



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 15, 2026 – 04:04 PM EDT

PDB ID : 12PL / pdb_000012pl
Title : Crystal Structure of serine/threonine-protein kinase (AEK1) from Trypanosoma cruzi in complex with LMS
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2026-04-14
Resolution : 2.82 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

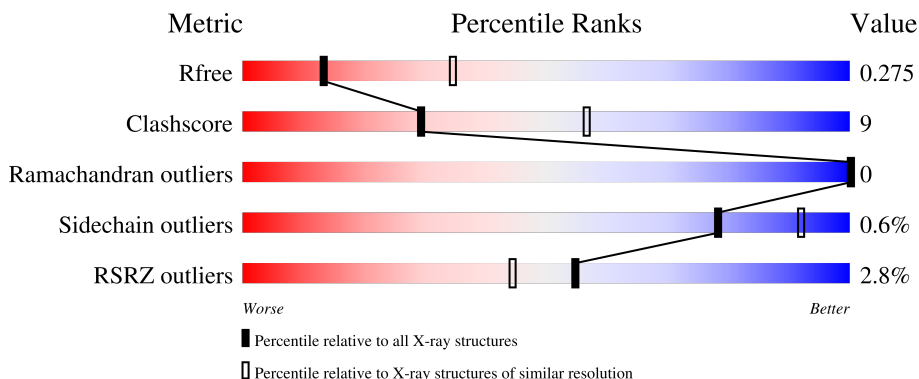
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	361	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>10%</div> </div> </div>
1	B	361	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5117 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.

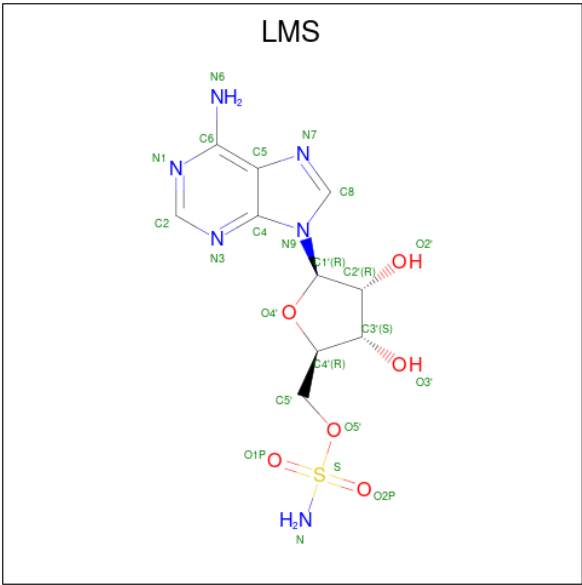
- Molecule 1 is a protein called Serine/threonine protein kinase, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	P	S	0	0	0
			2573	1662	427	470	2	12			
1	B	319	Total	C	N	O	P	S	0	0	0
			2498	1611	418	455	2	12			

There are 24 discrepancies between the modelled and reference sequences:

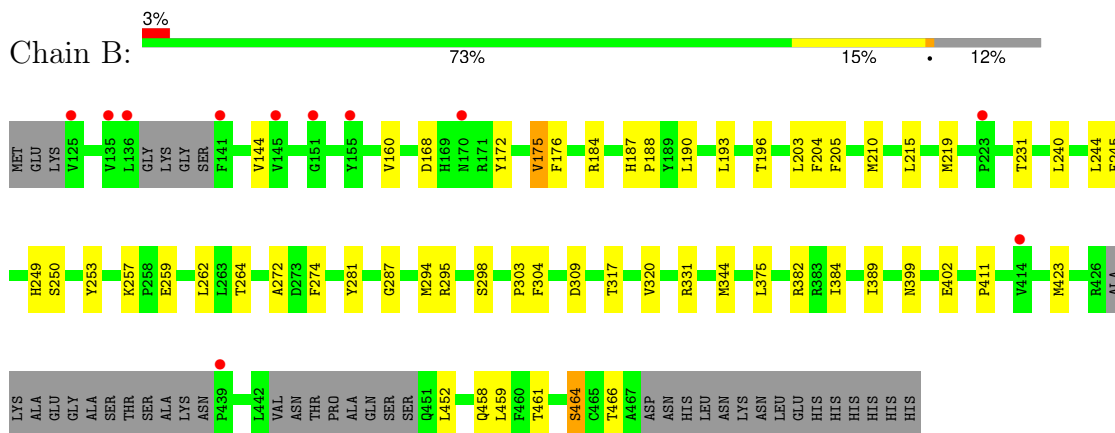
Chain	Residue	Modelled	Actual	Comment	Reference
A	122	MET	-	initiating methionine	UNP Q4E2L0
A	185	ILE	THR	engineered mutation	UNP Q4E2L0
A	227	PHE	VAL	engineered mutation	UNP Q4E2L0
A	314	SER	ASN	engineered mutation	UNP Q4E2L0
A	475	LEU	-	expression tag	UNP Q4E2L0
A	476	GLU	-	expression tag	UNP Q4E2L0
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 [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDRO-2-FURANYL]METHYL SULFAMATE (CCD ID: LMS) (formula: C₁₀H₁₄N₆O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	10	6	6	1		
2	B	1	Total	C	N	O	S	0	0
			23	10	6	6	1		

- Molecule 1: Serine/threonine protein kinase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.19Å 86.19Å 193.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.77 – 2.82 48.77 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.77-2.82) 99.9 (48.77-2.82)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.81Å)	Xtriage
Refinement program	PHENIX (2.1rc1_6025: ???)	Depositor
R, R_{free}	0.240 , 0.279 0.240 , 0.275	Depositor DCC
R_{free} test set	1004 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5117	wwPDB-VP
Average B, all atoms (Å ²)	94.0	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 38.24 % 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 3.7968e-04. 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: SEP, LMS

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	0.16	0/2615	0.33	0/3541
1	B	0.18	0/2540	0.36	0/3446
All	All	0.17	0/5155	0.34	0/6987

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	382	ARG	Sidechain

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	2573	0	2474	52	0
1	B	2498	0	2356	41	0
2	A	23	0	13	1	0
2	B	23	0	13	1	0
All	All	5117	0	4856	86	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 9.

The worst 5 of 86 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:189:TYR:C	1:A:270:VAL:HG23	2.09	0.78
1:B:375:LEU:HD21	1:B:389:ILE:HD13	1.76	0.68
1:B:423:MET:HA	1:B:423:MET:HE3	1.78	0.65
1:A:344:MET:HE2	1:A:459:LEU:HB3	1.80	0.64
1:A:375:LEU:HD21	1:A:389:ILE:CD1	2.30	0.61

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	315/361 (87%)	306 (97%)	9 (3%)	0	100	100
1	B	309/361 (86%)	303 (98%)	6 (2%)	0	100	100
All	All	624/722 (86%)	609 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	268/318 (84%)	267 (100%)	1 (0%)	84	94
1	B	254/318 (80%)	252 (99%)	2 (1%)	73	90
All	All	522/636 (82%)	519 (99%)	3 (1%)	78	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ASP
1	B	175	VAL
1	B	309	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	HIS
1	A	268	HIS
1	B	399	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	1.72	1 (12%)	7,12,14	1.30	1 (14%)
1	SEP	B	464	1	8,9,10	1.61	1 (12%)	7,12,14	0.94	0
1	SEP	B	298	1	8,9,10	1.55	1 (12%)	7,12,14	1.15	1 (14%)
1	SEP	A	464	1	8,9,10	1.68	1 (12%)	7,12,14	1.51	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	464	1	-	1/6/8/10	-

All (4) 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	A	464	SEP	P-O1P	3.66	1.61	1.50
1	B	464	SEP	P-O1P	3.44	1.61	1.50
1	B	298	SEP	P-O1P	3.36	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	SEP	OG-CB-CA	3.41	111.46	108.14
1	A	298	SEP	OG-CB-CA	2.96	111.03	108.14
1	B	298	SEP	OG-CB-CA	2.62	110.69	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	464	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	464	SEP	1	0

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	LMS	A	501	-	25,25,25	4.10	12 (48%)	38,38,38	2.58	13 (34%)
2	LMS	B	501	-	25,25,25	4.10	11 (44%)	38,38,38	2.59	10 (26%)

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	LMS	A	501	-	-	2/10/26/26	0/3/3/3
2	LMS	B	501	-	-	1/10/26/26	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LMS	O2P-S	8.78	1.51	1.42
2	A	501	LMS	O1P-S	8.77	1.51	1.42
2	B	501	LMS	O1P-S	8.70	1.51	1.42
2	B	501	LMS	O4'-C1'	8.62	1.61	1.42
2	B	501	LMS	O2P-S	8.60	1.51	1.42

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	LMS	O2P-S-O1P	-10.74	109.01	119.94
2	A	501	LMS	O2P-S-O1P	-9.63	110.14	119.94
2	A	501	LMS	N3-C2-N1	-5.68	119.98	128.58
2	B	501	LMS	N3-C2-N1	-5.56	120.17	128.58
2	B	501	LMS	C5-C4-N3	-4.76	120.17	126.72

There are no chirality outliers.

All (3) torsion outliers are listed below:

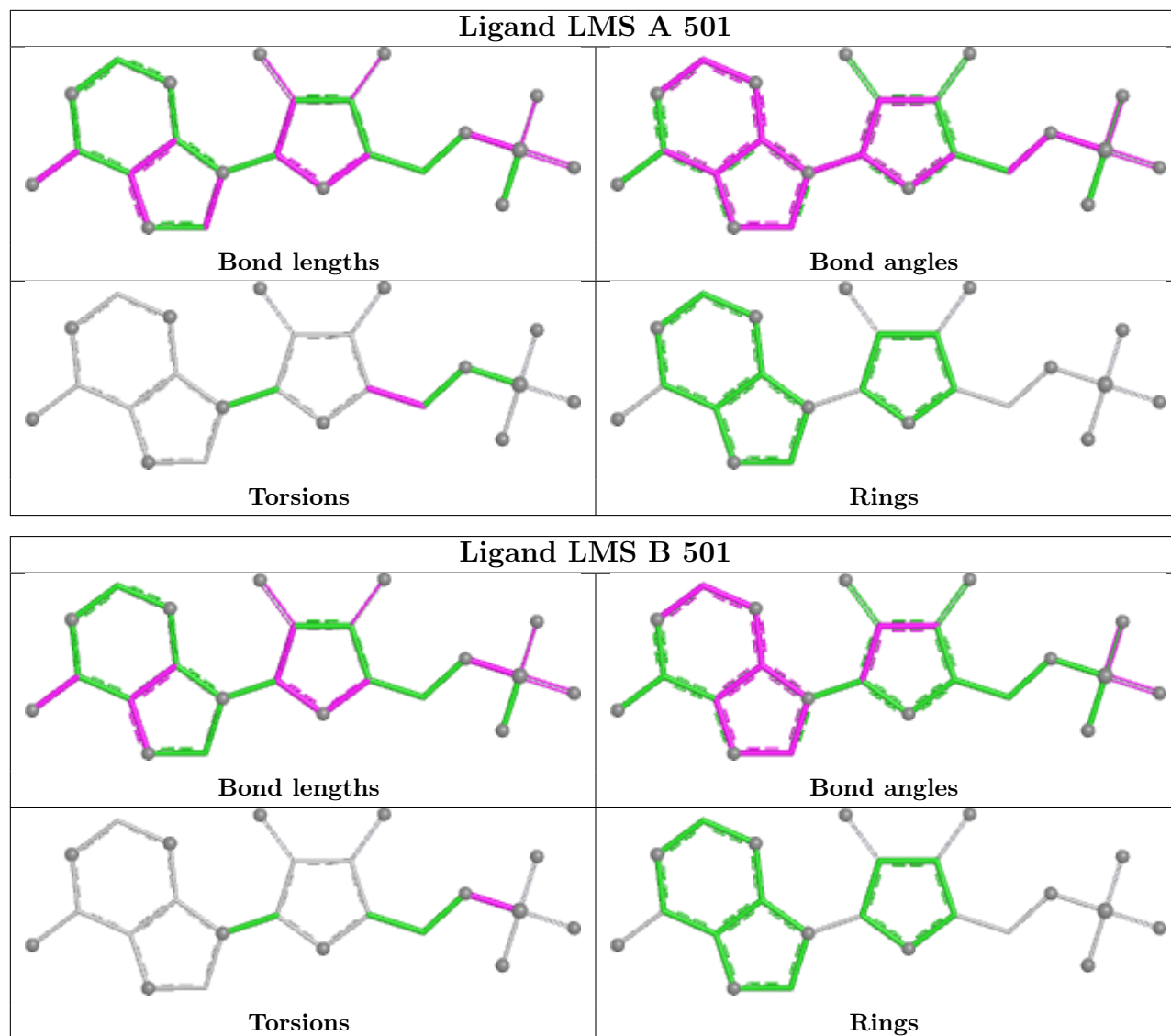
Mol	Chain	Res	Type	Atoms
2	A	501	LMS	O4'-C4'-C5'-O5'
2	A	501	LMS	C3'-C4'-C5'-O5'
2	B	501	LMS	C5'-O5'-S-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LMS	1	0
2	B	501	LMS	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 [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 [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, 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	323/361 (89%)	0.36	7 (2%) 62 52	64, 92, 129, 142	0
1	B	317/361 (87%)	0.44	11 (3%) 47 37	53, 94, 134, 158	0
All	All	640/722 (88%)	0.40	18 (2%) 55 44	53, 93, 132, 158	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	ASN	3.5
1	A	134	ASP	3.4
1	B	125	VAL	3.1
1	A	170	ASN	3.1
1	B	136	LEU	2.9

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	464	10/11	0.86	0.10	102,114,117,124	0
1	SEP	B	464	10/11	0.92	0.08	72,79,84,102	0
1	SEP	B	298	10/11	0.95	0.07	61,69,77,81	0
1	SEP	A	298	10/11	0.96	0.07	59,72,82,88	0

6.3 Carbohydrates [i](#)

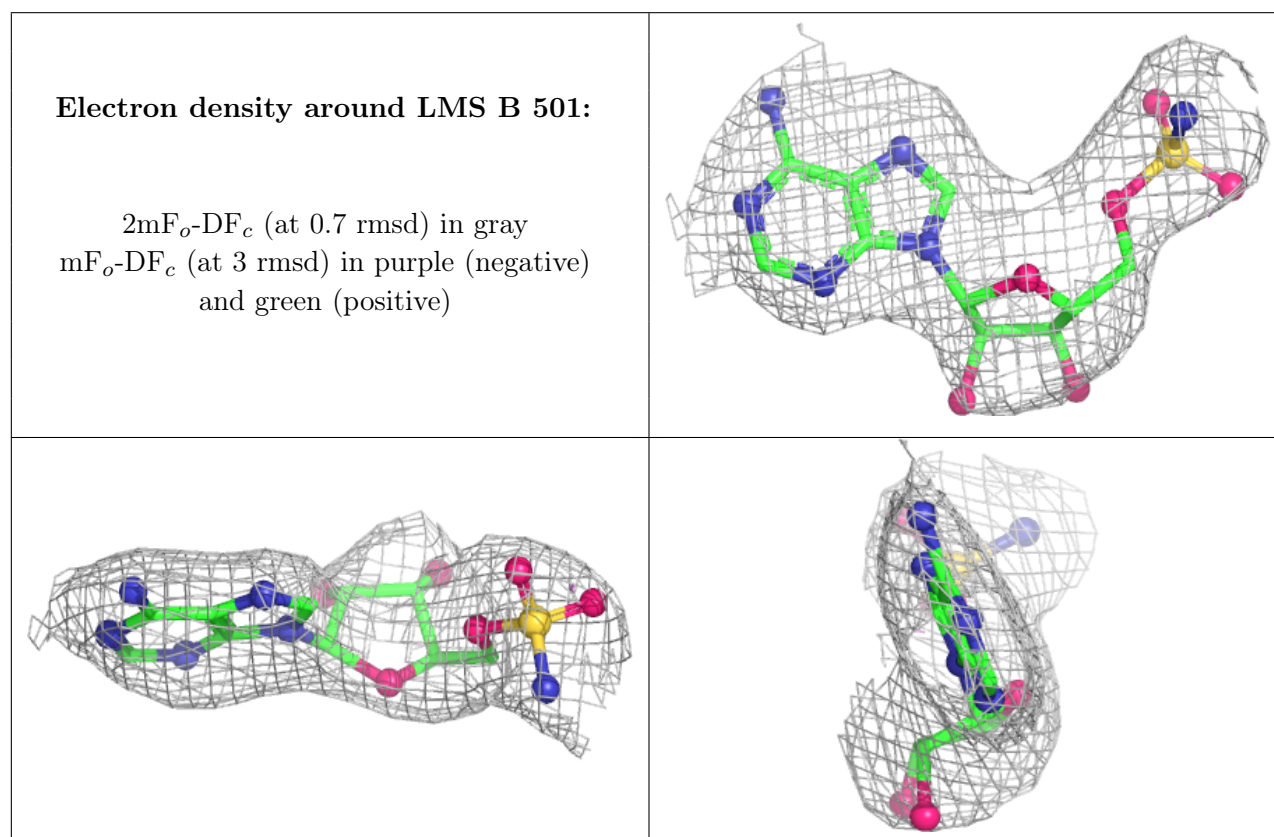
There are no oligosaccharides in this entry.

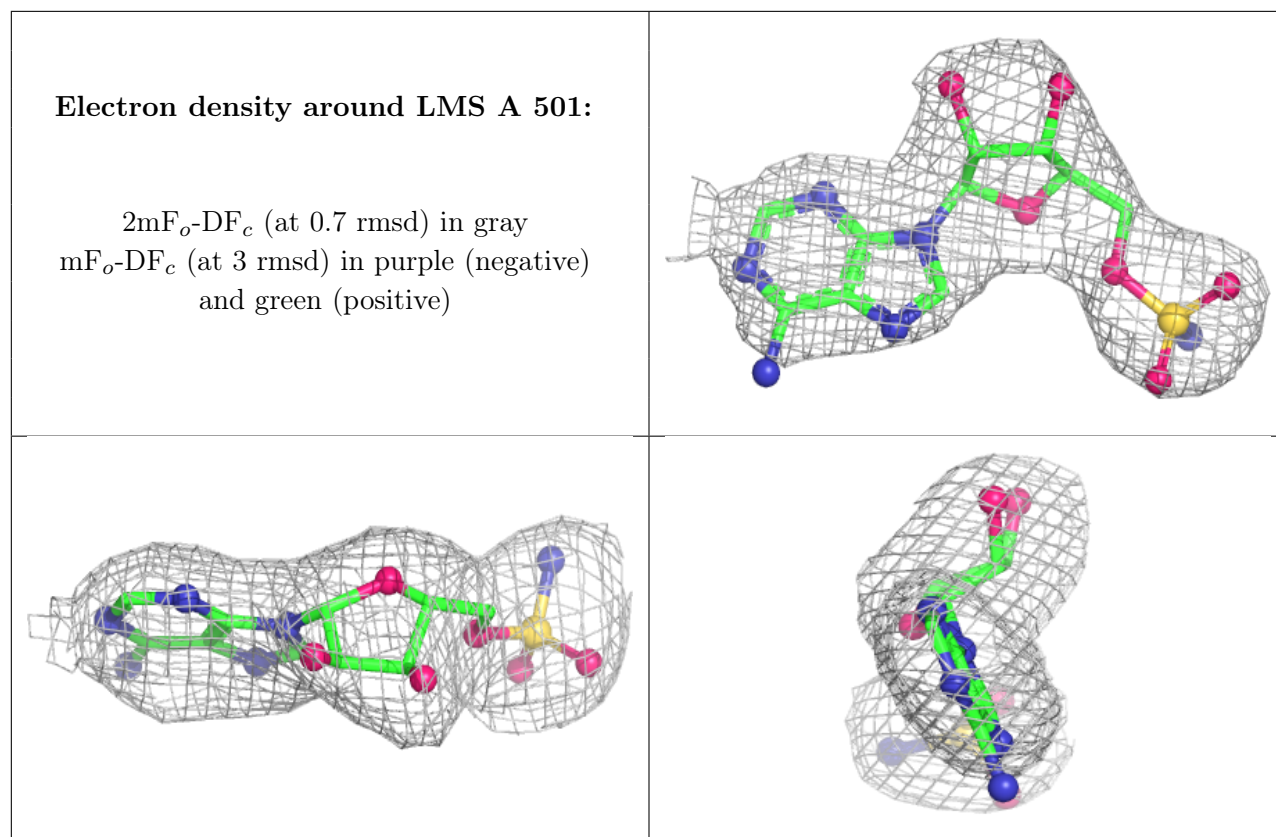
6.4 Ligands [i](#)

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, 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(\AA^2)	Q<0.9
2	LMS	B	501	23/23	0.83	0.12	94,112,136,141	0
2	LMS	A	501	23/23	0.91	0.09	70,81,98,105	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.