wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 06:43 PM EDT

PDB ID	:	6SY7
Title	:	Structure of Trypanosome Brucei Phosphofructokinase in complex with AMP.
Authors	:	McNae, I.W.; Vasquez-Valdivieso, M.G.; Walkinshaw, M.D.
Deposited on	:	2019-09-27
Resolution	:	2.75 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:

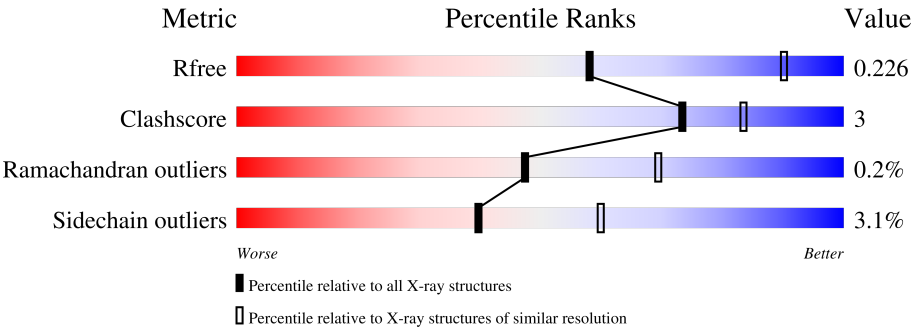
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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%

Mol	Chain	Length	Quality of chain
1	A	487	85% 7% • 7%
1	B	487	85% 8% 7%
1	C	487	82% 10% 7%
1	D	487	83% 9% 7%
1	E	487	83% 8% • 8%
1	F	487	83% 8% 8%
1	G	487	85% 7% • 7%

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Mol	Chain	Length	Quality of chain
1	H	487	

2 Entry composition (i)

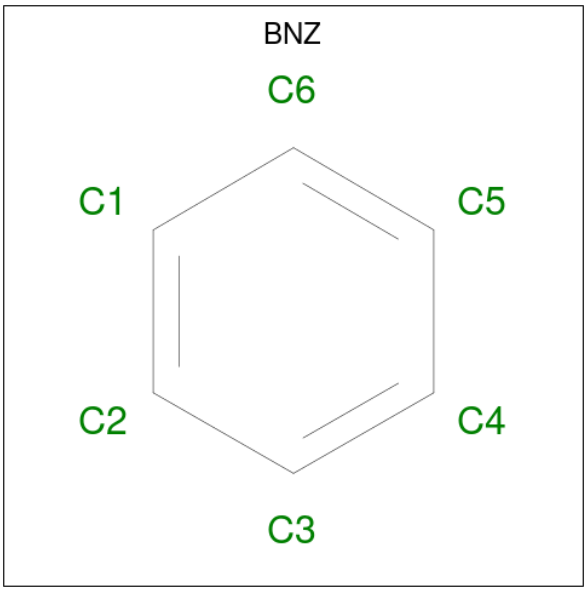
There are 5 unique types of molecules in this entry. The entry contains 28937 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent 6-phosphofructokinase.

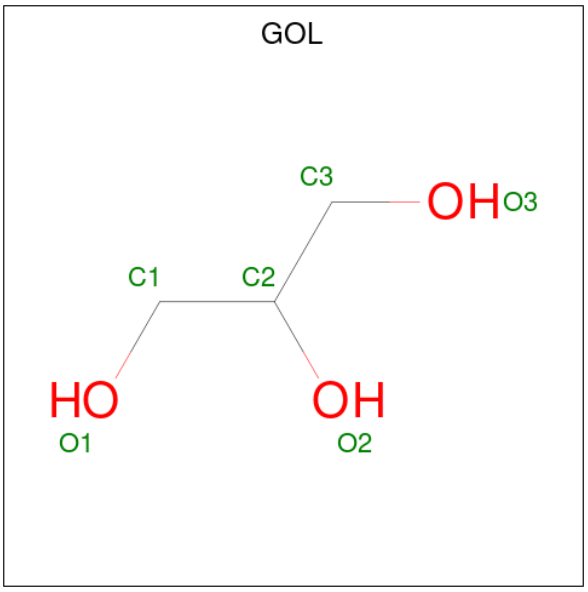
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3522	2208	643	654	17			
1	B	454	Total	C	N	O	S	0	0	0
			3514	2203	642	653	16			
1	C	451	Total	C	N	O	S	0	0	0
			3492	2190	638	648	16			
1	D	452	Total	C	N	O	S	0	0	0
			3498	2191	640	651	16			
1	E	450	Total	C	N	O	S	0	0	0
			3485	2185	637	647	16			
1	F	450	Total	C	N	O	S	0	0	0
			3486	2185	637	648	16			
1	G	452	Total	C	N	O	S	0	0	0
			3502	2195	640	651	16			
1	H	454	Total	C	N	O	S	0	0	0
			3518	2206	642	653	17			

- Molecule 2 is BENZENE (three-letter code: BNZ) (formula: C_6H_6).



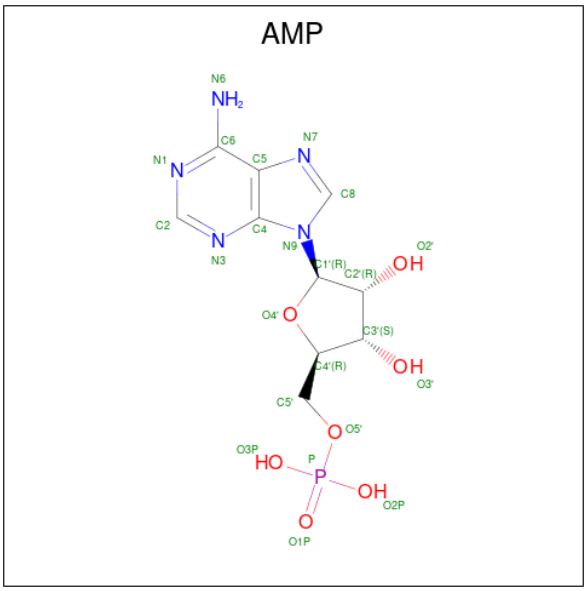
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 6 6	0	0
2	B	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	D	1	Total C 6 6	0	0
2	E	1	Total C 6 6	0	0
2	F	1	Total C 6 6	0	0
2	G	1	Total C 6 6	0	0
2	H	1	Total C 6 6	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	99	Total	O	0	0
			99	99		
5	B	96	Total	O	0	0
			96	96		
5	C	81	Total	O	0	0
			81	81		
5	D	74	Total	O	0	0
			74	74		

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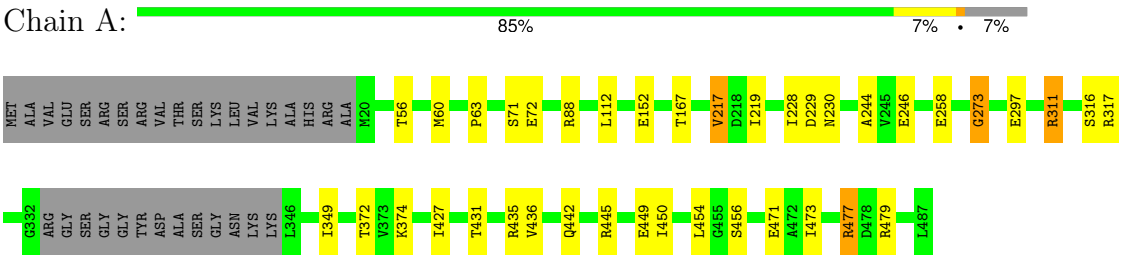
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	62	Total O 62 62	0	0
5	F	70	Total O 70 70	0	0
5	G	58	Total O 58 58	0	0
5	H	100	Total O 100 100	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

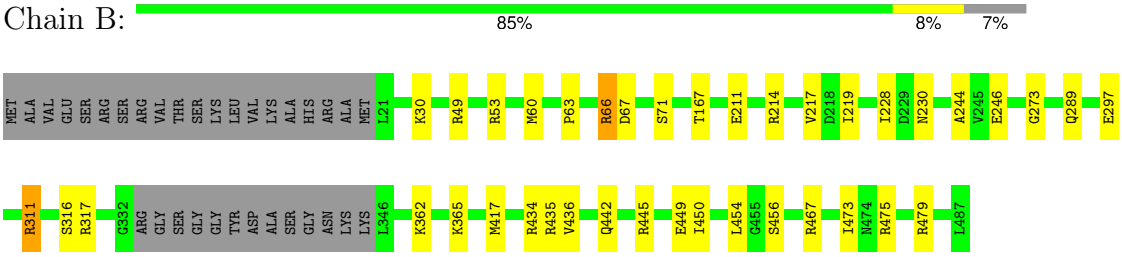
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain A:



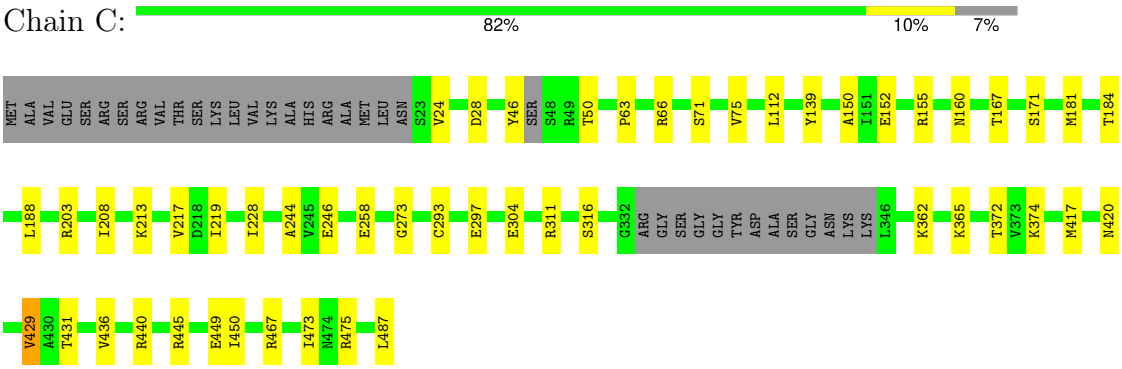
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain B:



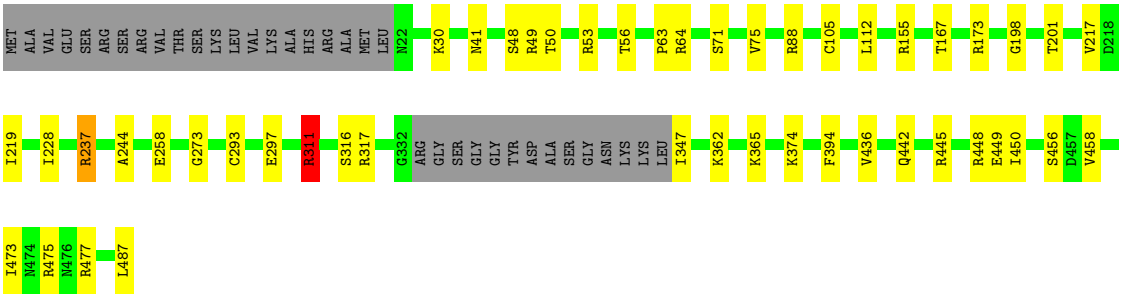
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain C:



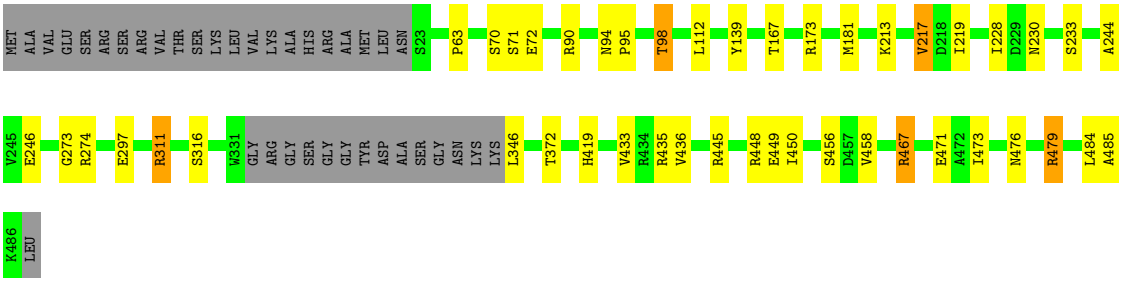
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain D:



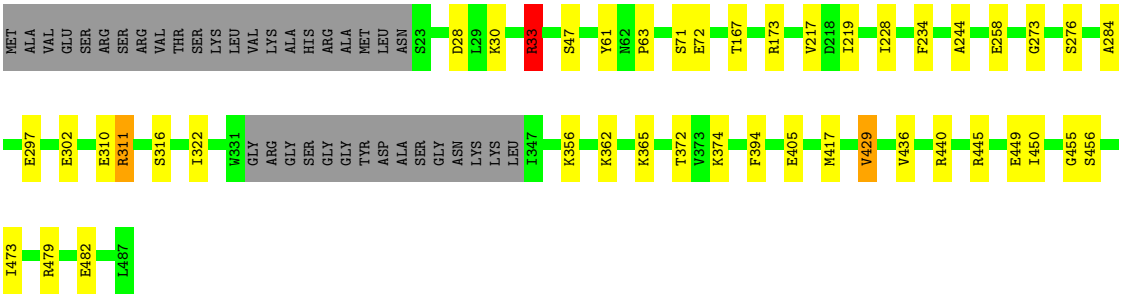
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain E:



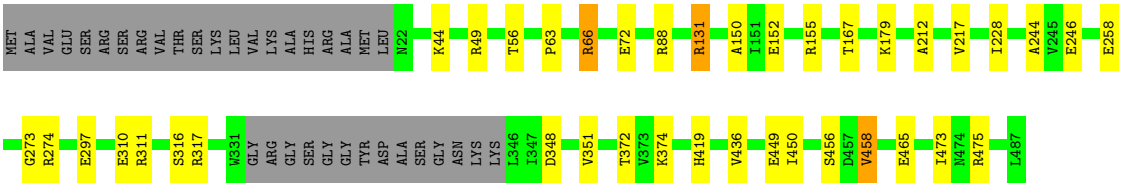
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain F:



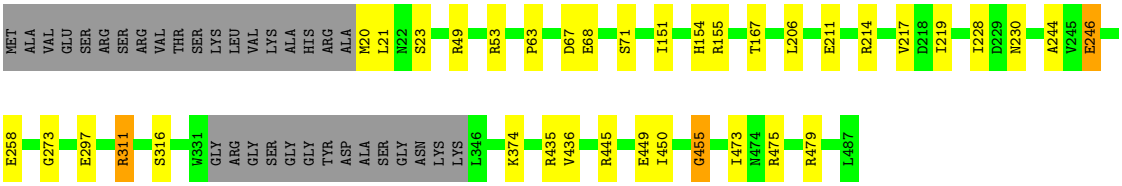
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain G:



• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain H:


MET ALA VAL GLU SER ARG SER ARG VAL THR SER LYS LEU VAL LYS ALA HIS ARG ALA M20 L21 N22 S23 R49 R53 P63 D67 E68 S71 I151 H154 R155 T167 L206 E211 R214 V217 D218 I219 I228 D229 N230 A244 V245 E246
E258 G273 E297 R311 S316 W331 GLY ARG GLY SER GLY GLY TYR ASP ALA SER GLY ASN LYS LYS L346 K374 R435 V436 R445 E449 I450 G455 I473 N474 R475 R479 L487

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.39Å 133.71Å 271.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 2.75 39.81 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.81-2.75) 98.8 (39.81-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	(Not available) , (Not available) 0.205 , 0.226	Depositor DCC
R_{free} test set	5586 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 27.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28937	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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: GOL, AMP, BNZ

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	0.69	2/3582 (0.1%)	0.81	1/4846 (0.0%)
1	B	0.68	2/3574 (0.1%)	0.82	2/4836 (0.0%)
1	C	0.66	0/3551	0.81	0/4803
1	D	0.68	0/3558	0.82	3/4814 (0.1%)
1	E	0.67	1/3545 (0.0%)	0.80	0/4798
1	F	0.66	0/3546	0.82	2/4798 (0.0%)
1	G	0.67	0/3562	0.81	3/4820 (0.1%)
1	H	0.69	1/3578 (0.0%)	0.81	1/4841 (0.0%)
All	All	0.68	6/28496 (0.0%)	0.81	12/38556 (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	F	0	1
1	H	0	1
All	All	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	246	GLU	CD-OE1	6.87	1.33	1.25
1	A	246	GLU	CD-OE2	6.60	1.32	1.25
1	B	246	GLU	CD-OE2	5.74	1.31	1.25
1	A	246	GLU	CD-OE1	5.42	1.31	1.25
1	E	246	GLU	CD-OE2	5.22	1.31	1.25

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	33	ARG	NE-CZ-NH1	-11.03	114.79	120.30
1	F	33	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	D	53	ARG	CB-CG-CD	6.78	129.22	111.60
1	D	237	ARG	CG-CD-NE	6.71	125.89	111.80
1	A	311	ARG	NE-CZ-NH2	-6.15	117.23	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	455	GLY	Peptide
1	H	455	GLY	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	3522	0	3573	25	0
1	B	3514	0	3564	23	0
1	C	3492	0	3541	34	0
1	D	3498	0	3542	34	0
1	E	3485	0	3533	32	0
1	F	3486	0	3533	23	0
1	G	3502	0	3550	22	0
1	H	3518	0	3570	24	0
2	A	6	0	6	0	0
2	B	6	0	6	0	0
2	C	6	0	6	0	0
2	D	6	0	6	0	0
2	E	6	0	6	0	0
2	F	6	0	6	0	0
2	G	6	0	6	0	0
2	H	6	0	6	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	1	0
3	D	6	0	8	1	0
3	E	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
4	A	23	0	12	1	0
4	B	23	0	12	2	0
4	C	23	0	12	2	0
4	D	23	0	12	1	0
4	F	46	0	24	2	0
4	G	23	0	12	2	0
4	H	23	0	12	1	0
5	A	99	0	0	1	0
5	B	96	0	0	1	0
5	C	81	0	0	3	0
5	D	74	0	0	2	0
5	E	62	0	0	5	0
5	F	70	0	0	0	0
5	G	58	0	0	3	0
5	H	100	0	0	3	0
All	All	28937	0	28614	190	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 3.

The worst 5 of 190 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:MET:HE1	1:B:60:MET:SD	1.99	1.01
1:A:60:MET:CE	1:B:60:MET:SD	2.53	0.96
1:D:105:CYS:HB2	1:D:201:THR:HG21	1.46	0.95
1:B:473:ILE:HG23	1:C:473:ILE:HG23	1.50	0.94
1:D:311:ARG:HG2	1:D:311:ARG:HH11	1.34	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	451/487 (93%)	441 (98%)	9 (2%)	1 (0%)	47	69
1	B	450/487 (92%)	440 (98%)	9 (2%)	1 (0%)	47	69
1	C	445/487 (91%)	435 (98%)	9 (2%)	1 (0%)	47	69
1	D	448/487 (92%)	438 (98%)	9 (2%)	1 (0%)	47	69
1	E	446/487 (92%)	436 (98%)	9 (2%)	1 (0%)	47	69
1	F	446/487 (92%)	436 (98%)	9 (2%)	1 (0%)	47	69
1	G	448/487 (92%)	437 (98%)	10 (2%)	1 (0%)	47	69
1	H	450/487 (92%)	437 (97%)	12 (3%)	1 (0%)	47	69
All	All	3584/3896 (92%)	3500 (98%)	76 (2%)	8 (0%)	47	69

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	273	GLY
1	F	273	GLY
1	A	273	GLY
1	B	273	GLY
1	D	273	GLY

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	381/405 (94%)	370 (97%)	11 (3%)	42	62
1	B	380/405 (94%)	369 (97%)	11 (3%)	42	62
1	C	377/405 (93%)	362 (96%)	15 (4%)	31	51
1	D	378/405 (93%)	367 (97%)	11 (3%)	42	62
1	E	377/405 (93%)	363 (96%)	14 (4%)	34	54
1	F	377/405 (93%)	363 (96%)	14 (4%)	34	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	379/405 (94%)	368 (97%)	11 (3%)	42 62
1	H	381/405 (94%)	373 (98%)	8 (2%)	53 71
All	All	3030/3240 (94%)	2935 (97%)	95 (3%)	40 60

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	311	ARG
1	F	372	THR
1	E	372	THR
1	F	72	GLU
1	F	482	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	154	HIS
1	H	364	ASN
1	C	176	GLN
1	D	22	ASN
1	D	250	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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	$\#\|Z\| > 2$
4	AMP	H	1001	-	21,25,25	0.62	0	23,38,38	0.78	1 (4%)
2	BNZ	A	501	-	6,6,6	0.75	0	6,6,6	0.43	0
3	GOL	G	502	-	5,5,5	0.13	0	5,5,5	0.45	0
3	GOL	F	1004	-	5,5,5	0.11	0	5,5,5	0.28	0
4	AMP	F	1002	-	21,25,25	0.65	0	23,38,38	0.94	1 (4%)
3	GOL	A	502	-	5,5,5	0.15	0	5,5,5	0.54	0
3	GOL	B	1003	-	5,5,5	0.19	0	5,5,5	0.53	0
4	AMP	A	503	-	21,25,25	0.64	0	23,38,38	1.00	1 (4%)
2	BNZ	E	501	-	6,6,6	0.78	0	6,6,6	0.42	0
3	GOL	D	1003	-	5,5,5	0.23	0	5,5,5	0.38	0
4	AMP	D	1001	-	21,25,25	0.69	0	23,38,38	1.13	2 (8%)
4	AMP	F	1001	-	21,25,25	0.57	0	23,38,38	0.81	1 (4%)
3	GOL	E	502	-	5,5,5	0.10	0	5,5,5	0.32	0
4	AMP	B	1001	-	21,25,25	0.61	0	23,38,38	1.05	1 (4%)
2	BNZ	B	1002	-	6,6,6	0.95	0	6,6,6	0.54	0
2	BNZ	F	1003	-	6,6,6	0.69	0	6,6,6	0.35	0
2	BNZ	H	1002	-	6,6,6	1.26	1 (16%)	6,6,6	1.03	0
2	BNZ	D	1002	-	6,6,6	0.66	0	6,6,6	0.52	0
4	AMP	G	503	-	21,25,25	0.58	0	23,38,38	0.84	1 (4%)
4	AMP	C	503	-	21,25,25	0.65	0	23,38,38	0.85	1 (4%)
2	BNZ	G	501	-	6,6,6	0.62	0	6,6,6	0.49	0
3	GOL	C	502	-	5,5,5	0.18	0	5,5,5	0.22	0
3	GOL	H	1003	-	5,5,5	0.21	0	5,5,5	0.34	0
2	BNZ	C	501	-	6,6,6	0.69	0	6,6,6	0.45	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
4	AMP	H	1001	-	-	3/6/26/26	0/3/3/3
2	BNZ	A	501	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	G	502	-	-	2/4/4/4	-
3	GOL	F	1004	-	-	4/4/4/4	-
4	AMP	F	1002	-	-	2/6/26/26	0/3/3/3
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	B	1003	-	-	2/4/4/4	-
4	AMP	A	503	-	-	3/6/26/26	0/3/3/3
2	BNZ	E	501	-	-	-	0/1/1/1
3	GOL	D	1003	-	-	0/4/4/4	-
4	AMP	D	1001	-	-	1/6/26/26	0/3/3/3
4	AMP	F	1001	-	-	2/6/26/26	0/3/3/3
3	GOL	E	502	-	-	2/4/4/4	-
4	AMP	B	1001	-	-	0/6/26/26	0/3/3/3
2	BNZ	B	1002	-	-	-	0/1/1/1
2	BNZ	F	1003	-	-	-	0/1/1/1
2	BNZ	H	1002	-	-	-	0/1/1/1
2	BNZ	D	1002	-	-	-	0/1/1/1
4	AMP	G	503	-	-	1/6/26/26	0/3/3/3
4	AMP	C	503	-	-	4/6/26/26	0/3/3/3
2	BNZ	G	501	-	-	-	0/1/1/1
3	GOL	C	502	-	-	0/4/4/4	-
3	GOL	H	1003	-	-	3/4/4/4	-
2	BNZ	C	501	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1002	BNZ	C2-C1	2.31	1.43	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1001	AMP	C5-C6-N6	2.96	124.82	120.31
4	A	503	AMP	C5-C6-N6	2.96	124.82	120.31
4	D	1001	AMP	C5-C6-N6	2.84	124.64	120.31
4	F	1002	AMP	C5-C6-N6	2.76	124.52	120.31
4	H	1001	AMP	C5-C6-N6	2.59	124.26	120.31

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
3	E	502	GOL	O1-C1-C2-C3
3	G	502	GOL	C1-C2-C3-O3
3	H	1003	GOL	C1-C2-C3-O3

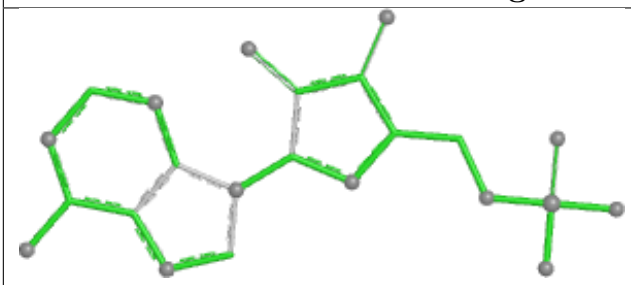
There are no ring outliers.

10 monomers are involved in 13 short contacts:

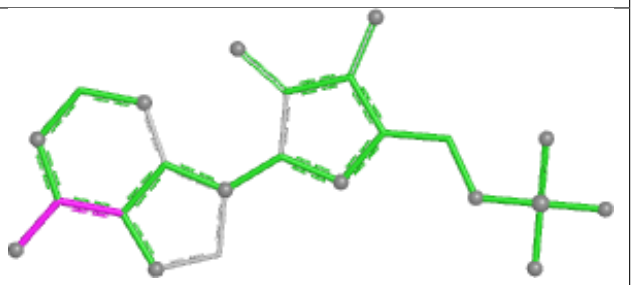
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1001	AMP	1	0
4	F	1002	AMP	1	0
4	A	503	AMP	1	0
3	D	1003	GOL	1	0
4	D	1001	AMP	1	0
4	F	1001	AMP	1	0
4	B	1001	AMP	2	0
4	G	503	AMP	2	0
4	C	503	AMP	2	0
3	C	502	GOL	1	0

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.

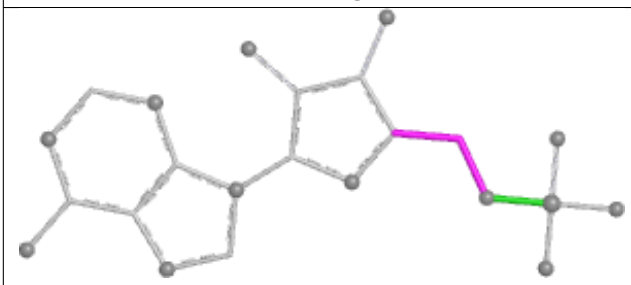
Ligand AMP H 1001



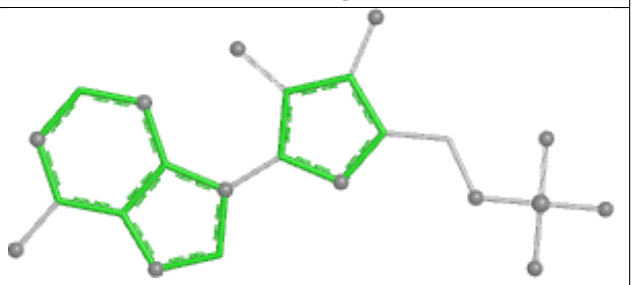
Bond lengths



Bond angles

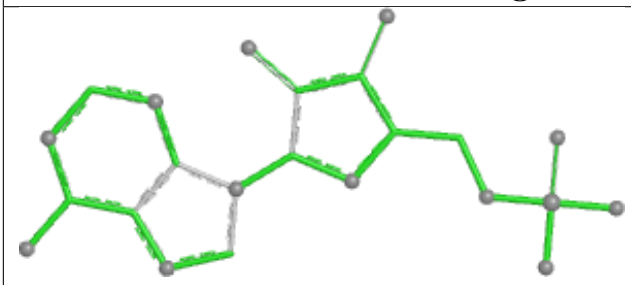


Torsions

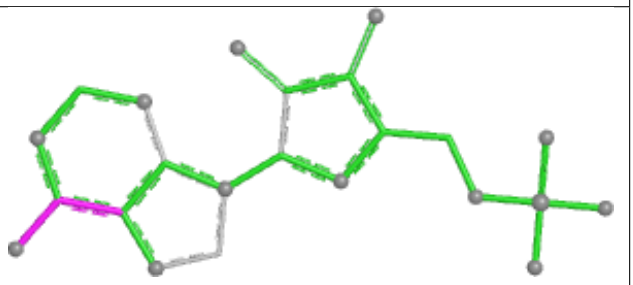


Rings

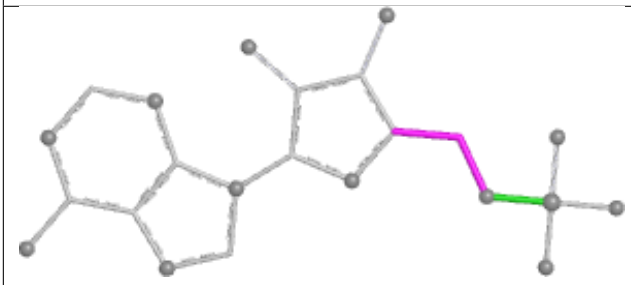
Ligand AMP F 1002



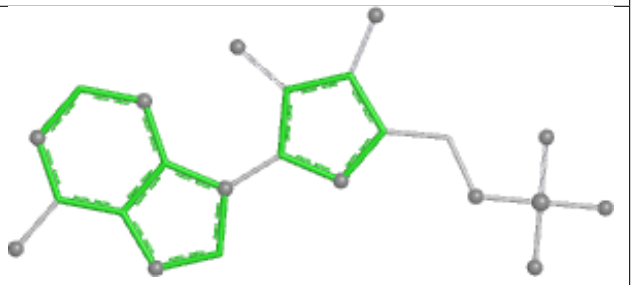
Bond lengths



Bond angles

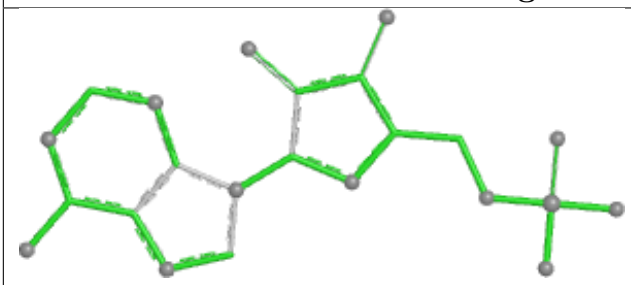


Torsions

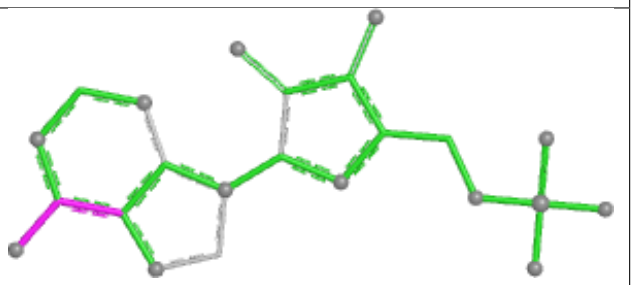


Rings

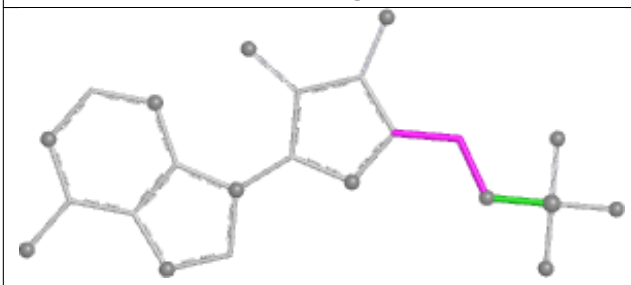
Ligand AMP A 503



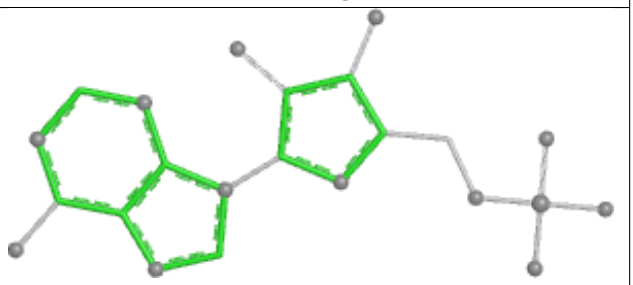
Bond lengths



Bond angles

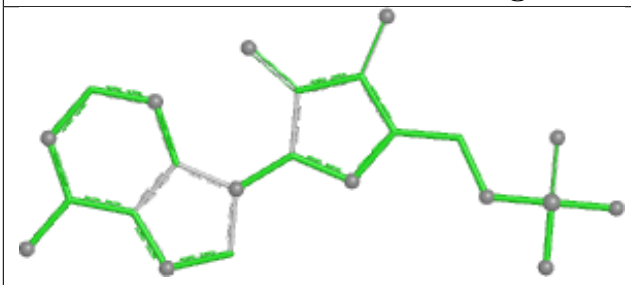


Torsions

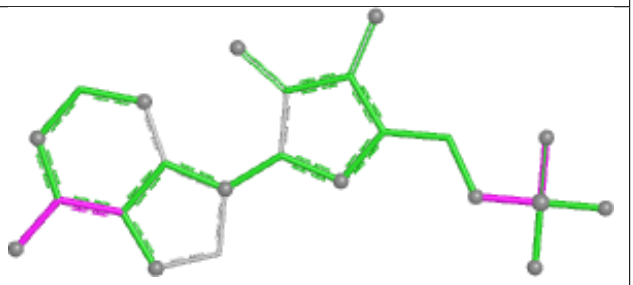


Rings

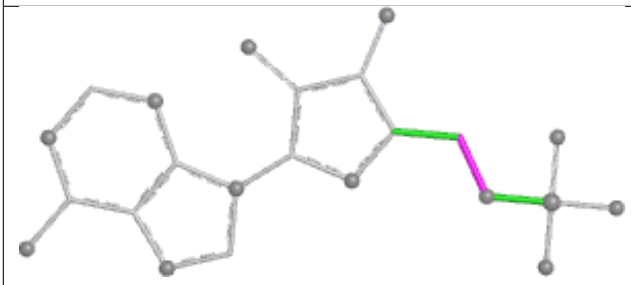
Ligand AMP D 1001



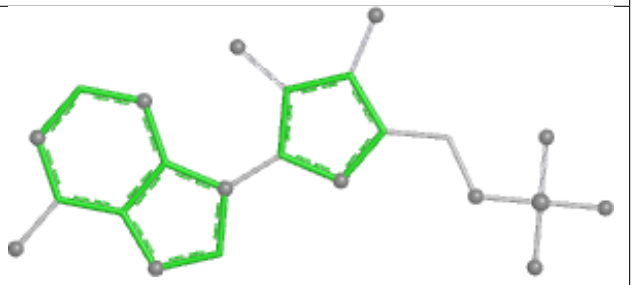
Bond lengths



Bond angles

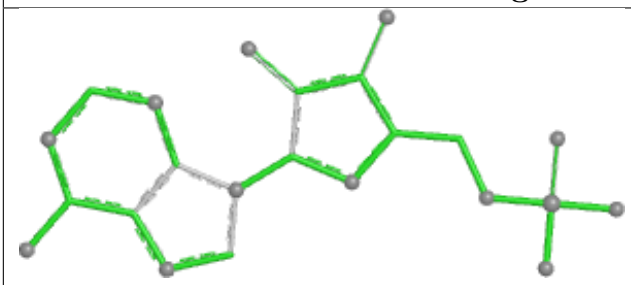


Torsions

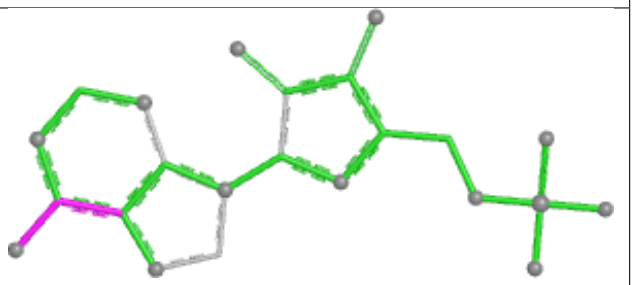


Rings

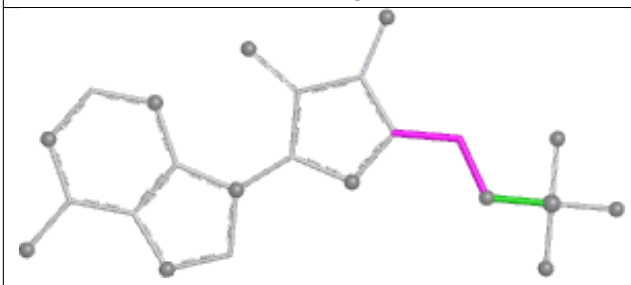
Ligand AMP F 1001



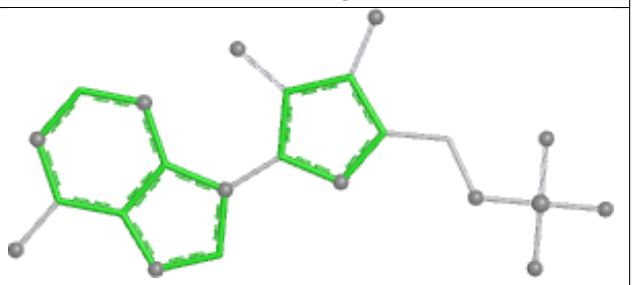
Bond lengths



Bond angles

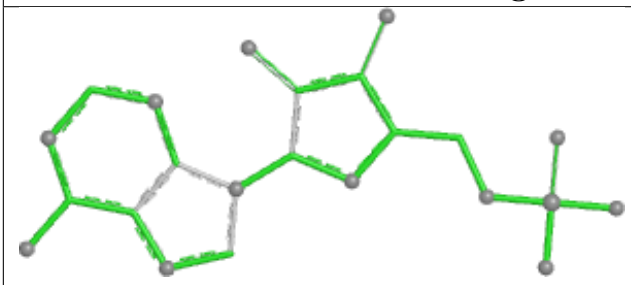


Torsions

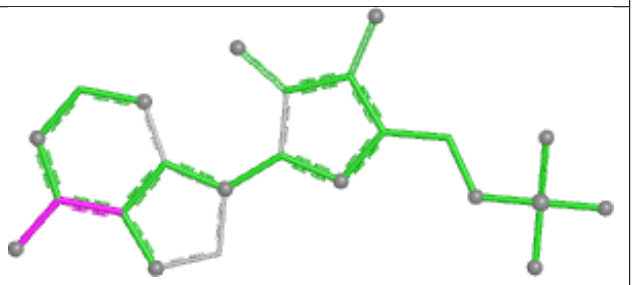


Rings

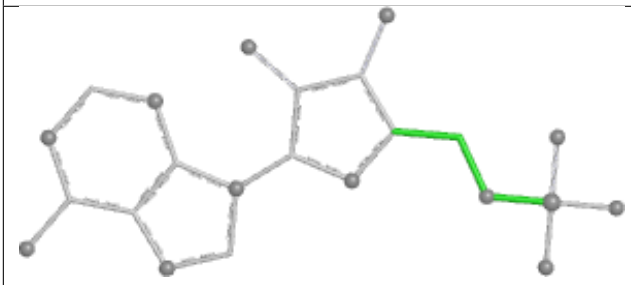
Ligand AMP B 1001



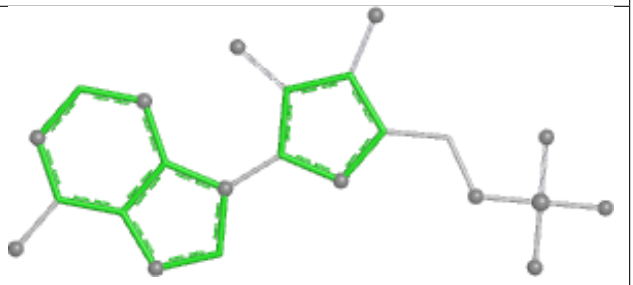
Bond lengths



Bond angles

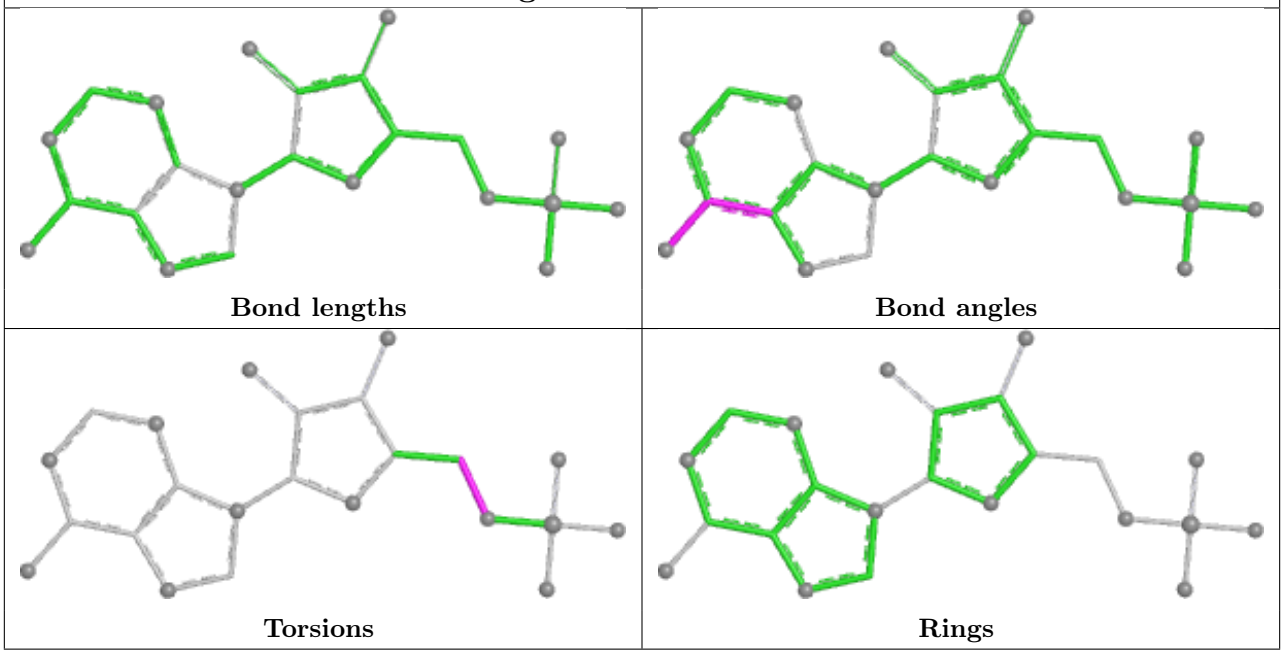


Torsions

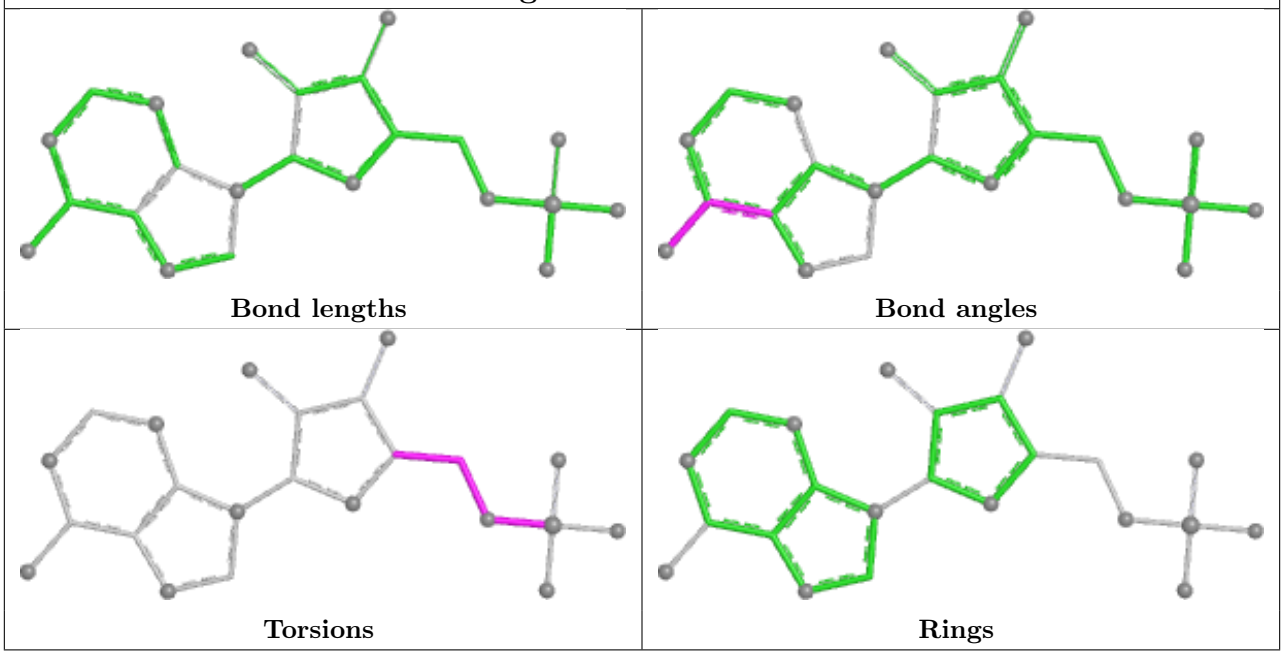


Rings

Ligand AMP G 503



Ligand AMP C 503



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

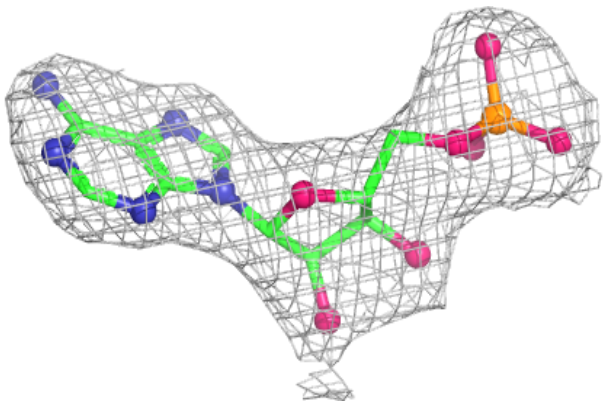
6.4 Ligands

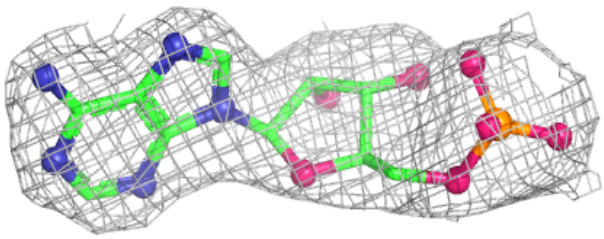
Unable to reproduce the depositors R factor - this section is therefore empty.

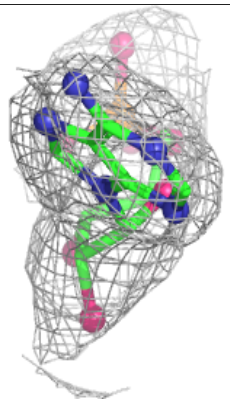
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP A 503:

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

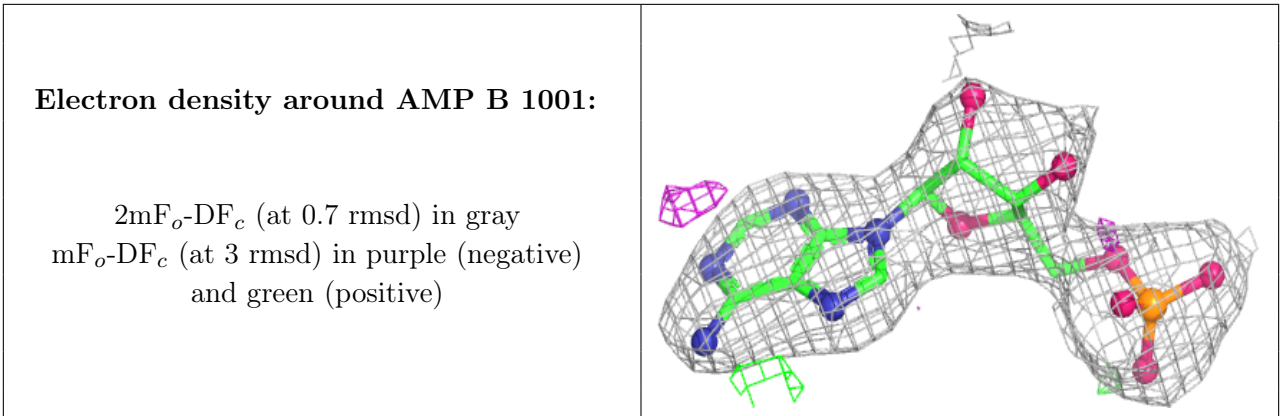


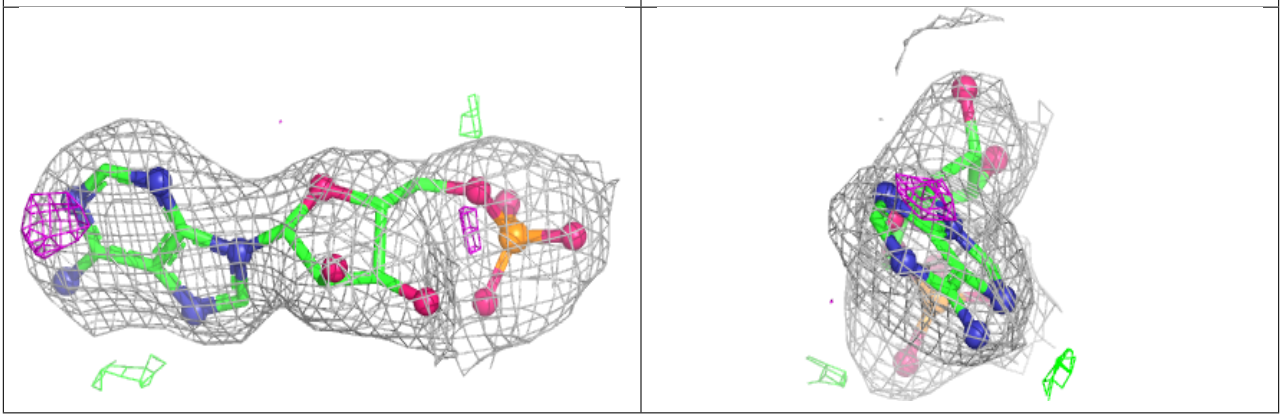




Electron density around AMP B 1001:

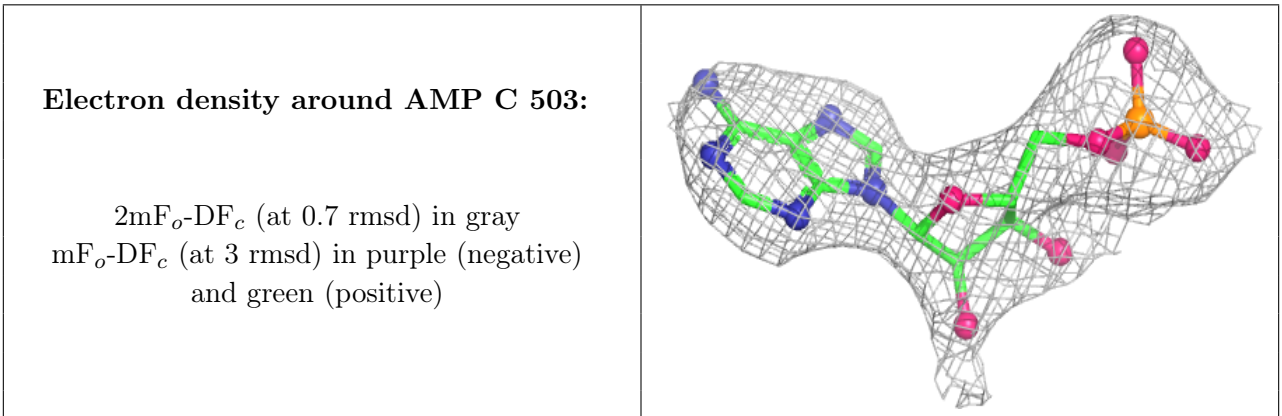
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

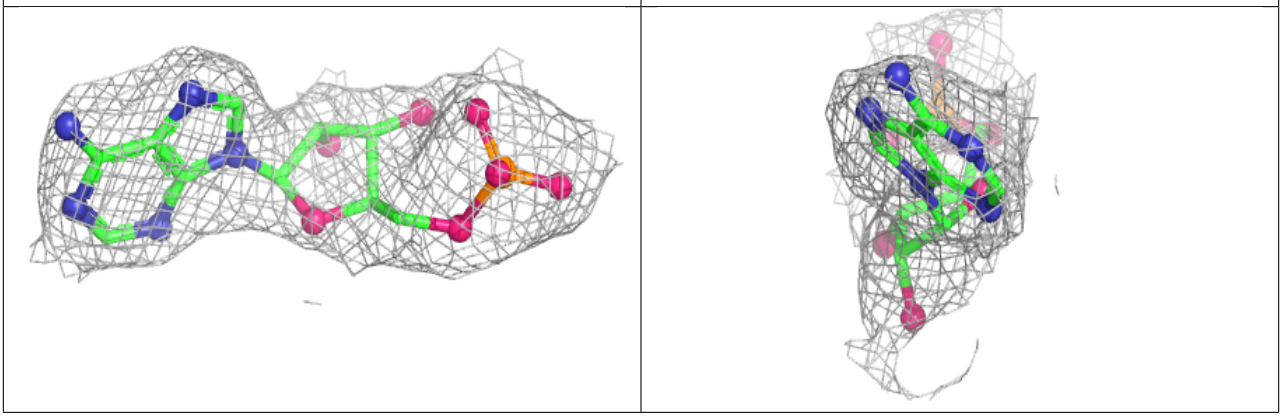




Electron density around AMP C 503:

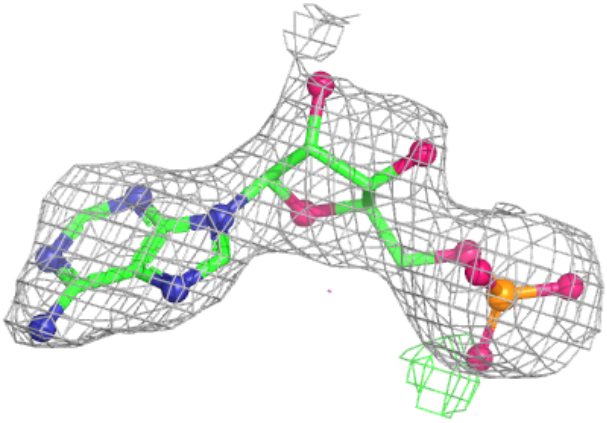
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

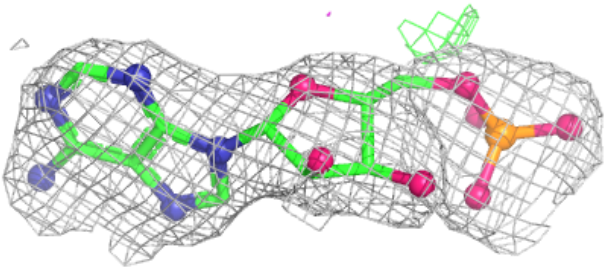


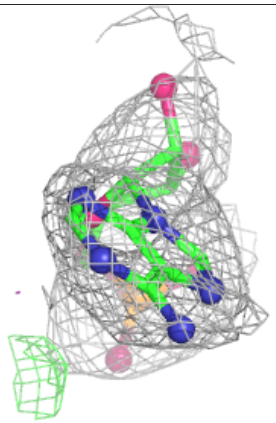


Electron density around AMP D 1001:

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

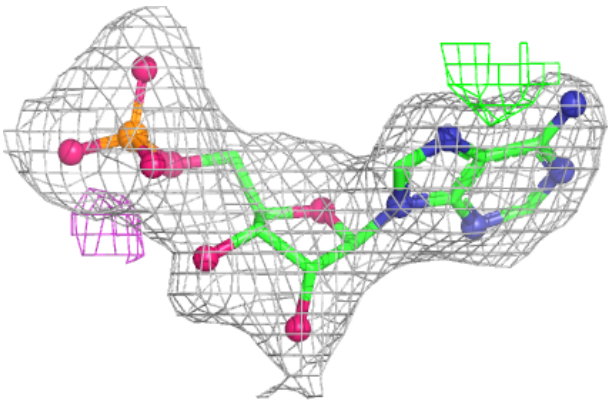


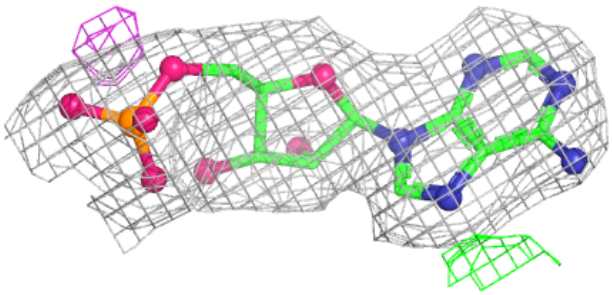


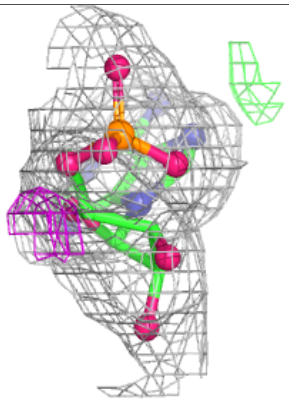


Electron density around AMP F 1001:

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

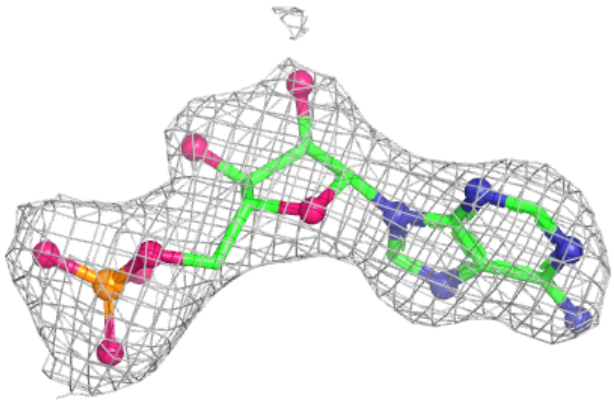


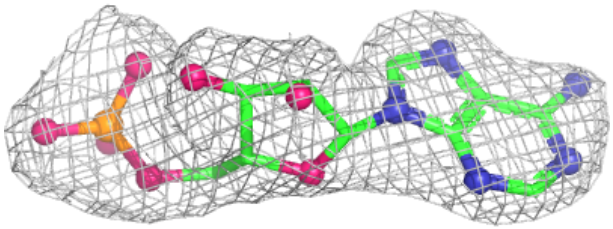


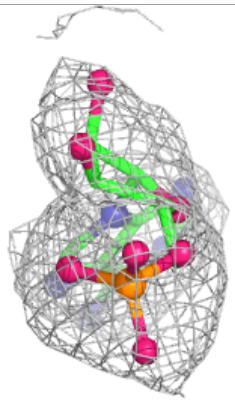


Electron density around AMP F 1002:

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

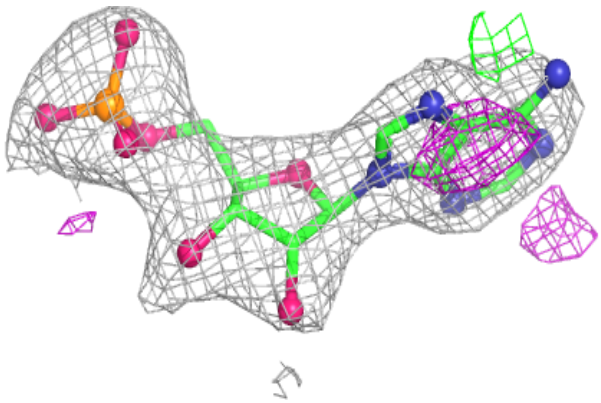


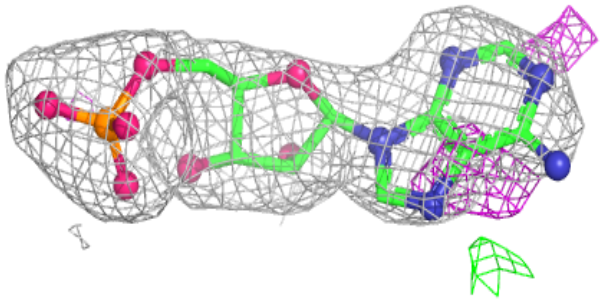


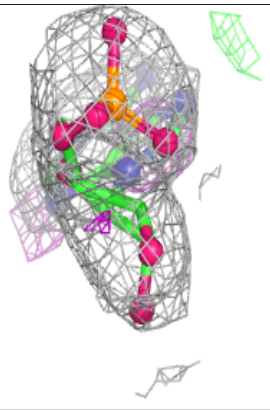


Electron density around AMP G 503:

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

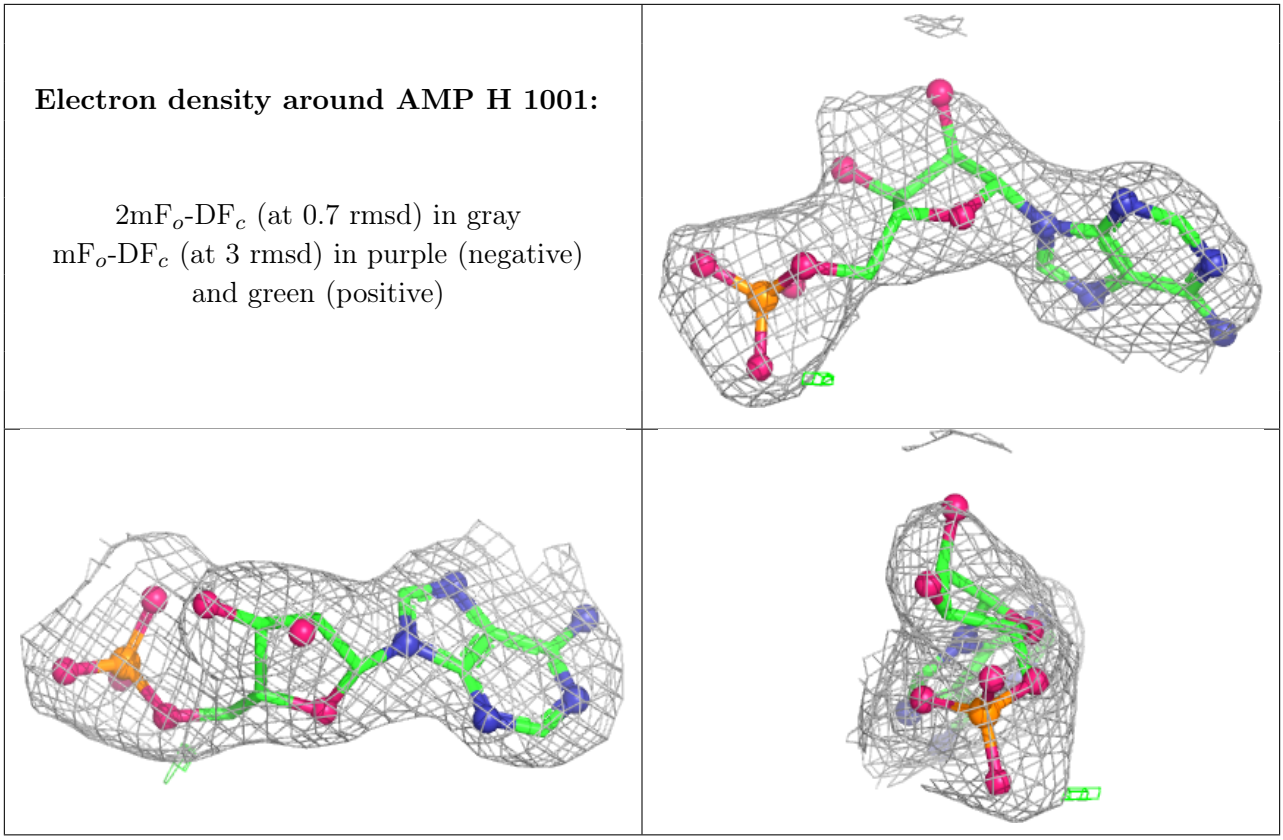






Electron density around AMP H 1001:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.