



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:24 PM UTC

PDB ID : 7L29 / pdb_00007L29
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 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

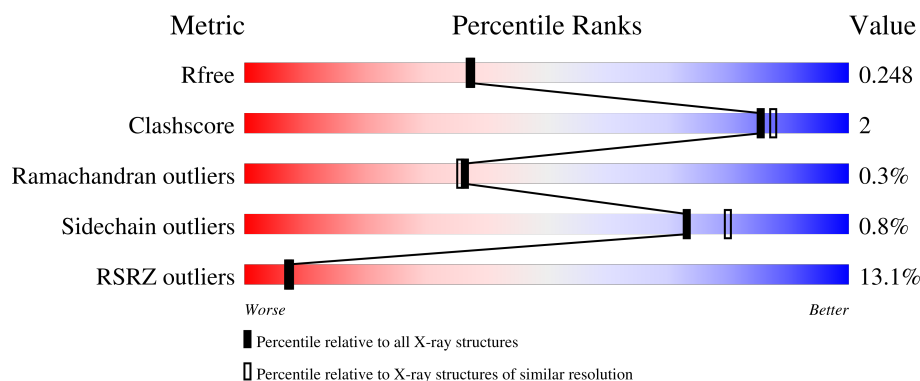
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (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 $\leq 5\%$. 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	380	
1	B	380	
1	C	380	
1	D	380	

2 Entry composition

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:

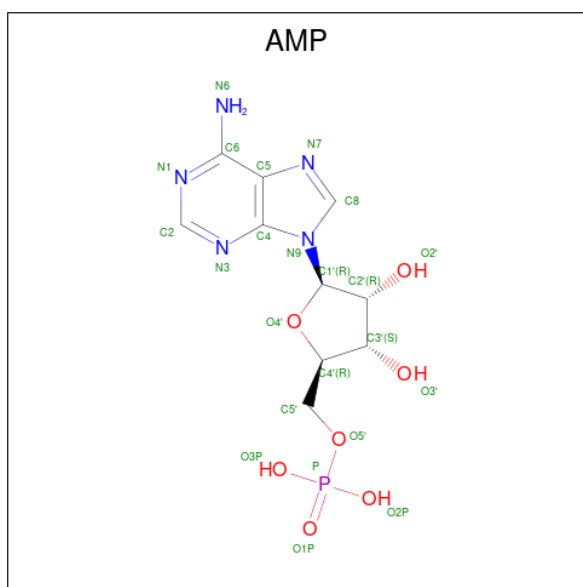
Chain	Residue	Modelled	Actual	Comment	Reference
A	668	GLY	-	expression tag	UNP Q14432
A	780	GLY	-	linker	UNP Q14432
A	796	GLY	-	linker	UNP Q14432
A	797	SER	-	linker	UNP Q14432
A	798	GLY	-	linker	UNP Q14432
A	799	GLY	-	linker	UNP Q14432
A	800	SER	-	linker	UNP Q14432
A	1062	GLY	-	linker	UNP Q14432
A	1063	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 (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

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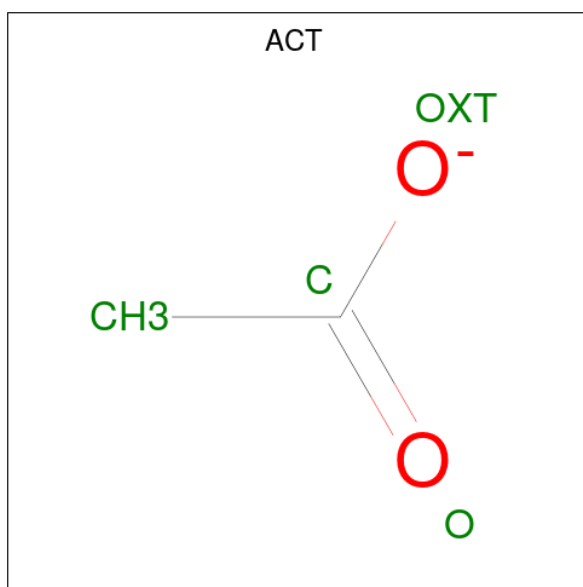
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

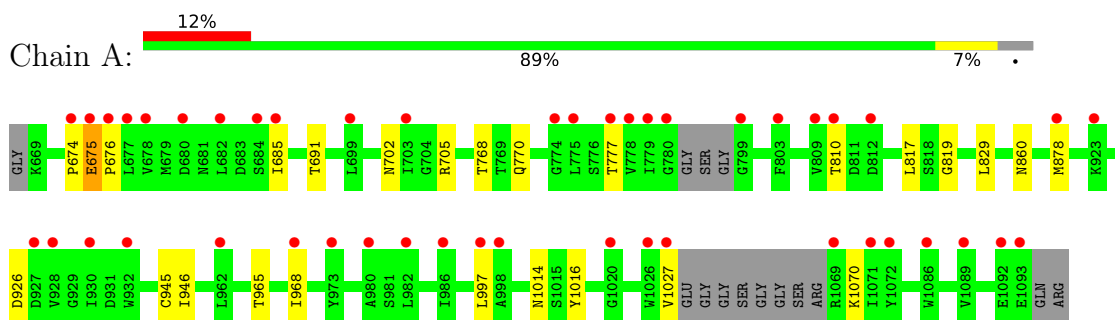
- Molecule 7 is water.

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

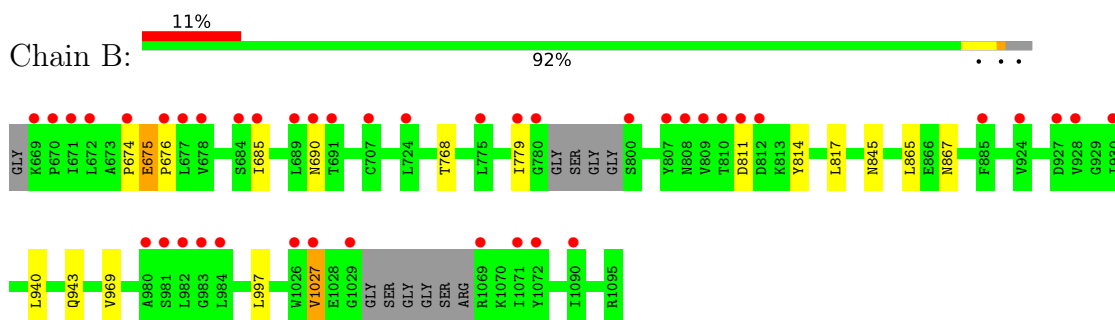
3 Residue-property plots [i](#)

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.

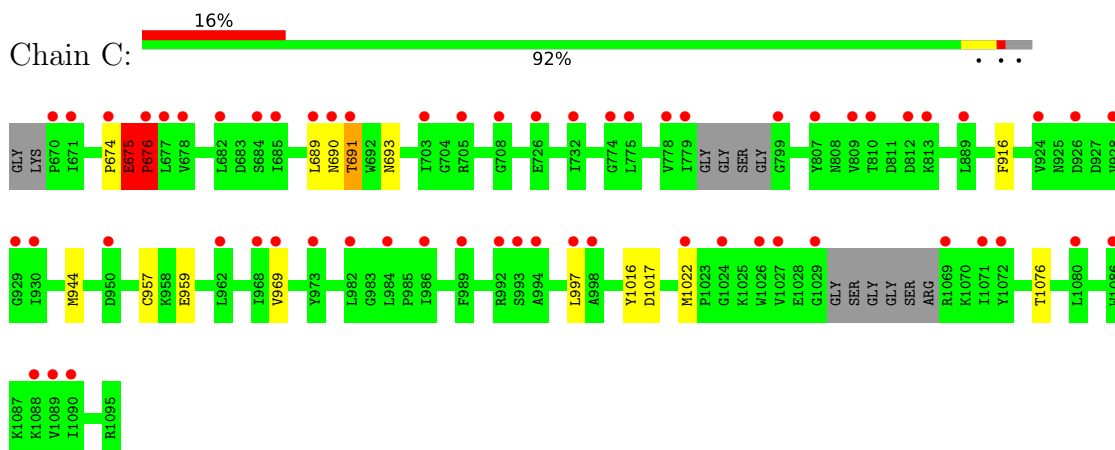
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



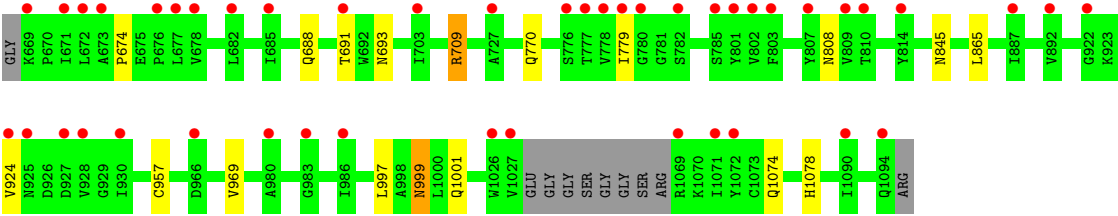
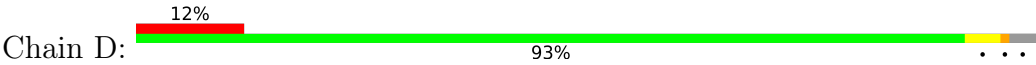
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



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



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



4 Data and refinement statistics

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 47.90 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.90-2.08) 93.3 (47.90-2.08)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.253 (Not available) , 0.248	Depositor DCC
R_{free} test set	4207 reflections (4.63%)	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)	0.33 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MN, MG, ACT, 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	0.76	0/3038	0.95	5/4125 (0.1%)
1	B	0.78	0/3068	0.97	1/4163 (0.0%)
1	C	0.84	2/3059 (0.1%)	0.99	4/4151 (0.1%)
1	D	0.81	0/3062	0.97	3/4158 (0.1%)
All	All	0.80	2/12227 (0.0%)	0.97	13/16597 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	676	PRO	N-CD	-11.77	1.31	1.47
1	C	691	THR	C-N	9.50	1.47	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	675	GLU	C-N-CD	-9.61	85.62	125.00
1	C	676	PRO	CB-CA-C	7.05	123.20	111.56
1	C	674	PRO	N-CA-C	6.94	120.94	111.22
1	D	770	GLN	CB-CA-C	6.21	118.42	109.11
1	A	674	PRO	N-CA-C	6.19	122.10	111.77
1	C	676	PRO	CA-N-CD	6.18	120.66	112.00
1	A	810	THR	N-CA-C	-6.08	105.15	113.30
1	A	770	GLN	CB-CA-C	5.58	117.48	109.11
1	A	705	ARG	N-CA-C	5.54	117.31	111.28
1	A	926	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	808	ASN	N-CA-C	-5.43	107.20	113.88
1	D	924	VAL	N-CA-C	-5.39	107.17	111.81
1	B	674	PRO	N-CA-C	5.25	120.44	111.68

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	12	0
1	B	2986	0	2910	12	0
1	C	2977	0	2898	15	0
1	D	2979	0	2903	12	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	51	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 (51) 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
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	1.69	0.75
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:C:959:GLU:H	1:C:959:GLU:CD	2.21	0.48
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:A:945[B]:CYS:HG	1:A:1016:TYR:HH	1.59	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:A:878:MET:HE3	1:A:878:MET:HB3	1.87	0.45
1:C:689:LEU:C	1:C:691:THR:H	2.26	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1022:MET:HE2	1:C:1076:THR:HG23	2.02	0.41
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: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%)	36	36
1	B	364/380 (96%)	355 (98%)	8 (2%)	1 (0%)	36	36
1	C	363/380 (96%)	351 (97%)	10 (3%)	2 (1%)	21	17
1	D	367/380 (97%)	359 (98%)	8 (2%)	0	100	100
All	All	1455/1520 (96%)	1416 (97%)	35 (2%)	4 (0%)	36	36

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 ⓘ

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%)	318 (99%)	3 (1%)	70	77
1	B	324/327 (99%)	321 (99%)	3 (1%)	70	77
1	C	323/327 (99%)	322 (100%)	1 (0%)	86	91
1	D	323/327 (99%)	320 (99%)	3 (1%)	70	77
All	All	1291/1308 (99%)	1281 (99%)	10 (1%)	73	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	691	THR
1	A	968	ILE
1	A	1014	ASN
1	B	685	ILE
1	B	690	ASN
1	B	1027	VAL
1	C	675	GLU
1	D	709	ARG
1	D	779	ILE
1	D	999	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	702	ASN
1	A	855	GLN
1	A	860	ASN
1	A	884	ASN
1	A	891	HIS
1	A	896	HIS
1	A	963	GLN
1	A	970	ASN
1	A	1014	ASN

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Mol	Chain	Res	Type
1	B	702	ASN
1	B	762	HIS
1	B	770	GLN
1	B	808	ASN
1	B	845	ASN
1	B	867	ASN
1	B	884	ASN
1	B	888	ASN
1	B	943	GLN
1	B	963	GLN
1	B	996	GLN
1	B	999	ASN
1	C	690	ASN
1	C	770	GLN
1	C	855	GLN
1	C	867	ASN
1	C	884	ASN
1	C	888	ASN
1	C	896	HIS
1	C	970	ASN
1	D	693	ASN
1	D	808	ASN
1	D	845	ASN
1	D	855	GLN
1	D	867	ASN
1	D	884	ASN
1	D	888	ASN
1	D	891	HIS
1	D	925	ASN
1	D	963	GLN
1	D	999	ASN
1	D	1001	GLN
1	D	1078	HIS
1	D	1081	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	AMP	C	1101	4,3	25,25,25	0.59	0	37,38,38	0.97	2 (5%)
6	ACT	A	1105	-	3,3,3	1.04	0	3,3,3	0.84	0
2	AMP	B	1101	4,3	25,25,25	0.44	0	37,38,38	0.47	0
2	AMP	A	1101	4,3	25,25,25	0.40	0	37,38,38	0.47	0
6	ACT	C	1104	-	3,3,3	0.96	0	3,3,3	0.91	0
6	ACT	B	1104	-	3,3,3	0.95	0	3,3,3	0.95	0
6	ACT	D	1104	-	3,3,3	0.98	0	3,3,3	0.77	0
2	AMP	D	1101	4,3	25,25,25	0.44	0	37,38,38	0.79	0

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	C	1101	4,3	-	3/10/26/26	0/3/3/3
2	AMP	B	1101	4,3	-	1/10/26/26	0/3/3/3
2	AMP	A	1101	4,3	-	4/10/26/26	0/3/3/3
2	AMP	D	1101	4,3	-	1/10/26/26	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	AMP	O3P-P-O5'	-3.19	98.34	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	AMP	O4'-C4'-C3'	-2.36	100.47	105.15

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
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'

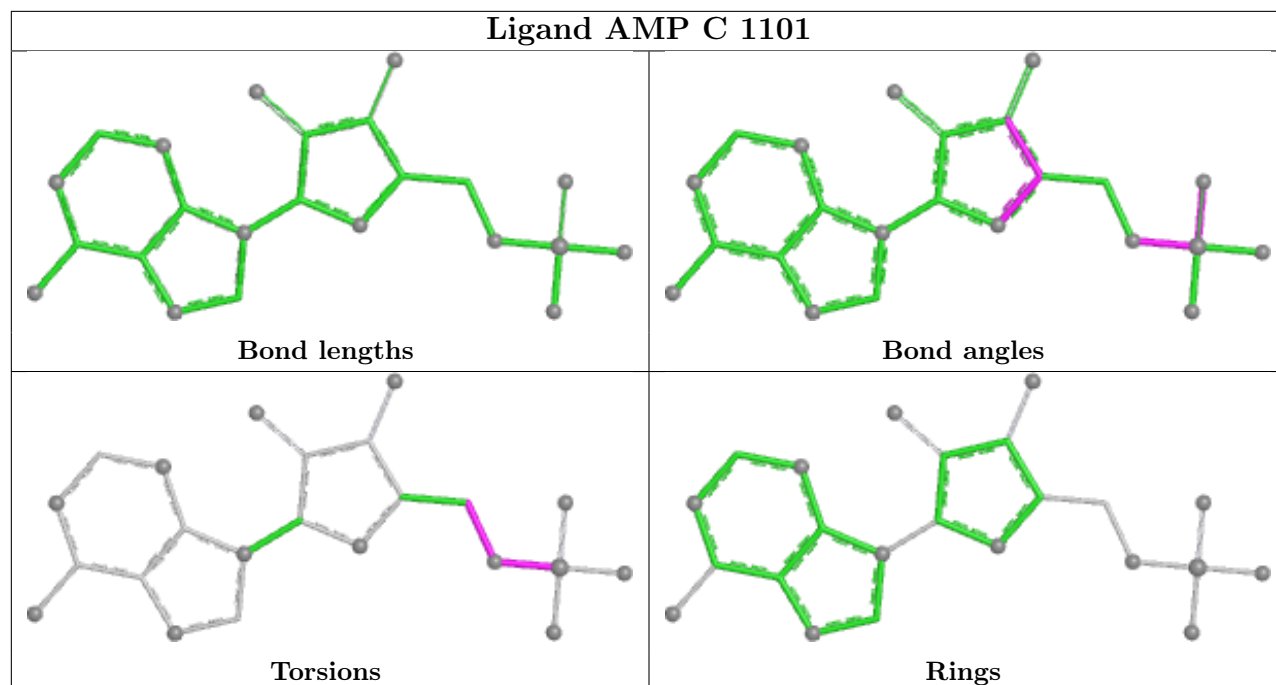
There are no ring outliers.

2 monomers are involved in 3 short contacts:

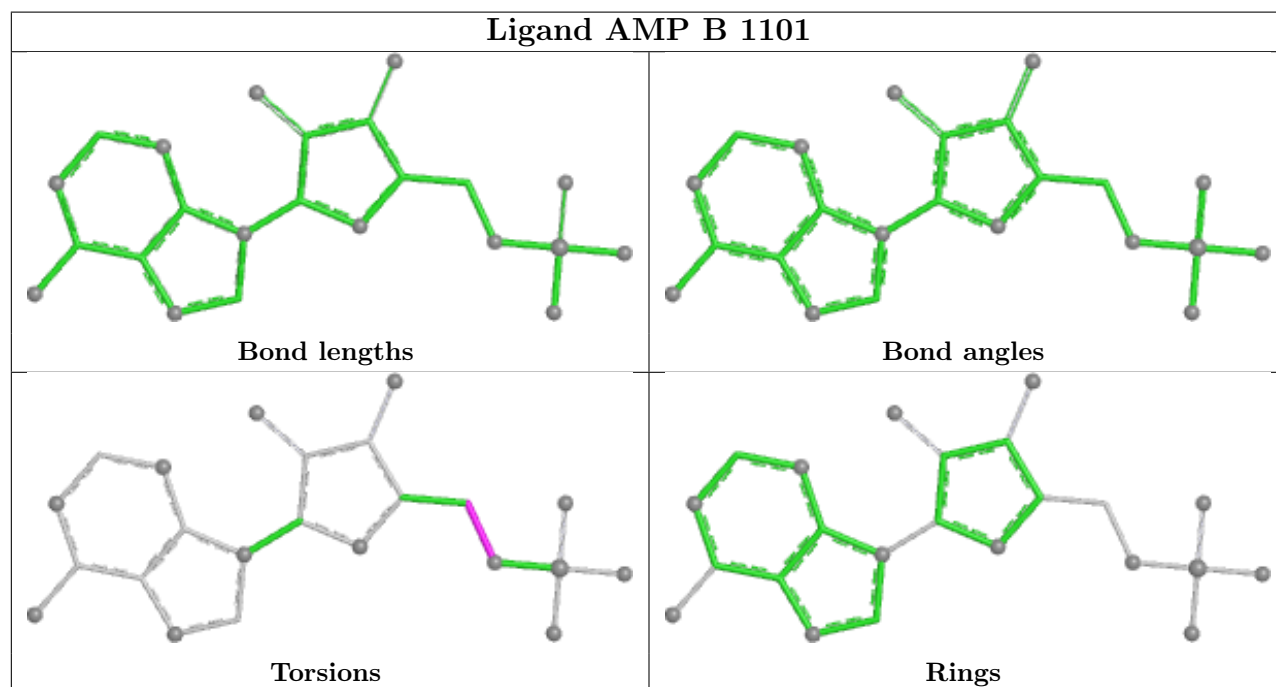
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	AMP	1	0
2	D	1101	AMP	2	0

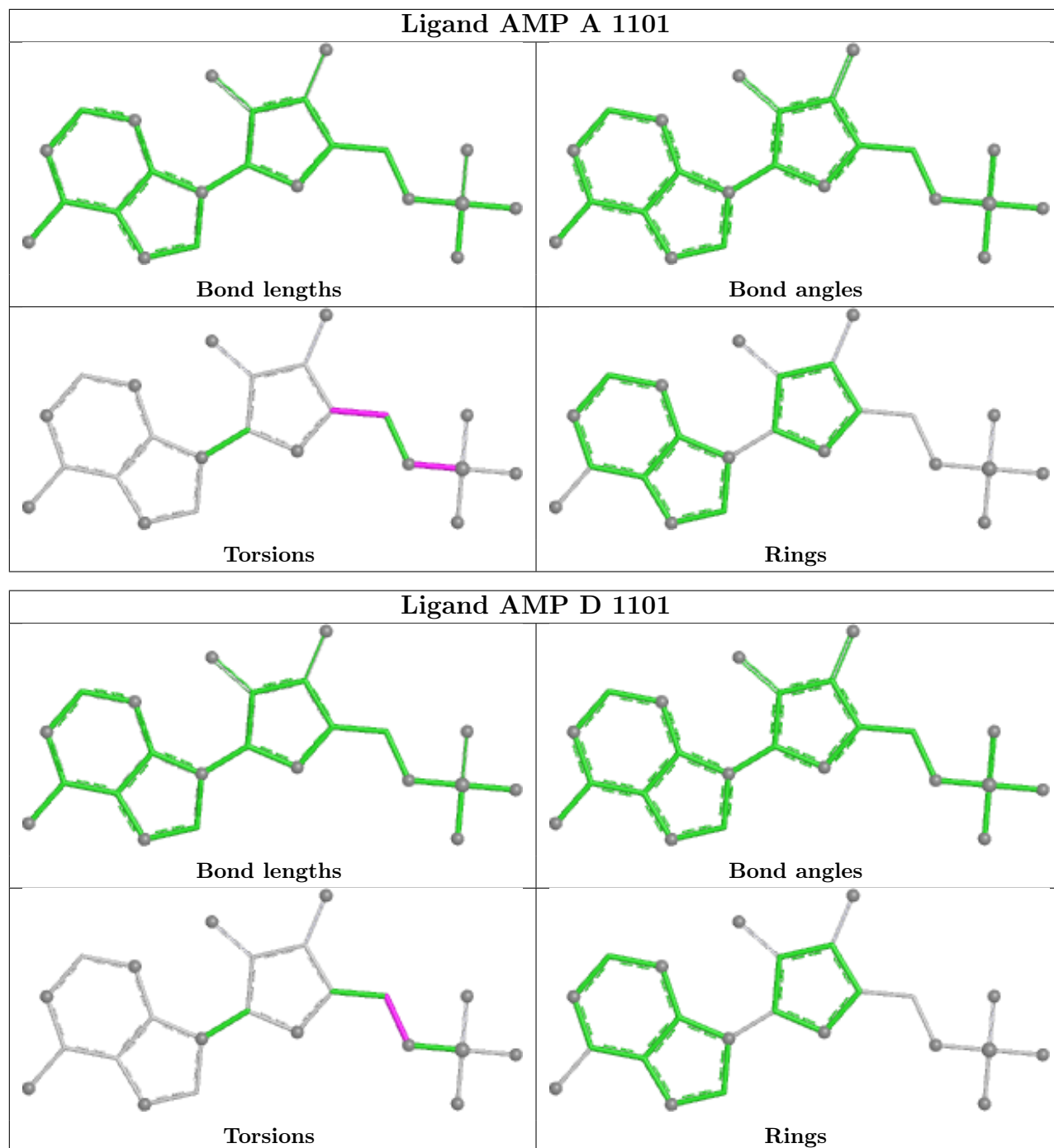
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 C 1101



Ligand AMP B 1101





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, 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	366/380 (96%)	1.09	46 (12%) 8 8	36, 80, 132, 175	1 (0%)
1	B	369/380 (97%)	1.01	42 (11%) 10 10	35, 77, 136, 187	1 (0%)
1	C	368/380 (96%)	1.07	60 (16%) 4 4	36, 73, 133, 206	1 (0%)
1	D	370/380 (97%)	0.95	45 (12%) 8 9	32, 71, 124, 158	1 (0%)
All	All	1473/1520 (96%)	1.03	193 (13%) 7 7	32, 75, 133, 206	4 (0%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	779	ILE	5.2
1	A	1027	VAL	4.9
1	C	779	ILE	4.8
1	B	780	GLY	4.6
1	C	1027	VAL	4.4
1	A	1071	ILE	4.3
1	D	1026	TRP	4.1
1	A	779	ILE	4.1
1	D	803	PHE	4.0
1	D	809	VAL	4.0
1	C	1029	GLY	4.0
1	A	1089	VAL	4.0
1	D	1027	VAL	3.7
1	C	986	ILE	3.7
1	C	809	VAL	3.7
1	B	779	ILE	3.7
1	C	997	LEU	3.6
1	B	685	ILE	3.5
1	B	809	VAL	3.5
1	C	1026	TRP	3.5
1	A	780	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	674	PRO	3.4
1	D	810	THR	3.4
1	A	799	GLY	3.3
1	B	674	PRO	3.3
1	B	1026	TRP	3.3
1	B	1029	GLY	3.3
1	D	676	PRO	3.3
1	B	928	VAL	3.3
1	A	928	VAL	3.3
1	D	1072	TYR	3.3
1	A	678	VAL	3.2
1	A	809	VAL	3.2
1	D	928	VAL	3.2
1	C	778	VAL	3.2
1	C	1022	MET	3.2
1	A	676	PRO	3.2
1	D	983	GLY	3.1
1	B	984	LEU	3.1
1	C	670	PRO	3.1
1	C	962	LEU	3.1
1	C	998	ALA	3.0
1	A	997	LEU	3.0
1	A	1026	TRP	3.0
1	C	926	ASP	3.0
1	C	677	LEU	3.0
1	C	1090	ILE	2.9
1	D	703	ILE	2.9
1	D	930	ILE	2.9
1	B	812	ASP	2.9
1	B	808	ASN	2.9
1	A	968	ILE	2.9
1	C	1071	ILE	2.9
1	D	1090	ILE	2.9
1	A	1093	GLU	2.9
1	A	778	VAL	2.8
1	C	691	THR	2.8
1	D	801	TYR	2.8
1	D	887	ILE	2.8
1	C	684	SER	2.8
1	D	925	ASN	2.8
1	B	980	ALA	2.8
1	B	670	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	685	ILE	2.8
1	A	998	ALA	2.8
1	A	962	LEU	2.8
1	C	1080	LEU	2.8
1	C	1089	VAL	2.8
1	A	1086	TRP	2.8
1	D	980	ALA	2.7
1	C	807	TYR	2.7
1	C	674	PRO	2.7
1	C	928	VAL	2.7
1	B	811	ASP	2.7
1	A	810	THR	2.7
1	B	810	THR	2.7
1	C	682	LEU	2.7
1	B	1069	ARG	2.7
1	A	980	ALA	2.6
1	C	685	ILE	2.6
1	C	703	ILE	2.6
1	D	677	LEU	2.6
1	D	671	ILE	2.6
1	B	677	LEU	2.6
1	C	950	ASP	2.6
1	C	982	LEU	2.6
1	D	777	THR	2.6
1	B	672	LEU	2.6
1	A	1072	TYR	2.5
1	B	690	ASN	2.5
1	B	678	VAL	2.5
1	D	927	ASP	2.5
1	C	994	ALA	2.5
1	A	677	LEU	2.5
1	A	982	LEU	2.5
1	B	982	LEU	2.5
1	D	1071	ILE	2.5
1	C	676	PRO	2.5
1	A	803	PHE	2.5
1	C	799	GLY	2.5
1	A	986	ILE	2.5
1	B	1071	ILE	2.5
1	C	732	ILE	2.5
1	C	930	ILE	2.5
1	C	1072	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	684	SER	2.4
1	B	800	SER	2.4
1	C	984	LEU	2.4
1	C	1069	ARG	2.4
1	B	885	PHE	2.4
1	A	675	GLU	2.4
1	B	671	ILE	2.4
1	B	1027	VAL	2.4
1	B	983	GLY	2.4
1	C	708	GLY	2.4
1	C	690	ASN	2.4
1	B	930	ILE	2.4
1	A	923	LYS	2.4
1	B	707	CYS	2.4
1	B	691	THR	2.4
1	C	973	TYR	2.4
1	A	812	ASP	2.4
1	A	775	LEU	2.3
1	D	780	GLY	2.3
1	D	778	VAL	2.3
1	D	892	VAL	2.3
1	B	676	PRO	2.3
1	A	774	GLY	2.3
1	C	689	LEU	2.3
1	C	775	LEU	2.3
1	A	878	MET	2.3
1	C	993	SER	2.3
1	D	776	SER	2.3
1	A	930	ILE	2.3
1	D	807	TYR	2.3
1	B	669	LYS	2.3
1	D	785	SER	2.3
1	C	671	ILE	2.3
1	D	691	THR	2.3
1	D	672	LEU	2.3
1	D	924	VAL	2.2
1	A	973	TYR	2.2
1	A	932	TRP	2.2
1	C	989	PHE	2.2
1	D	685	ILE	2.2
1	D	673	ALA	2.2
1	A	682	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	807	TYR	2.2
1	D	814	TYR	2.2
1	A	684	SER	2.2
1	A	680	ASP	2.2
1	C	968	ILE	2.2
1	C	929	GLY	2.2
1	C	810	THR	2.2
1	D	802	VAL	2.1
1	D	727	ALA	2.1
1	A	1069	ARG	2.1
1	B	775	LEU	2.1
1	B	1072	TYR	2.1
1	A	927	ASP	2.1
1	A	703	ILE	2.1
1	B	1090	ILE	2.1
1	B	924	VAL	2.1
1	C	969	VAL	2.1
1	C	1024	GLY	2.1
1	C	992	ARG	2.1
1	C	726	GLU	2.1
1	B	927	ASP	2.1
1	A	777	THR	2.1
1	C	813	LYS	2.1
1	C	1088	LYS	2.1
1	B	689	LEU	2.1
1	C	889	LEU	2.1
1	D	682	LEU	2.1
1	D	782	SER	2.1
1	A	1092	GLU	2.1
1	C	812	ASP	2.1
1	D	966	ASP	2.1
1	C	774	GLY	2.1
1	D	922	GLY	2.1
1	D	986	ILE	2.1
1	C	678	VAL	2.1
1	C	924	VAL	2.1
1	D	678	VAL	2.1
1	B	981	SER	2.1
1	A	699	LEU	2.0
1	B	724	LEU	2.0
1	D	1069	ARG	2.0
1	A	1020	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	1086	TRP	2.0
1	D	1094	GLN	2.0
1	C	705	ARG	2.0
1	D	669	LYS	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 oligosaccharides 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, 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.

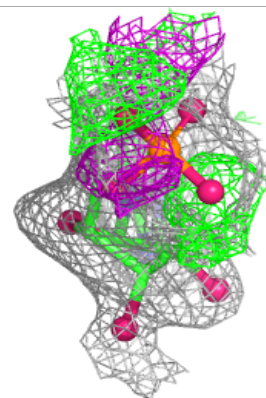
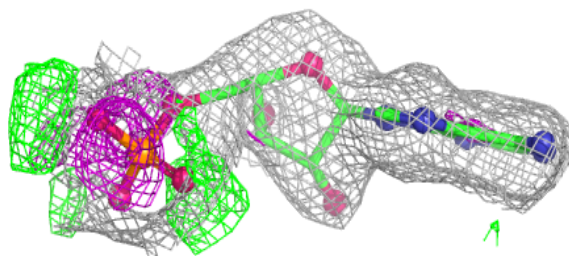
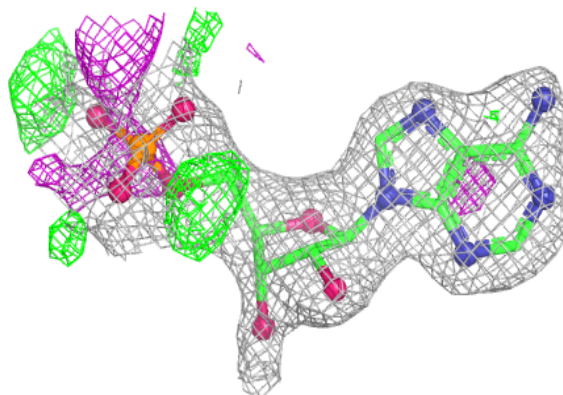
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AMP	A	1101	23/23	0.84	0.13	48,63,80,81	0
2	AMP	C	1101	23/23	0.84	0.14	38,61,88,103	0
6	ACT	B	1104	4/4	0.86	0.19	51,66,89,96	0
2	AMP	B	1101	23/23	0.88	0.13	39,60,72,88	0
6	ACT	C	1104	4/4	0.89	0.12	51,63,70,81	0
2	AMP	D	1101	23/23	0.90	0.12	38,46,71,85	0
6	ACT	A	1105	4/4	0.92	0.21	57,60,71,71	0
6	ACT	D	1104	4/4	0.93	0.16	45,45,48,50	0
4	MG	D	1103	1/1	0.96	0.09	25,25,25,25	0
4	MG	C	1103	1/1	0.97	0.07	27,27,27,27	0
5	CA	A	1104	1/1	0.97	0.39	30,30,30,30	0
4	MG	A	1103	1/1	0.98	0.06	27,27,27,27	0
4	MG	B	1103	1/1	0.98	0.07	27,27,27,27	0
3	MN	D	1102	1/1	0.98	0.12	29,29,29,29	0
3	MN	B	1102	1/1	0.99	0.12	33,33,33,33	0
3	MN	C	1102	1/1	0.99	0.09	33,33,33,33	0
3	MN	A	1102	1/1	0.99	0.12	34,34,34,34	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.

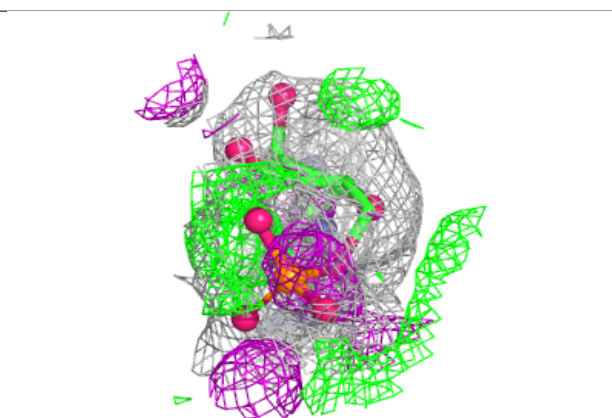
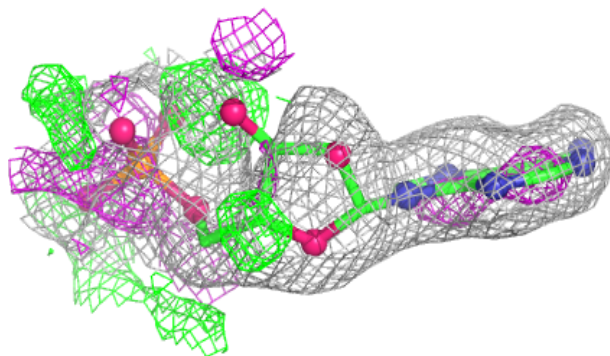
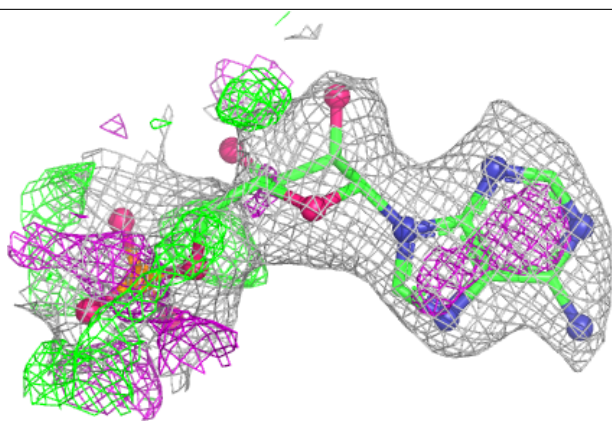
Electron density around AMP A 1101:

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

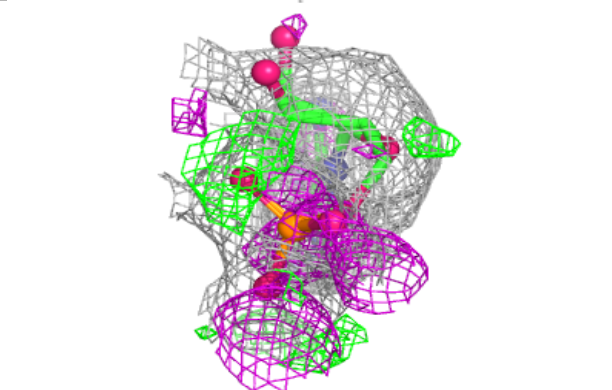
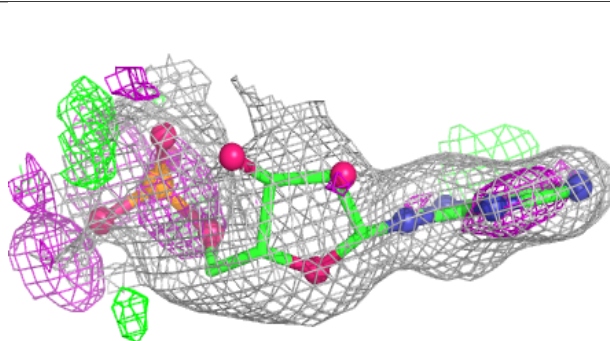
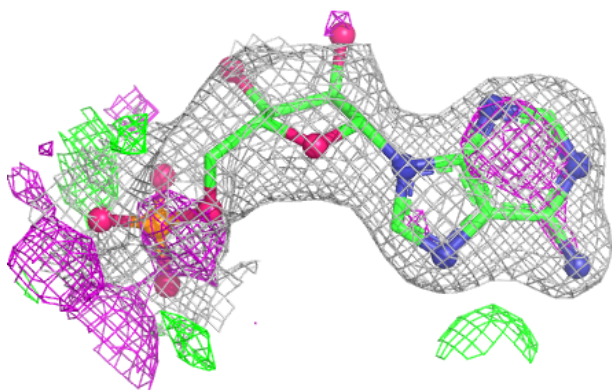


Electron density around AMP C 1101:

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

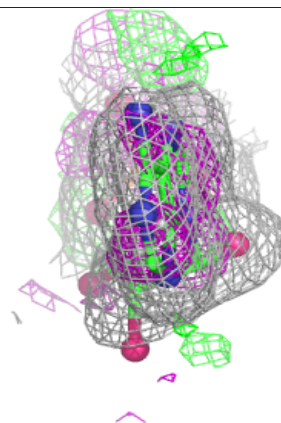
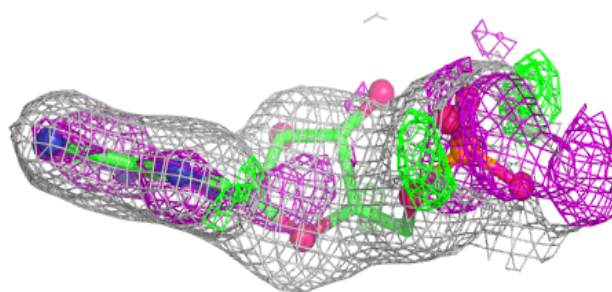
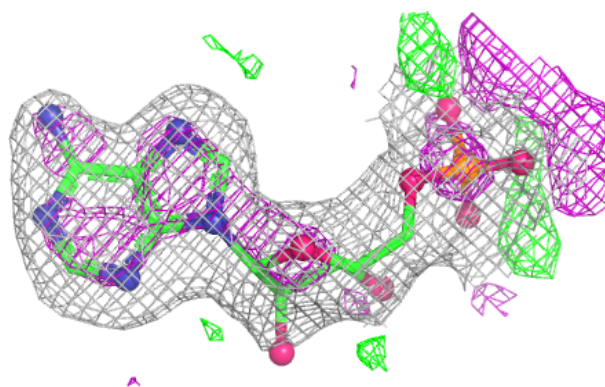
**Electron density around AMP B 1101:**

$2mF_o-DF_c$ (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.