wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2023 – 03:08 PM EDT

PDB ID	:	3E3N
Title	:	The Glycogen phosphorylase b R state- AMP complex
Authors	:	Leonidas, D.D.; Zographos, S.E.; Oikonomakos, N.G.
Deposited on	:	2008-08-07
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 (i) 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 (i)) were used in the production of this report:

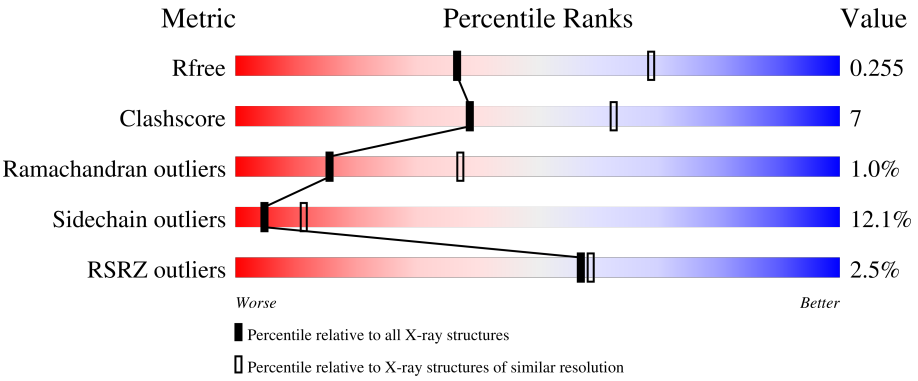
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	842	2% 72% 20% 5% ·
1	B	842	4% 71% 21% 5% ·
1	C	842	2% 76% 15% 5% 5%
1	D	842	% 76% 18% · ·
1	E	842	2% 73% 19% · 5%

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Mol	Chain	Length	Quality of chain
1	F	842	2% 74% 20%
1	G	842	2% 73% 19% 5%
1	H	842	4% 75% 19%

2 Entry composition (i)

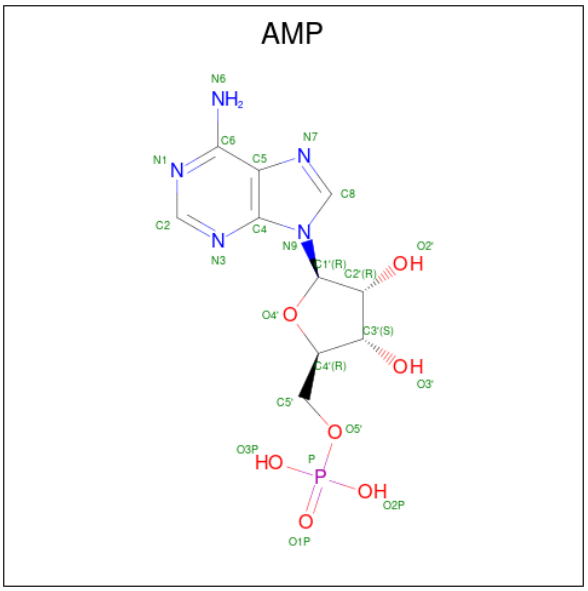
There are 4 unique types of molecules in this entry. The entry contains 53512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, muscle form.

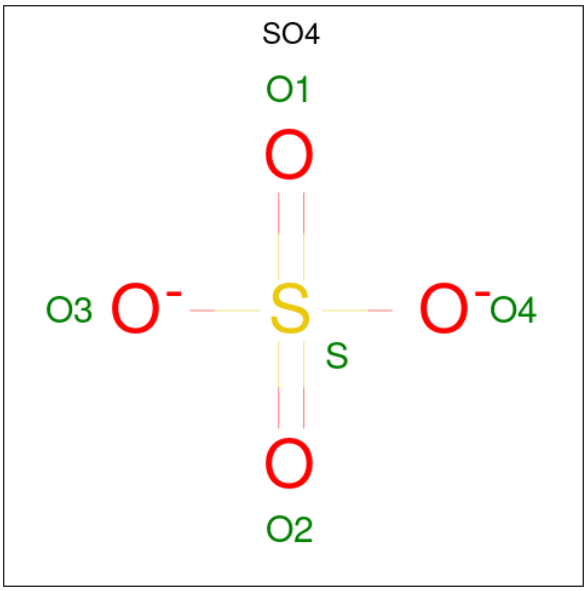
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	P	S	0	0	0
			6635	4225	1175	1204	1	30			
1	B	815	Total	C	N	O	P	S	0	0	0
			6642	4230	1176	1205	1	30			
1	C	802	Total	C	N	O	P	S	0	0	0
			6536	4165	1155	1186	1	29			
1	D	815	Total	C	N	O	P	S	0	0	0
			6643	4229	1176	1207	1	30			
1	E	803	Total	C	N	O	P	S	0	0	0
			6545	4170	1156	1189	1	29			
1	F	813	Total	C	N	O	P	S	0	0	0
			6626	4220	1173	1202	1	30			
1	G	814	Total	C	N	O	P	S	0	0	0
			6635	4225	1175	1204	1	30			
1	H	814	Total	C	N	O	P	S	0	0	0
			6636	4224	1175	1206	1	30			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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		
2	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

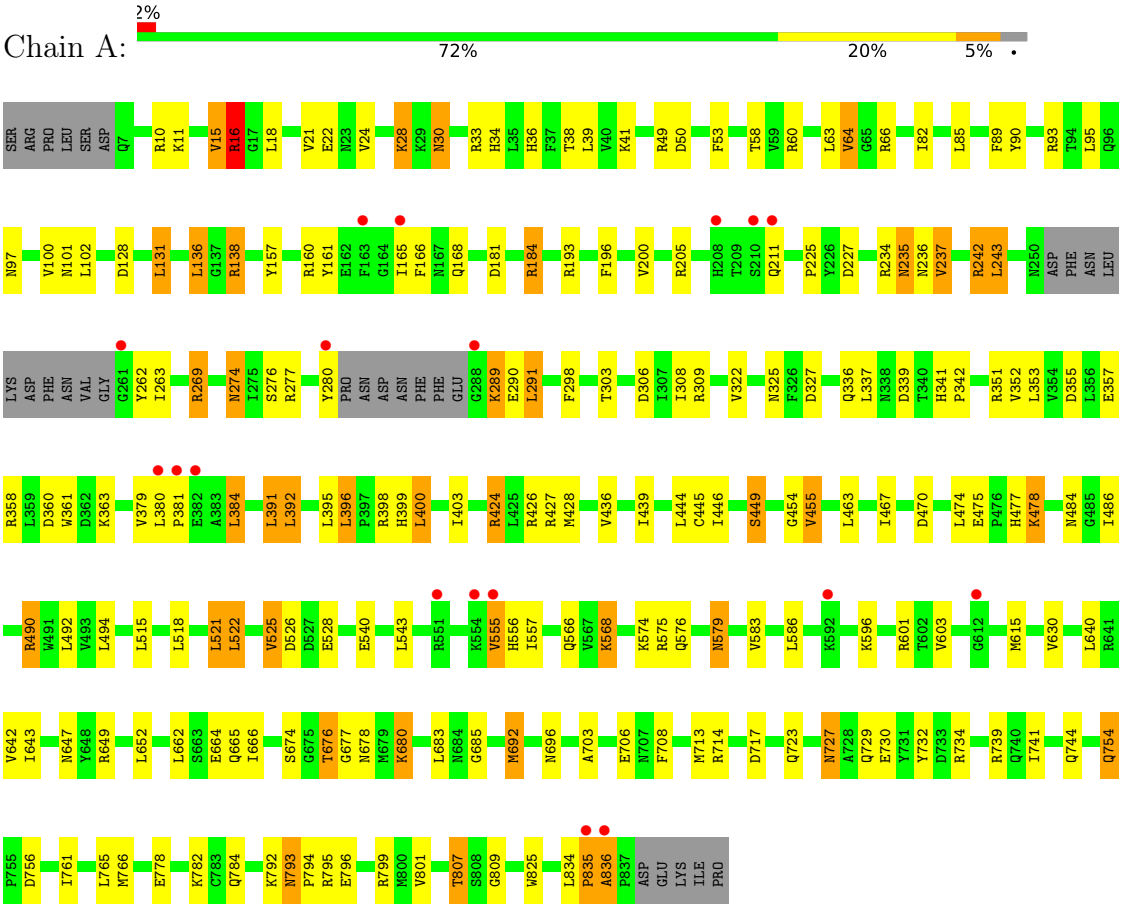
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	32	Total O 32 32	0	0
4	C	36	Total O 36 36	0	0
4	D	62	Total O 62 62	0	0
4	E	27	Total O 27 27	0	0
4	F	38	Total O 38 38	0	0
4	G	69	Total O 69 69	0	0
4	H	30	Total O 30 30	0	0

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.

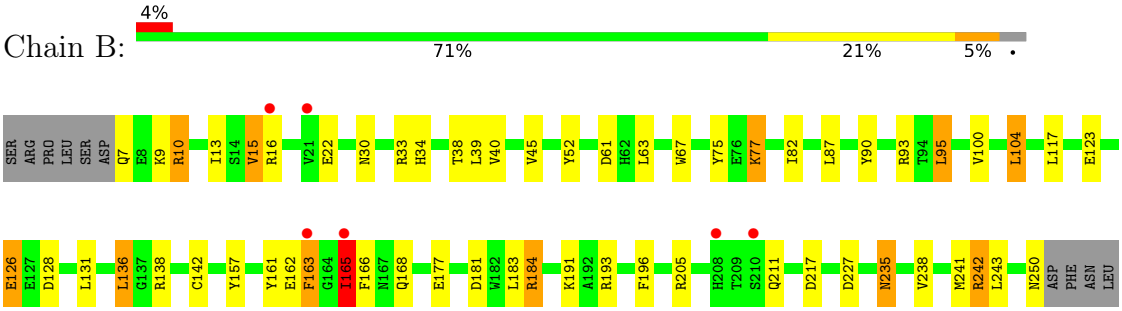
• Molecule 1: Glycogen phosphorylase, muscle form

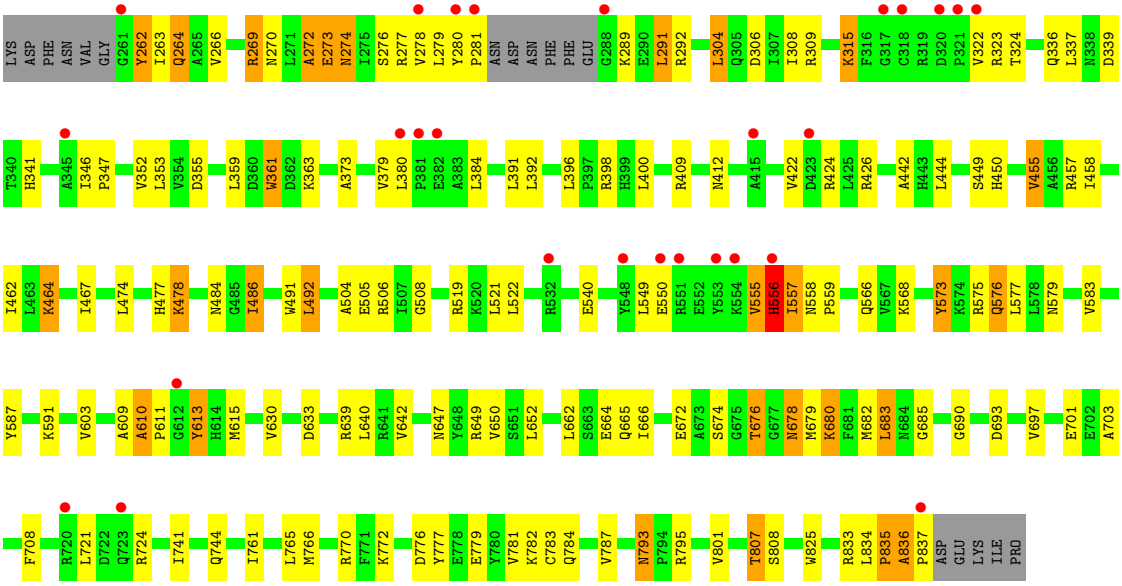
Chain A:



• Molecule 1: Glycogen phosphorylase, muscle form

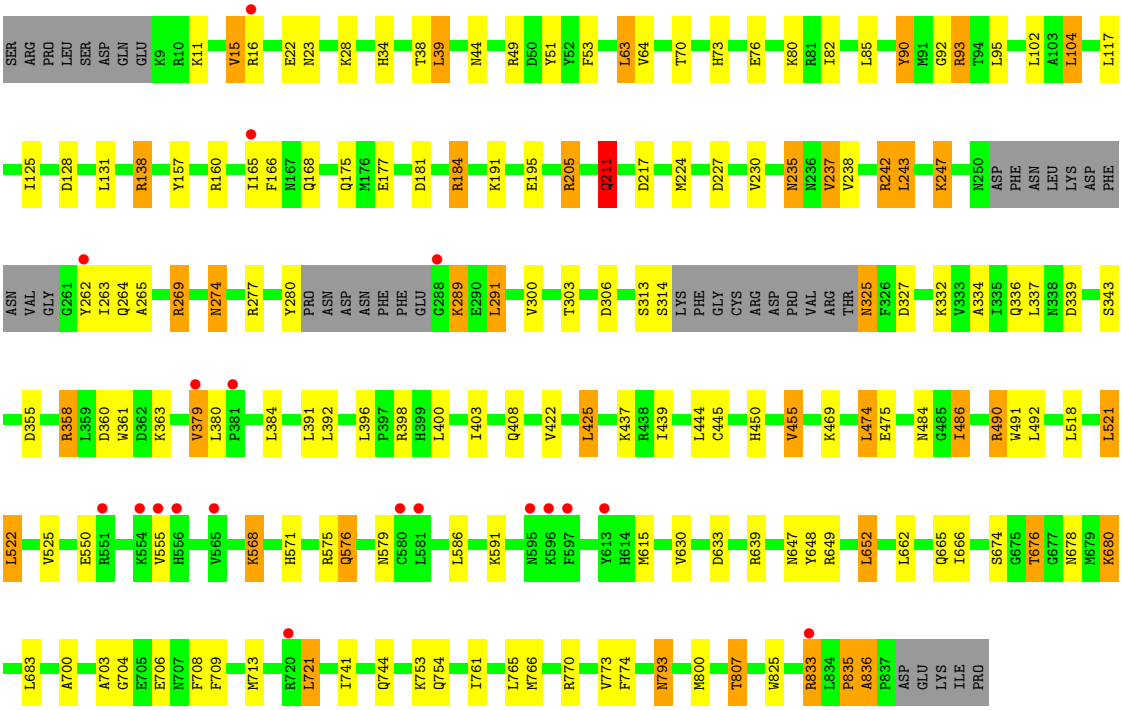
Chain B:





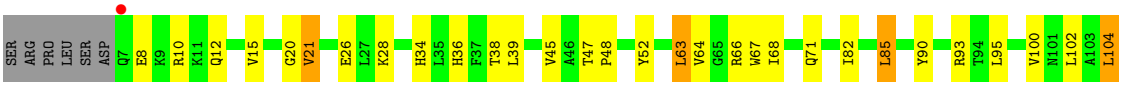
• Molecule 1: Glycogen phosphorylase, muscle form

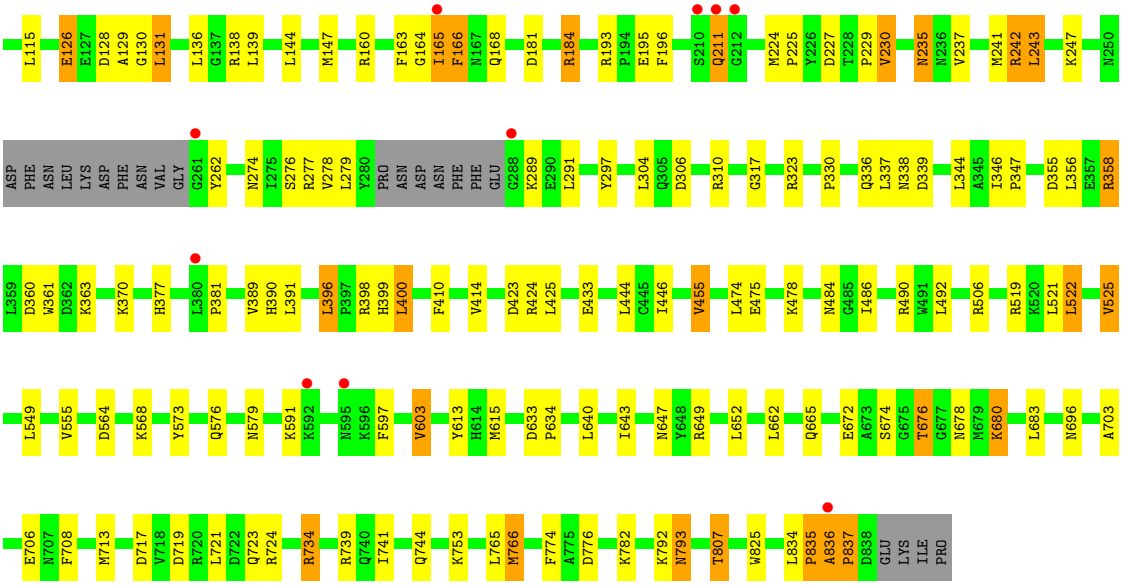
Chain C:



• Molecule 1: Glycogen phosphorylase, muscle form

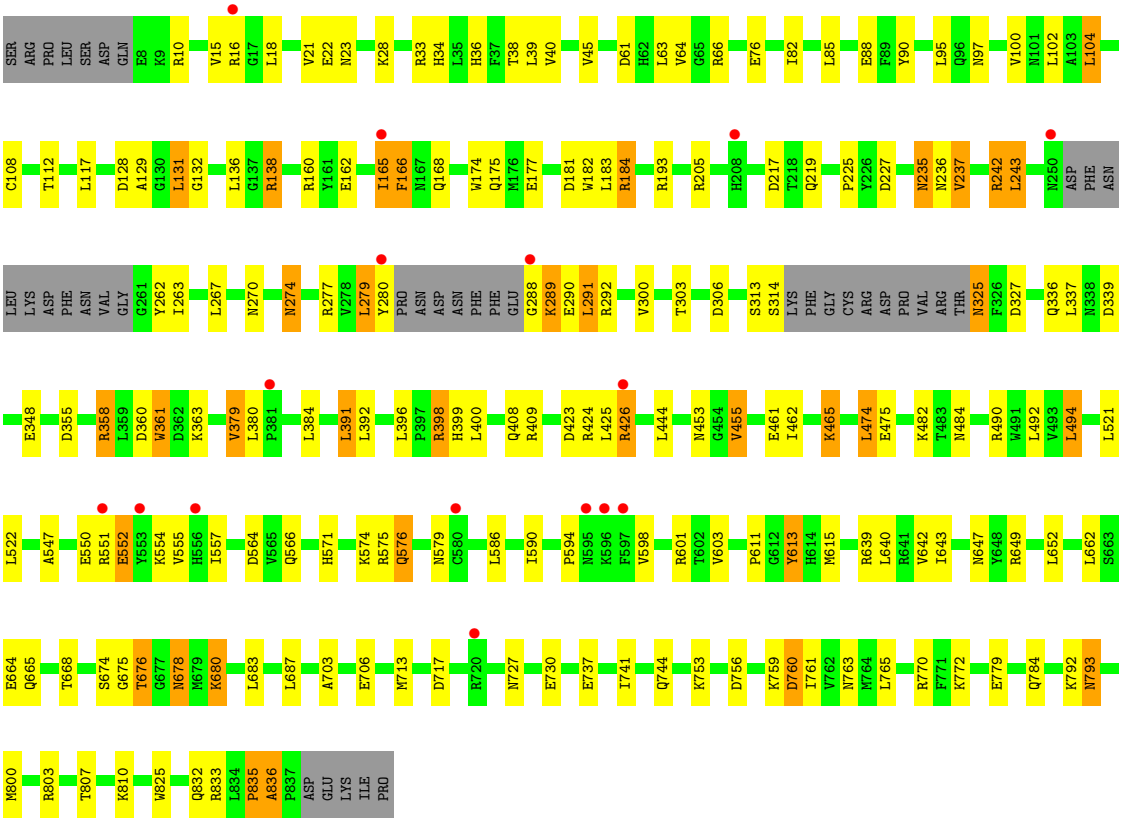
Chain D:





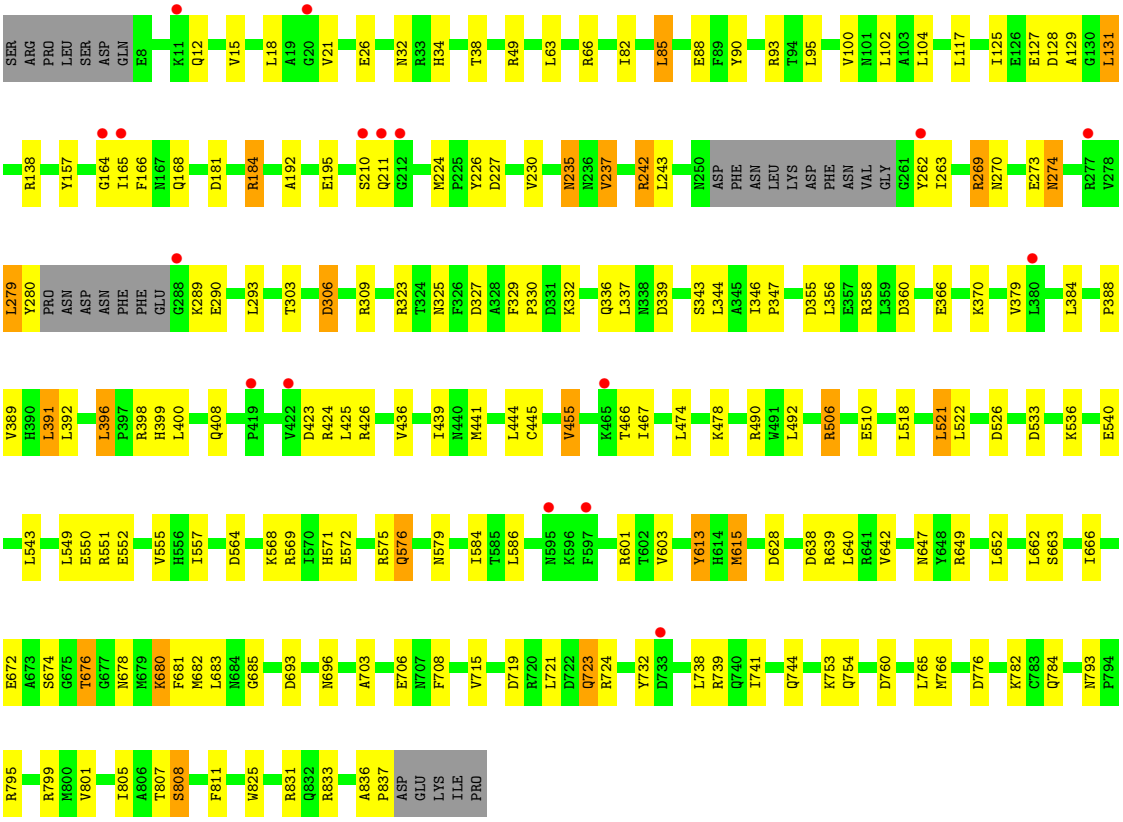
• Molecule 1: Glycogen phosphorylase, muscle form

Chain E:



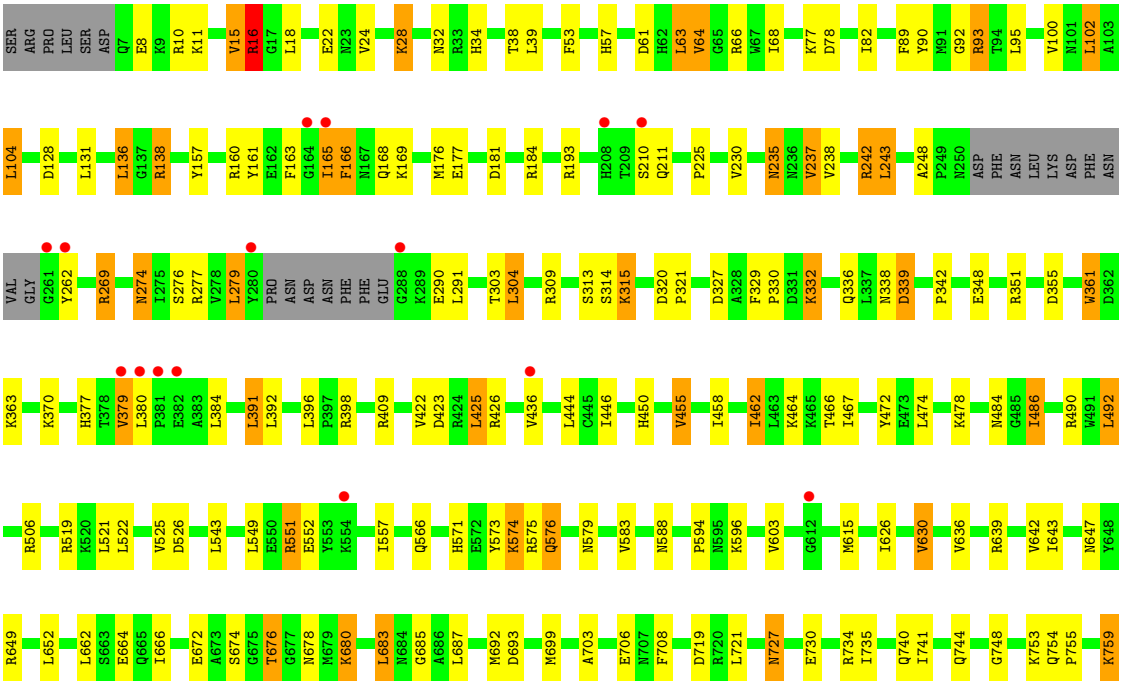
• Molecule 1: Glycogen phosphorylase, muscle form

Chain F:



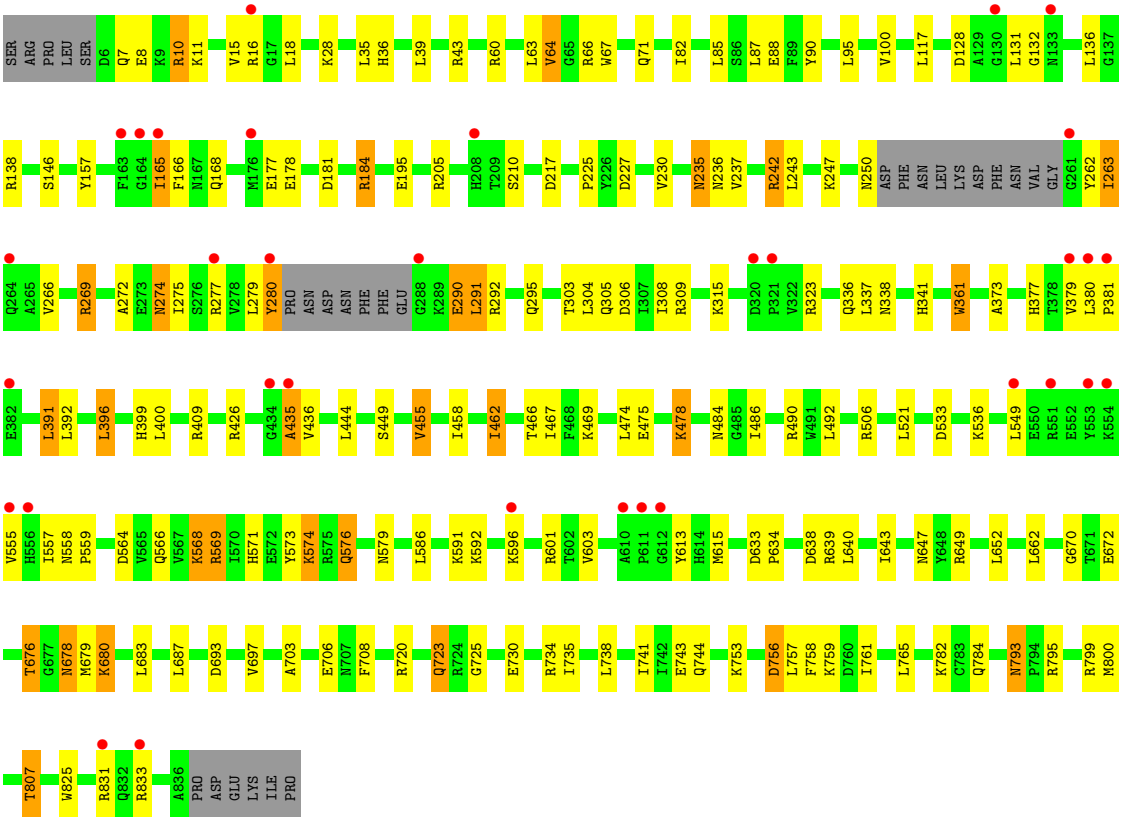
• Molecule 1: Glycogen phosphorylase, muscle form

Chain G:



• Molecule 1: Glycogen phosphorylase, muscle form

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.02Å 188.08Å 175.91Å 90.00° 108.92° 90.00°	Depositor
Resolution (Å)	29.79 – 2.70 29.79 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.79-2.70) 94.2 (29.79-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.256 0.193 , 0.255	Depositor DCC
R_{free} test set	9450 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	53512	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5777e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: AMP, SO4, LLP

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	0.46	0/6756	0.65	2/9137 (0.0%)
1	B	0.44	0/6764	0.62	2/9149 (0.0%)
1	C	0.44	0/6654	0.61	0/8999
1	D	0.46	0/6764	0.64	3/9148 (0.0%)
1	E	0.44	0/6663	0.61	1/9011 (0.0%)
1	F	0.46	0/6747	0.63	0/9125
1	G	0.47	0/6756	0.66	1/9137 (0.0%)
1	H	0.44	0/6756	0.61	0/9136
All	All	0.45	0/53860	0.63	9/72842 (0.0%)

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	H	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	LEU	CA-CB-CG	6.06	129.23	115.30
1	G	136	LEU	CA-CB-CG	5.78	128.58	115.30
1	A	136	LEU	CA-CB-CG	5.67	128.34	115.30
1	D	400	LEU	CA-CB-CG	5.53	128.02	115.30
1	B	556	HIS	CB-CA-C	5.50	121.39	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	454	GLY	Peptide
1	H	7	GLN	Peptide

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	6635	0	6598	107	0
1	B	6642	0	6605	125	0
1	C	6536	0	6500	88	0
1	D	6643	0	6602	81	0
1	E	6545	0	6506	102	0
1	F	6626	0	6590	90	0
1	G	6635	0	6598	120	0
1	H	6636	0	6595	103	0
2	A	23	0	12	1	0
2	B	23	0	12	2	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
2	E	23	0	12	0	0
2	F	23	0	12	0	0
2	G	23	0	12	1	0
2	H	23	0	12	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	1	0
3	G	10	0	0	1	0
3	H	10	0	0	0	0
4	A	56	0	0	1	0
4	B	32	0	0	1	0
4	C	36	0	0	3	0
4	D	62	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	27	0	0	2	0
4	F	38	0	0	0	0
4	G	69	0	0	1	0
4	H	30	0	0	3	0
All	All	53512	0	52690	793	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 7.

The worst 5 of 793 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ASN:HA	1:C:277:ARG:HG3	1.34	1.09
1:G:274:ASN:HA	1:G:277:ARG:HG3	1.42	1.01
1:D:336:GLN:HE21	1:D:825:TRP:HE1	0.99	0.98
1:H:336:GLN:HE21	1:H:825:TRP:HE1	1.08	0.94
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.48	0.92

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	807/842 (96%)	771 (96%)	27 (3%)	9 (1%)	14	34
1	B	808/842 (96%)	757 (94%)	39 (5%)	12 (2%)	10	26
1	C	793/842 (94%)	745 (94%)	40 (5%)	8 (1%)	15	37
1	D	808/842 (96%)	763 (94%)	38 (5%)	7 (1%)	17	40
1	E	794/842 (94%)	752 (95%)	36 (4%)	6 (1%)	19	43
1	F	806/842 (96%)	759 (94%)	42 (5%)	5 (1%)	25	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	807/842 (96%)	763 (94%)	34 (4%)	10 (1%)	13	32
1	H	807/842 (96%)	756 (94%)	44 (6%)	7 (1%)	17	40
All	All	6430/6736 (96%)	6066 (94%)	300 (5%)	64 (1%)	15	37

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	166	PHE
1	A	835	PRO
1	B	16	ARG
1	B	273	GLU

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	703/730 (96%)	613 (87%)	90 (13%)	4	10
1	B	704/730 (96%)	624 (89%)	80 (11%)	5	13
1	C	692/730 (95%)	609 (88%)	83 (12%)	5	11
1	D	704/730 (96%)	616 (88%)	88 (12%)	4	10
1	E	693/730 (95%)	609 (88%)	84 (12%)	5	11
1	F	702/730 (96%)	613 (87%)	89 (13%)	4	10
1	G	703/730 (96%)	618 (88%)	85 (12%)	5	11
1	H	703/730 (96%)	622 (88%)	81 (12%)	5	13
All	All	5604/5840 (96%)	4924 (88%)	680 (12%)	5	11

5 of 680 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	391	LEU
1	G	579	ASN

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Mol	Chain	Res	Type
1	F	492	LEU
1	F	389	VAL
1	G	64	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 182 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	34	HIS
1	G	168	GLN
1	F	235	ASN
1	F	566	GLN
1	G	541	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	G	680	1	23,24,25	1.58	3 (13%)	25,32,34	1.53	5 (20%)
1	LLP	A	680	1	23,24,25	1.84	4 (17%)	25,32,34	1.43	5 (20%)
1	LLP	E	680	1	23,24,25	1.67	3 (13%)	25,32,34	1.58	6 (24%)
1	LLP	F	680	1	23,24,25	1.60	3 (13%)	25,32,34	1.43	4 (16%)
1	LLP	B	680	1	23,24,25	1.75	5 (21%)	25,32,34	1.40	5 (20%)
1	LLP	D	680	1	23,24,25	1.74	4 (17%)	25,32,34	1.45	6 (24%)
1	LLP	C	680	1	23,24,25	1.67	3 (13%)	25,32,34	1.39	4 (16%)
1	LLP	H	680	1	23,24,25	1.72	4 (17%)	25,32,34	1.29	5 (20%)

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	LLP	G	680	1	-	0/16/17/19	0/1/1/1
1	LLP	A	680	1	-	2/16/17/19	0/1/1/1
1	LLP	E	680	1	-	1/16/17/19	0/1/1/1
1	LLP	F	680	1	-	2/16/17/19	0/1/1/1
1	LLP	B	680	1	-	3/16/17/19	0/1/1/1
1	LLP	D	680	1	-	4/16/17/19	0/1/1/1
1	LLP	C	680	1	-	3/16/17/19	0/1/1/1
1	LLP	H	680	1	-	3/16/17/19	0/1/1/1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O3-C3	-6.24	1.22	1.37
1	C	680	LLP	O3-C3	-5.77	1.23	1.37
1	B	680	LLP	O3-C3	-5.77	1.23	1.37
1	H	680	LLP	O3-C3	-5.73	1.23	1.37
1	E	680	LLP	O3-C3	-5.61	1.23	1.37

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	680	LLP	OP4-C5'-C5	3.63	116.27	109.35
1	B	680	LLP	OP4-C5'-C5	3.35	115.74	109.35
1	G	680	LLP	CE-NZ-C4'	-3.35	108.61	118.90
1	A	680	LLP	CE-NZ-C4'	-3.13	109.28	118.90
1	B	680	LLP	CE-NZ-C4'	-3.12	109.32	118.90

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	680	LLP	C5'-OP4-P-OP2
1	A	680	LLP	C5'-OP4-P-OP3
1	B	680	LLP	C5'-OP4-P-OP1
1	B	680	LLP	C5'-OP4-P-OP2
1	B	680	LLP	C5'-OP4-P-OP3

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	680	LLP	6	0
1	A	680	LLP	3	0
1	E	680	LLP	4	0
1	F	680	LLP	3	0
1	B	680	LLP	3	0
1	D	680	LLP	1	0
1	C	680	LLP	5	0
1	H	680	LLP	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AMP	A	843	-	22,25,25	1.10	3 (13%)	25,38,38	1.39	4 (16%)
3	SO4	C	844	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	H	844	-	4,4,4	0.13	0	6,6,6	0.18	0
3	SO4	A	845	-	4,4,4	0.13	0	6,6,6	0.15	0
3	SO4	E	845	-	4,4,4	0.14	0	6,6,6	0.08	0
2	AMP	G	843	-	22,25,25	0.96	1 (4%)	25,38,38	1.47	3 (12%)
3	SO4	D	845	-	4,4,4	0.11	0	6,6,6	0.17	0
2	AMP	H	843	-	22,25,25	1.00	2 (9%)	25,38,38	1.42	4 (16%)
2	AMP	E	843	-	22,25,25	1.05	2 (9%)	25,38,38	1.32	4 (16%)
3	SO4	A	844	-	4,4,4	0.12	0	6,6,6	0.20	0
2	AMP	D	843	-	22,25,25	1.09	3 (13%)	25,38,38	1.49	4 (16%)
3	SO4	E	844	-	4,4,4	0.12	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	H	899	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	G	845	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	D	844	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	F	845	-	4,4,4	0.12	0	6,6,6	0.18	0
2	AMP	F	843	-	22,25,25	1.04	2 (9%)	25,38,38	1.46	4 (16%)
2	AMP	C	843	-	22,25,25	1.07	2 (9%)	25,38,38	1.31	4 (16%)
3	SO4	B	845	-	4,4,4	0.12	0	6,6,6	0.16	0
3	SO4	C	845	-	4,4,4	0.15	0	6,6,6	0.21	0
2	AMP	B	843	-	22,25,25	1.02	1 (4%)	25,38,38	1.29	2 (8%)
3	SO4	G	844	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	F	844	-	4,4,4	0.15	0	6,6,6	0.22	0
3	SO4	B	844	-	4,4,4	0.15	0	6,6,6	0.14	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	A	843	-	-	0/6/26/26	0/3/3/3
2	AMP	H	843	-	-	0/6/26/26	0/3/3/3
2	AMP	F	843	-	-	0/6/26/26	0/3/3/3
2	AMP	C	843	-	-	0/6/26/26	0/3/3/3
2	AMP	E	843	-	-	0/6/26/26	0/3/3/3
2	AMP	B	843	-	-	0/6/26/26	0/3/3/3
2	AMP	D	843	-	-	0/6/26/26	0/3/3/3
2	AMP	G	843	-	-	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)
2	B	843	AMP	C5-C4	2.67	1.48	1.40
2	H	843	AMP	C5-C4	2.67	1.48	1.40
2	D	843	AMP	C5-C4	2.66	1.48	1.40
2	E	843	AMP	C5-C4	2.65	1.48	1.40
2	C	843	AMP	C5-C4	2.64	1.47	1.40

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	843	AMP	N3-C2-N1	-3.68	122.92	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	843	AMP	N3-C2-N1	-3.61	123.04	128.68
2	B	843	AMP	N3-C2-N1	-3.60	123.05	128.68
2	G	843	AMP	O5'-P-O1P	-3.53	96.57	106.47
2	D	843	AMP	N3-C2-N1	-3.47	123.26	128.68

There are no chirality outliers.

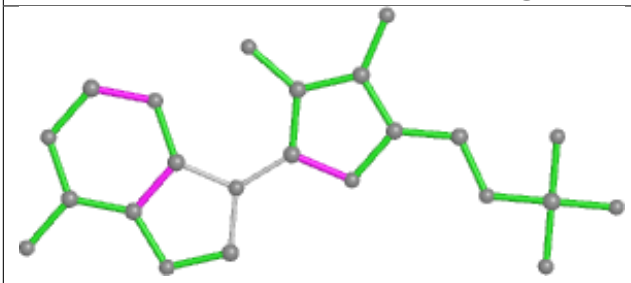
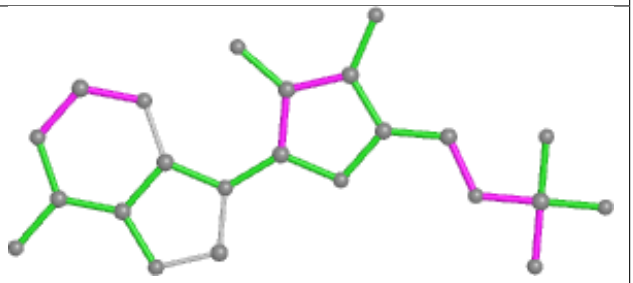
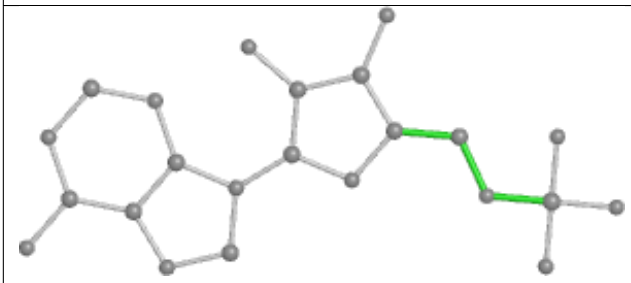
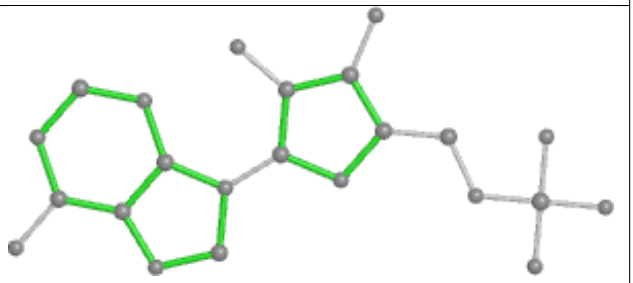
There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	843	AMP	1	0
2	G	843	AMP	1	0
2	H	843	AMP	1	0
3	F	845	SO4	1	0
2	B	843	AMP	2	0
3	G	844	SO4	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 A 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

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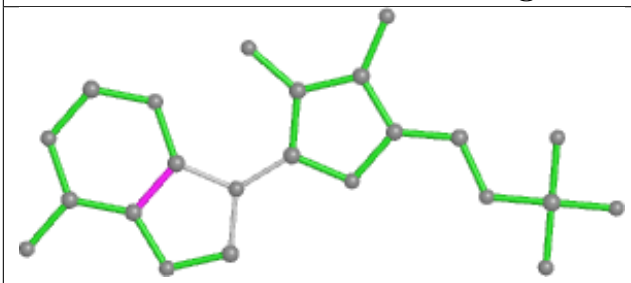
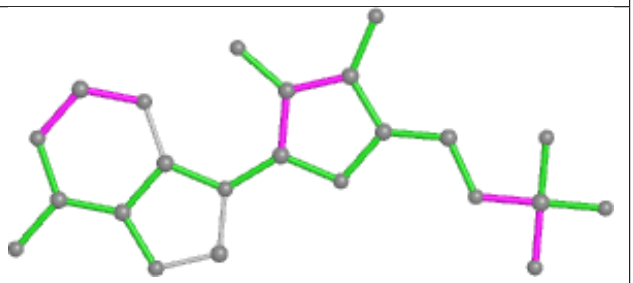
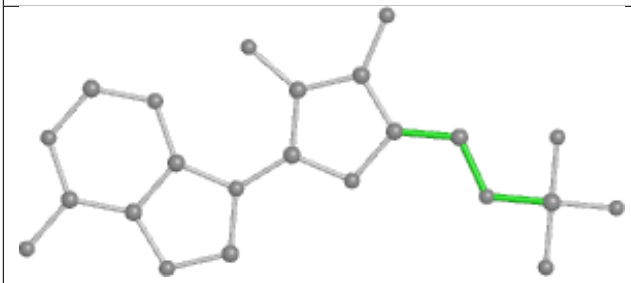
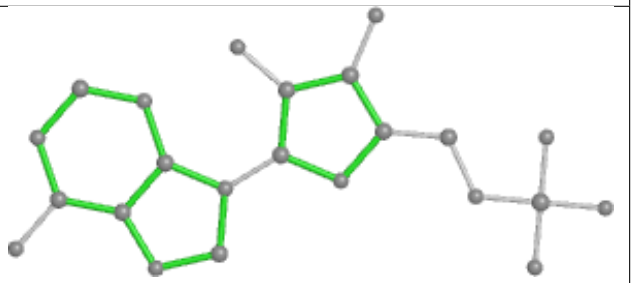
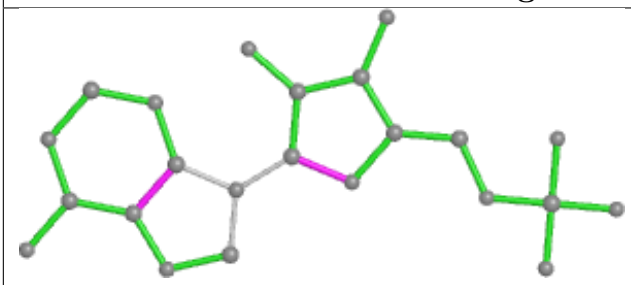
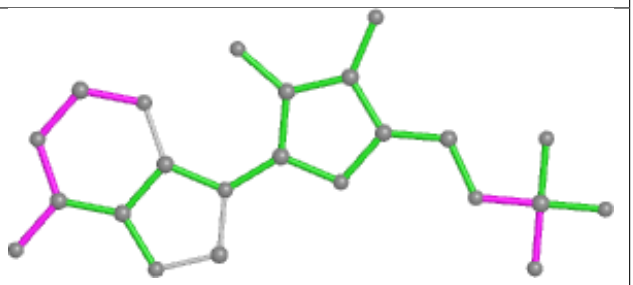
 Bond lengths	 Bond angles
 Torsions	 Rings

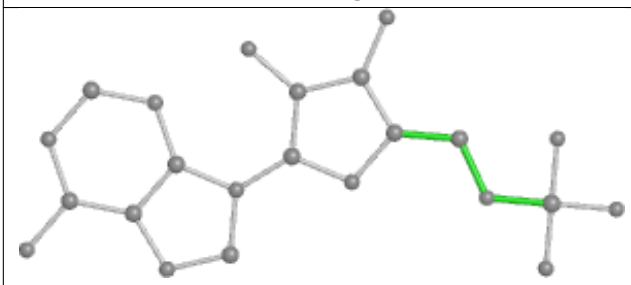
Ligand AMP H 843



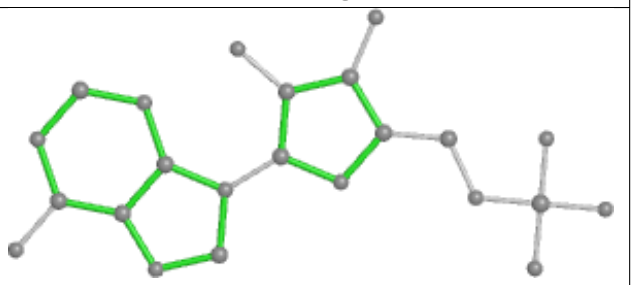
Bond lengths



Bond angles



Torsions



Rings

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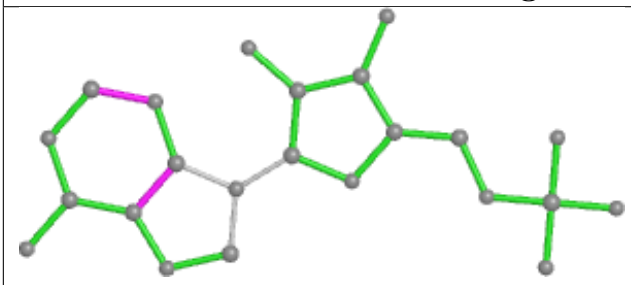
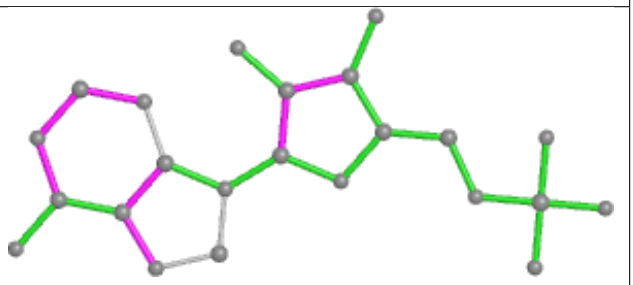
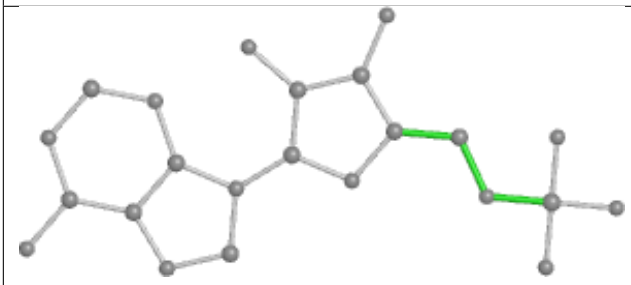


Bond lengths



Bond angles



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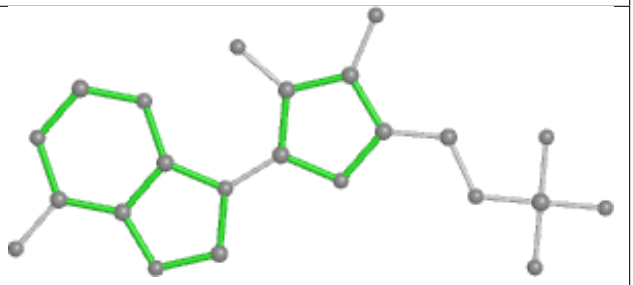

Rings

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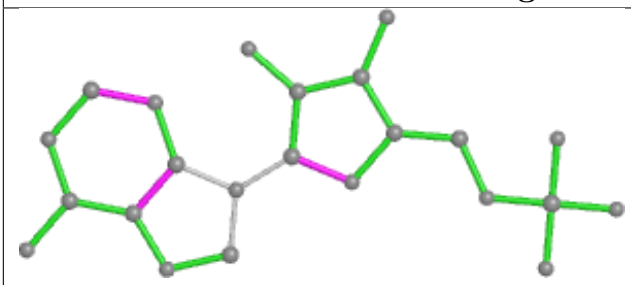
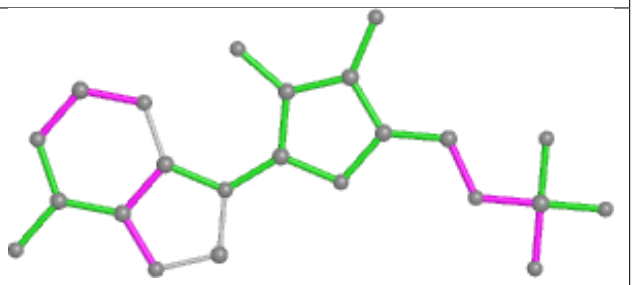
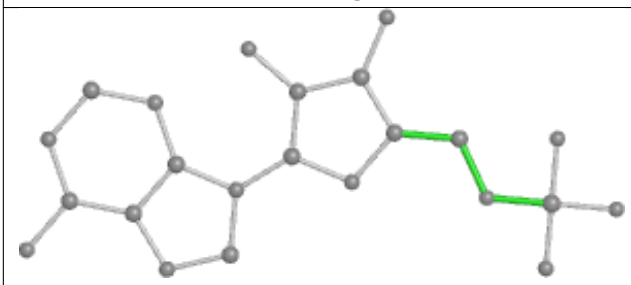


Bond lengths



Bond angles



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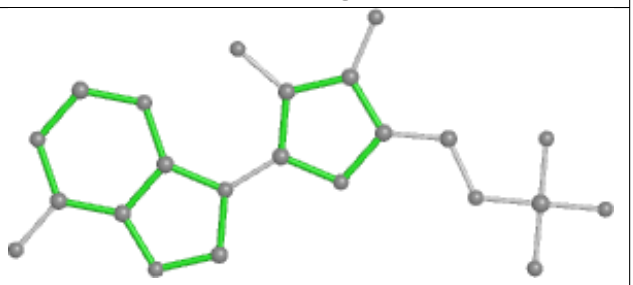

Rings

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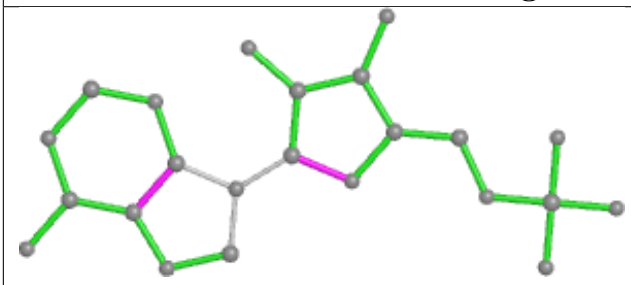
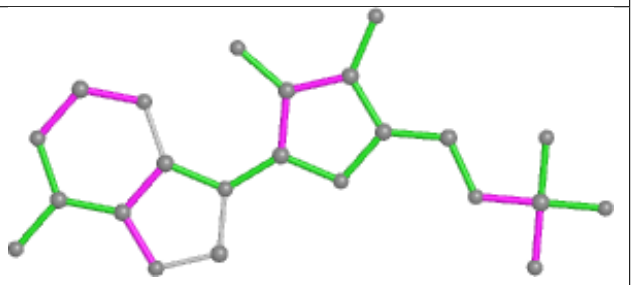
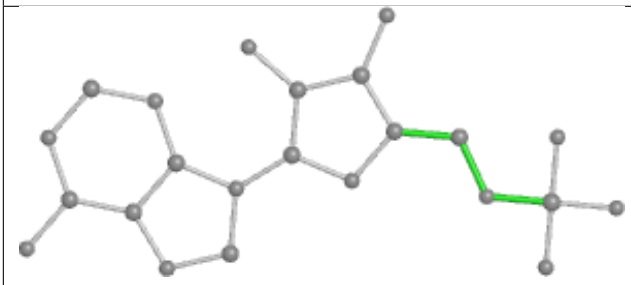


Bond lengths



Bond angles



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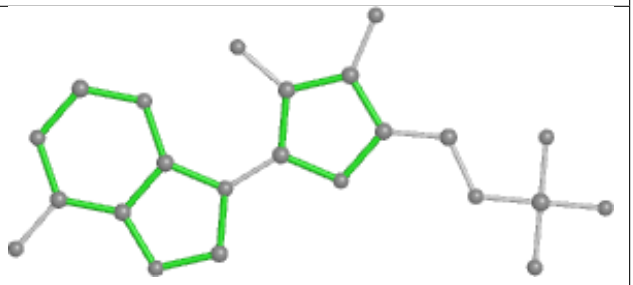

Rings

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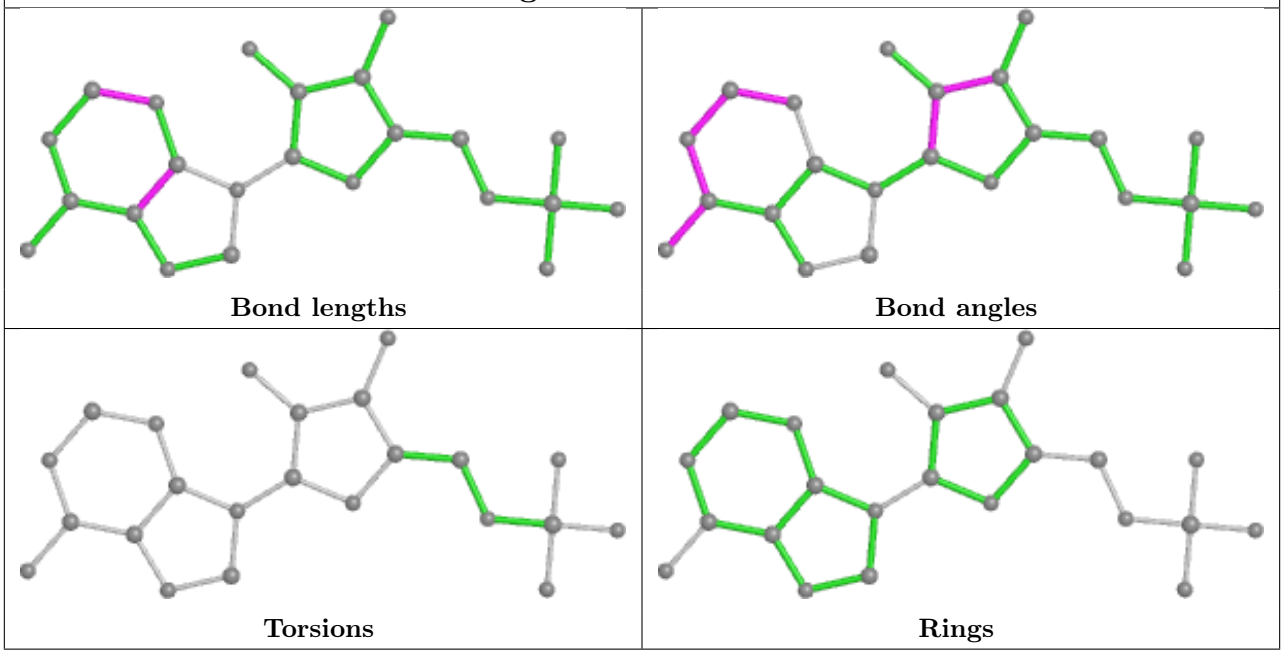

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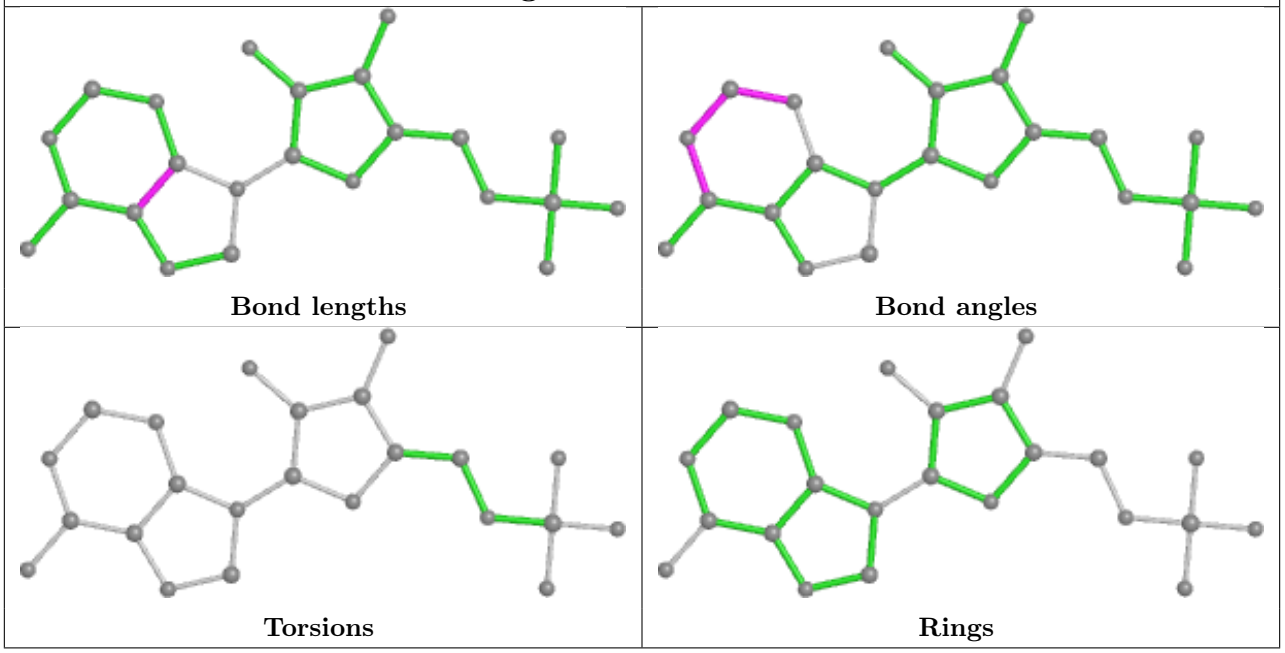

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	813/842 (96%)	-0.33	18 (2%)	62	63	7, 21, 42, 58	0
1	B	814/842 (96%)	-0.04	33 (4%)	37	36	4, 25, 50, 75	0
1	C	801/842 (95%)	-0.18	19 (2%)	59	60	3, 21, 41, 54	0
1	D	814/842 (96%)	-0.23	11 (1%)	75	77	6, 22, 38, 54	0
1	E	802/842 (95%)	-0.17	16 (1%)	65	67	5, 23, 43, 54	0
1	F	812/842 (96%)	-0.22	17 (2%)	63	65	3, 20, 38, 57	0
1	G	813/842 (96%)	-0.29	16 (1%)	65	67	7, 21, 41, 57	0
1	H	813/842 (96%)	-0.04	33 (4%)	37	36	8, 28, 54, 69	0
All	All	6482/6736 (96%)	-0.19	163 (2%)	57	59	3, 23, 44, 75	0

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	288	GLY	6.8
1	A	288	GLY	6.5
1	B	210	SER	6.3
1	C	288	GLY	6.3
1	H	380	LEU	5.8

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

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
1	LLP	B	680	24/25	0.96	0.18	19,27,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	F	680	24/25	0.96	0.15	15,17,22,23	0
1	LLP	D	680	24/25	0.97	0.15	16,17,21,24	0
1	LLP	E	680	24/25	0.97	0.14	16,19,22,23	0
1	LLP	C	680	24/25	0.97	0.14	13,16,23,23	0
1	LLP	G	680	24/25	0.97	0.17	17,18,21,23	0
1	LLP	H	680	24/25	0.97	0.14	22,25,27,27	0
1	LLP	A	680	24/25	0.98	0.14	17,19,22,24	0

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, 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
3	SO4	E	845	5/5	0.82	0.19	95,95,96,96	0
3	SO4	C	844	5/5	0.90	0.15	88,88,88,88	0
3	SO4	A	845	5/5	0.90	0.15	97,98,98,98	0
3	SO4	F	845	5/5	0.90	0.18	86,86,87,87	0
3	SO4	B	845	5/5	0.91	0.18	90,90,90,91	0
3	SO4	D	845	5/5	0.92	0.15	83,84,84,85	0
3	SO4	G	845	5/5	0.94	0.16	82,83,83,84	0
3	SO4	H	899	5/5	0.94	0.13	80,80,80,81	0
3	SO4	C	845	5/5	0.95	0.16	58,59,60,60	0
3	SO4	B	844	5/5	0.95	0.14	67,67,68,68	0
2	AMP	E	843	23/23	0.97	0.10	33,37,39,39	0
2	AMP	F	843	23/23	0.97	0.12	20,26,27,27	0
2	AMP	G	843	23/23	0.97	0.10	23,28,30,30	0
3	SO4	E	844	5/5	0.97	0.10	71,72,73,73	0
2	AMP	H	843	23/23	0.97	0.13	28,34,34,36	0
3	SO4	F	844	5/5	0.97	0.15	58,59,59,60	0
2	AMP	B	843	23/23	0.97	0.11	26,35,36,36	0
2	AMP	C	843	23/23	0.97	0.10	28,32,34,34	0
2	AMP	D	843	23/23	0.97	0.13	27,29,31,31	0
2	AMP	A	843	23/23	0.98	0.10	25,27,29,29	0
3	SO4	D	844	5/5	0.98	0.08	66,66,66,67	0

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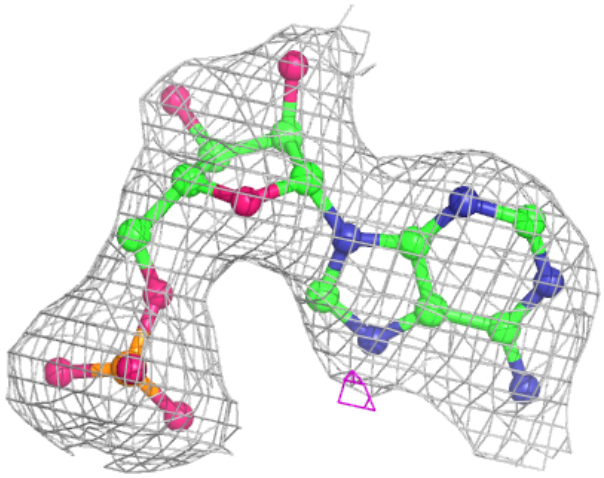
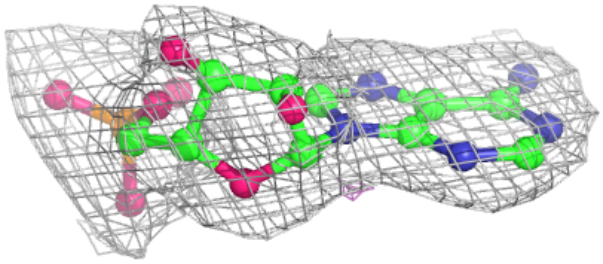
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	H	844	5/5	0.98	0.11	46,46,46,47	0
3	SO4	A	844	5/5	0.98	0.07	47,47,48,48	0
3	SO4	G	844	5/5	0.99	0.09	40,41,42,42	0

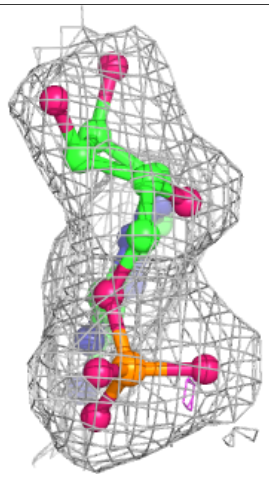
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP E 843:

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

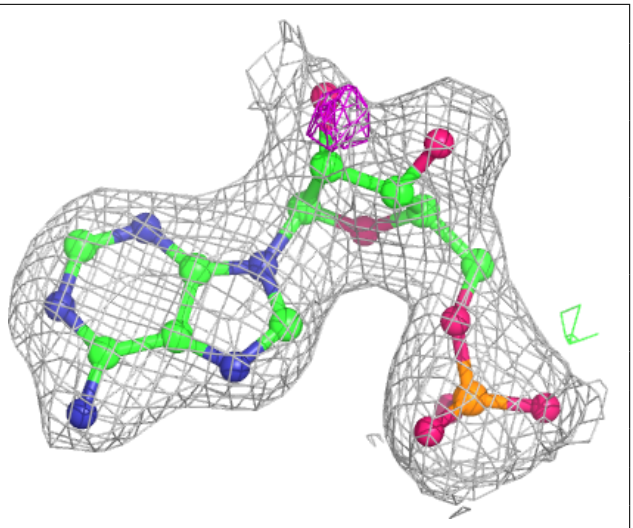


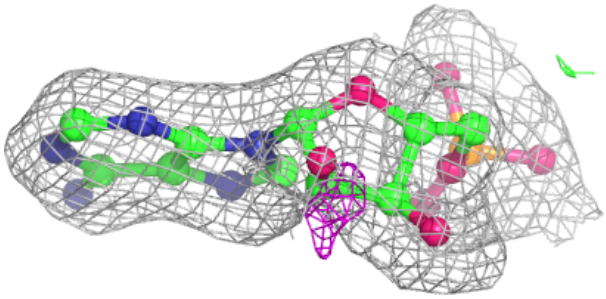


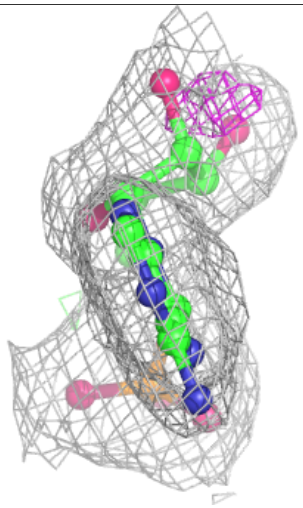


Electron density around AMP F 843:

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

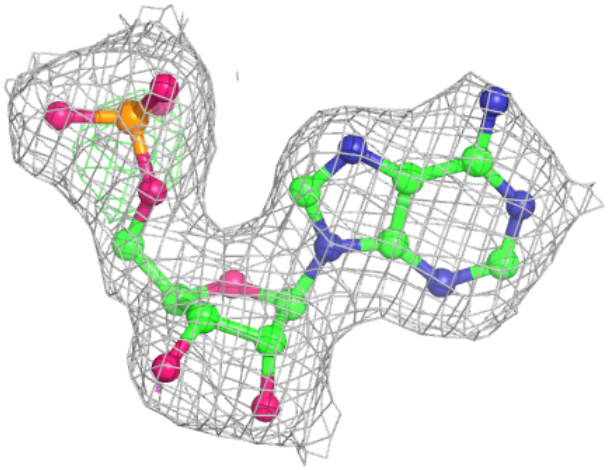


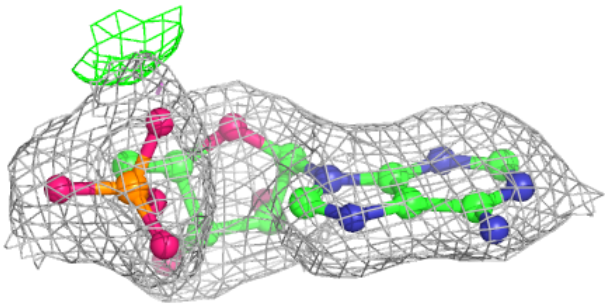




Electron density around AMP G 843:

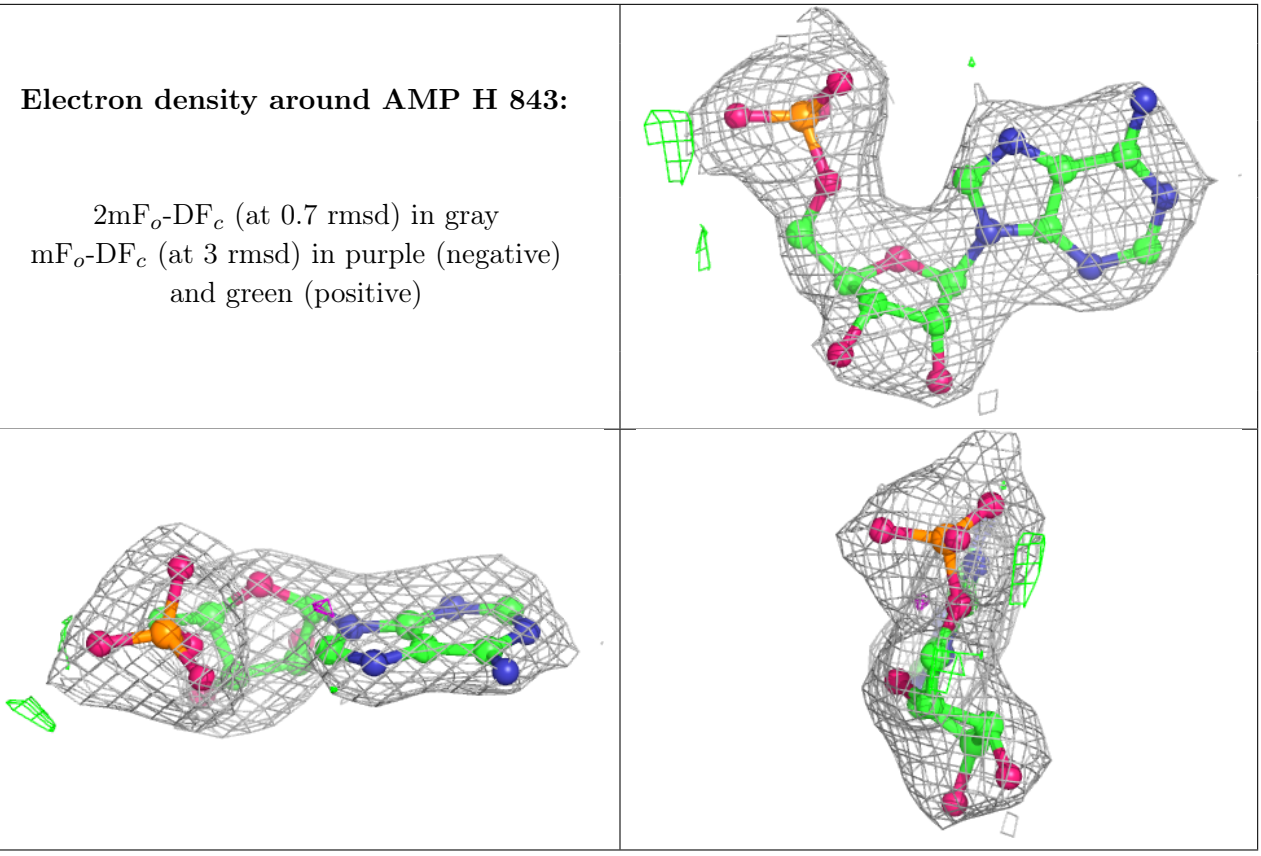
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





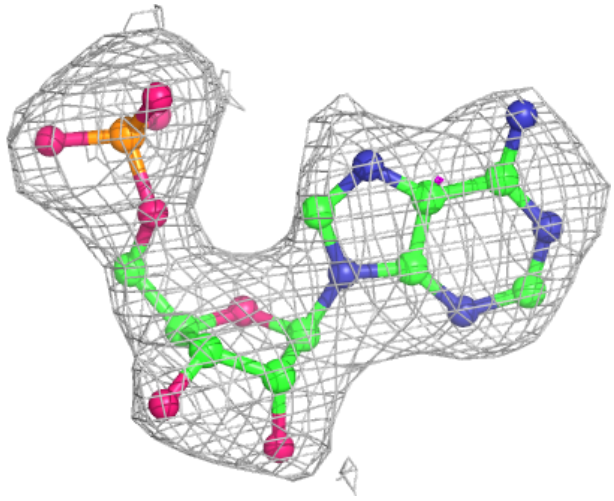
Electron density around AMP H 843:

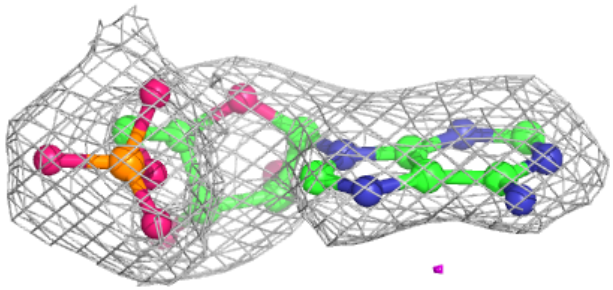
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

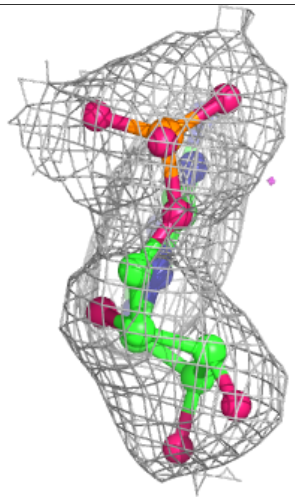


Electron density around AMP B 843:

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

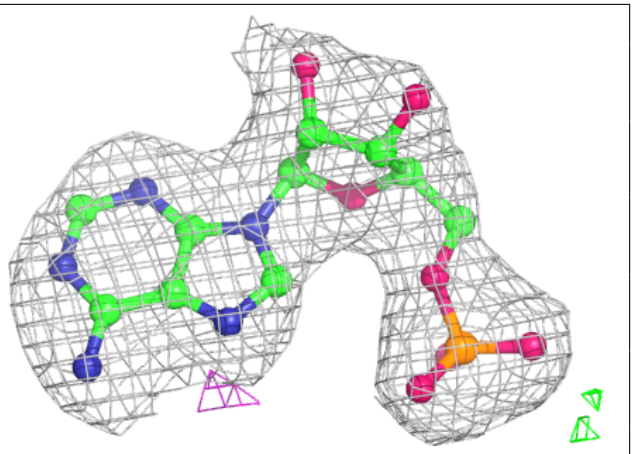


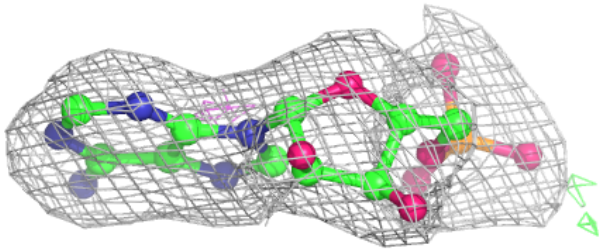


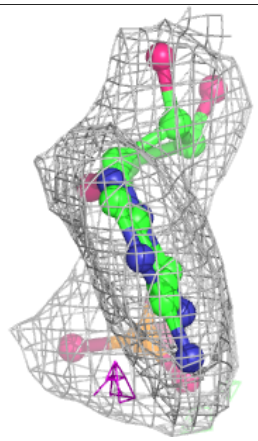


Electron density around AMP C 843:

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

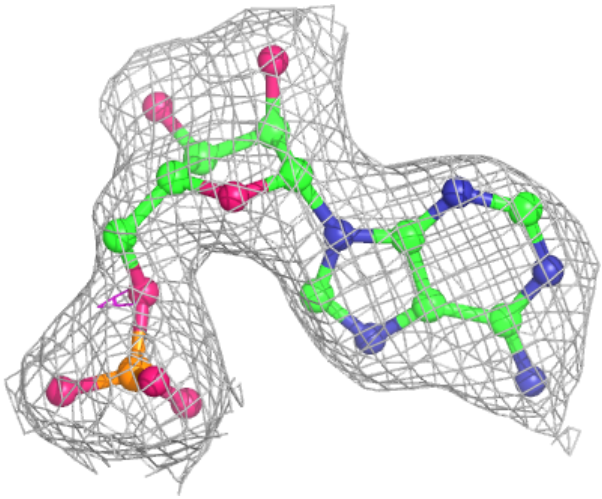


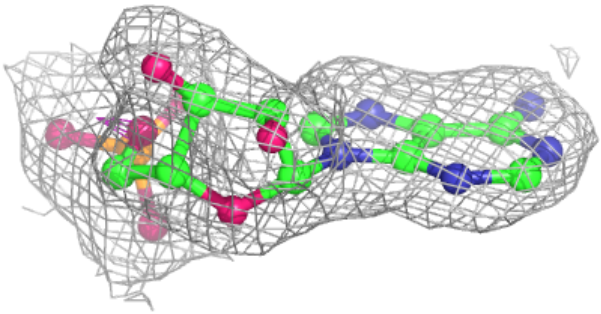


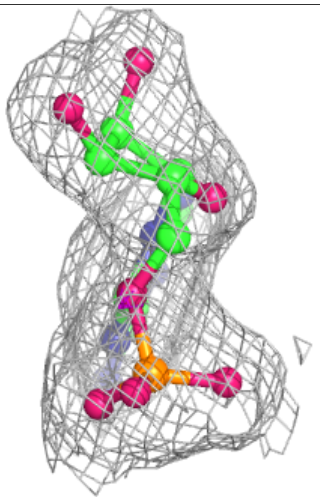


Electron density around AMP D 843:

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

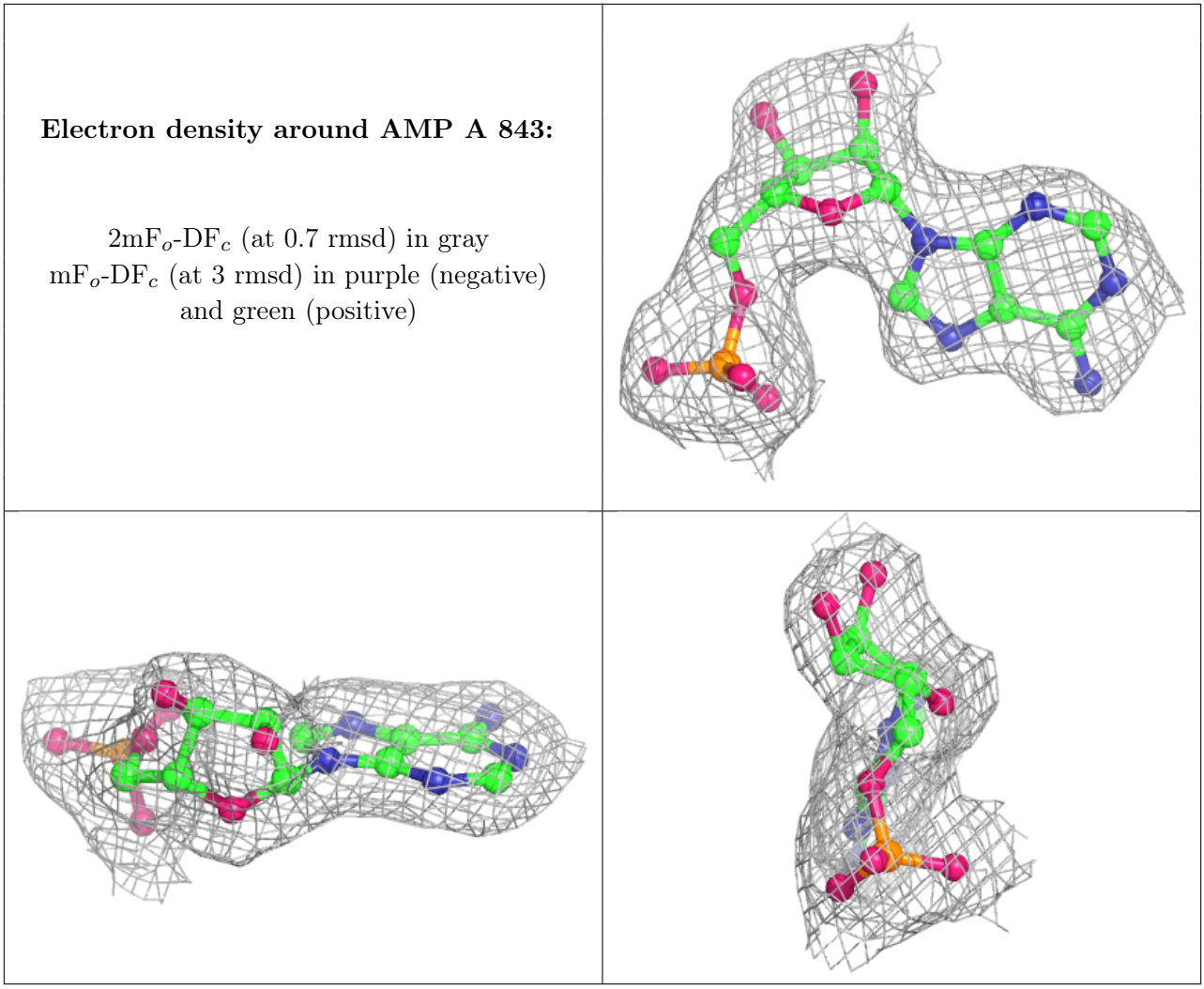






Electron density around AMP A 843:

$2mF_o$-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.