



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:14 PM UTC

PDB ID : 10BL / pdb\_000010bl  
Title : Crystal Structure of serine/threonine-protein kinase (AEK1) from Trypanosoma cruzi in complex ADP  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2026-01-09  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

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

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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

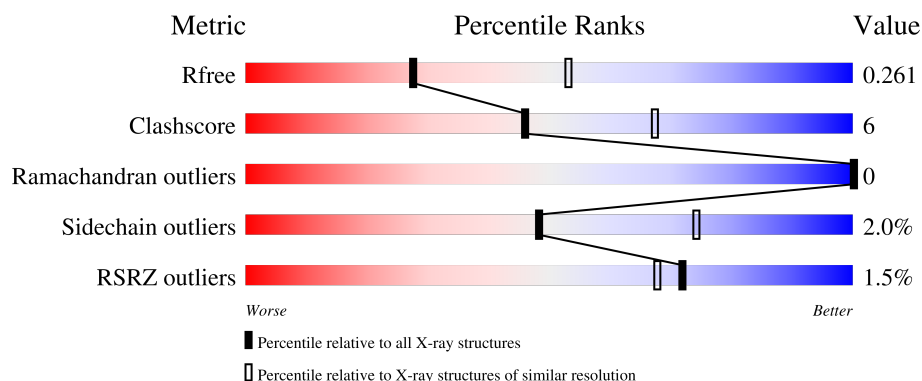
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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  $\geq 3$ , 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	361	<div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	B	361	<div> <div> <div>2%</div> <div>77%</div> <div>13%</div> <div>10%</div> </div> </div>

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
4	MLI	A	504	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5409 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 Putative rac serine-threonine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	P	S	0	0	0
			2716	1741	457	502	4	12			
1	B	326	Total	C	N	O	P	S	0	0	0
			2624	1686	441	482	3	12			

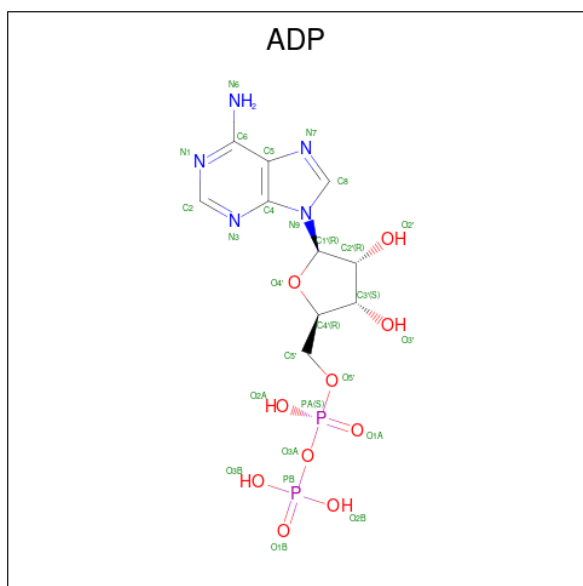
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	MET	-	initiating methionine	UNP Q4E2L0
A	185	ILE	THR	engineered mutation	UNP Q4E2L0
A	227	PHE	VAL	engineered mutation	UNP Q4E2L0
A	314	SER	ASN	engineered mutation	UNP Q4E2L0
A	475	LEU	-	expression tag	UNP Q4E2L0
A	476	GLU	-	expression tag	UNP Q4E2L0
A	477	HIS	-	expression tag	UNP Q4E2L0
A	478	HIS	-	expression tag	UNP Q4E2L0
A	479	HIS	-	expression tag	UNP Q4E2L0
A	480	HIS	-	expression tag	UNP Q4E2L0
A	481	HIS	-	expression tag	UNP Q4E2L0
A	482	HIS	-	expression tag	UNP Q4E2L0
B	122	MET	-	initiating methionine	UNP Q4E2L0
B	185	ILE	THR	engineered mutation	UNP Q4E2L0
B	227	PHE	VAL	engineered mutation	UNP Q4E2L0
B	314	SER	ASN	engineered mutation	UNP Q4E2L0
B	475	LEU	-	expression tag	UNP Q4E2L0
B	476	GLU	-	expression tag	UNP Q4E2L0
B	477	HIS	-	expression tag	UNP Q4E2L0
B	478	HIS	-	expression tag	UNP Q4E2L0
B	479	HIS	-	expression tag	UNP Q4E2L0
B	480	HIS	-	expression tag	UNP Q4E2L0
B	481	HIS	-	expression tag	UNP Q4E2L0
B	482	HIS	-	expression tag	UNP Q4E2L0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

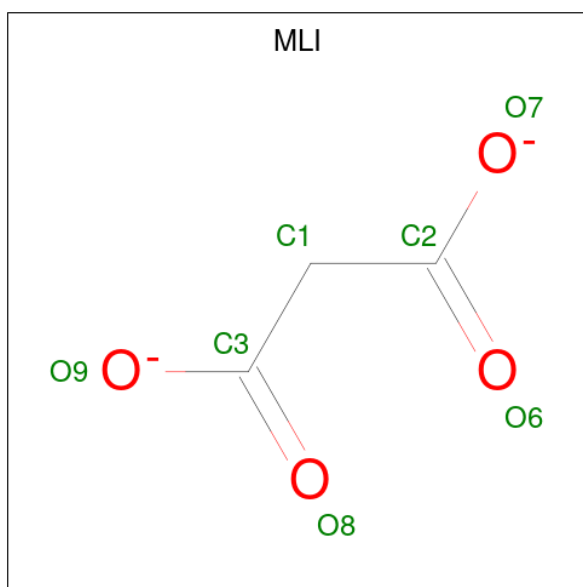
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	B	1	Total Cl 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula:  $\text{C}_3\text{H}_2\text{O}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		

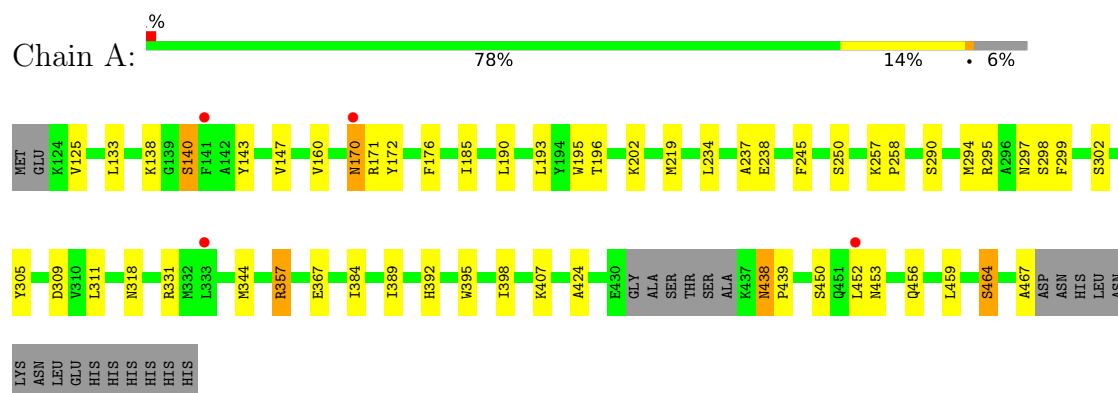
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	1	Total	O	0	0
			1	1		

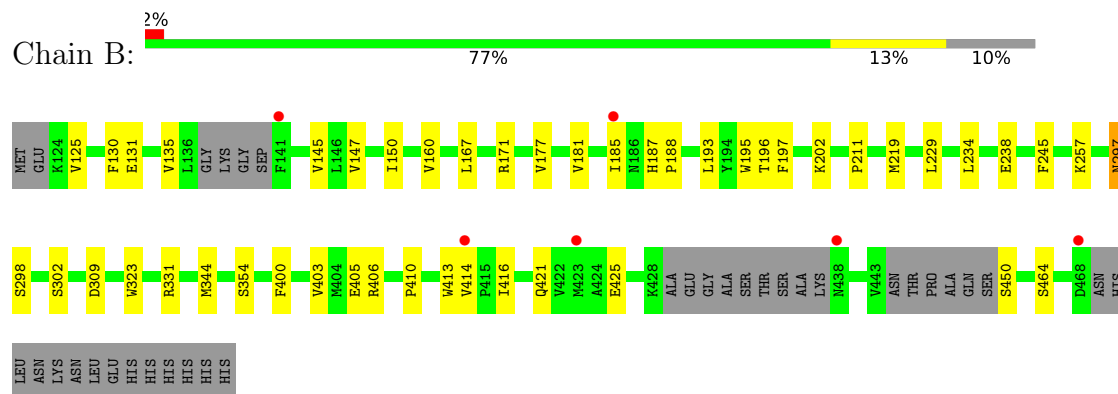
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Putative rac serine-threonine kinase



- Molecule 1: Putative rac serine-threonine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.17Å 86.17Å 192.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.69 – 2.60 48.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.69-2.60) 99.9 (48.69-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.61Å)	Xtriage
Refinement program	PHENIX (2.0_5904: ???)	Depositor
R, $R_{free}$	0.215 , 0.265 0.216 , 0.261	Depositor DCC
$R_{free}$ test set	1345 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.9	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 74.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5409	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	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 40.60 % 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 2.6723e-04. 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SEP, CL, MLI

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	0.36	0/2740	0.52	0/3704
1	B	0.38	0/2656	0.56	0/3594
All	All	0.37	0/5396	0.54	0/7298

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2716	0	2640	33	0
1	B	2624	0	2544	35	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	7	0	2	1	0
5	A	4	0	0	0	0
5	B	1	0	0	0	0
All	All	5409	0	5210	62	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 6.

All (62) 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:B:125:VAL:HG21	1:B:195:TRP:CD1	2.31	0.65
1:B:193:LEU:HD21	1:B:196:THR:HG23	1.82	0.62
1:A:185:ILE:HG23	1:A:245:PHE:HE2	1.65	0.60
1:B:400:PHE:HA	1:B:403:VAL:HG12	1.84	0.58
1:B:160:VAL:CG1	1:B:202:LYS:HD3	2.34	0.58
1:A:219:MET:HE1	1:A:331:ARG:HG3	1.90	0.54
1:B:414:VAL:HG23	1:B:414:VAL:O	2.08	0.54
1:B:160:VAL:HG12	1:B:202:LYS:HD3	1.91	0.53
1:A:219:MET:HE1	1:A:331:ARG:CG	2.39	0.53
1:A:407:LYS:HE2	1:A:407:LYS:HA	1.91	0.53
1:A:295:ARG:HG2	1:A:295:ARG:HH11	1.75	0.51
1:B:297:ASN:ND2	1:B:297:ASN:N	2.60	0.50
1:A:464:SEP:OG	1:B:197:PHE:HA	2.12	0.49
1:A:138:LYS:HD2	1:A:143:TYR:HB3	1.95	0.49
1:B:187:HIS:CG	1:B:188:PRO:HD2	2.48	0.49
1:A:140:SEP:O1P	1:B:171:ARG:HD2	2.13	0.48
1:A:438:ASN:OD1	1:A:438:ASN:C	2.57	0.48
1:B:131:GLU:HB2	1:B:150:ILE:HD11	1.94	0.48
1:A:237:ALA:HB2	1:A:395:TRP:CZ3	2.50	0.47
1:A:133:LEU:HD12	1:A:147:VAL:HA	1.97	0.47
1:A:257:LYS:HD3	1:A:302:SER:OG	2.15	0.46
1:B:188:PRO:HA	1:B:406:ARG:HH21	1.79	0.46
1:B:130:PHE:HB3	1:B:147:VAL:HB	1.98	0.46
1:B:185:ILE:HG23	1:B:245:PHE:HE2	1.79	0.46
1:A:424:ALA:O	4:A:504:MLI:H11	2.17	0.45
1:A:299:PHE:HE1	1:A:311:LEU:HD23	1.82	0.45
1:B:405:GLU:O	1:B:406:ARG:HB2	2.16	0.45
1:A:384:ILE:HG12	1:A:389:ILE:HG13	1.99	0.45
1:B:421:GLN:O	1:B:425:GLU:HG3	2.17	0.44
1:A:234:LEU:O	1:A:238:GLU:HG3	2.17	0.44
1:A:170:ASN:HA	1:A:172:TYR:CE1	2.53	0.44
1:A:344:MET:HE3	1:A:459:LEU:HB3	1.99	0.44
1:A:176:PHE:CD2	1:B:344:MET:HE2	2.53	0.44
1:A:176:PHE:CE2	1:B:344:MET:HE2	2.53	0.43
1:B:193:LEU:HD21	1:B:196:THR:CG2	2.47	0.43
1:B:257:LYS:HD3	1:B:302:SER:OG	2.18	0.43
1:B:135:VAL:O	1:B:135:VAL:HG13	2.18	0.43
1:B:400:PHE:HA	1:B:403:VAL:CG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:HG11	1:B:202:LYS:HD3	1.99	0.43
1:A:125:VAL:HG21	1:A:195:TRP:CG	2.54	0.43
1:B:211:PRO:HB2	1:B:416:ILE:HG21	2.00	0.43
1:A:171:ARG:NH2	1:B:171:ARG:HG3	2.34	0.42
1:A:160:VAL:CG1	1:A:202:LYS:HD3	2.49	0.42
1:B:135:VAL:HA	1:B:145:VAL:HG12	2.00	0.42
1:A:258:PRO:HD3	1:A:305:TYR:CZ	2.55	0.42
1:A:467:ALA:HB3	1:B:193:LEU:O	2.18	0.42
1:B:219:MET:HE3	1:B:331:ARG:CZ	2.50	0.42
1:B:135:VAL:HG23	1:B:145:VAL:HG12	2.02	0.41
1:A:438:ASN:HA	1:A:439:PRO:HD3	1.95	0.41
1:A:453:ASN:OD1	1:A:456:GLN:HB2	2.20	0.41
1:B:229:LEU:HD23	1:B:229:LEU:O	2.20	0.41
1:B:234:LEU:O	1:B:238:GLU:HG3	2.20	0.41
1:B:323:TRP:CD1	1:B:323:TRP:C	2.98	0.41
1:A:367:GLU:O	1:A:392:HIS:HE1	2.03	0.41
1:A:357:ARG:CZ	1:A:357:ARG:HB2	2.50	0.41
1:A:193:LEU:HD21	1:A:196:THR:HG23	2.03	0.41
1:B:167:LEU:H	1:B:167:LEU:HD22	1.86	0.41
1:B:177:VAL:O	1:B:181:VAL:HG23	2.22	0.40
1:A:185:ILE:HG21	1:A:190:LEU:HD13	2.02	0.40
1:A:250:SER:HA	1:A:294:MET:SD	2.60	0.40
1:B:410:PRO:HB2	1:B:413:TRP:HB2	2.03	0.40
1:A:318:ASN:OD1	1:A:318:ASN:C	2.63	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/361 (91%)	324 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	316/361 (88%)	310 (98%)	6 (2%)	0	100	100
All	All	646/722 (90%)	634 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	286/316 (90%)	278 (97%)	8 (3%)	38	66
1	B	277/316 (88%)	274 (99%)	3 (1%)	65	84
All	All	563/632 (89%)	552 (98%)	11 (2%)	48	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	290	SER
1	A	297	ASN
1	A	309	ASP
1	A	357	ARG
1	A	398	ILE
1	A	438	ASN
1	A	452	LEU
1	B	297	ASN
1	B	309	ASP
1	B	354	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	381	ASN

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Mol	Chain	Res	Type
1	B	164	GLN
1	B	297	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	SEP	A	298	1	8,9,10	1.74	1 (12%)	7,12,14	1.02	0
1	SEP	B	464	1	8,9,10	1.70	2 (25%)	7,12,14	0.64	0
1	SEP	B	298	1	8,9,10	1.54	2 (25%)	7,12,14	1.27	1 (14%)
1	SEP	A	140	1	8,9,10	1.63	1 (12%)	7,12,14	1.49	1 (14%)
1	SEP	A	450	1	8,9,10	1.66	1 (12%)	7,12,14	1.61	2 (28%)
1	SEP	B	450	1	8,9,10	1.63	1 (12%)	7,12,14	1.27	1 (14%)
1	SEP	A	464	1	8,9,10	1.68	2 (25%)	7,12,14	1.59	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	298	1	-	0/6/8/10	-
1	SEP	B	464	1	-	0/6/8/10	-
1	SEP	B	298	1	-	0/6/8/10	-
1	SEP	A	140	1	-	3/6/8/10	-
1	SEP	A	450	1	-	4/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	450	1	-	3/6/8/10	-
1	SEP	A	464	1	-	0/6/8/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	SEP	P-O1P	3.77	1.62	1.50
1	B	464	SEP	P-O1P	3.75	1.62	1.50
1	A	450	SEP	P-O1P	3.59	1.61	1.50
1	A	464	SEP	P-O1P	3.56	1.61	1.50
1	B	450	SEP	P-O1P	3.44	1.61	1.50
1	A	140	SEP	P-O1P	3.44	1.61	1.50
1	B	298	SEP	P-O1P	3.12	1.60	1.50
1	A	464	SEP	P-O2P	2.07	1.62	1.54
1	B	464	SEP	P-O3P	2.01	1.62	1.54
1	B	298	SEP	P-O2P	2.00	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	SEP	OG-CB-CA	3.55	111.60	108.14
1	A	140	SEP	OG-CB-CA	3.30	111.36	108.14
1	A	450	SEP	OG-CB-CA	3.16	111.22	108.14
1	B	298	SEP	OG-CB-CA	2.70	110.77	108.14
1	B	450	SEP	OG-CB-CA	2.36	110.44	108.14
1	A	450	SEP	O3P-P-OG	2.08	112.10	106.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	140	SEP	CB-OG-P-O1P
1	A	140	SEP	CB-OG-P-O2P
1	A	140	SEP	CB-OG-P-O3P
1	A	450	SEP	N-CA-CB-OG
1	A	450	SEP	C-CA-CB-OG
1	B	450	SEP	N-CA-CB-OG
1	B	450	SEP	C-CA-CB-OG
1	A	450	SEP	CB-OG-P-O2P
1	A	450	SEP	CA-CB-OG-P
1	B	450	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	140	SEP	1	0
1	A	464	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	MLI	A	504	-	6,6,6	1.67	1 (16%)	7,7,7	1.49	2 (28%)
3	ADP	B	502	-	28,29,29	1.49	4 (14%)	43,45,45	1.85	11 (25%)
3	ADP	A	503	-	28,29,29	1.50	5 (17%)	43,45,45	1.86	11 (25%)

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	MLI	A	504	-	-	4/4/4/4	-
3	ADP	B	502	-	-	6/16/32/32	0/3/3/3
3	ADP	A	503	-	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	ADP	C5-C4	5.01	1.48	1.39
3	B	502	ADP	C5-C4	4.79	1.47	1.39
3	B	502	ADP	PA-O3A	3.44	1.63	1.59
3	A	503	ADP	PA-O3A	2.64	1.62	1.59
3	A	503	ADP	C8-N7	2.60	1.36	1.31
3	B	502	ADP	C5-C6	2.57	1.48	1.41
3	B	502	ADP	C8-N7	2.51	1.36	1.31
3	A	503	ADP	C5-N7	-2.47	1.34	1.39
3	A	503	ADP	C5-C6	2.47	1.47	1.41
4	A	504	MLI	C1-C3	2.26	1.54	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	ADP	C5-C4-N3	-5.84	118.68	126.72
3	B	502	ADP	C5-C4-N3	-5.12	119.67	126.72
3	A	503	ADP	N3-C4-N9	5.03	135.72	127.17
3	B	502	ADP	N3-C4-N9	4.45	134.74	127.17
3	B	502	ADP	N3-C2-N1	-3.68	123.01	128.58
3	A	503	ADP	C2-N3-C4	3.65	120.75	111.83
3	A	503	ADP	N3-C2-N1	-3.62	123.10	128.58
3	B	502	ADP	C4-N9-C8	3.49	109.40	105.74
3	B	502	ADP	C2-N3-C4	3.47	120.32	111.83
3	B	502	ADP	C4-C5-N7	-3.18	106.95	110.58
3	B	502	ADP	C2-N1-C6	2.77	123.28	118.73
3	A	503	ADP	C4-C5-N7	-2.65	107.55	110.58
3	A	503	ADP	C4-N9-C8	2.58	108.44	105.74
3	B	502	ADP	C5-N7-C8	2.53	107.42	103.45
3	A	503	ADP	C2-N1-C6	2.47	122.78	118.73
3	B	502	ADP	N9-C8-N7	-2.33	110.64	113.94
3	B	502	ADP	C6-C5-N7	2.32	136.57	132.09
3	A	503	ADP	C5-N7-C8	2.26	107.01	103.45
3	A	503	ADP	C2'-C3'-C4'	2.18	106.81	102.61
3	A	503	ADP	C3'-C2'-C1'	2.17	105.58	101.46
3	B	502	ADP	C3'-C2'-C1'	2.16	105.55	101.46
4	A	504	MLI	O6-C2-C1	-2.15	116.00	122.11
3	A	503	ADP	N6-C6-N1	2.13	123.12	118.38
4	A	504	MLI	O9-C3-O8	2.11	128.77	123.33

There are no chirality outliers.

All (12) torsion outliers are listed below:



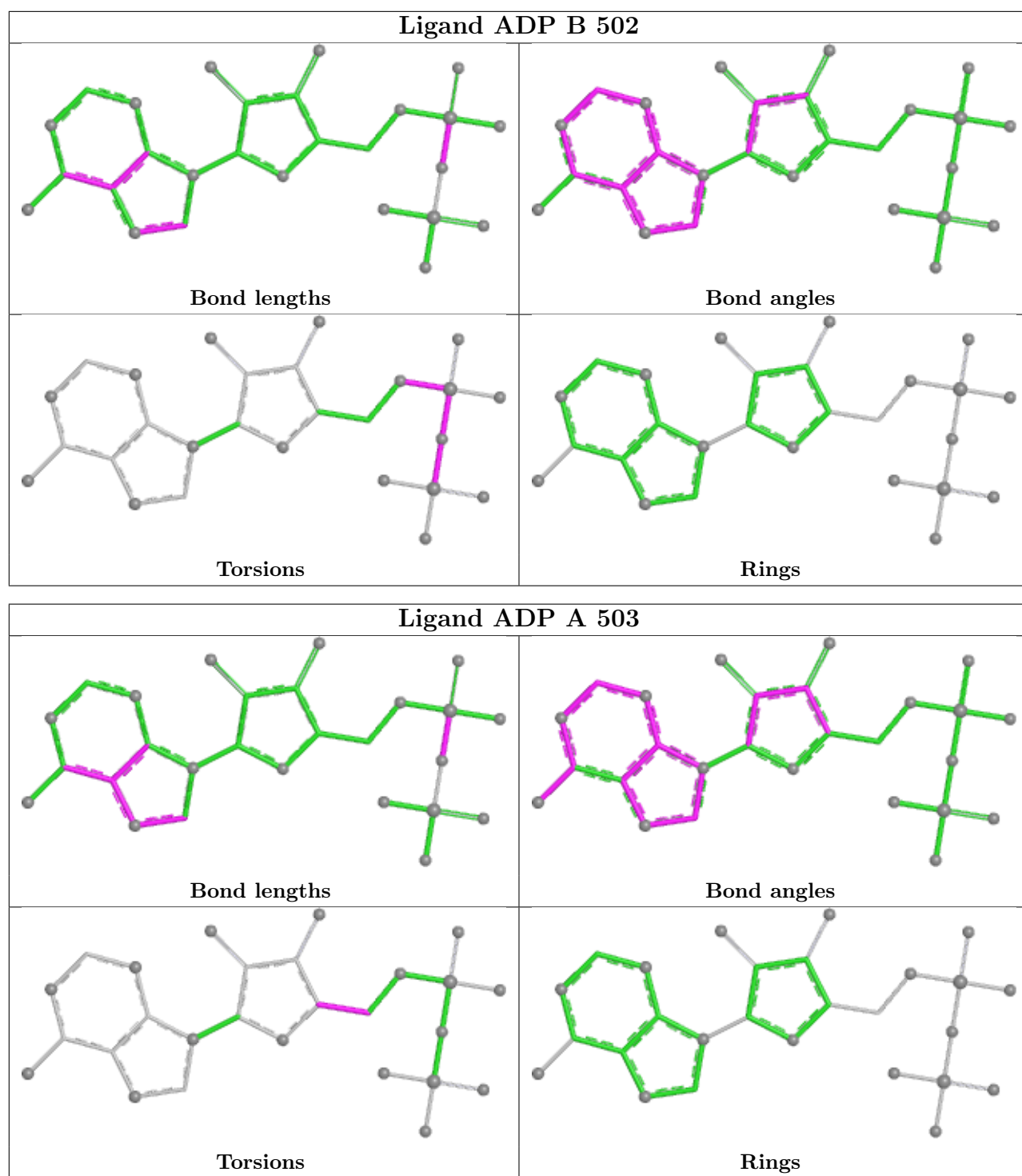
Mol	Chain	Res	Type	Atoms
3	B	502	ADP	C5'-O5'-PA-O1A
4	A	504	MLI	C3-C1-C2-O6
4	A	504	MLI	C2-C1-C3-O8
4	A	504	MLI	C2-C1-C3-O9
3	B	502	ADP	PA-O3A-PB-O2B
4	A	504	MLI	C3-C1-C2-O7
3	B	502	ADP	C5'-O5'-PA-O2A
3	B	502	ADP	C5'-O5'-PA-O3A
3	A	503	ADP	O4'-C4'-C5'-O5'
3	B	502	ADP	PA-O3A-PB-O3B
3	A	503	ADP	C3'-C4'-C5'-O5'
3	B	502	ADP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	MLI	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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	334/361 (92%)	0.02	4 (1%) 76 73	55, 83, 122, 154	0
1	B	323/361 (89%)	0.12	6 (1%) 66 61	50, 87, 136, 168	0
All	All	657/722 (90%)	0.07	10 (1%) 72 68	50, 85, 132, 168	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	468	ASP	3.1
1	B	414	VAL	2.6
1	A	141	PHE	2.6
1	B	438	ASN	2.5
1	A	170	ASN	2.4
1	B	141	PHE	2.4
1	B	423	MET	2.2
1	A	333	LEU	2.1
1	A	452	LEU	2.0
1	B	185	ILE	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	SEP	B	450	10/11	0.39	0.13	127,139,151,160	0
1	SEP	A	140	10/11	0.63	0.13	153,159,171,173	0
1	SEP	A	450	10/11	0.67	0.12	127,137,155,158	0
1	SEP	A	464	10/11	0.91	0.07	82,88,100,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SEP	B	464	10/11	0.95	0.06	59,64,80,83	0
1	SEP	A	298	10/11	0.97	0.07	62,72,76,80	0
1	SEP	B	298	10/11	0.97	0.07	58,67,72,76	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

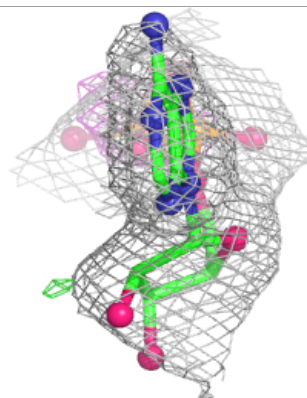
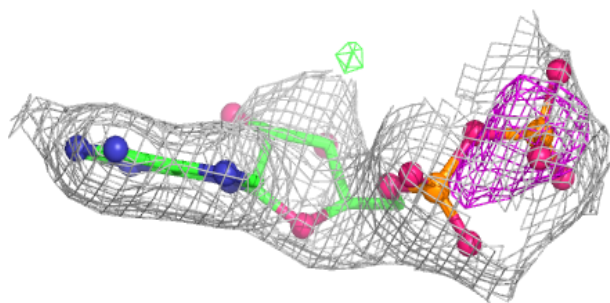
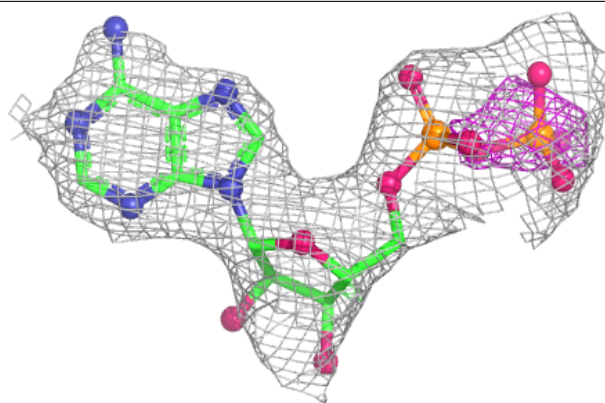
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	ADP	A	503	27/27	0.81	0.10	65,93,117,126	0
2	CL	B	501	1/1	0.83	0.25	91,91,91,91	0
3	ADP	B	502	27/27	0.88	0.09	89,107,120,138	0
2	CL	A	501	1/1	0.89	0.38	98,98,98,98	0
4	MLI	A	504	7/7	0.89	0.09	62,71,76,79	0
2	CL	A	502	1/1	0.91	0.10	89,89,89,89	0

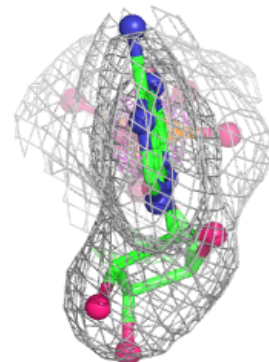
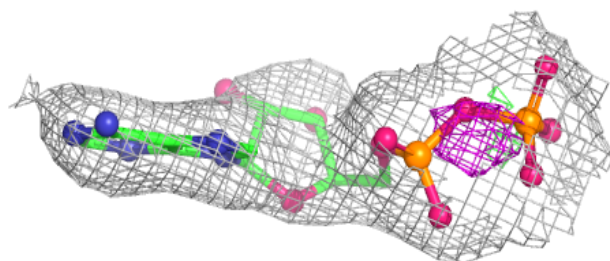
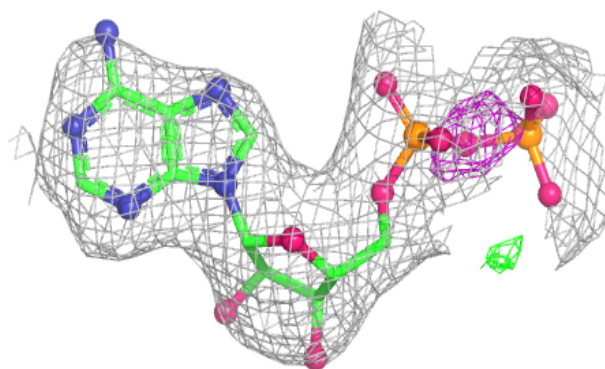
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP 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 ADP B 502:**

$2mF_o-DF_c$  (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.