



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 03:54 AM UTC

PDB ID : 6P6U / pdb_00006p6u
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

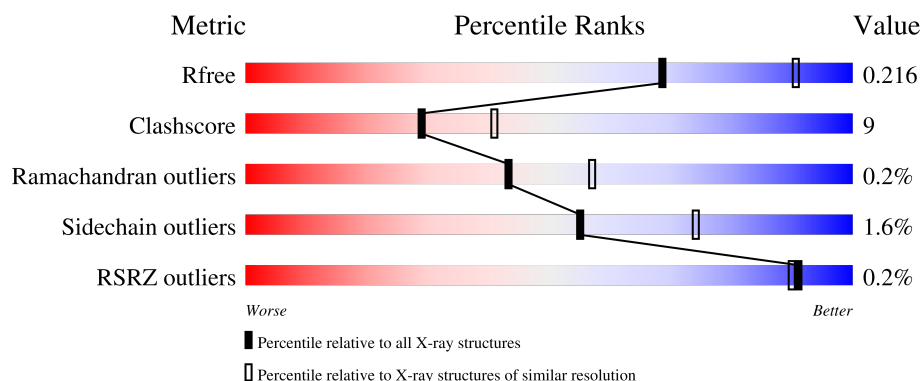
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	332	90% 10%
1	B	332	87% 11% .
1	C	332	86% 11% .
1	D	332	86% 13% .
1	E	332	85% 14% .

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Mol	Chain	Length	Quality of chain
1	F	332	 83% 16% .
1	G	332	 88% 11% .
1	H	332	 81% 18% .
1	I	332	 86% 13% .
1	J	332	 82% 18% .
1	K	332	 85% 14% .
1	L	332	 86% 13% .
1	M	332	 83% 16% .
1	N	332	 86% 13% .
1	O	332	 81% 17% .
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	-
2	AMP	E	401	-	-	X	-

2 Entry composition

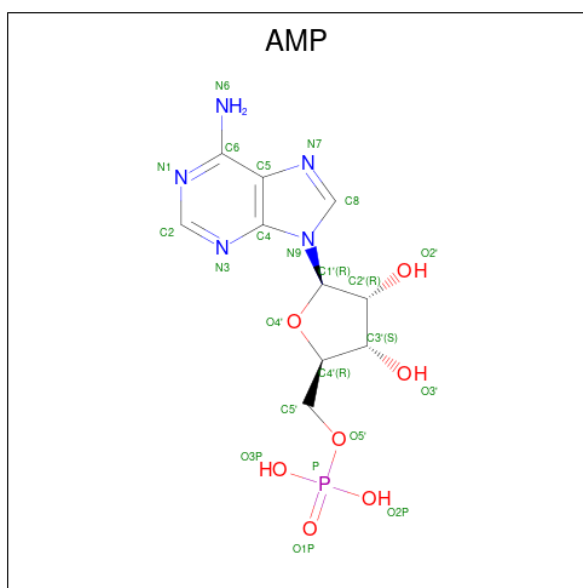
There are 3 unique types of molecules in this entry. The entry contains 42467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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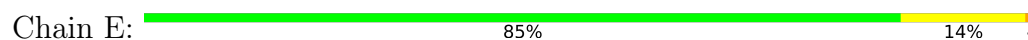
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	54	Total 54	O 54	0	0
3	K	65	Total 65	O 65	0	0
3	L	77	Total 77	O 77	0	0
3	M	66	Total 66	O 66	0	0
3	N	72	Total 72	O 72	0	0
3	O	61	Total 61	O 61	0	0
3	P	83	Total 83	O 83	0	0

- Molecule 1: L-lactate dehydrogenase A chain

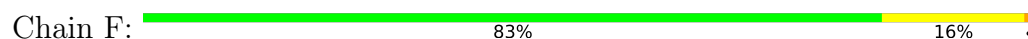




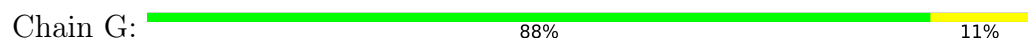
- Molecule 1: L-lactate dehydrogenase A chain



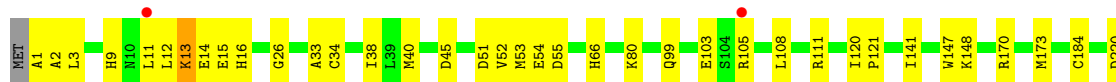
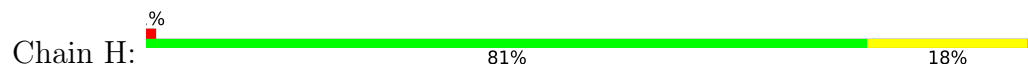
- Molecule 1: L-lactate dehydrogenase A chain



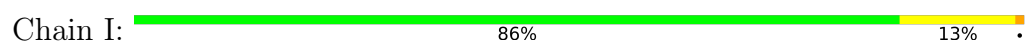
- Molecule 1: L-lactate dehydrogenase A chain

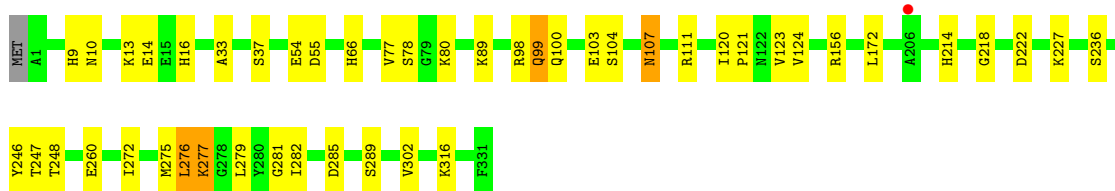


- Molecule 1: L-lactate dehydrogenase A chain



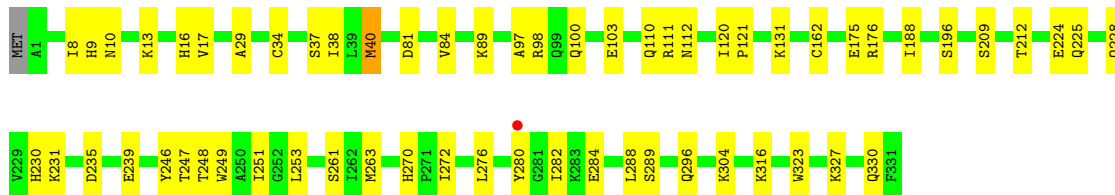
- Molecule 1: L-lactate dehydrogenase A chain





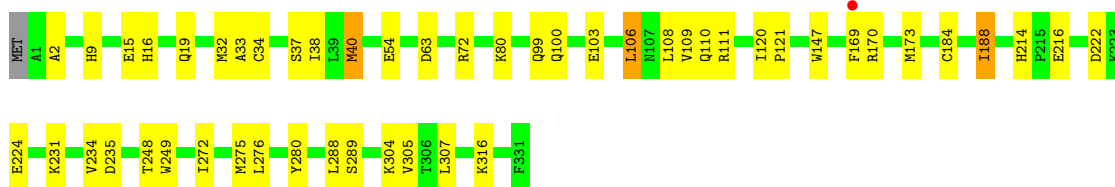
- Molecule 1: L-lactate dehydrogenase A chain

Chain J: 82% 18%



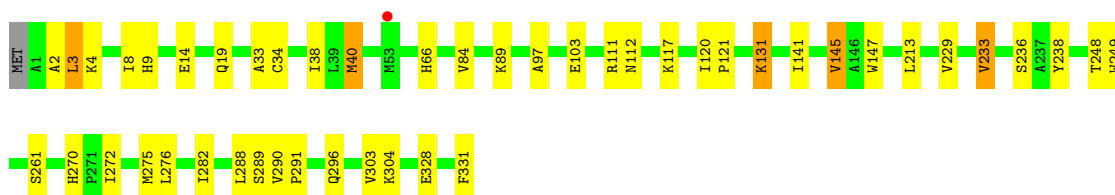
- Molecule 1: L-lactate dehydrogenase A chain

Chain K: 85% 14%



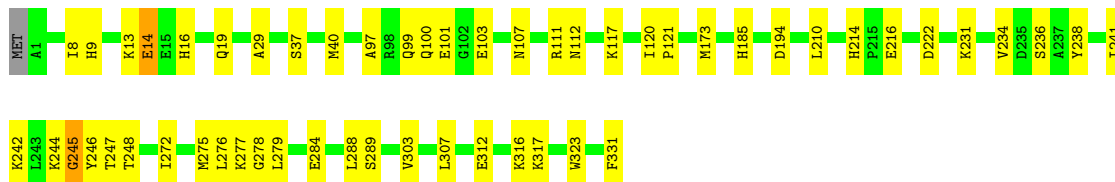
- Molecule 1: L-lactate dehydrogenase A chain

Chain L: 86% 13%



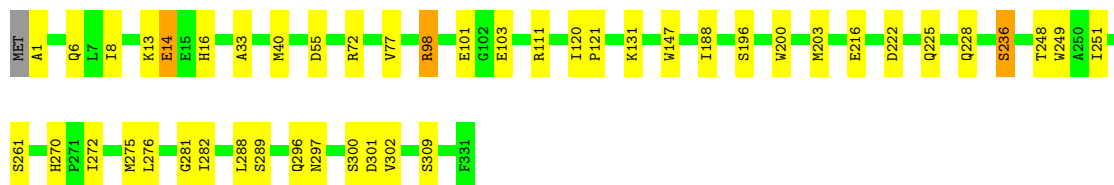
- Molecule 1: L-lactate dehydrogenase A chain

Chain M: 83% 16%



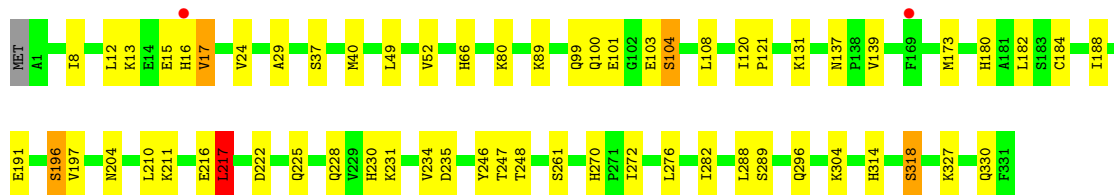
- Molecule 1: L-lactate dehydrogenase A chain

Chain N:  86% 13% .



- Molecule 1: L-lactate dehydrogenase A chain

Chain O:  81% 17% .



- Molecule 1: L-lactate dehydrogenase A chain

Chain P:  85% 14% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	160.57Å 100.84Å 223.10Å 90.00° 101.23° 90.00°	Depositor
Resolution (Å)	60.00 – 2.42 60.00 – 2.42	Depositor EDS
% Data completeness (in resolution range)	51.5 (60.00-2.42) 51.5 (60.00-2.42)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	42467	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.61	0/2614	0.81	2/3535 (0.1%)
1	B	0.63	0/2605	0.80	1/3523 (0.0%)
1	C	0.62	0/2605	0.80	2/3523 (0.1%)
1	D	0.62	0/2613	0.81	1/3533 (0.0%)
1	E	0.59	0/2625	0.81	1/3549 (0.0%)
1	F	0.60	0/2633	0.81	2/3560 (0.1%)
1	G	0.62	0/2612	0.81	3/3533 (0.1%)
1	H	0.61	0/2613	0.82	1/3534 (0.0%)
1	I	0.60	0/2605	0.83	2/3523 (0.1%)
1	J	0.60	0/2616	0.82	1/3537 (0.0%)
1	K	0.60	0/2614	0.81	0/3535
1	L	0.59	0/2619	0.83	3/3541 (0.1%)
1	M	0.59	0/2605	0.83	2/3523 (0.1%)
1	N	0.61	0/2605	0.81	3/3523 (0.1%)
1	O	0.60	0/2627	0.85	4/3552 (0.1%)
1	P	0.61	0/2614	0.86	4/3535 (0.1%)
All	All	0.61	0/41825	0.82	32/56559 (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

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	245	GLY	N-CA-C	-10.53	101.99	111.67
1	I	277	LYS	CA-C-O	-8.76	111.11	120.92
1	P	192	HIS	N-CA-C	8.49	125.30	111.37
1	P	192	HIS	CA-C-O	-8.18	111.45	121.02
1	O	17	VAL	N-CA-C	7.87	116.02	107.60

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	32	0
1	B	2559	0	2639	54	0
1	C	2559	0	2639	50	0
1	D	2564	0	2648	39	0
1	E	2573	0	2658	63	0
1	F	2578	0	2662	63	0
1	G	2563	0	2648	32	0
1	H	2564	0	2650	54	1
1	I	2559	0	2639	46	0
1	J	2567	0	2652	60	0
1	K	2565	0	2647	59	0
1	L	2567	0	2653	34	1
1	M	2559	0	2639	50	0
1	N	2559	0	2639	40	0
1	O	2574	0	2659	66	0
1	P	2565	0	2645	49	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	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	113	0	0	8	0
3	E	93	0	0	5	0
3	F	96	0	0	11	0
3	G	122	0	0	5	0
3	H	117	0	0	10	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	723	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 9.

The worst 5 of 723 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:O:173:MET:HE2	1:O:184:CYS:HB3	1.22	1.14
1:C:242:LYS:HB2	2:C:401:AMP:C2	1.87	1.09
1:I:275:MET:HE3	1:I:277:LYS:CB	1.82	1.09

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 [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	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%)	36	49
1	I	329/332 (99%)	318 (97%)	10 (3%)	1 (0%)	36	49
1	J	330/332 (99%)	323 (98%)	7 (2%)	0	100	100
1	K	330/332 (99%)	321 (97%)	8 (2%)	1 (0%)	36	49
1	L	331/332 (100%)	322 (97%)	8 (2%)	1 (0%)	36	49
1	M	329/332 (99%)	321 (98%)	7 (2%)	1 (0%)	36	49
1	N	329/332 (99%)	317 (96%)	11 (3%)	1 (0%)	36	49
1	O	331/332 (100%)	319 (96%)	10 (3%)	2 (1%)	21	30
1	P	330/332 (99%)	322 (98%)	8 (2%)	0	100	100
All	All	5280/5312 (99%)	5152 (98%)	120 (2%)	8 (0%)	43	57

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%)	283 (99%)	2 (1%)	76	87
1	B	284/285 (100%)	278 (98%)	6 (2%)	47	67
1	C	284/285 (100%)	277 (98%)	7 (2%)	42	62
1	D	285/285 (100%)	278 (98%)	7 (2%)	42	62
1	E	286/285 (100%)	281 (98%)	5 (2%)	53	73
1	F	287/285 (101%)	283 (99%)	4 (1%)	59	77
1	G	285/285 (100%)	280 (98%)	5 (2%)	51	71
1	H	285/285 (100%)	280 (98%)	5 (2%)	51	71
1	I	284/285 (100%)	279 (98%)	5 (2%)	51	71
1	J	285/285 (100%)	283 (99%)	2 (1%)	76	87
1	K	285/285 (100%)	281 (99%)	4 (1%)	59	77
1	L	286/285 (100%)	280 (98%)	6 (2%)	47	67
1	M	284/285 (100%)	281 (99%)	3 (1%)	65	81
1	N	284/285 (100%)	281 (99%)	3 (1%)	65	81
1	O	286/285 (100%)	280 (98%)	6 (2%)	47	67
1	P	285/285 (100%)	280 (98%)	5 (2%)	51	71
All	All	4560/4560 (100%)	4485 (98%)	75 (2%)	55	74

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	233	VAL
1	P	99	GLN
1	M	16	HIS
1	O	188	ILE
1	E	16	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	107	ASN
1	P	192	HIS
1	M	214	HIS
1	O	180	HIS
1	F	19	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 oligosaccharides 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	C	401	-	25,25,25	1.60	4 (16%)	37,38,38	2.17	9 (24%)
2	AMP	E	401	-	25,25,25	1.50	3 (12%)	37,38,38	2.11	12 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	C	401	-	-	7/10/26/26	0/3/3/3
2	AMP	E	401	-	-	7/10/26/26	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	AMP	C5-C4	5.25	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	AMP	C5-C4	4.84	1.47	1.39
2	C	401	AMP	C5-C6	3.29	1.50	1.41
2	E	401	AMP	C5-C6	3.14	1.49	1.41
2	E	401	AMP	C8-N7	2.74	1.36	1.31

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	AMP	C5-C4-N3	-6.75	117.43	126.72
2	E	401	AMP	C5-C4-N3	-5.77	118.78	126.72
2	C	401	AMP	N3-C4-N9	4.69	135.14	127.17
2	C	401	AMP	O4'-C1'-N9	4.29	116.32	108.09
2	C	401	AMP	C4-C5-N7	-4.26	105.71	110.58

There are no chirality outliers.

5 of 14 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'

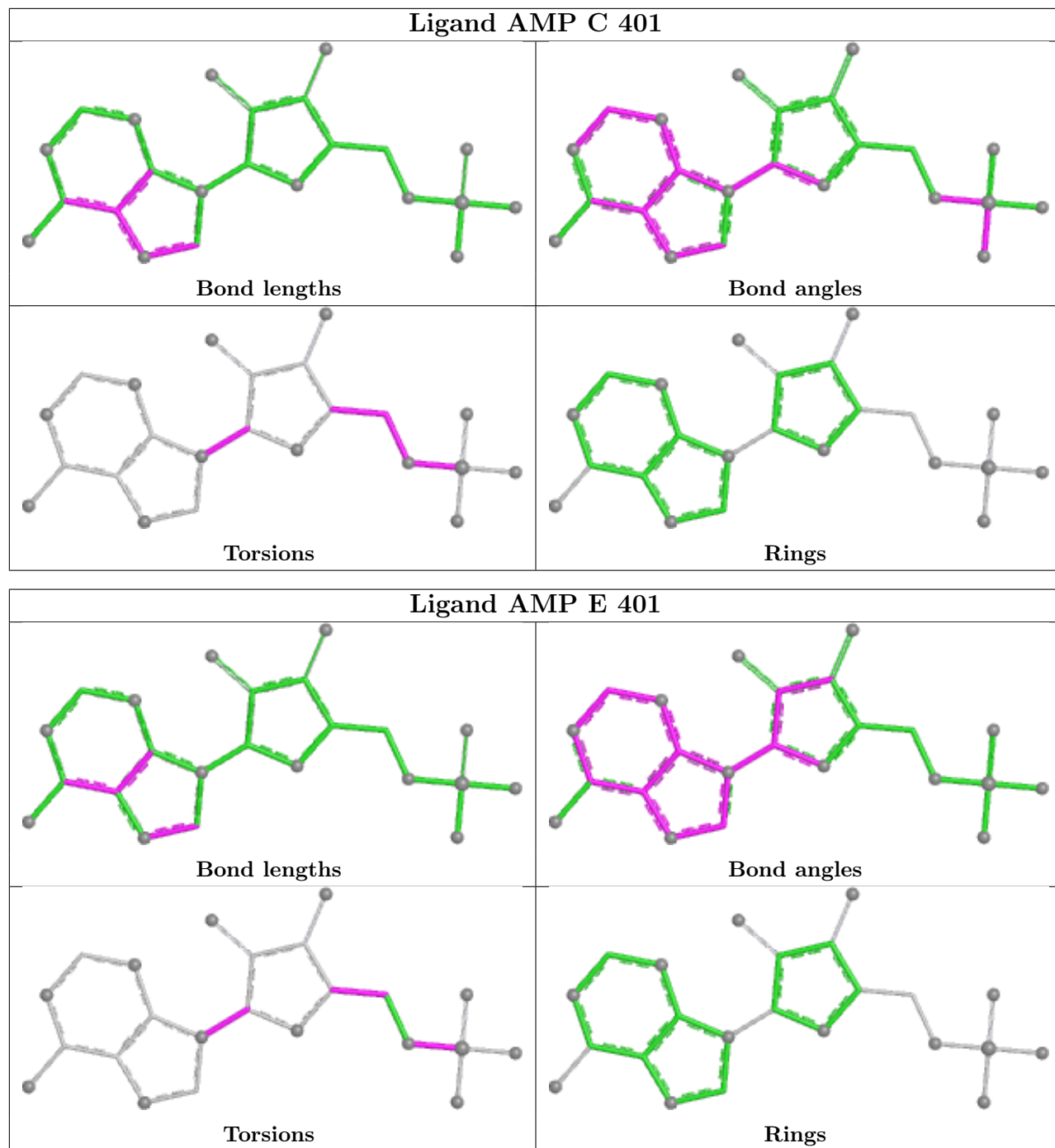
There are no ring outliers.

2 monomers are involved in 17 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/332 (99%)	-0.38	1 (0%) 90 88	23, 43, 86, 129	1 (0%)
1	B	331/332 (99%)	-0.48	1 (0%) 90 88	25, 39, 75, 110	0
1	C	331/332 (99%)	-0.46	1 (0%) 90 88	25, 39, 77, 133	0
1	D	331/332 (99%)	-0.47	1 (0%) 90 88	25, 39, 74, 160	1 (0%)
1	E	331/332 (99%)	-0.39	1 (0%) 90 88	14, 40, 84, 136	2 (0%)
1	F	331/332 (99%)	-0.51	0 100 100	14, 38, 75, 110	3 (0%)
1	G	331/332 (99%)	-0.48	0 100 100	17, 36, 79, 120	1 (0%)
1	H	331/332 (99%)	-0.49	2 (0%) 85 84	23, 39, 75, 184	1 (0%)
1	I	331/332 (99%)	-0.22	1 (0%) 90 88	28, 53, 104, 144	0
1	J	331/332 (99%)	-0.27	1 (0%) 90 88	18, 50, 91, 114	1 (0%)
1	K	331/332 (99%)	-0.22	1 (0%) 90 88	29, 52, 103, 169	1 (0%)
1	L	331/332 (99%)	-0.40	1 (0%) 90 88	30, 46, 84, 120	2 (0%)
1	M	331/332 (99%)	-0.24	0 100 100	33, 54, 104, 139	0
1	N	331/332 (99%)	-0.26	0 100 100	33, 52, 92, 110	0
1	O	331/332 (99%)	-0.18	2 (0%) 85 84	23, 53, 104, 167	2 (0%)
1	P	331/332 (99%)	-0.37	0 100 100	30, 49, 82, 123	1 (0%)
All	All	5296/5312 (99%)	-0.36	13 (0%) 91 90	14, 46, 91, 184	16 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	105	ARG	3.2
1	H	105	ARG	3.0
1	B	275	MET	2.9
1	A	1	ALA	2.7
1	C	238	TYR	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

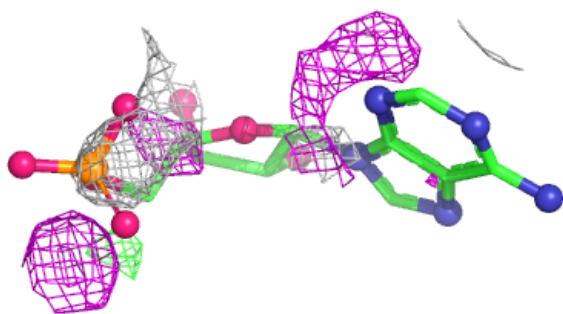
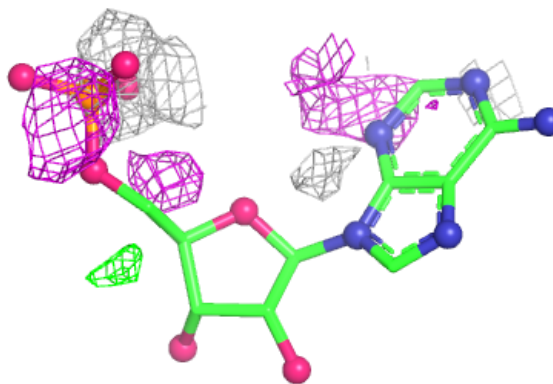
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AMP	C	401	23/23	0.51	0.20	108,120,131,142	23
2	AMP	E	401	23/23	0.54	0.17	87,109,126,133	23

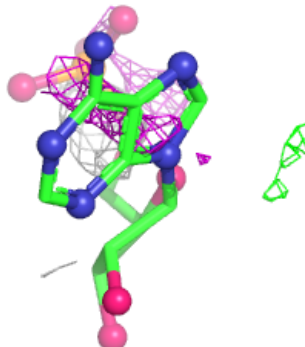
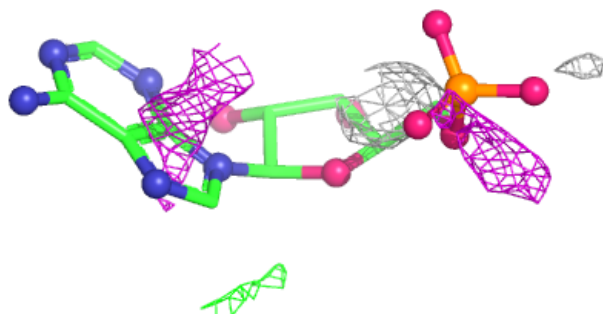
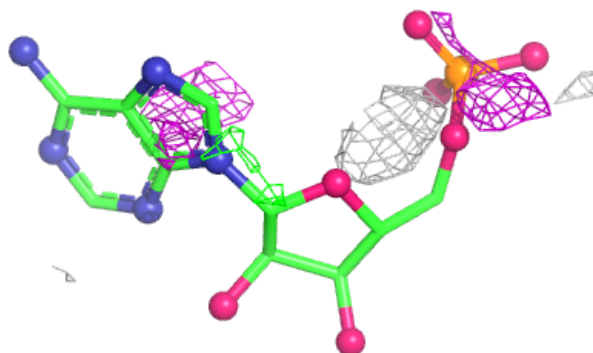
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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