Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2021 – 10:08 AM EDT

PDB ID	:	7L29
Title	:	Crystal structure of the catalytic domain of human PDE3A bound to AMP
Authors	:	Horner, S.W.; Garvie, C.
Deposited on	:	2020-12-16
Resolution	:	2.08 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 following versions of software and data (see references ⓘ) were used in the production of this report:

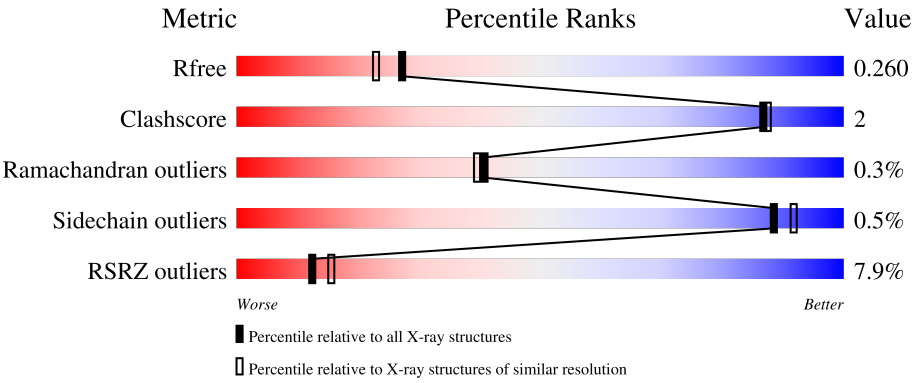
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 <=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	380	7% 91% 5% .
1	B	380	11% 92% 5% .
1	C	380	7% 93% . . .
1	D	380	7% 93% . .

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12288 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 cGMP-inhibited 3',5'-cyclic phosphodiesterase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	1	0
			2956	1906	495	536	19			
1	B	369	Total	C	N	O	S	0	1	0
			2986	1922	502	543	19			
1	C	368	Total	C	N	O	S	0	1	0
			2977	1916	500	542	19			
1	D	370	Total	C	N	O	S	0	1	0
			2979	1918	500	542	19			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	GLY	-	expression tag	UNP Q14432
A	780	GLY	-	linker	UNP Q14432
A	796	GLY	-	linker	UNP Q14432
A	797	SER	-	linker	UNP Q14432
A	798	GLY	-	linker	UNP Q14432
A	799	GLY	-	linker	UNP Q14432
A	800	SER	-	linker	UNP Q14432
A	1062	GLY	-	linker	UNP Q14432
A	1063	GLY	-	linker	UNP Q14432
A	1064	SER	-	linker	UNP Q14432
A	1065	GLY	-	linker	UNP Q14432
A	1066	GLY	-	linker	UNP Q14432
A	1067	SER	-	linker	UNP Q14432
B	668	GLY	-	expression tag	UNP Q14432
B	780	GLY	-	linker	UNP Q14432
B	796	GLY	-	linker	UNP Q14432
B	797	SER	-	linker	UNP Q14432
B	798	GLY	-	linker	UNP Q14432
B	799	GLY	-	linker	UNP Q14432
B	800	SER	-	linker	UNP Q14432
B	1029	GLY	-	linker	UNP Q14432

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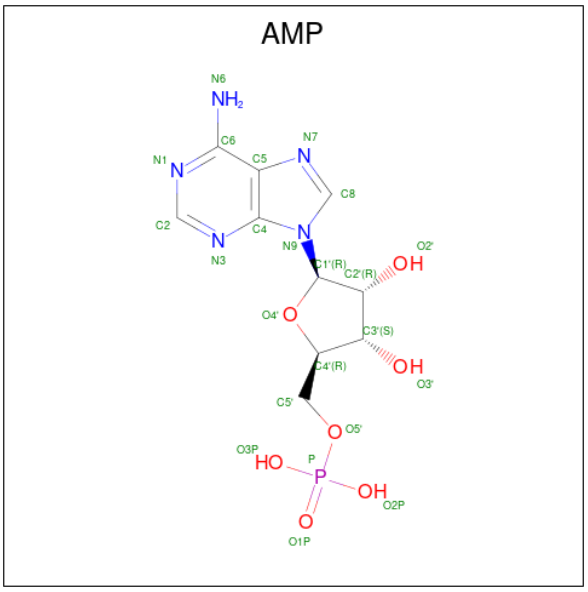
Chain	Residue	Modelled	Actual	Comment	Reference
B	1063	GLY	-	linker	UNP Q14432
B	1064	SER	-	linker	UNP Q14432
B	1065	GLY	-	linker	UNP Q14432
B	1066	GLY	-	linker	UNP Q14432
B	1067	SER	-	linker	UNP Q14432
C	668	GLY	-	expression tag	UNP Q14432
C	795	GLY	-	linker	UNP Q14432
C	796	GLY	-	linker	UNP Q14432
C	797	SER	-	linker	UNP Q14432
C	798	GLY	-	linker	UNP Q14432
C	799	GLY	-	linker	UNP Q14432
C	800	SER	-	linker	UNP Q14432
C	1029	GLY	-	linker	UNP Q14432
C	1063	GLY	-	linker	UNP Q14432
C	1064	SER	-	linker	UNP Q14432
C	1065	GLY	-	linker	UNP Q14432
C	1066	GLY	-	linker	UNP Q14432
C	1067	SER	-	linker	UNP Q14432
D	668	GLY	-	expression tag	UNP Q14432
D	780	GLY	-	linker	UNP Q14432
D	781	GLY	-	linker	UNP Q14432
D	782	SER	-	linker	UNP Q14432
D	783	GLY	-	linker	UNP Q14432
D	784	GLY	-	linker	UNP Q14432
D	785	SER	-	linker	UNP Q14432
D	1062	GLY	-	linker	UNP Q14432
D	1063	GLY	-	linker	UNP Q14432
D	1064	SER	-	linker	UNP Q14432
D	1065	GLY	-	linker	UNP Q14432
D	1066	GLY	-	linker	UNP Q14432
D	1067	SER	-	linker	UNP Q14432

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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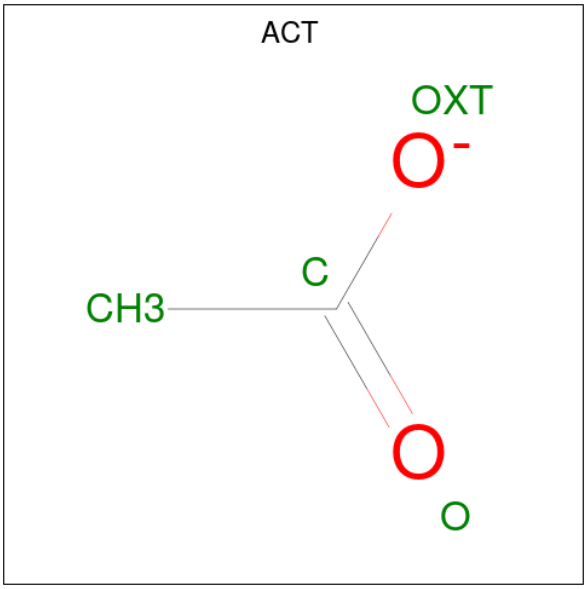
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

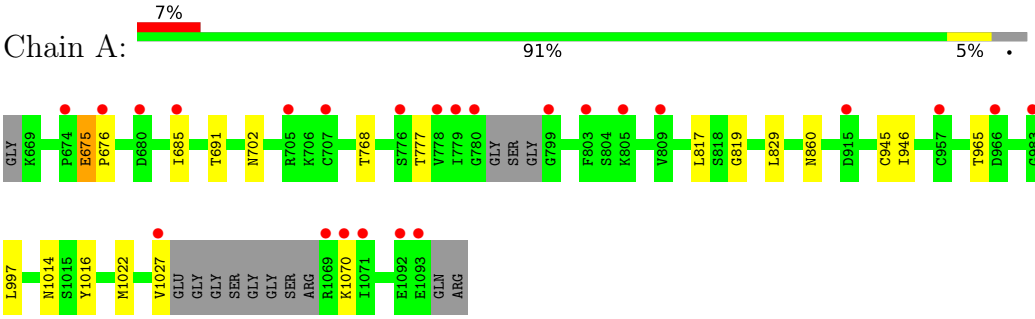
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	61	Total O 61 61	0	0
7	B	60	Total O 60 60	0	0
7	C	72	Total O 72 72	0	0
7	D	80	Total O 80 80	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

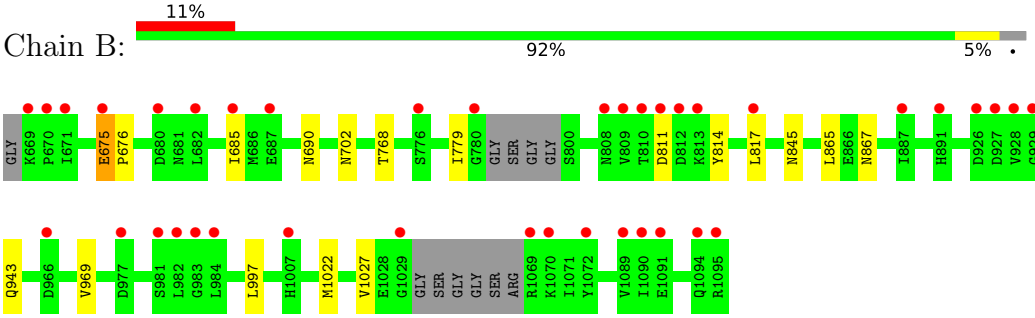
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A

Chain A:



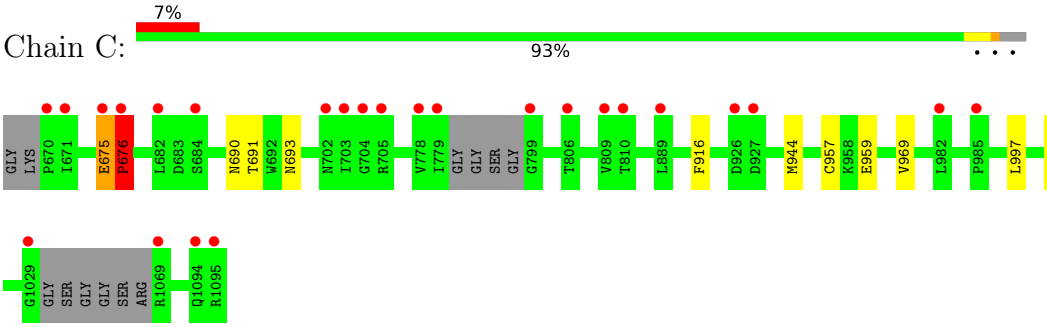
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A

Chain B:



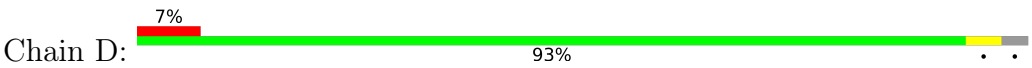
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A

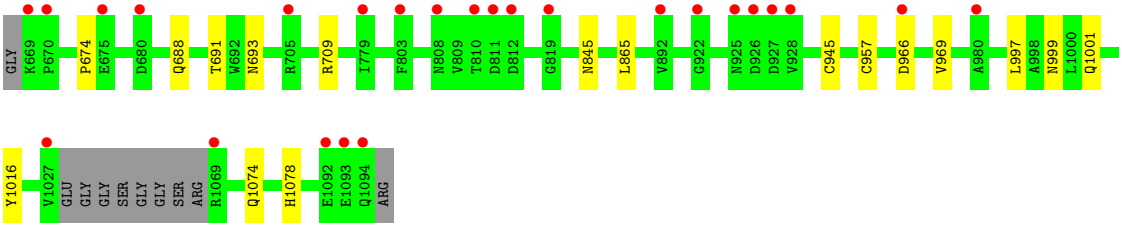
Chain C:



• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A

Chain D:




GLY
K669
P670
P674
E675
D680
Q688
T691
W692
N693
R705
R709
I779
F803
N808
V809
T810
D811
D812
G819
N845
L865
V892
G922
N925
D926
D927
Y928
C945
C957
D966
V969
A980
L997
A998
N999
L1000
Q1001
Y1016
V1027
GLU
GLY
GLY
SER
GLY
GLY
SER
ARG
R1069
Q1074
H1078
E1092
E1093
Q1094
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.42Å 58.78Å 157.00Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	47.90 – 2.08 47.86 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.90-2.08) 99.5 (47.86-2.08)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.253 0.242 , 0.260	Depositor DCC
R_{free} test set	4207 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12288	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, CA, ACT, AMP, MG

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	0.54	0/3038	0.70	1/4125 (0.0%)
1	B	0.56	0/3068	0.70	1/4163 (0.0%)
1	C	0.63	2/3059 (0.1%)	0.77	3/4151 (0.1%)
1	D	0.59	0/3062	0.70	0/4158
All	All	0.58	2/12227 (0.0%)	0.72	5/16597 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	676	PRO	N-CD	-11.84	1.31	1.47
1	C	691	THR	C-N	5.74	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	675	GLU	C-N-CD	-15.90	85.62	120.60
1	C	676	PRO	CA-N-CD	6.40	120.66	111.70
1	A	1022	MET	CG-SD-CE	-5.57	91.30	100.20
1	C	1022	MET	CG-SD-CE	5.25	108.60	100.20
1	B	1022	MET	CG-SD-CE	-5.05	92.12	100.20

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	2956	0	2883	11	0
1	B	2986	0	2910	12	0
1	C	2977	0	2898	13	0
1	D	2979	0	2903	13	0
2	A	23	0	12	0	0
2	B	23	0	12	1	0
2	C	23	0	12	0	0
2	D	23	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
6	C	4	0	3	0	0
6	D	4	0	3	0	0
7	A	61	0	0	0	0
7	B	60	0	0	1	0
7	C	72	0	0	0	0
7	D	80	0	0	0	0
All	All	12288	0	11654	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (49) 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)
2:B:1101:AMP:O2P	7:B:1201:HOH:O	1.68	1.12
1:D:688:GLN:O	1:D:691:THR:HG22	1.52	1.06
1:A:685:ILE:HD12	1:A:702:ASN:HD22	1.23	1.04
1:C:675:GLU:CB	1:C:676:PRO:HD2	1.93	0.96
1:C:675:GLU:HB2	1:C:676:PRO:HD2	1.46	0.96
1:D:845:ASN:HD21	1:D:865:LEU:H	1.15	0.90
1:B:845:ASN:HD21	1:B:865:LEU:H	1.13	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:GLU:CB	1:C:676:PRO:CD	2.55	0.85
1:A:675:GLU:HB3	1:A:676:PRO:HD2	1.63	0.78
1:A:685:ILE:HD12	1:A:702:ASN:ND2	1.99	0.78
1:D:1001:GLN:HE22	2:D:1101:AMP:HN62	1.32	0.77
1:C:916:PHE:HB3	1:C:944:MET:HE1	1.67	0.76
1:A:860:ASN:HD22	1:B:867:ASN:HD22	1.39	0.71
1:B:675:GLU:HB3	1:B:676:PRO:HD2	1.73	0.69
1:C:1017:ASP:HA	1:C:1022:MET:HG2	1.74	0.68
1:A:777:THR:HG23	1:A:819:GLY:HA3	1.77	0.67
1:C:916:PHE:HB3	1:C:944:MET:CE	2.24	0.66
1:B:969:VAL:HG11	1:B:997:LEU:HD13	1.78	0.65
1:B:969:VAL:HG11	1:B:997:LEU:CD1	2.32	0.59
1:B:845:ASN:ND2	1:B:865:LEU:H	1.94	0.56
1:D:845:ASN:ND2	1:D:865:LEU:H	1.96	0.54
1:B:811:ASP:HB3	1:B:814:TYR:HB2	1.90	0.53
1:D:674:PRO:HG2	1:D:709:ARG:HD3	1.91	0.52
1:C:675:GLU:HB3	1:C:676:PRO:HD3	1.92	0.51
1:A:965:THR:CG2	1:A:997:LEU:HD11	2.40	0.51
1:A:675:GLU:HB3	1:A:676:PRO:CD	2.40	0.51
1:C:675:GLU:CB	1:C:676:PRO:HD3	2.40	0.50
1:C:1016:TYR:HD2	1:C:1022:MET:SD	2.35	0.49
1:D:1074:GLN:HE21	1:D:1078:HIS:HE1	1.59	0.49
1:B:675:GLU:HB3	1:B:676:PRO:CD	2.42	0.49
1:D:969:VAL:HG11	1:D:997:LEU:HD13	1.96	0.48
1:A:1027:VAL:HG23	1:A:1070:LYS:HG3	1.94	0.48
1:C:957:CYS:SG	1:C:959:GLU:OE1	2.72	0.47
1:D:1001:GLN:HE22	2:D:1101:AMP:N6	2.07	0.47
1:D:999:ASN:H	1:D:999:ASN:HD22	1.61	0.46
1:B:1027:VAL:O	1:B:1027:VAL:CG2	2.63	0.46
1:C:959:GLU:H	1:C:959:GLU:CD	2.21	0.44
1:D:945[B]:CYS:HG	1:D:1016:TYR:HH	1.66	0.43
1:C:693:ASN:ND2	1:C:957:CYS:H	2.16	0.42
1:A:829:LEU:HD11	1:A:946:ILE:HB	2.01	0.42
1:D:969:VAL:HG11	1:D:997:LEU:CD1	2.48	0.42
1:C:969:VAL:HG11	1:C:997:LEU:CD1	2.50	0.42
1:B:768:THR:HA	1:B:817:LEU:HB2	2.01	0.41
1:B:779:ILE:N	1:B:779:ILE:HD12	2.36	0.41
1:A:768:THR:HA	1:A:817:LEU:HB2	2.03	0.41
1:D:693:ASN:ND2	1:D:957:CYS:H	2.19	0.41
1:D:1074:GLN:HE21	1:D:1078:HIS:CE1	2.38	0.41
1:A:945[B]:CYS:HG	1:A:1016:TYR:HH	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:LEU:HA	1:B:943:GLN:HE21	1.86	0.40

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	361/380 (95%)	351 (97%)	9 (2%)	1 (0%)	41	39
1	B	364/380 (96%)	355 (98%)	8 (2%)	1 (0%)	41	39
1	C	363/380 (96%)	351 (97%)	10 (3%)	2 (1%)	25	20
1	D	367/380 (97%)	359 (98%)	8 (2%)	0	100	100
All	All	1455/1520 (96%)	1416 (97%)	35 (2%)	4 (0%)	41	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	676	PRO
1	A	675	GLU
1	B	675	GLU
1	C	690	ASN

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	321/327 (98%)	319 (99%)	2 (1%)	86 89
1	B	324/327 (99%)	321 (99%)	3 (1%)	78 83
1	C	323/327 (99%)	323 (100%)	0	100 100
1	D	323/327 (99%)	322 (100%)	1 (0%)	92 95
All	All	1291/1308 (99%)	1285 (100%)	6 (0%)	88 92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	691	THR
1	A	1014	ASN
1	B	685	ILE
1	B	690	ASN
1	B	702	ASN
1	D	966	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	702	ASN
1	A	896	HIS
1	A	1014	ASN
1	B	702	ASN
1	B	762	HIS
1	B	845	ASN
1	B	860	ASN
1	B	867	ASN
1	B	888	ASN
1	B	925	ASN
1	B	943	GLN
1	B	996	GLN
1	C	693	ASN
1	C	860	ASN
1	C	867	ASN
1	C	888	ASN
1	C	896	HIS
1	D	693	ASN
1	D	845	ASN
1	D	860	ASN
1	D	867	ASN

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Mol	Chain	Res	Type
1	D	888	ASN
1	D	925	ASN
1	D	999	ASN
1	D	1001	GLN
1	D	1078	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	ACT	A	1105	-	1,3,3	4.02	1 (100%)	0,3,3	0.00	-
2	AMP	D	1101	4,3	22,25,25	0.70	0	25,38,38	1.05	1 (4%)
2	AMP	C	1101	4,3	22,25,25	0.79	0	25,38,38	1.25	3 (12%)
2	AMP	A	1101	4,3	22,25,25	0.68	0	25,38,38	0.77	1 (4%)
6	ACT	B	1104	-	1,3,3	3.82	1 (100%)	0,3,3	0.00	-
2	AMP	B	1101	4,3	22,25,25	0.67	0	25,38,38	0.81	1 (4%)
6	ACT	C	1104	-	1,3,3	3.51	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ACT	D	1104	-	1,3,3	3.18	1 (100%)	0,3,3	0.00	-

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
2	AMP	A	1101	4,3	-	4/6/26/26	0/3/3/3
2	AMP	D	1101	4,3	-	1/6/26/26	0/3/3/3
2	AMP	C	1101	4,3	-	3/6/26/26	0/3/3/3
2	AMP	B	1101	4,3	-	1/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1105	ACT	CH3-C	4.02	1.53	1.48
6	B	1104	ACT	CH3-C	3.82	1.53	1.48
6	C	1104	ACT	CH3-C	3.51	1.53	1.48
6	D	1104	ACT	CH3-C	3.18	1.52	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1101	AMP	O3P-P-O5'	-3.15	98.34	106.73
2	C	1101	AMP	C5-C6-N6	2.41	124.02	120.35
2	B	1101	AMP	C5-C6-N6	2.41	124.01	120.35
2	C	1101	AMP	O4'-C4'-C3'	-2.35	100.47	105.11
2	D	1101	AMP	C5-C6-N6	2.28	123.82	120.35
2	A	1101	AMP	C5-C6-N6	2.24	123.76	120.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	AMP	C5'-O5'-P-O1P
2	A	1101	AMP	C5'-O5'-P-O2P
2	A	1101	AMP	C5'-O5'-P-O3P
2	C	1101	AMP	C5'-O5'-P-O2P
2	C	1101	AMP	C5'-O5'-P-O3P

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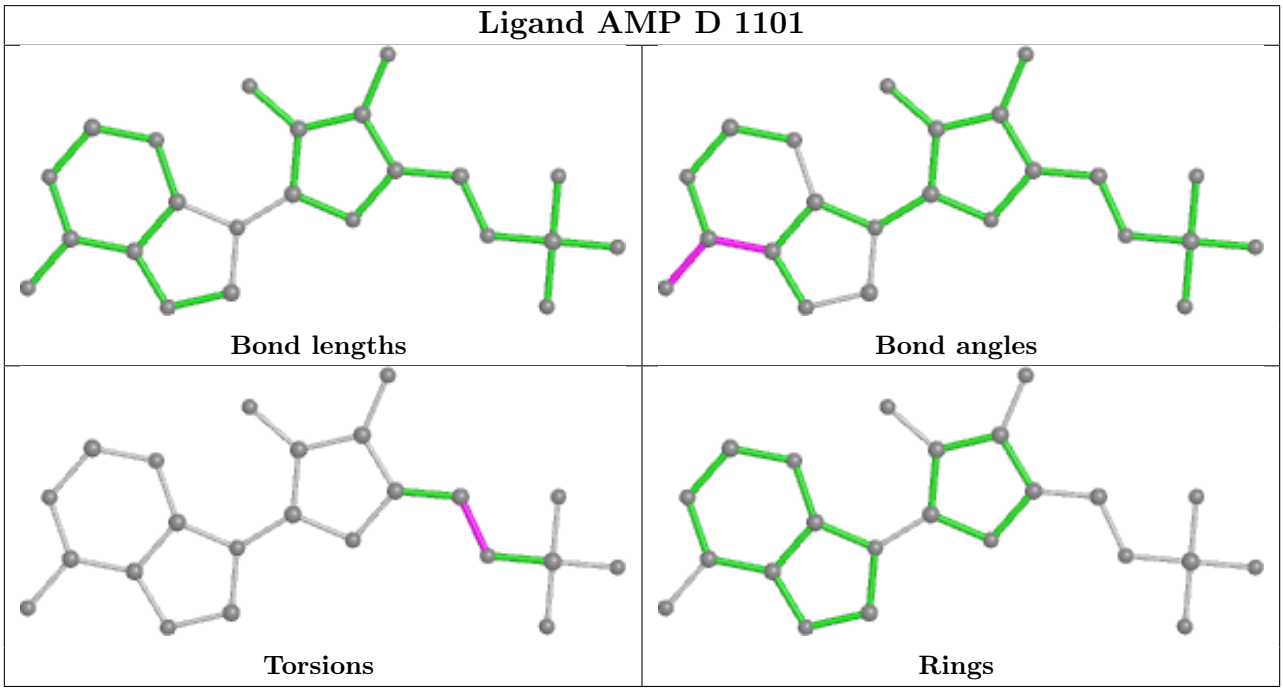
Mol	Chain	Res	Type	Atoms
2	B	1101	AMP	C4'-C5'-O5'-P
2	C	1101	AMP	C4'-C5'-O5'-P
2	D	1101	AMP	C4'-C5'-O5'-P
2	A	1101	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

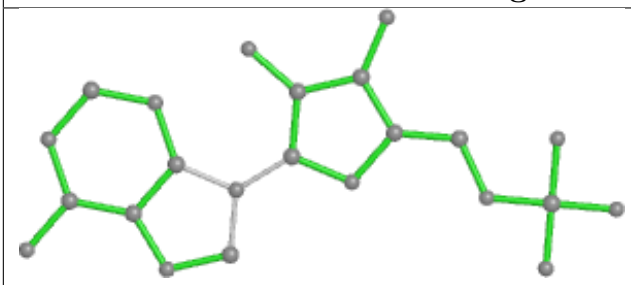
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1101	AMP	2	0
2	B	1101	AMP	1	0

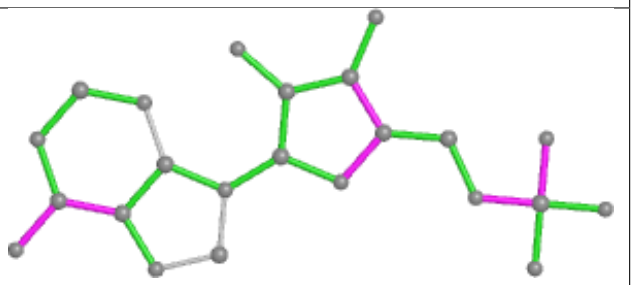
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



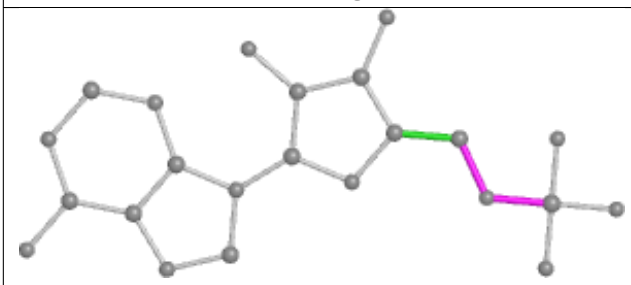
Ligand AMP C 1101



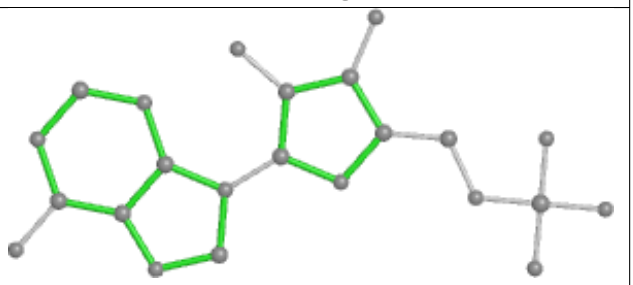
Bond lengths



Bond angles

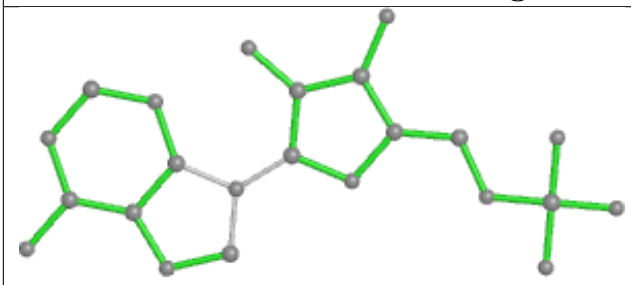


Torsions

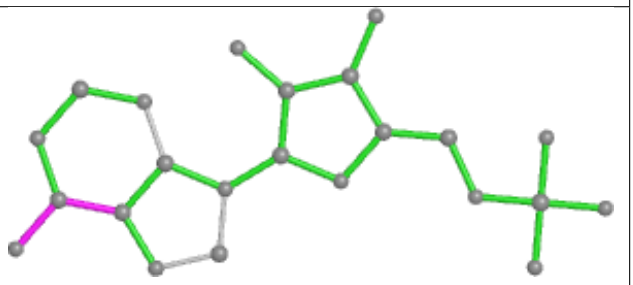


Rings

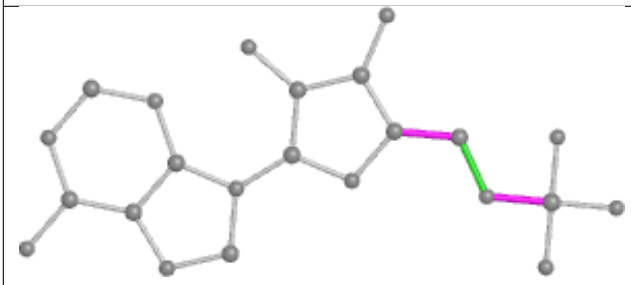
Ligand AMP A 1101



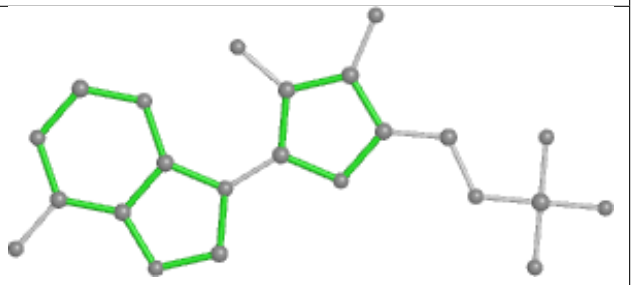
Bond lengths



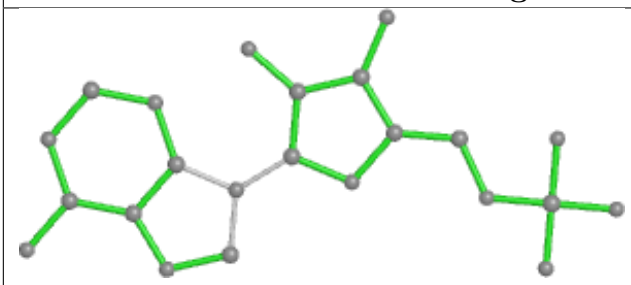
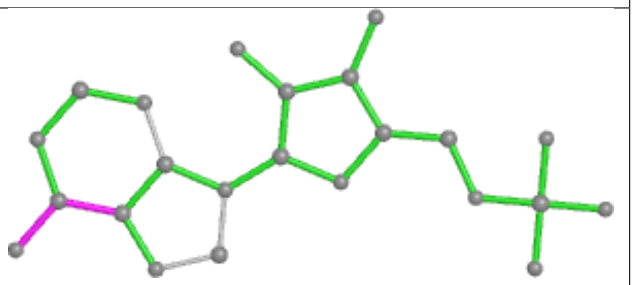
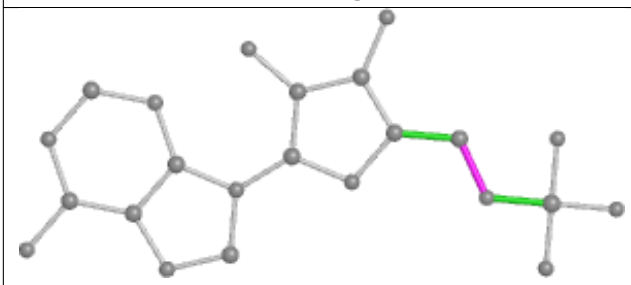
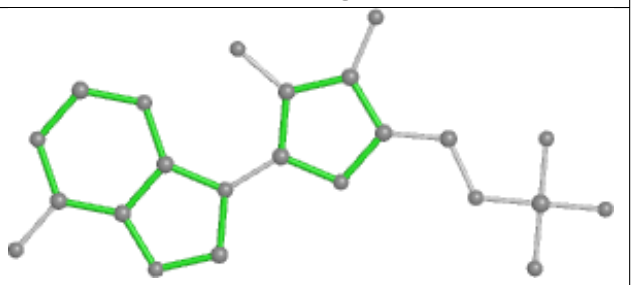
Bond angles



Torsions



Rings

Ligand AMP B 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	366/380 (96%)	0.69	26 (7%) 16 19	42, 80, 132, 175	0
1	B	369/380 (97%)	0.77	40 (10%) 5 7	42, 77, 136, 187	0
1	C	368/380 (96%)	0.69	25 (6%) 17 21	41, 73, 133, 206	0
1	D	370/380 (97%)	0.66	25 (6%) 17 21	38, 71, 124, 158	0
All	All	1473/1520 (96%)	0.70	116 (7%) 12 15	38, 75, 133, 206	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	928	VAL	12.1
1	B	811	ASP	11.2
1	A	779	ILE	10.1
1	C	779	ILE	10.0
1	C	1094	GLN	9.8
1	B	669	LYS	8.9
1	C	810	THR	7.9
1	D	927	ASP	7.5
1	B	929	GLY	7.4
1	A	705	ARG	7.2
1	C	675	GLU	6.9
1	C	1095	ARG	6.9
1	B	927	ASP	6.9
1	D	1094	GLN	6.8
1	B	680	ASP	6.6
1	C	705	ARG	6.3
1	B	982	LEU	5.8
1	B	670	PRO	5.6
1	B	808	ASN	5.3
1	A	1027	VAL	5.0
1	D	1069	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1069	ARG	4.7
1	D	669	LYS	4.6
1	A	707	CYS	4.5
1	B	809	VAL	4.4
1	D	812	ASP	4.3
1	B	810	THR	4.3
1	D	811	ASP	4.2
1	A	984	LEU	4.2
1	B	926	ASP	4.1
1	B	1029	GLY	4.1
1	B	1090	ILE	4.1
1	D	675	GLU	4.0
1	D	810	THR	4.0
1	C	670	PRO	3.9
1	A	780	GLY	3.8
1	D	1093	GLU	3.7
1	D	926	ASP	3.7
1	A	1070	LYS	3.6
1	D	803	PHE	3.5
1	C	704	GLY	3.5
1	D	1027	VAL	3.4
1	D	779	ILE	3.4
1	D	1092	GLU	3.4
1	B	1095	ARG	3.4
1	A	799	GLY	3.3
1	B	1069	ARG	3.3
1	C	926	ASP	3.2
1	A	778	VAL	3.1
1	C	778	VAL	3.1
1	D	892	VAL	3.1
1	B	780	GLY	3.0
1	D	670	PRO	3.0
1	C	684	SER	2.9
1	C	1029	GLY	2.9
1	C	809	VAL	2.9
1	A	674	PRO	2.9
1	B	966	ASP	2.9
1	C	703	ILE	2.9
1	B	812	ASP	2.8
1	B	685	ILE	2.8
1	A	1093	GLU	2.7
1	D	680	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	983	GLY	2.7
1	B	1070	LYS	2.7
1	B	984	LEU	2.7
1	A	680	ASP	2.7
1	A	1092	GLU	2.7
1	C	806	THR	2.6
1	B	928	VAL	2.6
1	A	957	CYS	2.6
1	B	675	GLU	2.6
1	B	930	ILE	2.6
1	A	676	PRO	2.6
1	A	809	VAL	2.6
1	A	986	ILE	2.5
1	B	891	HIS	2.5
1	C	682	LEU	2.5
1	C	1069	ARG	2.5
1	C	799	GLY	2.5
1	C	927	ASP	2.5
1	D	922	GLY	2.4
1	A	915	ASP	2.4
1	B	977	ASP	2.4
1	C	676	PRO	2.4
1	C	985	PRO	2.4
1	B	981	SER	2.4
1	D	705	ARG	2.4
1	B	1072	TYR	2.4
1	C	982	LEU	2.3
1	B	671	ILE	2.3
1	B	983	GLY	2.3
1	A	776	SER	2.3
1	C	671	ILE	2.3
1	B	887	ILE	2.3
1	B	1089	VAL	2.2
1	D	819	GLY	2.2
1	B	1091	GLU	2.2
1	B	813	LYS	2.2
1	A	1071	ILE	2.2
1	B	817	LEU	2.2
1	A	966	ASP	2.2
1	A	805	LYS	2.2
1	B	1007	HIS	2.2
1	C	889	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	776	SER	2.1
1	C	702	ASN	2.1
1	B	1094	GLN	2.1
1	B	687	GLU	2.1
1	A	685	ILE	2.1
1	D	808	ASN	2.1
1	D	980	ALA	2.1
1	A	803	PHE	2.1
1	D	925	ASN	2.0
1	D	966	ASP	2.0
1	B	682	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 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^{th} 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
2	AMP	A	1101	23/23	0.76	0.25	48,63,80,81	0
2	AMP	C	1101	23/23	0.79	0.30	38,61,88,103	0
2	AMP	B	1101	23/23	0.88	0.18	39,60,72,88	0
4	MG	D	1103	1/1	0.88	0.08	25,25,25,25	0
2	AMP	D	1101	23/23	0.89	0.19	38,46,71,85	0
6	ACT	B	1104	4/4	0.89	0.24	51,66,89,96	0
4	MG	C	1103	1/1	0.91	0.07	27,27,27,27	0
4	MG	A	1103	1/1	0.93	0.04	27,27,27,27	0
6	ACT	C	1104	4/4	0.93	0.21	51,63,70,81	0
6	ACT	D	1104	4/4	0.94	0.15	45,45,48,50	0
6	ACT	A	1105	4/4	0.97	0.09	57,60,71,71	0
3	MN	B	1102	1/1	0.98	0.04	33,33,33,33	0

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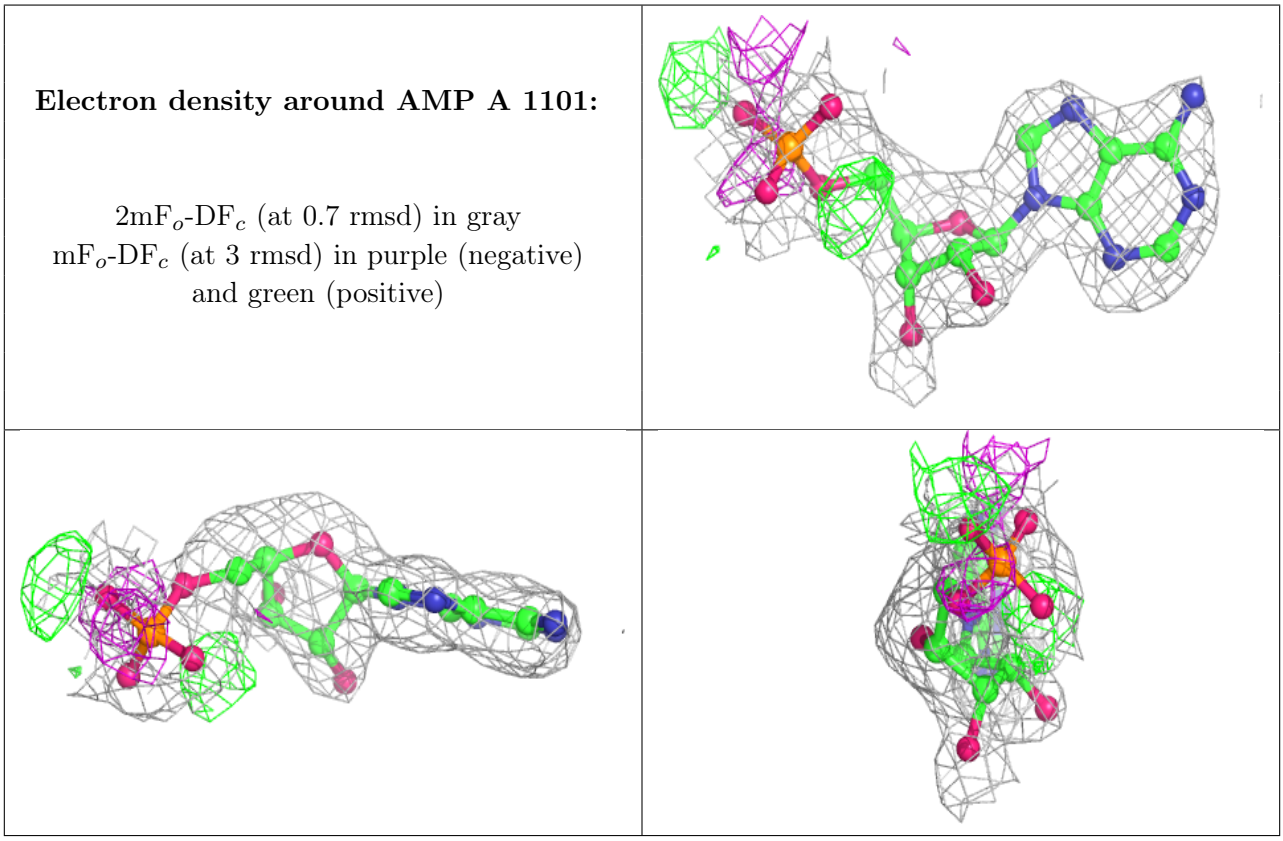
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	A	1102	1/1	0.98	0.05	34,34,34,34	0
4	MG	B	1103	1/1	0.98	0.07	27,27,27,27	0
3	MN	D	1102	1/1	0.99	0.05	29,29,29,29	0
5	CA	A	1104	1/1	0.99	0.32	30,30,30,30	0
3	MN	C	1102	1/1	0.99	0.03	33,33,33,33	0

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.

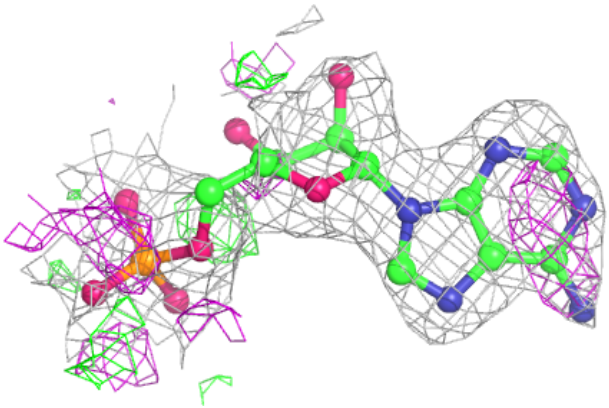
Electron density around AMP A 1101:

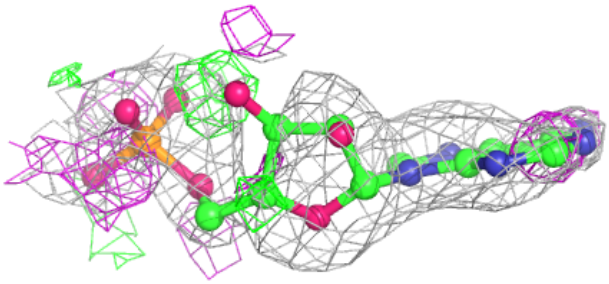
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

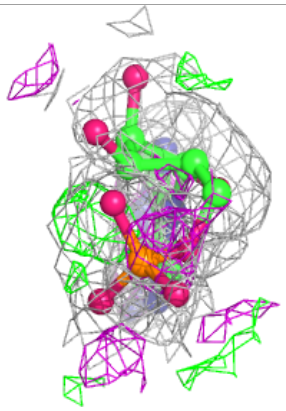


Electron density around AMP C 1101:

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

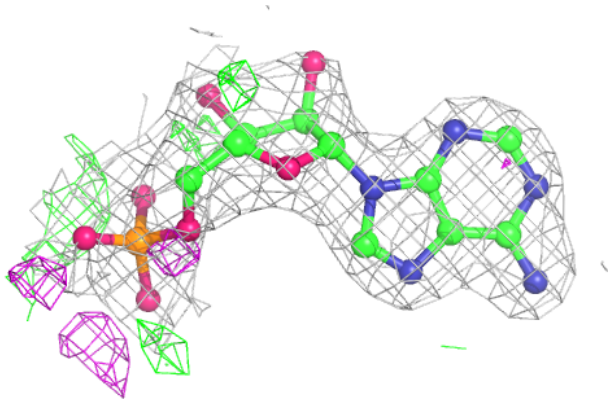


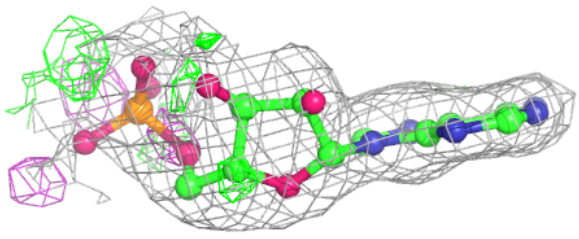


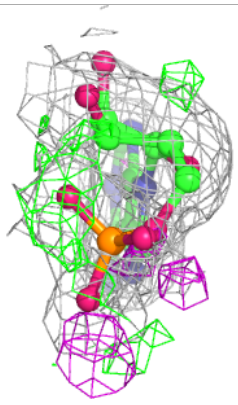


Electron density around AMP B 1101:

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

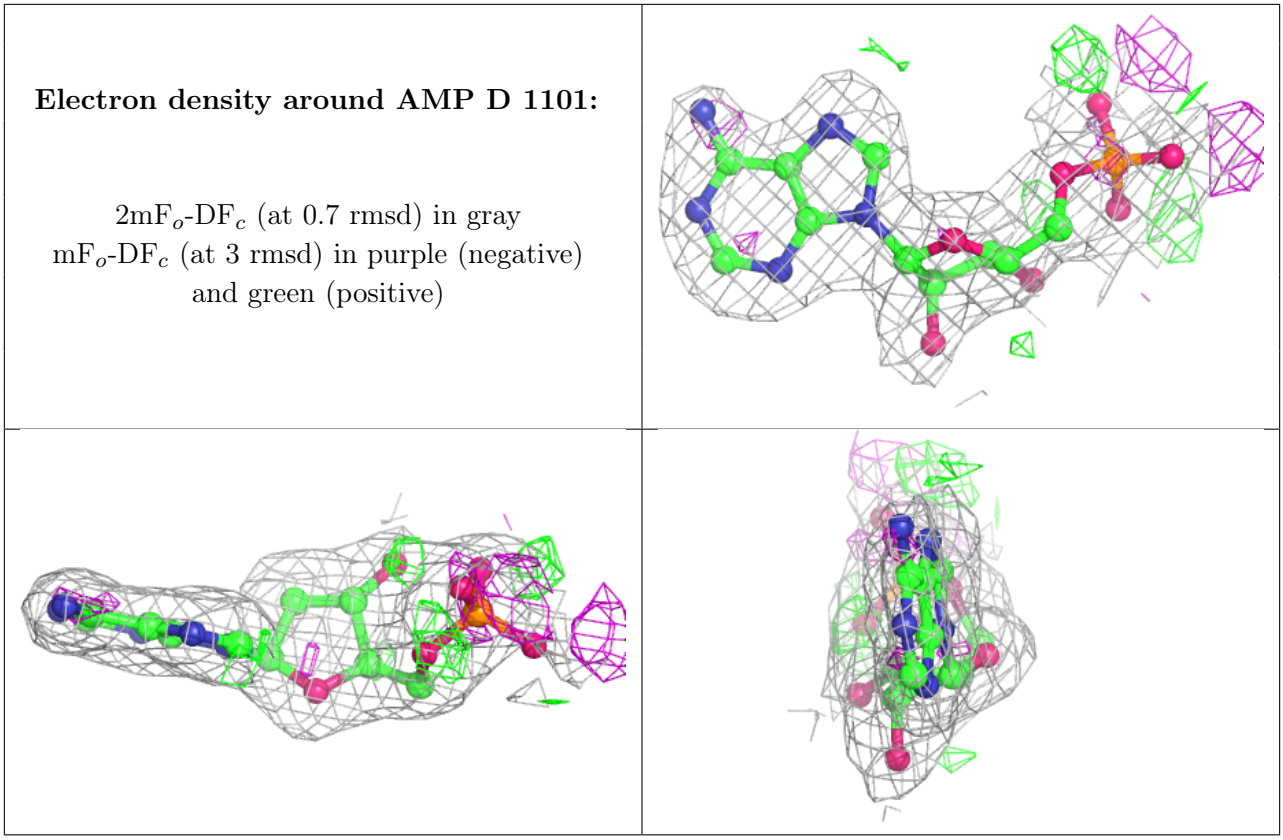






Electron density around AMP D 1101:

$2mF_o$-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.