



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2019 – 06:44 AM EST

PDB ID : 6C9G
Title : AMP-activated protein kinase bound to pharmacological activator R739
Authors : Yan, Y.; Zhou, X.E.; Novick, S.; Shaw, S.J.; Li, Y.; Hitoshi, Y.; Brunzelle, J.S.; Griffin, P.R.; Xu, H.E.; Melcher, K.
Deposited on : 2018-01-26
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

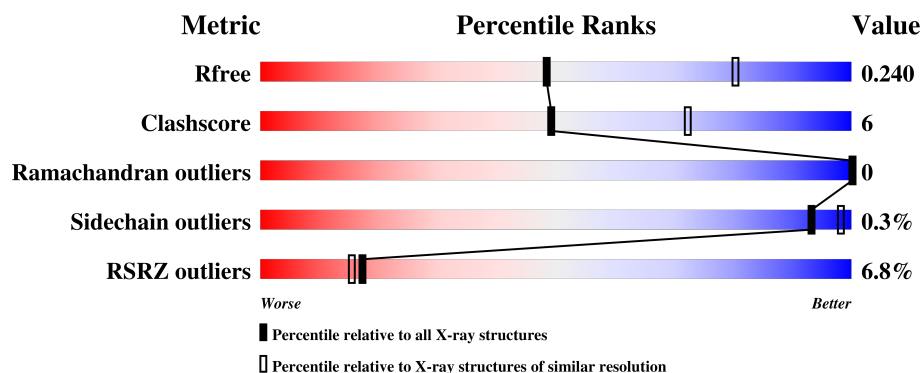
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	494	 6% 68% 10% 22%
2	B	204	 11% 77% 9% 13%
3	C	331	 3% 76% 15% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7170 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 5'-AMP-activated protein kinase catalytic subunit alpha-1,5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	P	S	0	0	0
			3140	2009	551	560	1	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	expression tag	UNP Q13131
A	4	GLY	-	expression tag	UNP Q13131
A	5	HIS	-	expression tag	UNP Q13131
A	6	HIS	-	expression tag	UNP Q13131
A	7	HIS	-	expression tag	UNP Q13131
A	8	HIS	-	expression tag	UNP Q13131
A	9	HIS	-	expression tag	UNP Q13131
A	10	HIS	-	expression tag	UNP Q13131
A	11	GLY	-	expression tag	UNP Q13131
A	12	SER	-	expression tag	UNP Q13131

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1419	918	241	255	5			

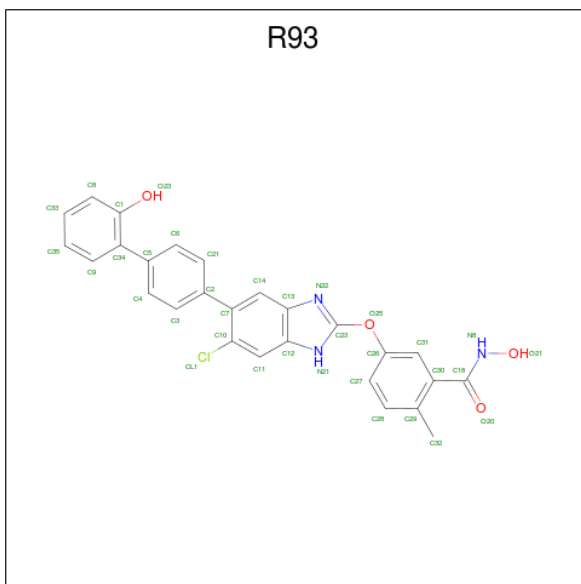
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	initiating methionine	UNP Q9Y478
B	108	ASP	SER	engineered mutation	UNP Q9Y478

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

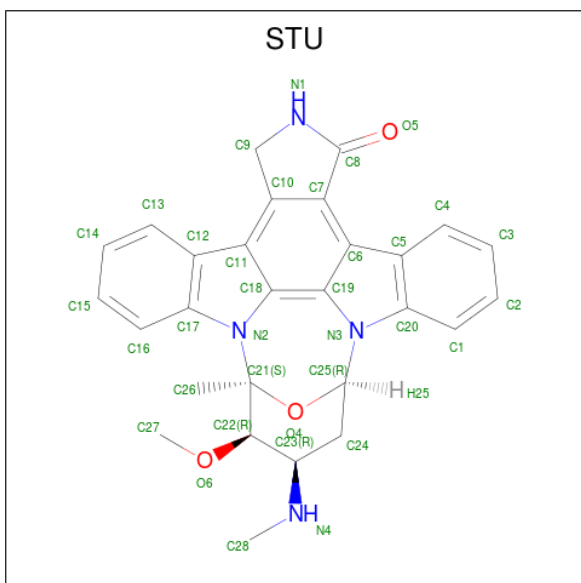
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	300	Total	C	N	O	S	0	0	0
			2420	1572	402	439	7			

- Molecule 4 is 5-[6-chloro-5-(2'-hydroxy[1,1'-biphenyl]-4-yl)-1H-benzimidazol-2-yl]oxy}-N-hydroxy-2-methylbenzamide (three-letter code: R93) (formula: $C_{27}H_{20}ClN_3O_4$).



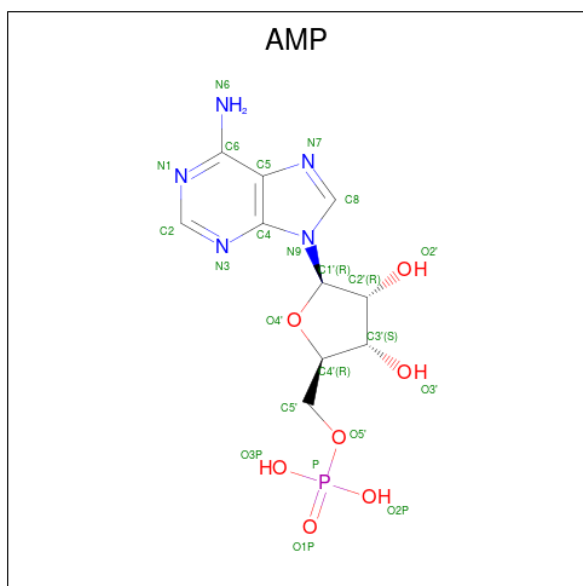
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 35	C 27	Cl 1	N 3	O 4	0	0

- Molecule 5 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 6 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

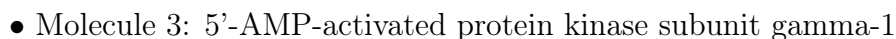


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	41	Total	O	0	0
			41	41		
7	B	7	Total	O	0	0
			7	7		
7	C	4	Total	O	0	0
			4	4		

● Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1, 5'-AMP-activated protein kinase catalytic subunit alpha-1



T324
GLY
GLY
GLU
LYS
LYS
PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.99Å 122.99Å 406.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.56 – 2.70 49.56 – 2.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.56-2.70) 100.0 (49.56-2.57)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.240 0.204 , 0.240	Depositor DCC
R_{free} test set	4168 reflections (7.11%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: TPO, STU, R93, 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	0.35	0/3198	0.50	0/4310
2	B	0.31	0/1459	0.47	0/1986
3	C	0.28	0/2471	0.46	0/3355
All	All	0.32	0/7128	0.48	0/9651

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

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	3140	0	3177	51	0
2	B	1419	0	1418	17	0
3	C	2420	0	2489	36	0
4	A	35	0	0	2	0
5	A	35	0	26	3	0
6	C	69	0	36	0	0
7	A	41	0	0	2	0
7	B	7	0	0	2	0
7	C	4	0	0	0	0
All	All	7170	0	7146	91	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 6.

The worst 5 of 91 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:342:PHE:CZ	3:C:174:PHE:HA	2.12	0.84
1:A:29:PHE:HZ	1:A:59:VAL:HG21	1.43	0.84
1:A:29:PHE:CZ	1:A:59:VAL:HG21	2.13	0.84
1:A:342:PHE:CD1	3:C:173:LYS:HG3	2.15	0.81
1:A:342:PHE:HD1	3:C:173:LYS:HG3	1.48	0.79

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	379/494 (77%)	374 (99%)	5 (1%)	0	100	100
2	B	171/204 (84%)	168 (98%)	3 (2%)	0	100	100
3	C	298/331 (90%)	295 (99%)	3 (1%)	0	100	100
All	All	848/1029 (82%)	837 (99%)	11 (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	347/447 (78%)	347 (100%)	0	100	100
2	B	160/185 (86%)	160 (100%)	0	100	100
3	C	276/304 (91%)	274 (99%)	2 (1%)	85	95
All	All	783/936 (84%)	781 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	175	LEU
3	C	298	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
2	B	212	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TPO	A	174	1	9,10,11	1.63	3 (33%)	11,14,16	2.25	2 (18%)

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	TPO	A	174	1	-	1/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	TPO	P-O1P	3.08	1.60	1.50
1	A	174	TPO	CA-C	2.42	1.53	1.50
1	A	174	TPO	P-O2P	-2.01	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	TPO	P-OG1-CB	-6.37	103.97	123.21
1	A	174	TPO	C-CA-N	2.56	115.09	109.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	174	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	174	TPO	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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
4	R93	A	601	-	39,39,39	2.23	6 (15%)	49,56,56	1.23	4 (8%)
5	STU	A	602	-	31,42,42	2.83	7 (22%)	31,68,68	1.49	6 (19%)
6	AMP	C	1101	-	21,25,25	0.98	1 (4%)	23,38,38	1.25	2 (8%)
6	AMP	C	1102	-	21,25,25	0.99	1 (4%)	23,38,38	1.25	4 (17%)
6	AMP	C	1103	-	21,25,25	0.99	1 (4%)	23,38,38	1.28	3 (13%)

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	R93	A	601	-	-	0/16/18/18	0/5/5/5
5	STU	A	602	-	-	1/4/42/42	-
6	AMP	C	1101	-	-	3/6/26/26	0/3/3/3
6	AMP	C	1102	-	-	3/6/26/26	0/3/3/3
6	AMP	C	1103	-	-	0/6/26/26	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	STU	C8-N1	10.81	1.43	1.35
4	A	601	R93	C18-N8	10.44	1.46	1.32
5	A	602	STU	O5-C8	8.32	1.40	1.23
4	A	601	R93	C7-C2	4.15	1.56	1.49
4	A	601	R93	O21-N8	3.81	1.46	1.39

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	STU	C9-N1-C8	-4.71	109.32	113.85
4	A	601	R93	O21-N8-C18	-3.89	109.66	119.67
6	C	1102	AMP	N3-C2-N1	-3.06	123.75	128.68
6	C	1101	AMP	N3-C2-N1	-3.05	123.77	128.68
6	C	1103	AMP	N3-C2-N1	-3.00	123.85	128.68

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

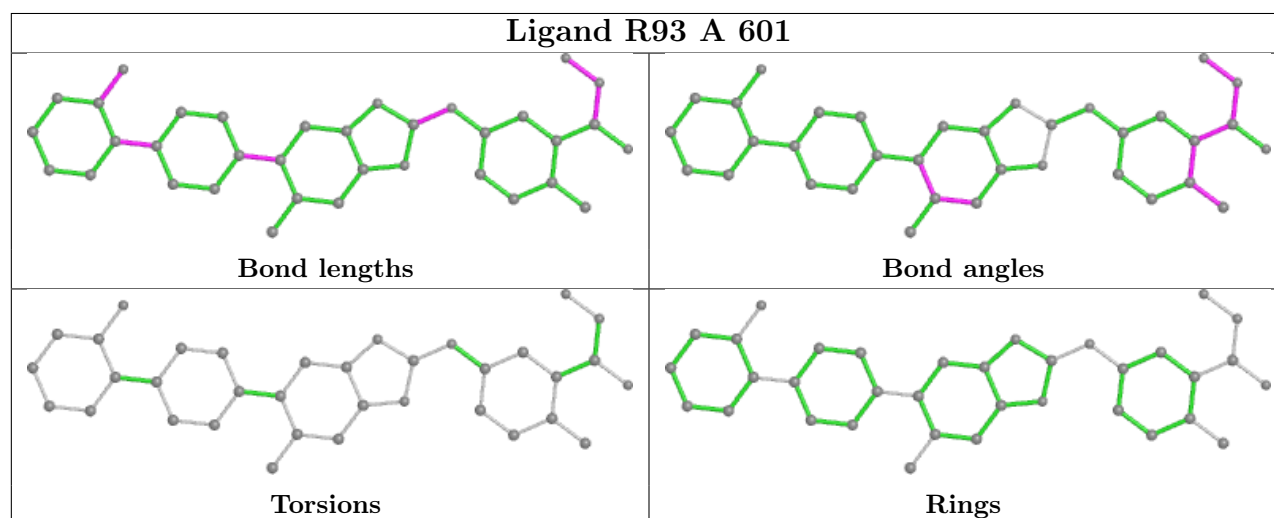
Mol	Chain	Res	Type	Atoms
6	C	1102	AMP	C5'-O5'-P-O3P
6	C	1101	AMP	C5'-O5'-P-O2P
6	C	1101	AMP	C5'-O5'-P-O3P
6	C	1102	AMP	O4'-C4'-C5'-O5'
6	C	1102	AMP	C3'-C4'-C5'-O5'

There are no ring outliers.

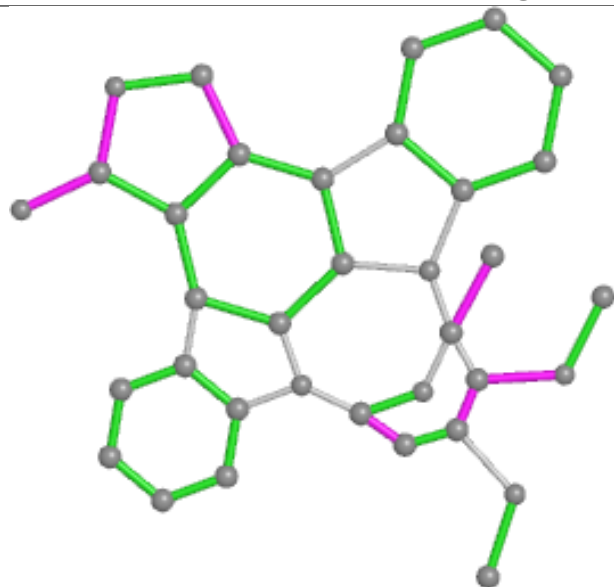
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	R93	2	0
5	A	602	STU	3	0

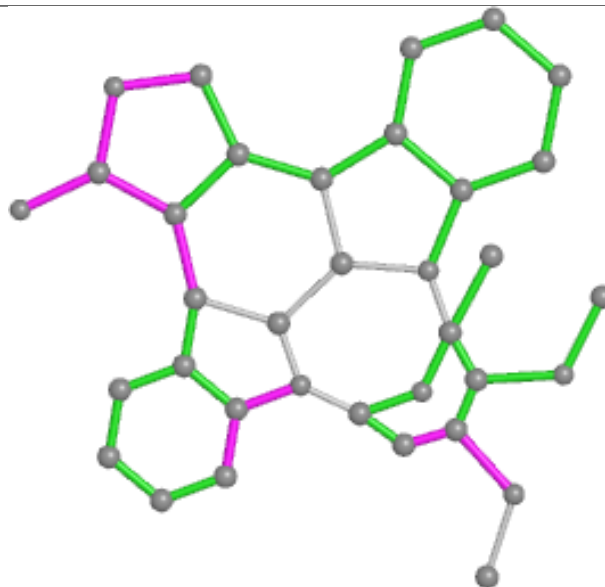
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



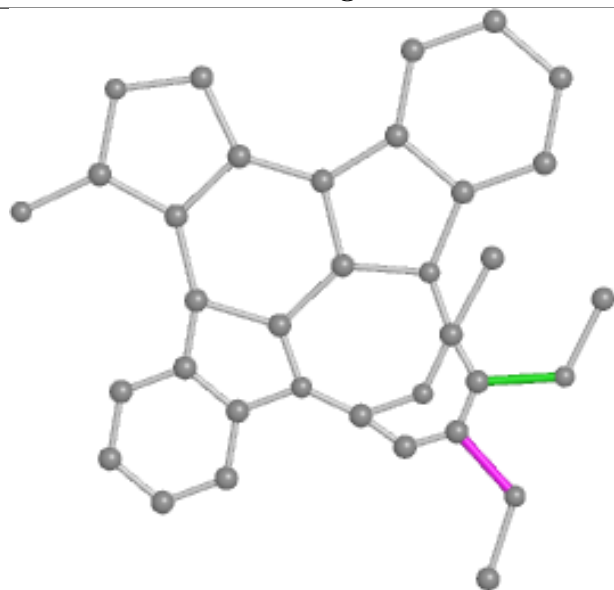
Ligand STU A 602



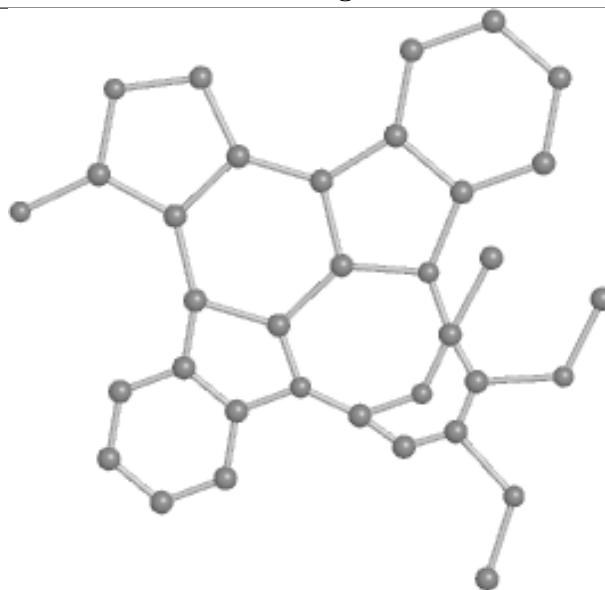
Bond lengths



Bond angles

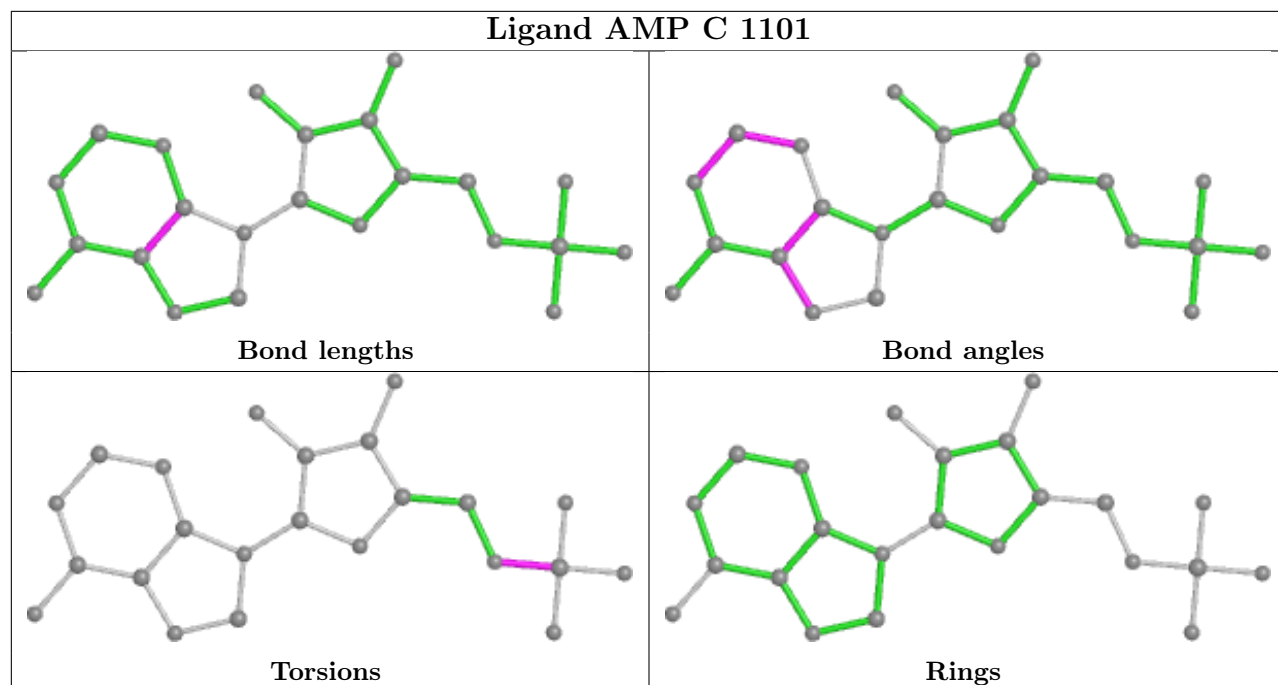


Torsions

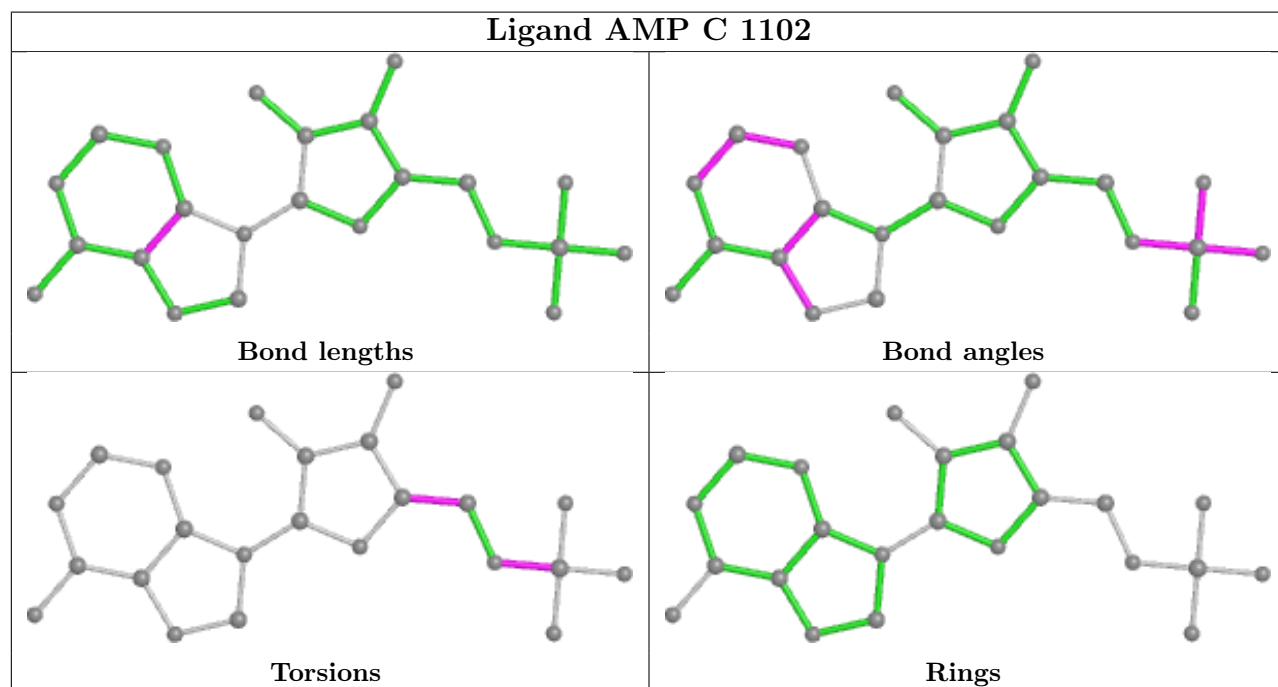


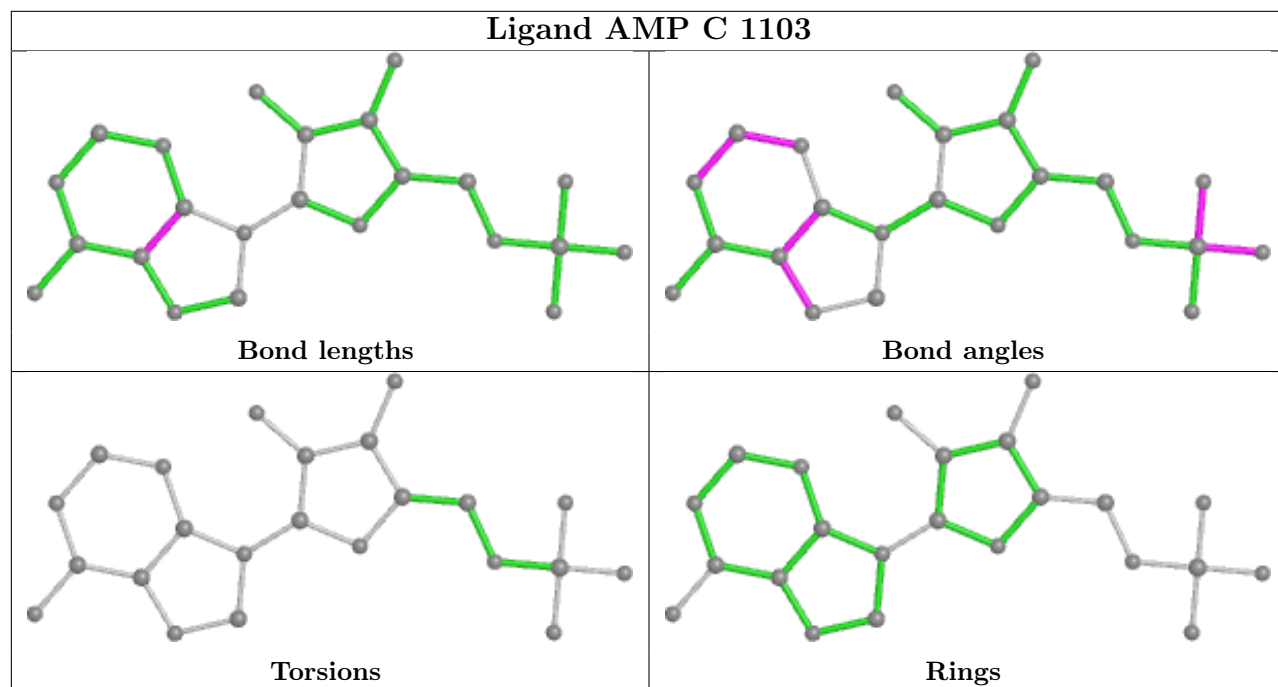
Rings

Ligand AMP C 1101



Ligand AMP C 1102





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	385/494 (77%)	0.22	28 (7%)	15 13	36, 68, 157, 242	0
2	B	177/204 (86%)	0.65	22 (12%)	4 3	45, 84, 160, 191	0
3	C	300/331 (90%)	0.08	9 (3%)	50 50	56, 93, 143, 182	0
All	All	862/1029 (83%)	0.26	59 (6%)	17 15	36, 83, 154, 242	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	222	SER	10.9
2	B	221	ILE	9.6
2	B	220	GLY	8.5
2	B	219	THR	8.5
2	B	76	GLN	7.6

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	TPO	A	174	11/12	0.89	0.19	43,57,115,153	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

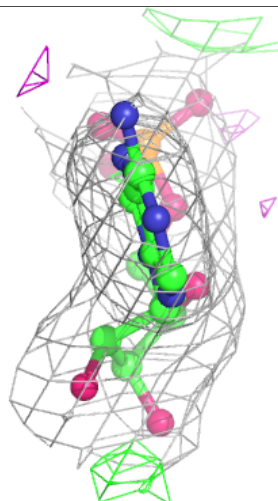
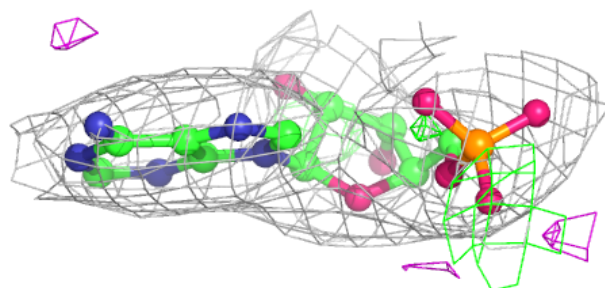
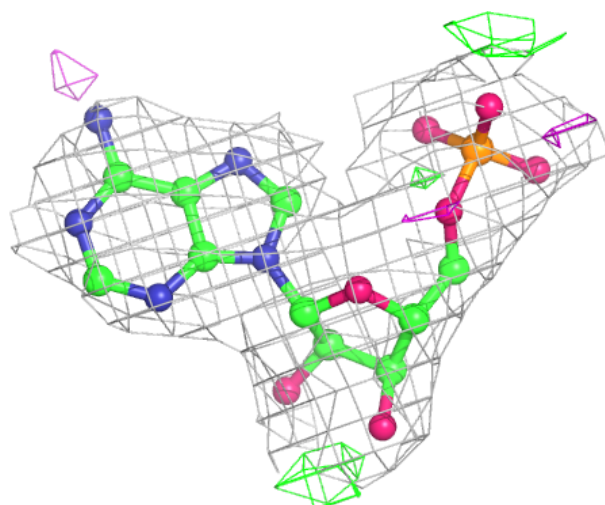
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	AMP	C	1102	23/23	0.92	0.17	65,85,117,131	0
6	AMP	C	1103	23/23	0.95	0.15	72,94,104,117	0
6	AMP	C	1101	23/23	0.96	0.16	80,112,118,121	0
4	R93	A	601	35/35	0.96	0.17	35,54,156,177	0
5	STU	A	602	35/35	0.98	0.19	25,40,45,56	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.

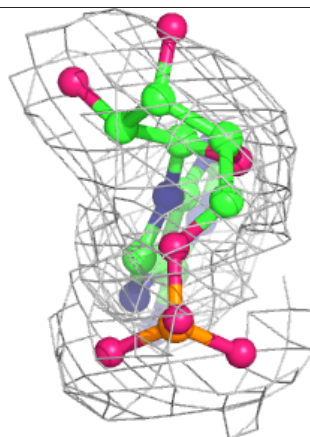
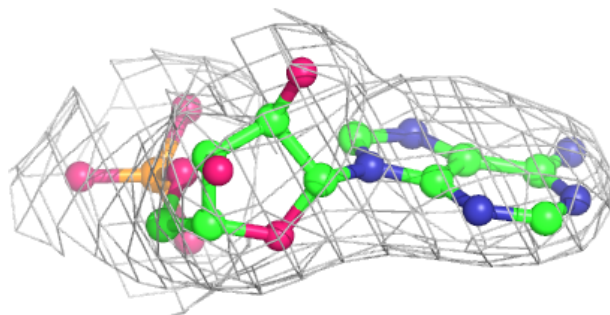
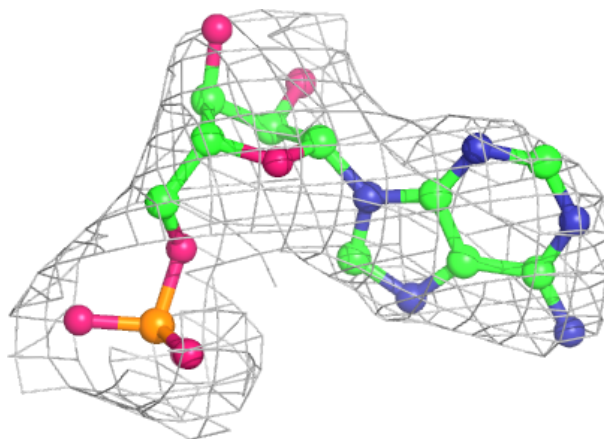
Electron density around AMP C 1102:

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



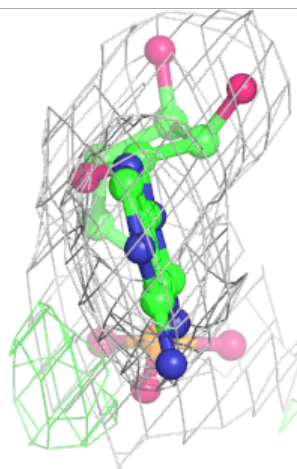
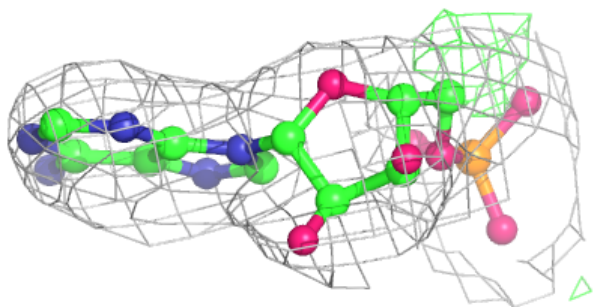
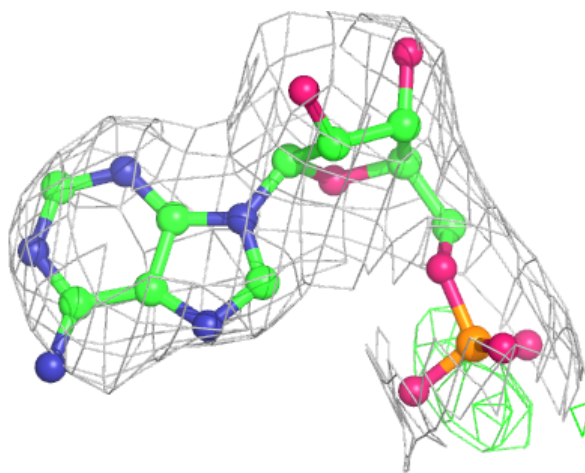
Electron density around AMP C 1103:

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



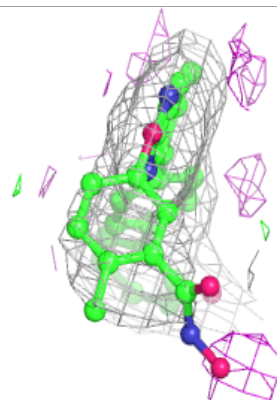
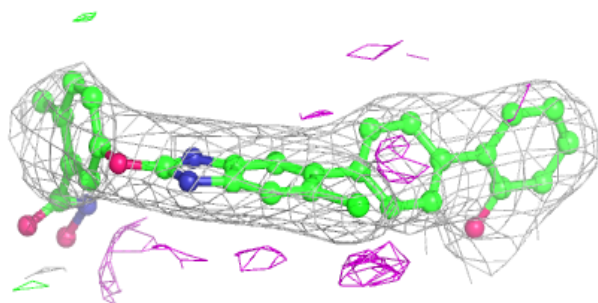
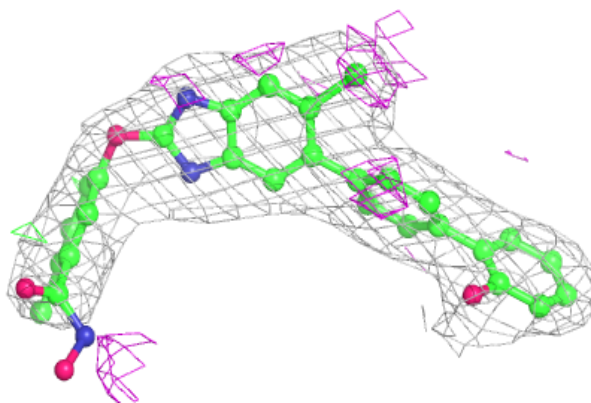
Electron density around AMP C 1101:

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



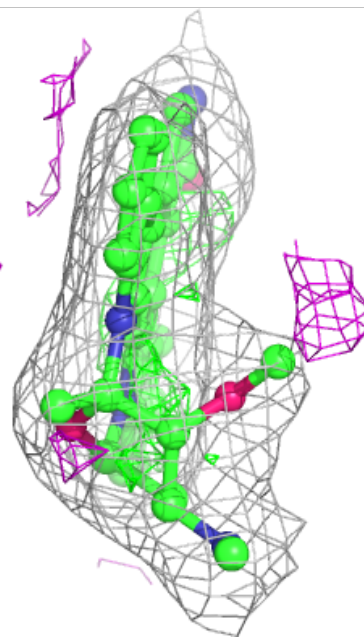
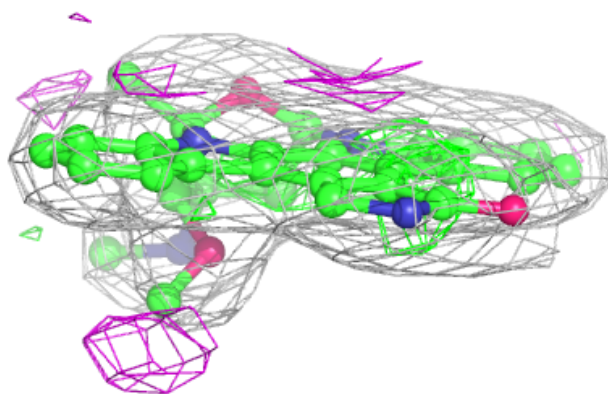
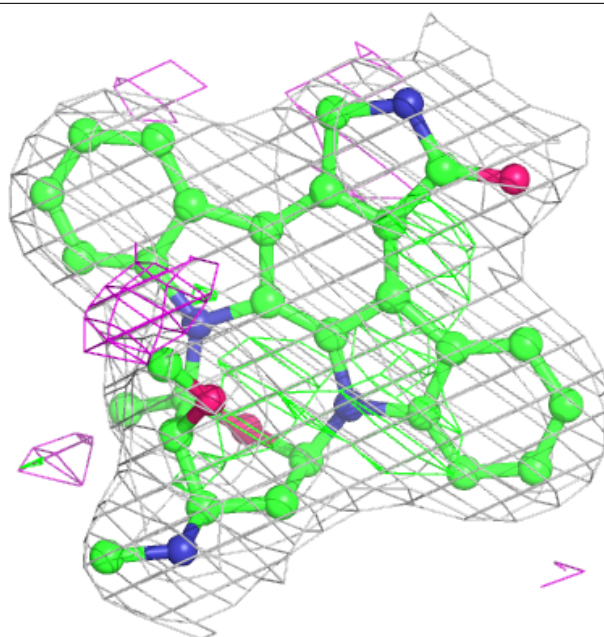
Electron density around R93 A 601:

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



Electron density around STU A 602:

$2mF_o-DF_c$ (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.