



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2024 – 06:33 PM EST

PDB ID : 4BRE  
Title : Legionella pneumophila NTPDase1 crystal form II (closed) in complex with transition state mimic adenosine 5'phosphovanadate  
Authors : Zebisch, M.; Schaefer, P.; Lauble, P.; Straeter, N.  
Deposited on : 2013-06-04  
Resolution : 1.60 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.

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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

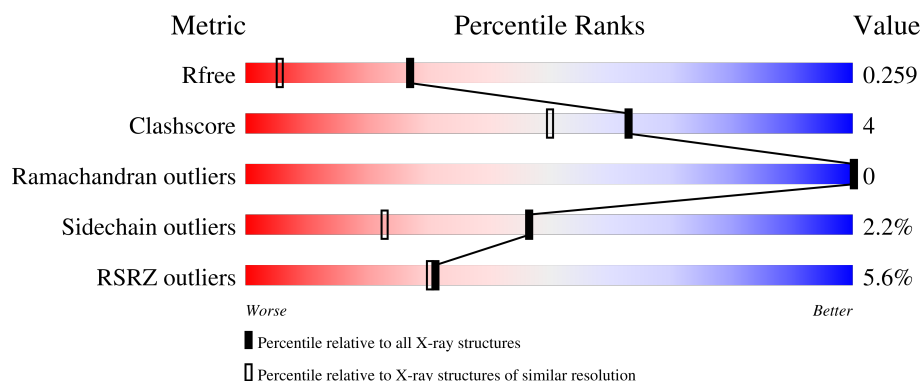
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6544 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 ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	23	0
			2984	1908	486	574	16			
1	B	358	Total	C	N	O	S	0	23	0
			2984	1904	489	575	16			

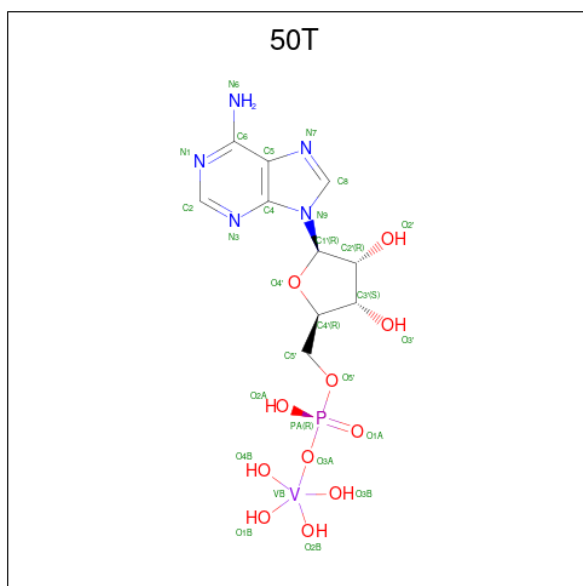
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	-	expression tag	UNP Q5ZUA2
A	137	ASP	GLU	conflict	UNP Q5ZUA2
A	149	VAL	ALA	conflict	UNP Q5ZUA2
A	394	LEU	-	expression tag	UNP Q5ZUA2
A	395	GLU	-	expression tag	UNP Q5ZUA2
A	396	HIS	-	expression tag	UNP Q5ZUA2
A	397	HIS	-	expression tag	UNP Q5ZUA2
A	398	HIS	-	expression tag	UNP Q5ZUA2
A	399	HIS	-	expression tag	UNP Q5ZUA2
A	400	HIS	-	expression tag	UNP Q5ZUA2
A	401	HIS	-	expression tag	UNP Q5ZUA2
B	34	MET	-	expression tag	UNP Q5ZUA2
B	137	ASP	GLU	conflict	UNP Q5ZUA2
B	149	VAL	ALA	conflict	UNP Q5ZUA2
B	394	LEU	-	expression tag	UNP Q5ZUA2
B	395	GLU	-	expression tag	UNP Q5ZUA2
B	396	HIS	-	expression tag	UNP Q5ZUA2
B	397	HIS	-	expression tag	UNP Q5ZUA2
B	398	HIS	-	expression tag	UNP Q5ZUA2
B	399	HIS	-	expression tag	UNP Q5ZUA2
B	400	HIS	-	expression tag	UNP Q5ZUA2
B	401	HIS	-	expression tag	UNP Q5ZUA2

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-PHOSPHOVANADATE (three-letter code: 50T) (formula:  $C_{10}H_{17}N_5O_{11}PV$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	V	0	0
			28	10	5	11	1	1		
3	B	1	Total	C	N	O	P	V	0	1
			47	20	10	15	1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		


- Molecule 6 is water.

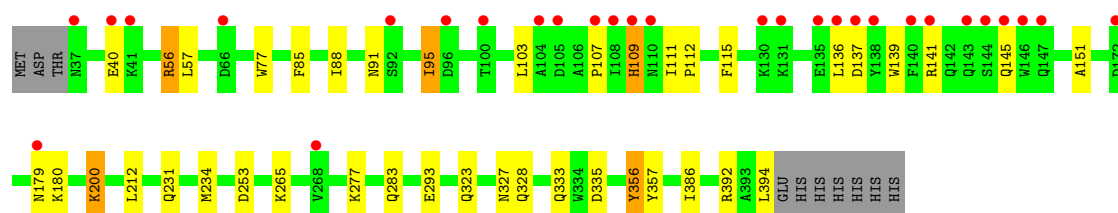
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	237	Total	O	0	3
			240	240		
6	B	232	Total	O	0	2
			234	234		

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


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

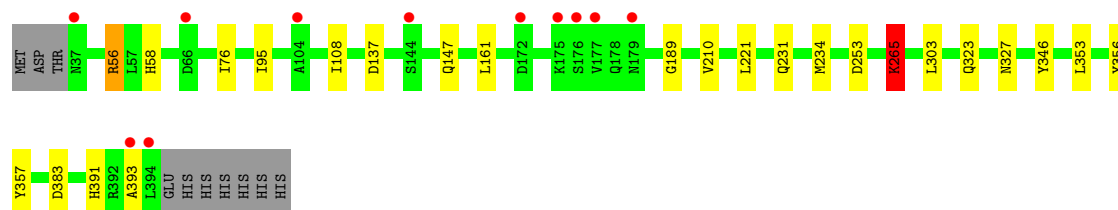
#### • Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE I

Chain A: 



#### • Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE I

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.68Å 86.20Å 70.88Å 90.00° 105.94° 90.00°	Depositor
Resolution (Å)	29.33 – 1.60 29.33 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.33-1.60) 99.9 (29.33-1.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.172 , 0.208 0.226 , 0.259	Depositor DCC
$R_{free}$ test set	1404 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: 50T, NA, MES, MG

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	0.90	0/3128	0.93	4/4262 (0.1%)
1	B	0.91	1/3125 (0.0%)	0.95	5/4256 (0.1%)
All	All	0.90	1/6253 (0.0%)	0.94	9/8518 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	GLY	N-CA	5.41	1.54	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASP	CB-CG-OD2	7.26	124.83	118.30
1	A	356	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	A	277	LYS	CD-CE-NZ	-6.12	97.62	111.70
1	B	56	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	A	56	ARG	NE-CZ-NH2	-5.92	117.34	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	391[B]	HIS	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	2984	0	2893	26	0
1	B	2984	0	2889	19	0
2	A	1	0	0	0	0
3	A	28	0	12	1	0
3	B	47	0	24	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	13	1	0
5	B	12	0	13	0	0
6	A	240	0	0	9	0
6	B	234	0	0	3	0
All	All	6544	0	5844	47	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 4.

The worst 5 of 47 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:333[B]:GLN:OE1	1:A:335[B]:ASP:OD1	1.55	1.24
1:B:323[B]:GLN:OE1	1:B:327:ASN:ND2	1.73	1.19
1:A:392[B]:ARG:NH2	6:A:2238:HOH:O	1.90	1.03
1:A:283[B]:GLN:OE1	6:A:2168:HOH:O	2.02	0.76
1:B:323[B]:GLN:CD	1:B:327:ASN:HD22	1.92	0.73

There are no symmetry-related clashes.

## 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	379/368 (103%)	365 (96%)	14 (4%)	0	100	100
1	B	379/368 (103%)	365 (96%)	14 (4%)	0	100	100
All	All	758/736 (103%)	730 (96%)	28 (4%)	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	341/328 (104%)	330 (97%)	11 (3%)	34	12
1	B	341/328 (104%)	336 (98%)	5 (2%)	60	39
All	All	682/656 (104%)	666 (98%)	16 (2%)	47	21

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	147[B]	GLN
1	B	147[A]	GLN
1	A	234[B]	MET
1	B	95	ILE
1	A	234[A]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	B	319	GLN
1	B	370	ASN
1	B	327	ASN
1	A	327	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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$
3	50T	A	1396	4	20,30,30	1.46	3 (15%)	21,49,49	1.75	2 (9%)
3	50T	B	1395[B]	-	20,30,30	1.37	3 (15%)	21,49,49	2.64	4 (19%)
5	MES	A	1398	-	12,12,12	2.09	2 (16%)	15,16,16	2.80	7 (46%)
3	50T	B	1395[A]	-	20,30,30	1.39	2 (10%)	21,49,49	1.86	5 (23%)
5	MES	B	1397	-	12,12,12	2.05	1 (8%)	15,16,16	2.74	5 (33%)

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
3	50T	A	1396	4	-	0/6/33/33	0/3/3/3
3	50T	B	1395[B]	-	-	0/6/33/33	0/3/3/3
5	MES	A	1398	-	-	5/6/14/14	0/1/1/1
3	50T	B	1395[A]	-	-	0/6/33/33	0/3/3/3
5	MES	B	1397	-	-	3/6/14/14	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1397	MES	C8-S	-6.60	1.68	1.77
5	A	1398	MES	C8-S	-6.27	1.68	1.77
3	B	1395[B]	50T	C6-N6	4.63	1.50	1.34
3	A	1396	50T	C6-N6	3.82	1.47	1.34
3	B	1395[A]	50T	C6-N6	3.74	1.47	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1395[B]	50T	O4'-C1'-N9	6.58	117.47	108.75
5	B	1397	MES	O1S-S-C8	-6.56	96.81	106.73
3	B	1395[B]	50T	N3-C2-N1	-6.29	120.13	128.67
5	A	1398	MES	O2S-S-C8	5.80	115.49	106.73
5	A	1398	MES	O3S-S-C8	-5.72	94.81	106.00

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1398	MES	N4-C7-C8-S
5	A	1398	MES	C7-C8-S-O2S
5	A	1398	MES	C7-C8-S-O3S
5	B	1397	MES	C8-C7-N4-C5
5	B	1397	MES	N4-C7-C8-S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

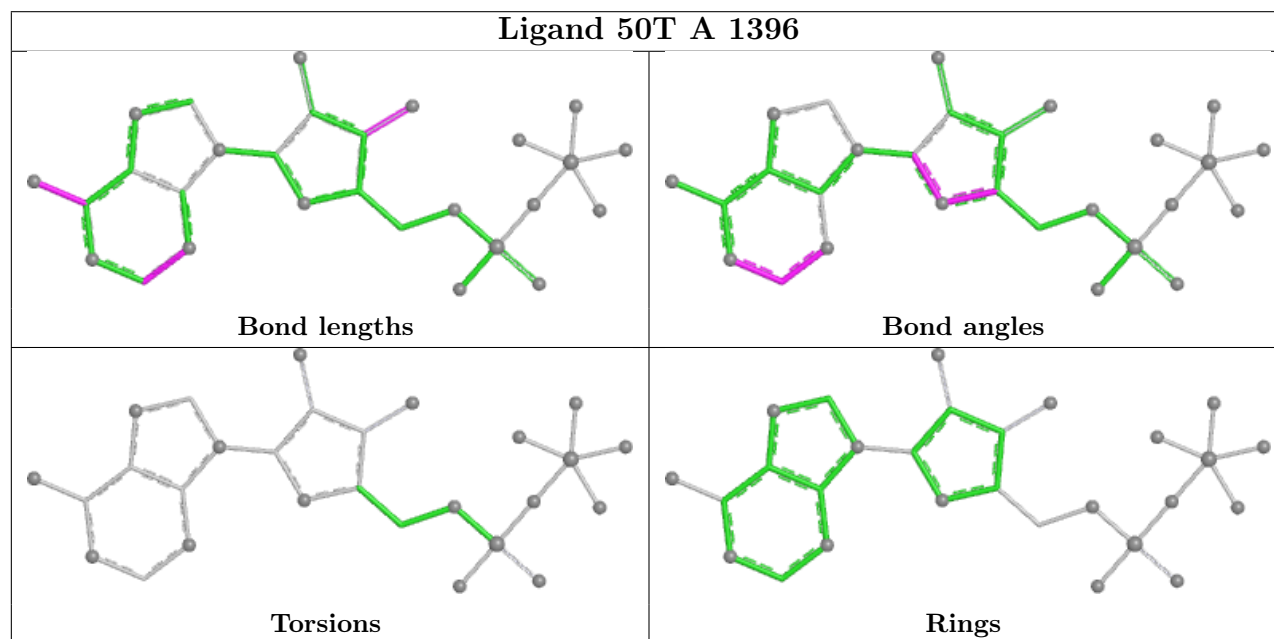
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1396	50T	1	0

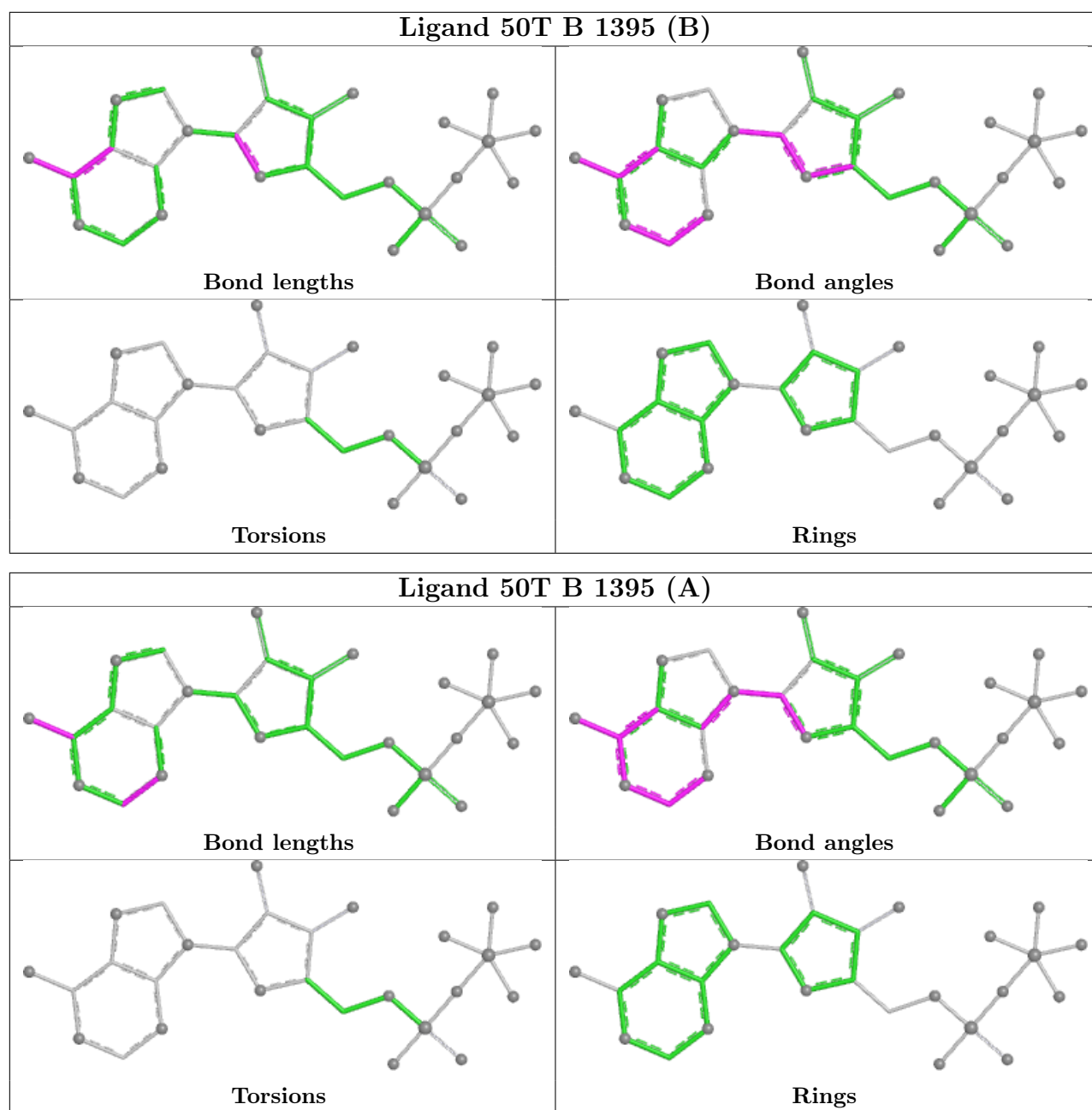
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1398	MES	1	0

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](#)

**Warning:** The R factor obtained from EDS is 0.2266, which does not match the depositor's R factor of 0.17211. Please interpret the results in this section carefully.

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	358/368 (97%)	0.38	29 (8%) 19 18	3, 7, 18, 30	23 (6%)
1	B	358/368 (97%)	0.06	11 (3%) 51 52	3, 7, 17, 27	23 (6%)
All	All	716/736 (97%)	0.22	40 (5%) 31 30	3, 7, 18, 30	46 (6%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	SER	4.4
1	A	138	TYR	4.3
1	A	104	ALA	4.1
1	B	66	ASP	4.0
1	A	107	PRO	3.6

### 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](#)

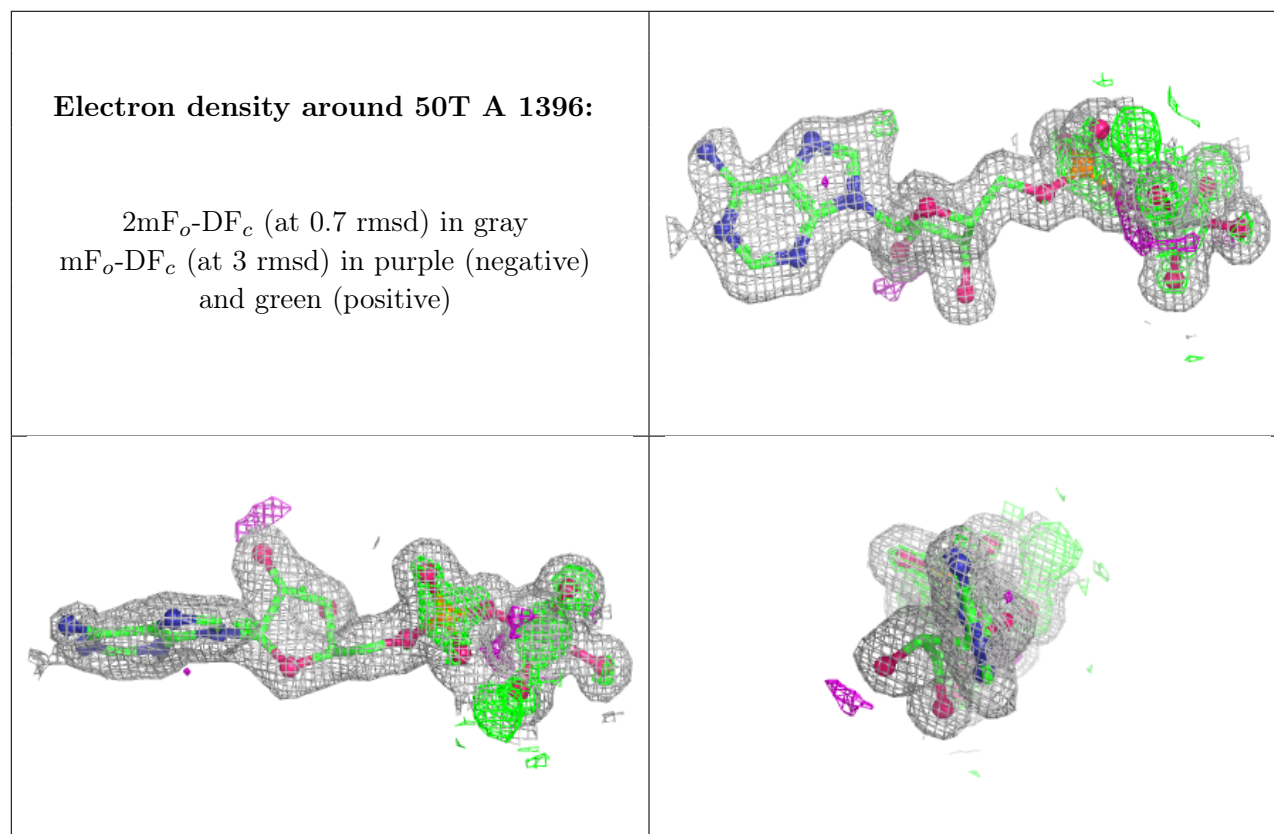
There are no monosaccharides in this entry.

### 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
5	MES	A	1398	12/12	0.86	0.19	24,34,41,43	12
5	MES	B	1397	12/12	0.88	0.21	25,32,38,40	12
2	NA	A	1395	1/1	0.95	0.12	37,37,37,37	0
3	50T	A	1396	28/28	0.96	0.14	14,23,34,38	0
3	50T	B	1395[A]	28/28	0.97	0.14	14,19,21,24	19
3	50T	B	1395[B]	28/28	0.97	0.14	14,17,18,19	19
4	MG	A	1397	1/1	0.99	0.19	16,16,16,16	0
4	MG	B	1396	1/1	0.99	0.13	15,15,15,15	0

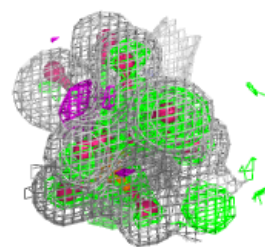
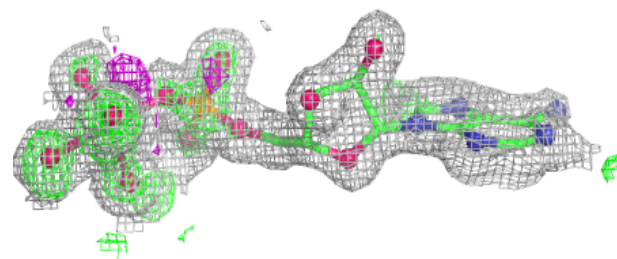
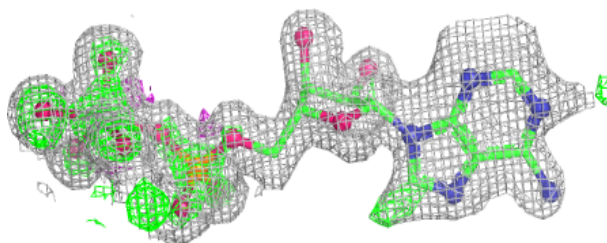
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



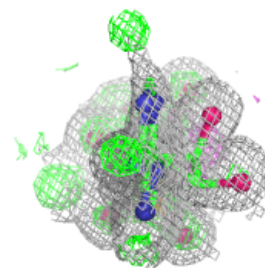
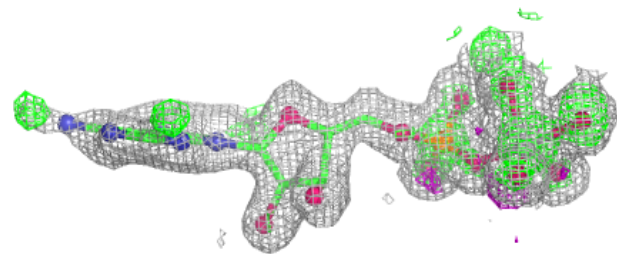
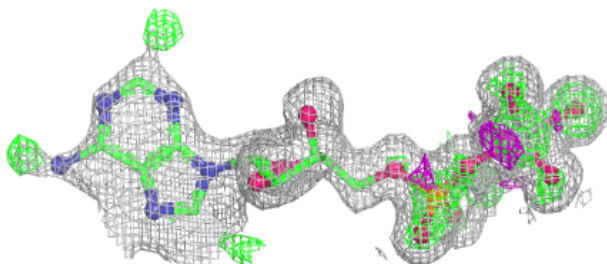


**Electron density around 50T B 1395 (A):**

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

**Electron density around 50T B 1395 (B):**

$2mF_o-DF_c$  (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.