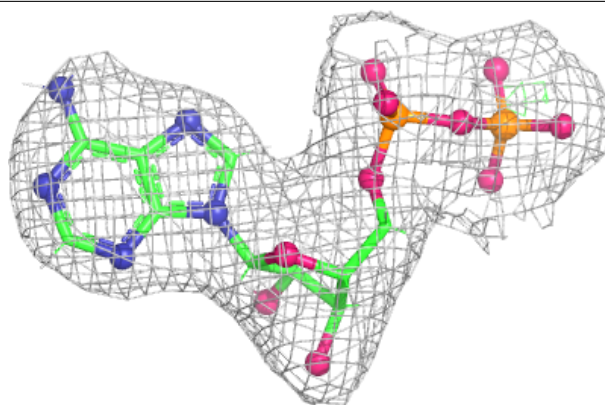
6.4 Ligands

EDS was not executed - this section is therefore empty.

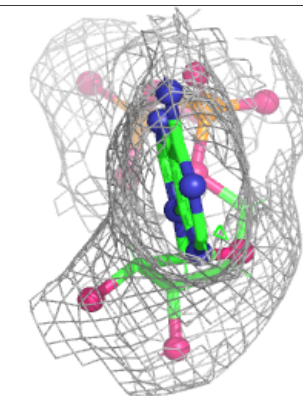
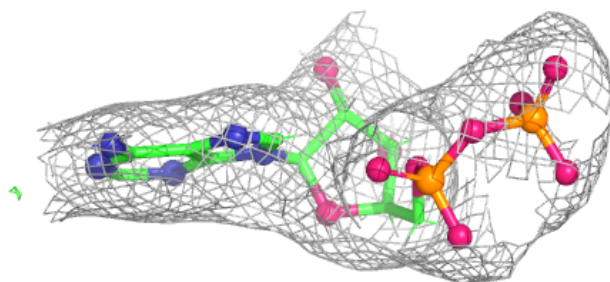
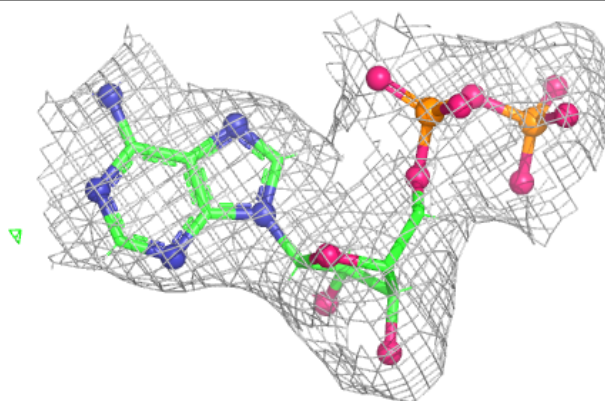
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 301:

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

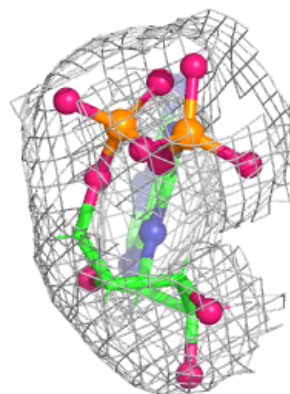
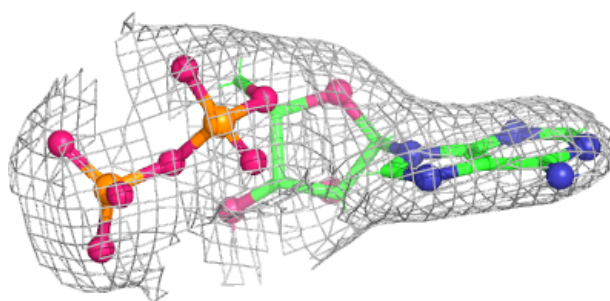
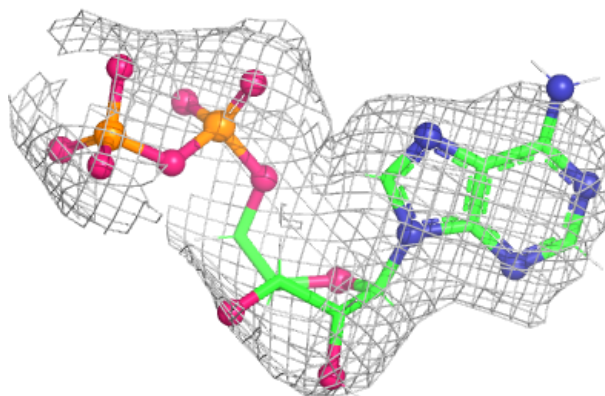
**Electron density around ADP B 301:**

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

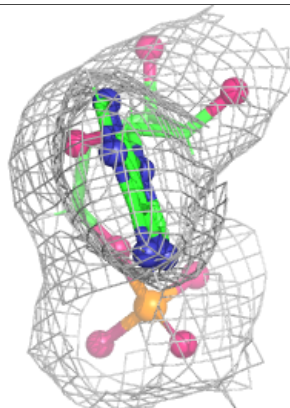
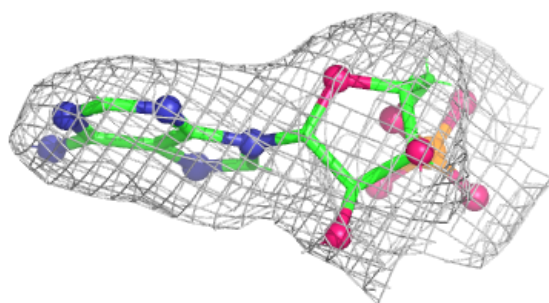
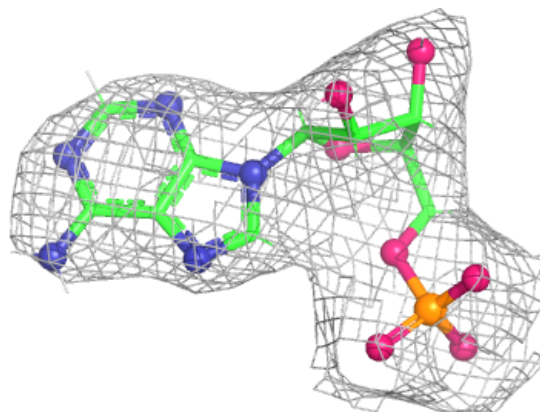


Electron density around ADP C 301:

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

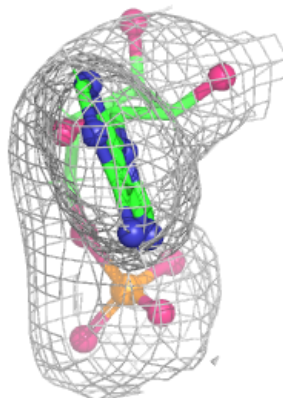
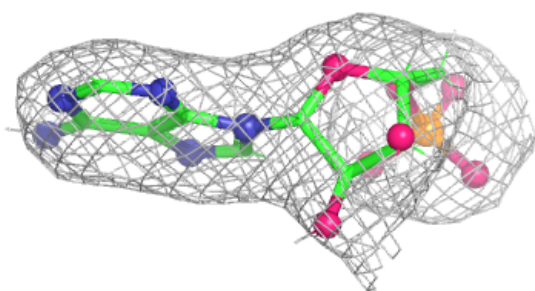
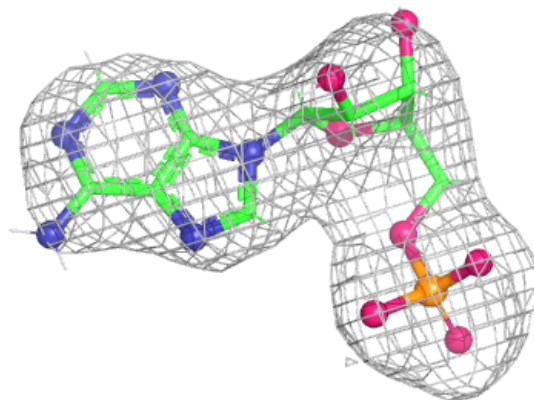
**Electron density around AMP A 302:**

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

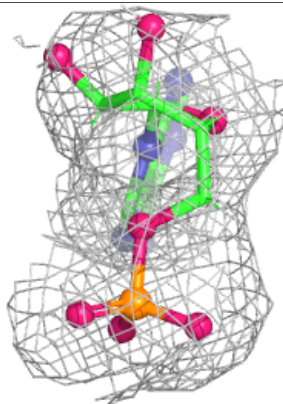
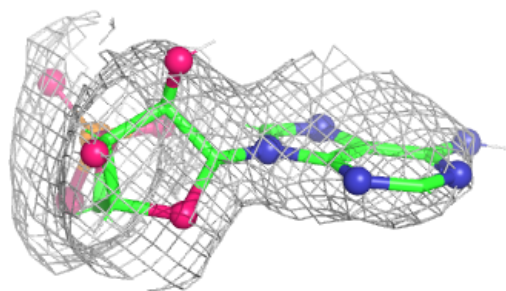
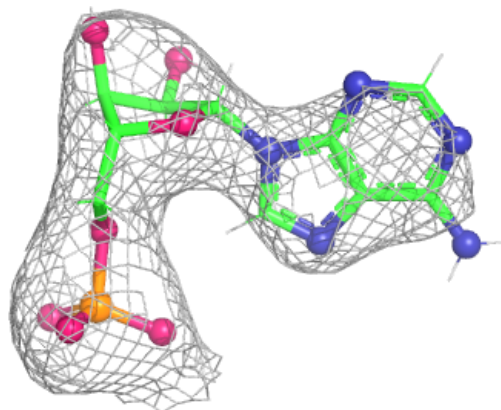


Electron density around AMP B 302:

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

**Electron density around AMP C 302:**

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



6.5 Other polymers

EDS was not executed - this section is therefore empty.