



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 06:30 AM BST

PDB ID : 6P6U  
Title : Crystal Structure of Monoclinic Rabbit Muscle Lactate Dehydrogenase with Four Tetramers as the Asymmetric Unit  
Authors : McPherson, A.  
Deposited on : 2019-06-04  
Resolution : 2.42 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

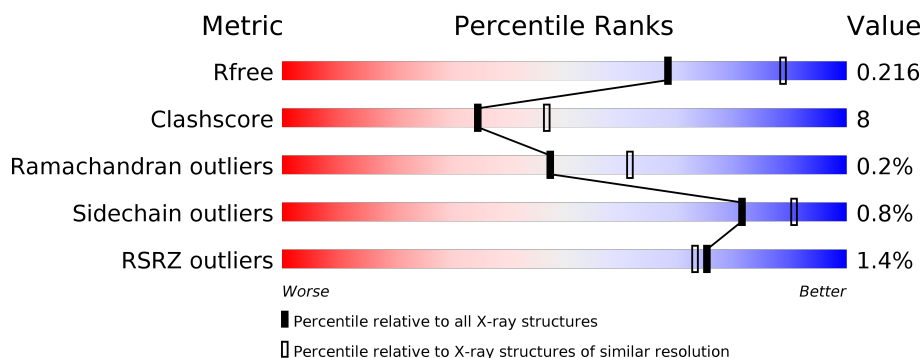
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	332	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	332	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>11%</div> </div> </div>
1	C	332	<div> <div></div> <div> <div></div> <div>86%</div> <div>12%</div> </div> </div>
1	D	332	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
1	E	332	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>
1	F	332	<div> <div></div> <div> <div></div> <div>84%</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	332	 89% 10% •
1	H	332	 82% 18%
1	I	332	 86% 13% •
1	J	332	 82% 17%
1	K	332	 85% 15%
1	L	332	 86% 13% •
1	M	332	 86% 14%
1	N	332	 87% 12% •
1	O	332	 82% 16% •
1	P	332	 85% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AMP	C	401	-	-	X	X
2	AMP	E	401	-	-	X	X

## 2 Entry composition [i](#)

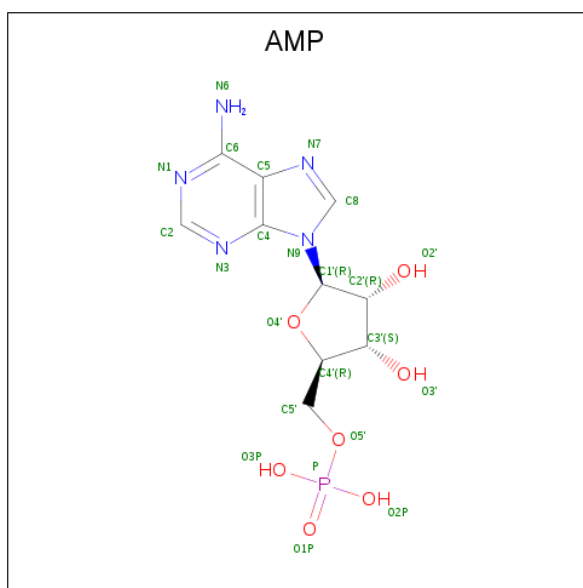
There are 3 unique types of molecules in this entry. The entry contains 42467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	1	0
			2565	1637	442	472	14			
1	B	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	C	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	D	331	Total	C	N	O	S	0	1	0
			2564	1637	441	471	15			
1	E	331	Total	C	N	O	S	0	2	0
			2573	1642	444	473	14			
1	F	331	Total	C	N	O	S	0	3	0
			2578	1645	444	475	14			
1	G	331	Total	C	N	O	S	0	1	0
			2563	1637	441	471	14			
1	H	331	Total	C	N	O	S	0	1	0
			2564	1638	441	471	14			
1	I	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	J	331	Total	C	N	O	S	0	1	0
			2567	1638	444	471	14			
1	K	331	Total	C	N	O	S	0	1	0
			2565	1637	442	472	14			
1	L	331	Total	C	N	O	S	0	2	0
			2567	1639	441	472	15			
1	M	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	N	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	O	331	Total	C	N	O	S	0	2	0
			2574	1643	446	471	14			
1	P	331	Total	C	N	O	S	0	1	0
			2565	1637	441	473	14			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	107	Total	O	0	0
			107	107		
3	C	94	Total	O	0	0
			94	94		
3	D	113	Total	O	0	0
			113	113		
3	E	93	Total	O	0	0
			93	93		
3	F	95	Total	O	0	1
			96	96		
3	G	122	Total	O	0	0
			122	122		
3	H	117	Total	O	0	0
			117	117		
3	I	61	Total	O	0	0
			61	61		

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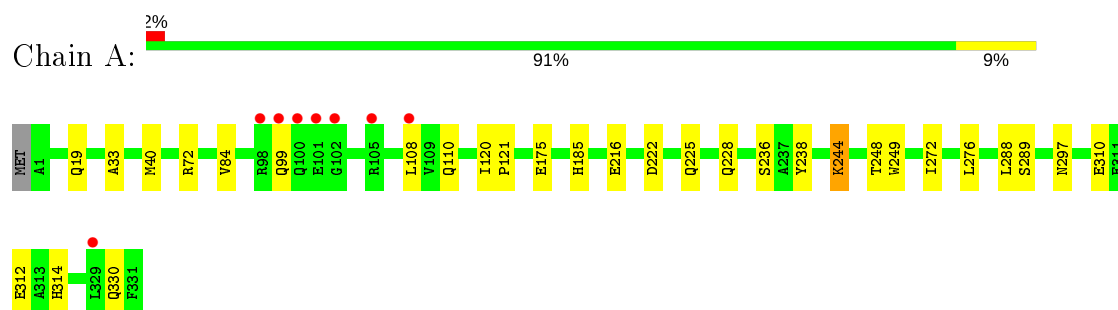
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	54	Total 54	O 54	0	0
3	K	65	Total 65	O 65	0	0
3	L	77	Total 77	O 77	0	0
3	M	66	Total 66	O 66	0	0
3	N	72	Total 72	O 72	0	0
3	O	61	Total 61	O 61	0	0
3	P	83	Total 83	O 83	0	0

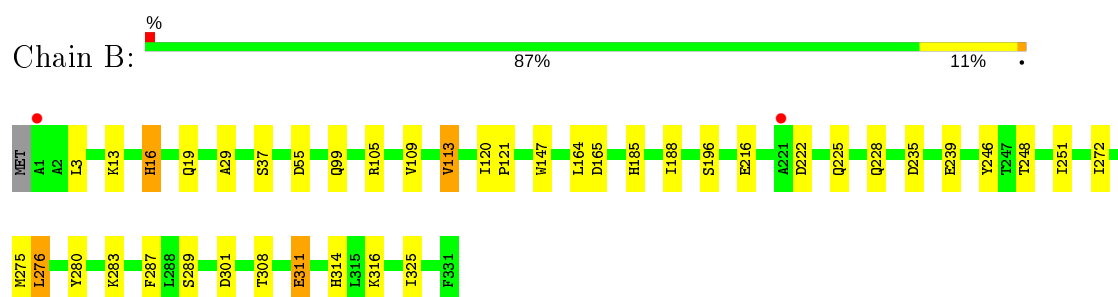
### 3 Residue-property plots

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.

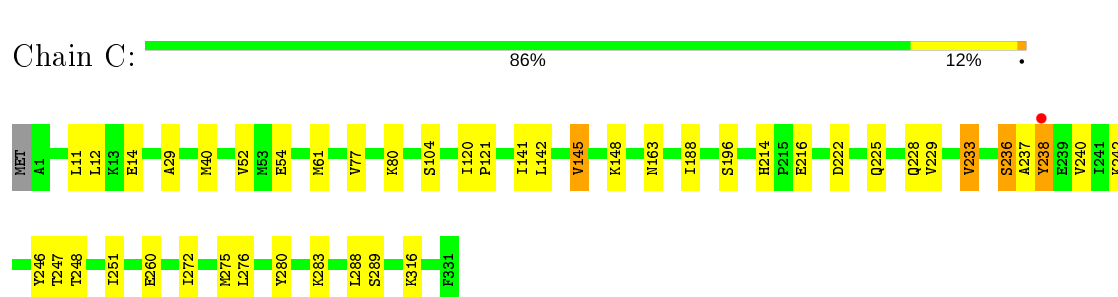
- Molecule 1: L-lactate dehydrogenase A chain



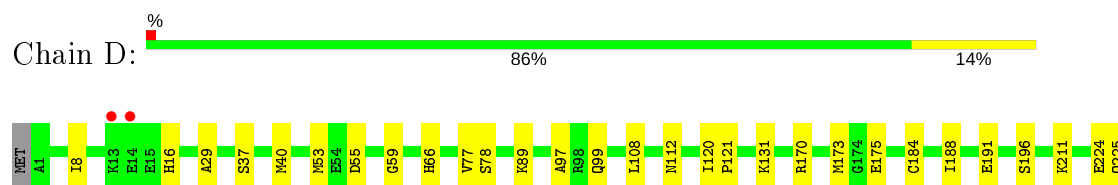
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain

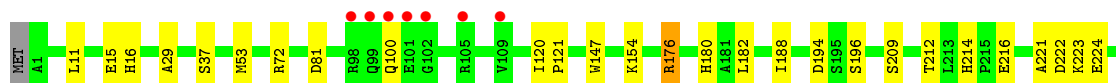
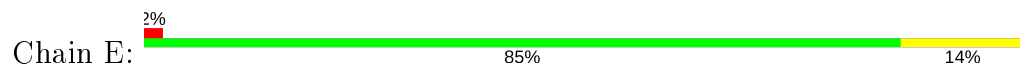


- Molecule 1: L-lactate dehydrogenase A chain

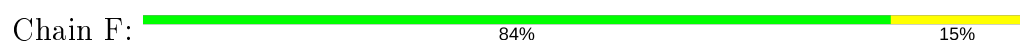




- Molecule 1: L-lactate dehydrogenase A chain



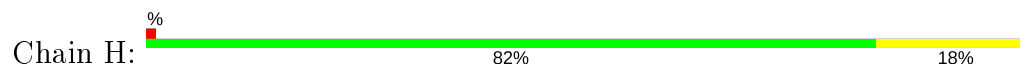
- Molecule 1: L-lactate dehydrogenase A chain



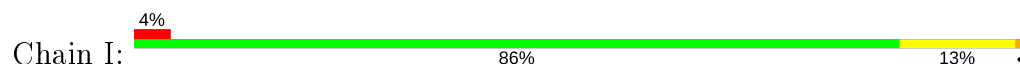
- Molecule 1: L-lactate dehydrogenase A chain



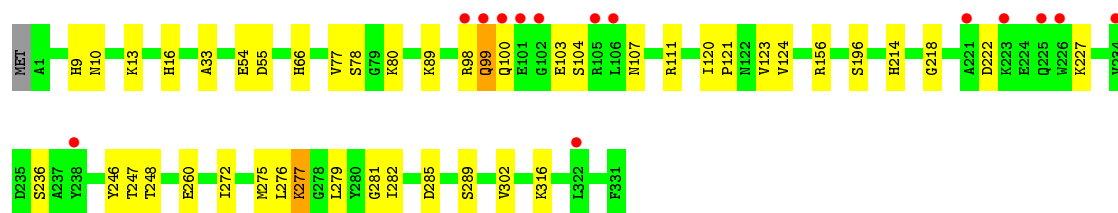
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain

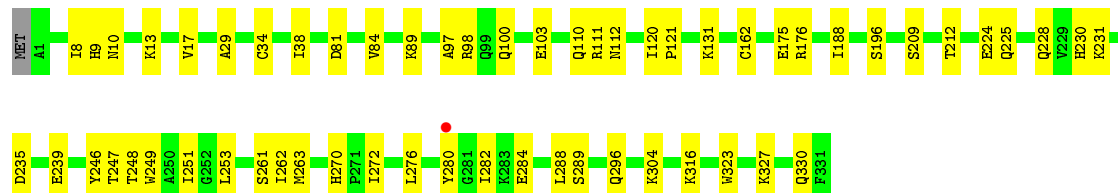






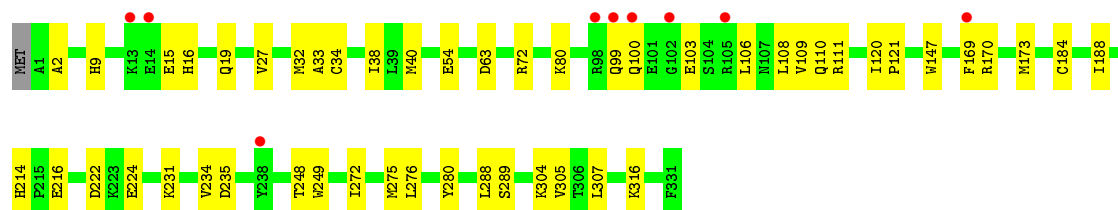
- Molecule 1: L-lactate dehydrogenase A chain

Chain J: 82% 17%



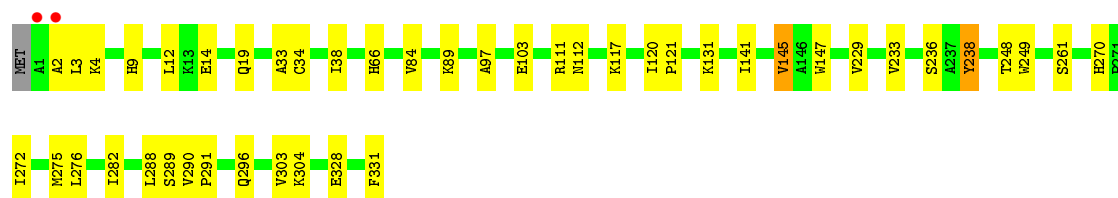
- Molecule 1: L-lactate dehydrogenase A chain

Chain K: 85% 15%



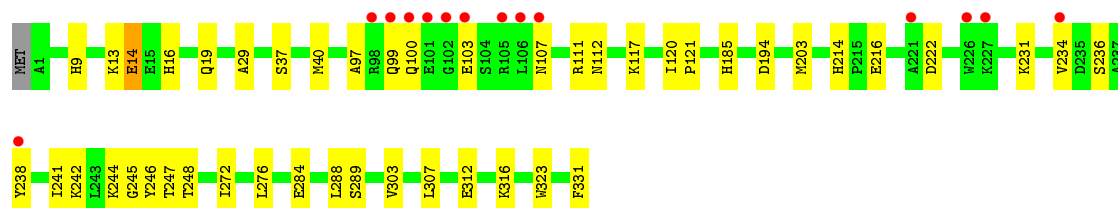
- Molecule 1: L-lactate dehydrogenase A chain

Chain L: 86% 13%

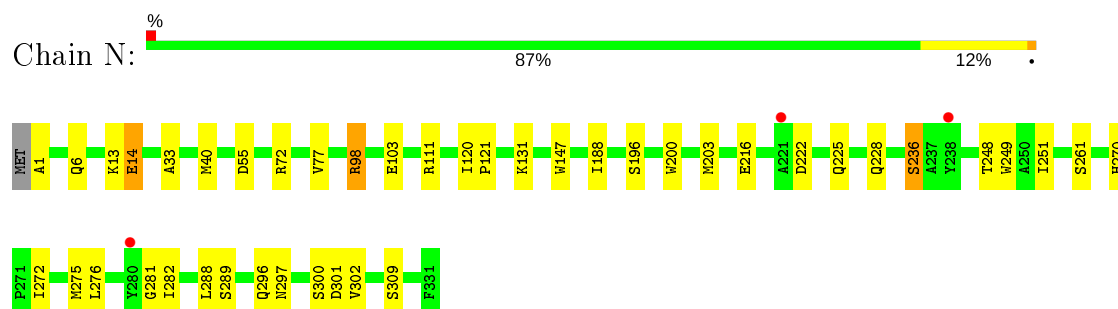


- Molecule 1: L-lactate dehydrogenase A chain

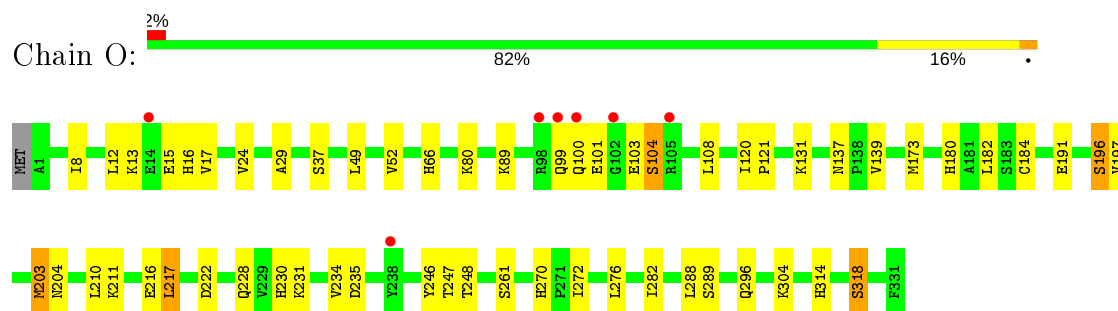
Chain M: 86% 14%



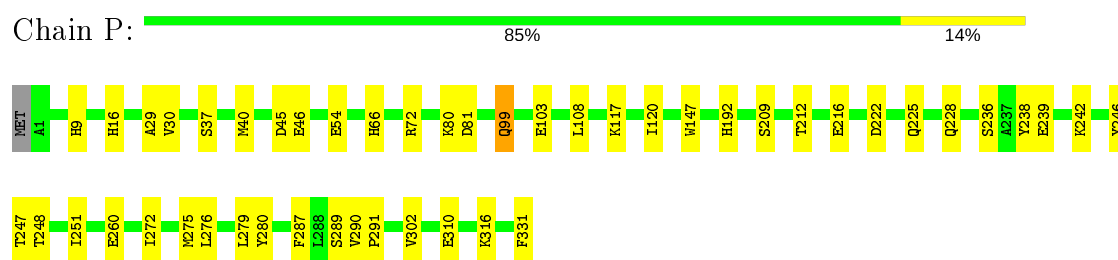
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.57Å 100.84Å 223.10Å 90.00° 101.23° 90.00°	Depositor
Resolution (Å)	60.00 – 2.42 62.27 – 2.42	Depositor EDS
% Data completeness (in resolution range)	51.5 (60.00-2.42) 51.5 (62.27-2.42)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.181 , 0.213 0.186 , 0.216	Depositor DCC
$R_{free}$ test set	13994 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	42467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	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 93.04 % 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 6.7009e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/2614	0.65	1/3535 (0.0%)
1	B	0.46	0/2605	0.66	3/3523 (0.1%)
1	C	0.48	1/2605 (0.0%)	0.65	2/3523 (0.1%)
1	D	0.46	0/2613	0.65	1/3533 (0.0%)
1	E	0.46	0/2625	0.68	3/3549 (0.1%)
1	F	0.46	0/2633	0.66	3/3560 (0.1%)
1	G	0.46	0/2612	0.66	2/3533 (0.1%)
1	H	0.45	0/2613	0.65	1/3534 (0.0%)
1	I	0.45	1/2605 (0.0%)	0.66	1/3523 (0.0%)
1	J	0.46	0/2616	0.67	1/3537 (0.0%)
1	K	0.45	0/2614	0.64	1/3535 (0.0%)
1	L	0.44	0/2619	0.68	3/3541 (0.1%)
1	M	0.44	0/2605	0.65	0/3523
1	N	0.45	0/2605	0.65	2/3523 (0.1%)
1	O	0.45	0/2627	0.67	2/3552 (0.1%)
1	P	0.46	0/2614	0.71	5/3535 (0.1%)
All	All	0.46	2/41825 (0.0%)	0.66	31/56559 (0.1%)

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	I	0	1
1	N	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	196	SER	CB-OG	-5.68	1.34	1.42
1	C	236	SER	CB-OG	-5.01	1.35	1.42

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	ASP	CB-CG-OD2	-10.78	108.60	118.30
1	P	120	ILE	CG1-CB-CG2	-10.35	88.64	111.40
1	E	81	ASP	CB-CG-OD1	8.91	126.32	118.30
1	E	81	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	P	81	ASP	CB-CG-OD1	7.52	125.07	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	156	ARG	Mainchain
1	N	281	GLY	Peptide

## 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	2565	0	2647	30	0
1	B	2559	0	2639	50	0
1	C	2559	0	2639	49	0
1	D	2564	0	2648	38	0
1	E	2573	0	2658	61	0
1	F	2578	0	2662	59	0
1	G	2563	0	2648	28	0
1	H	2564	0	2650	52	1
1	I	2559	0	2639	45	0
1	J	2567	0	2652	58	0
1	K	2565	0	2647	58	0
1	L	2567	0	2653	34	1
1	M	2559	0	2639	46	0
1	N	2559	0	2639	37	0
1	O	2574	0	2659	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	2565	0	2645	44	0
2	C	23	0	12	9	0
2	E	23	0	12	8	0
3	A	100	0	0	5	0
3	B	107	0	0	11	0
3	C	94	0	0	6	0
3	D	113	0	0	8	0
3	E	93	0	0	6	0
3	F	96	0	0	11	0
3	G	122	0	0	5	0
3	H	117	0	0	9	0
3	I	61	0	0	2	0
3	J	54	0	0	4	0
3	K	65	0	0	1	0
3	L	77	0	0	3	0
3	M	66	0	0	4	0
3	N	72	0	0	5	0
3	O	61	0	0	2	0
3	P	83	0	0	5	0
All	All	42467	0	42388	695	1

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 8.

The worst 5 of 695 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:I:275:MET:CE	1:I:277:LYS:HB2	1.58	1.34
1:C:238:TYR:HB2	2:C:401:AMP:O1P	1.39	1.23
1:B:147:TRP:CH2	1:B:275:MET:HE1	1.77	1.19
1:B:147:TRP:CZ3	1:B:275:MET:HE1	1.76	1.19
1:I:275:MET:HE2	1:I:277:LYS:HB2	1.27	1.10

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:LYS:NZ	1:L:328:GLU:OE2[2_645]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	330/332 (99%)	325 (98%)	5 (2%)	0	100	100
1	B	329/332 (99%)	323 (98%)	6 (2%)	0	100	100
1	C	329/332 (99%)	323 (98%)	6 (2%)	0	100	100
1	D	330/332 (99%)	323 (98%)	7 (2%)	0	100	100
1	E	331/332 (100%)	325 (98%)	6 (2%)	0	100	100
1	F	332/332 (100%)	326 (98%)	6 (2%)	0	100	100
1	G	330/332 (99%)	323 (98%)	7 (2%)	0	100	100
1	H	330/332 (99%)	321 (97%)	8 (2%)	1 (0%)	41	54
1	I	329/332 (99%)	318 (97%)	10 (3%)	1 (0%)	41	54
1	J	330/332 (99%)	323 (98%)	7 (2%)	0	100	100
1	K	330/332 (99%)	321 (97%)	8 (2%)	1 (0%)	41	54
1	L	331/332 (100%)	322 (97%)	8 (2%)	1 (0%)	41	54
1	M	329/332 (99%)	321 (98%)	7 (2%)	1 (0%)	41	54
1	N	329/332 (99%)	317 (96%)	11 (3%)	1 (0%)	41	54
1	O	331/332 (100%)	319 (96%)	10 (3%)	2 (1%)	25	35
1	P	330/332 (99%)	322 (98%)	8 (2%)	0	100	100
All	All	5280/5312 (99%)	5152 (98%)	120 (2%)	8 (0%)	47	61

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	99	GLN
1	L	3	LEU
1	M	14	GLU
1	N	14	GLU
1	O	217	LEU

### 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	285/285 (100%)	284 (100%)	1 (0%)	91	96
1	B	284/285 (100%)	282 (99%)	2 (1%)	84	92
1	C	284/285 (100%)	280 (99%)	4 (1%)	67	81
1	D	285/285 (100%)	280 (98%)	5 (2%)	59	75
1	E	286/285 (100%)	284 (99%)	2 (1%)	84	92
1	F	287/285 (101%)	285 (99%)	2 (1%)	84	92
1	G	285/285 (100%)	282 (99%)	3 (1%)	73	86
1	H	285/285 (100%)	281 (99%)	4 (1%)	67	81
1	I	284/285 (100%)	283 (100%)	1 (0%)	91	96
1	J	285/285 (100%)	285 (100%)	0	100	100
1	K	285/285 (100%)	284 (100%)	1 (0%)	91	96
1	L	286/285 (100%)	284 (99%)	2 (1%)	84	92
1	M	284/285 (100%)	282 (99%)	2 (1%)	84	92
1	N	284/285 (100%)	283 (100%)	1 (0%)	91	96
1	O	286/285 (100%)	283 (99%)	3 (1%)	76	87
1	P	285/285 (100%)	282 (99%)	3 (1%)	73	86
All	All	4560/4560 (100%)	4524 (99%)	36 (1%)	81	91

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	16	HIS
1	H	194	ASP
1	P	99	GLN
1	G	225	GLN
1	H	238	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:



Mol	Chain	Res	Type
1	H	228	GLN
1	J	112	ASN
1	O	230	HIS
1	I	114	ASN
1	I	192	HIS

### 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](#)

2 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	E	401	-	22,25,25	1.07	2 (9%)	25,38,38	1.56	3 (12%)
2	AMP	C	401	-	22,25,25	1.22	3 (13%)	25,38,38	1.54	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
2	AMP	E	401	-	-	5/6/26/26	0/3/3/3
2	AMP	C	401	-	-	4/6/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	AMP	C5-C4	2.85	1.48	1.40
2	C	401	AMP	O4'-C1'	2.80	1.45	1.41
2	E	401	AMP	C5-C4	2.57	1.47	1.40
2	E	401	AMP	O4'-C1'	2.56	1.44	1.41
2	C	401	AMP	C2-N3	2.36	1.35	1.32

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	AMP	C4-C5-N7	-3.54	105.71	109.40
2	E	401	AMP	N3-C2-N1	-3.53	123.16	128.68
2	E	401	AMP	C4-C5-N7	-3.44	105.81	109.40
2	C	401	AMP	N3-C2-N1	-3.16	123.73	128.68
2	E	401	AMP	C3'-C2'-C1'	2.96	105.44	100.98

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	AMP	C5'-O5'-P-O1P
2	E	401	AMP	C5'-O5'-P-O2P
2	E	401	AMP	C5'-O5'-P-O3P
2	C	401	AMP	C3'-C4'-C5'-O5'
2	E	401	AMP	O4'-C4'-C5'-O5'

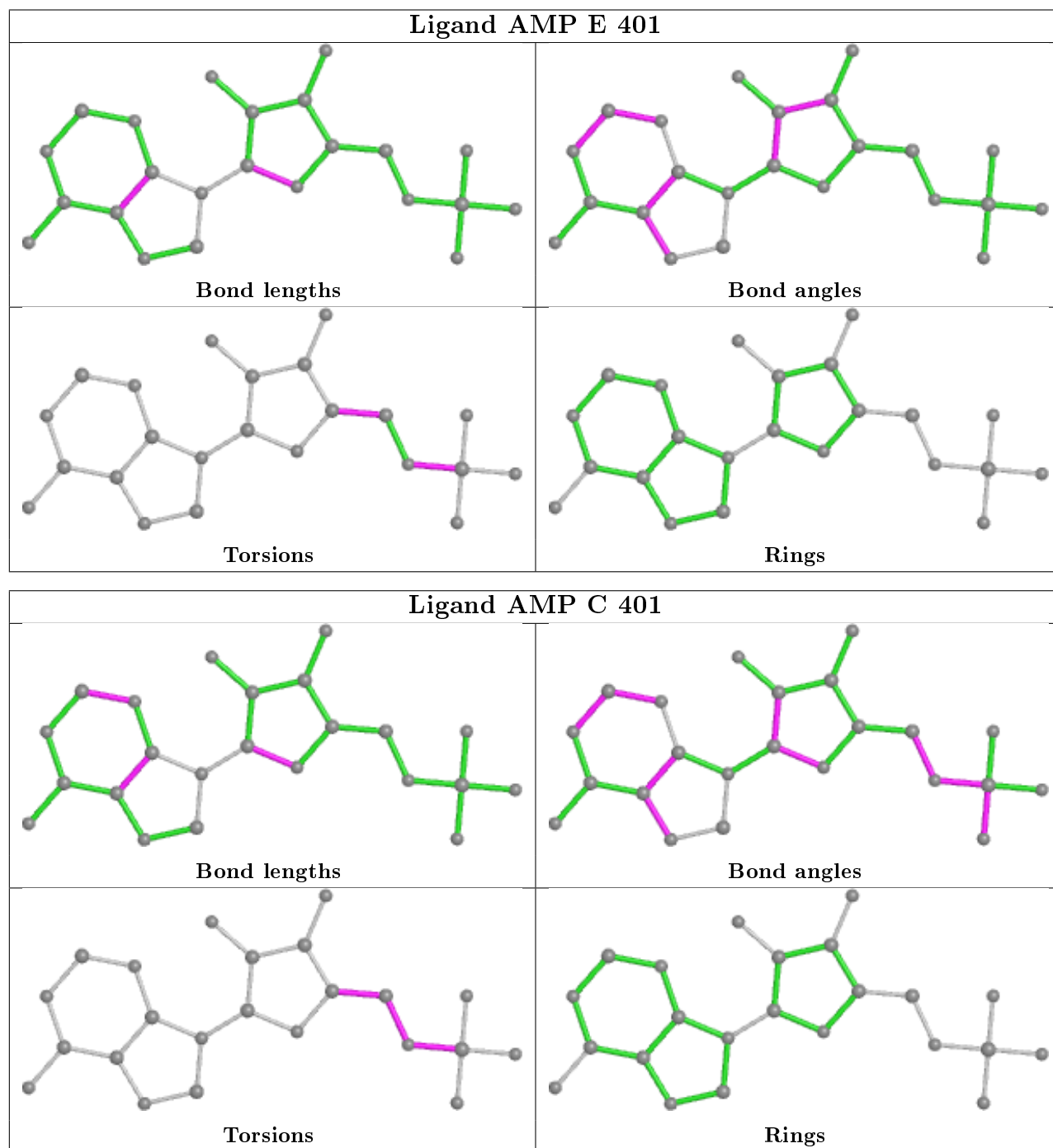
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	AMP	8	0
2	C	401	AMP	9	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.



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/332 (99%)	-0.20	8 (2%) 59 56	24, 43, 86, 129	0
1	B	331/332 (99%)	-0.39	2 (0%) 89 88	25, 39, 75, 110	0
1	C	331/332 (99%)	-0.41	1 (0%) 94 93	25, 39, 77, 133	0
1	D	331/332 (99%)	-0.35	3 (0%) 84 82	25, 39, 74, 160	0
1	E	331/332 (99%)	-0.22	8 (2%) 59 56	24, 41, 84, 136	0
1	F	331/332 (99%)	-0.42	1 (0%) 94 93	21, 39, 75, 110	0
1	G	331/332 (99%)	-0.45	0 100 100	20, 36, 79, 120	0
1	H	331/332 (99%)	-0.33	3 (0%) 84 82	23, 39, 75, 184	0
1	I	331/332 (99%)	0.03	14 (4%) 36 34	28, 53, 104, 144	0
1	J	331/332 (99%)	-0.49	1 (0%) 94 93	30, 50, 91, 114	0
1	K	331/332 (99%)	-0.26	9 (2%) 54 52	29, 52, 105, 169	0
1	L	331/332 (99%)	-0.52	2 (0%) 89 88	30, 46, 84, 120	0
1	M	331/332 (99%)	0.07	14 (4%) 36 34	33, 54, 104, 139	0
1	N	331/332 (99%)	-0.46	3 (0%) 84 82	33, 52, 92, 110	0
1	O	331/332 (99%)	-0.24	7 (2%) 63 60	29, 54, 104, 167	0
1	P	331/332 (99%)	-0.52	0 100 100	30, 49, 82, 123	0
All	All	5296/5312 (99%)	-0.32	76 (1%) 75 73	20, 46, 92, 184	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	13	LYS	7.4
1	M	102	GLY	5.7
1	H	14	GLU	5.3
1	I	102	GLY	5.2
1	O	102	GLY	5.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

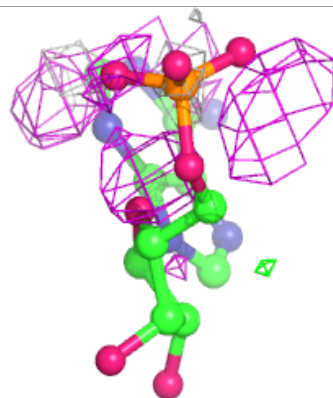
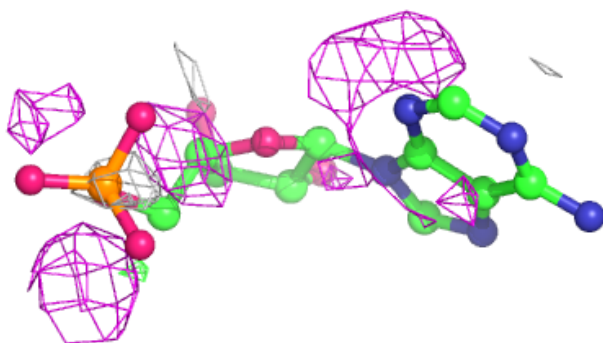
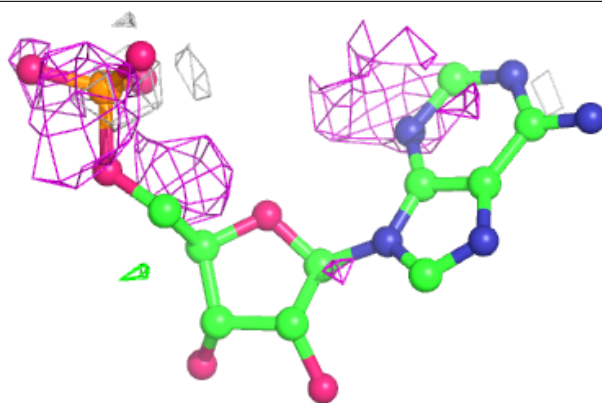
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	C	401	23/23	0.56	1.15	108,120,131,142	23
2	AMP	E	401	23/23	0.60	0.94	87,109,126,133	23

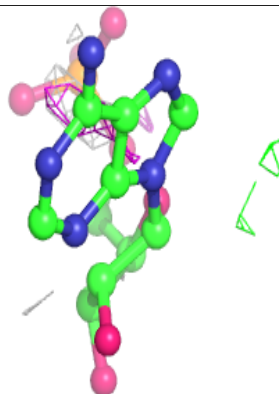
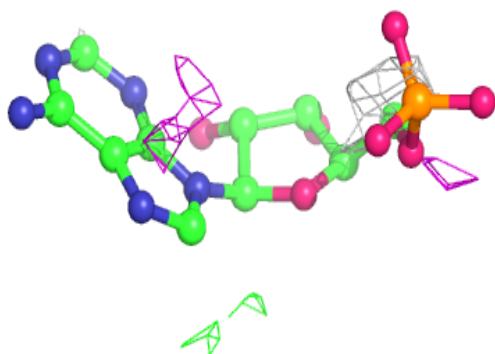
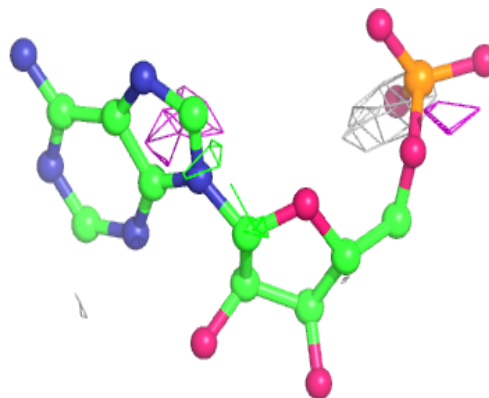
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AMP C 401:**

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

**Electron density around AMP E 401:**

$2mF_o-DF_c$  (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.