



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2025 – 05:06 PM EDT

PDB ID : 9NA3 / pdb\_00009na3  
Title : IRAK4 in Complex with Compound 15  
Authors : Ferrao, R.; Lansdon, E.B.  
Deposited on : 2025-02-11  
Resolution : 2.10 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

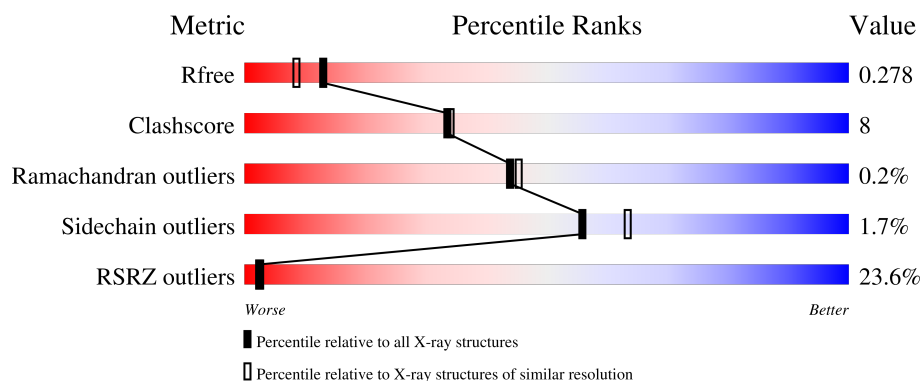
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	304	<div> <div>21%</div> <div>74%</div> <div>19%</div> <div>7%</div> </div>
1	H0A0	304	<div> <div>22%</div> <div>88%</div> <div>9%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4614 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.

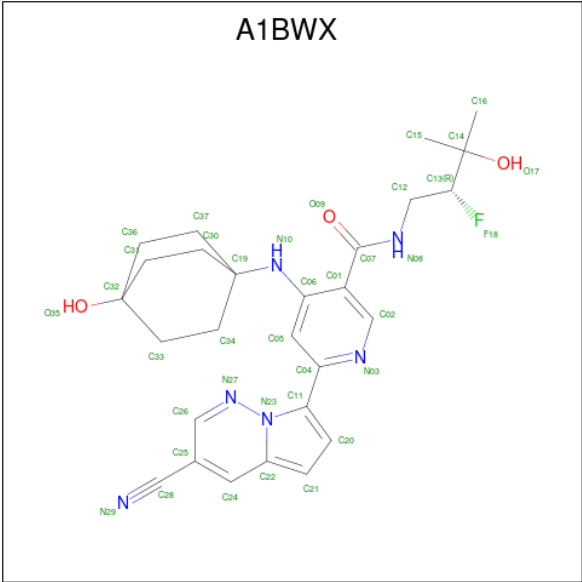
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	P	S	0	0	0
			2237	1406	376	438	3	14			
1	H0A0	277	Total	C	N	O	P	S	0	1	0
			2183	1375	364	426	3	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	GLY	-	expression tag	UNP Q9NWZ3
A	158	ALA	-	expression tag	UNP Q9NWZ3
A	159	MET	-	expression tag	UNP Q9NWZ3
H0A0	157	GLY	-	expression tag	UNP Q9NWZ3
H0A0	158	ALA	-	expression tag	UNP Q9NWZ3
H0A0	159	MET	-	expression tag	UNP Q9NWZ3

- Molecule 2 is (6P)-6-[(8R)-3-cyanopyrrolo[1,2-b]pyridazin-7-yl]-N-[(2S)-2-fluoro-3-hydroxy-3-methylbutyl]-4-[(4-hydroxybicyclo[2.2.2]octan-1-yl)amino]pyridine-3-carboxamide (CCD ID: A1BWX) (formula: C<sub>27</sub>H<sub>31</sub>FN<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			37	27	1	6	3		
2	H0A0	1	Total	C	F	N	O	0	0
			37	27	1	6	3		

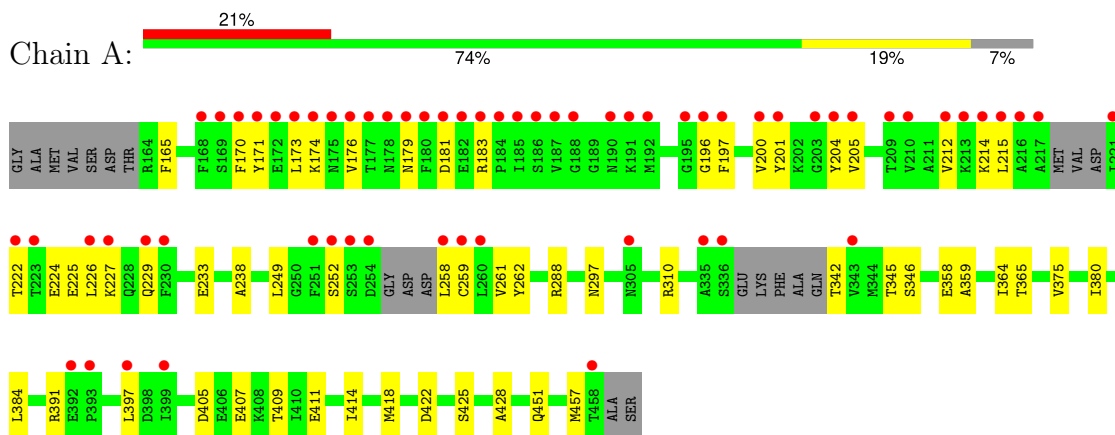
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	H0A0	60	Total	O	0	0
			60	60		

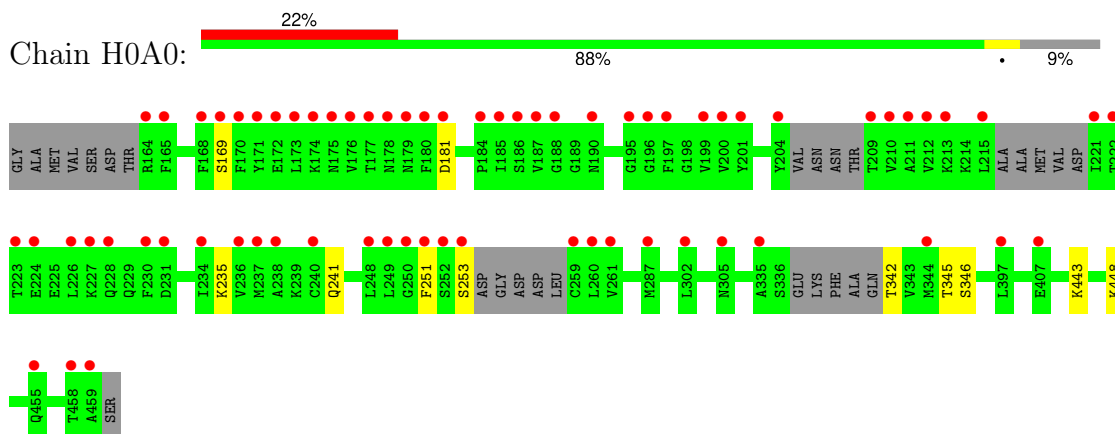
### 3 Residue-property plots [i](#)

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: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.67Å 110.43Å 140.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.10 49.09 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.09-2.10) 92.1 (49.09-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.243 , 0.277 0.243 , 0.278	Depositor DCC
$R_{free}$ test set	37946 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	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 27.86 % 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 2.0410e-03. 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: SEP, A1BWX, TPO

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	0.11	0/2240	0.33	0/3016
1	H0A0	0.12	0/2188	0.30	0/2943
All	All	0.12	0/4428	0.32	0/5959

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	2237	0	2207	32	0
1	H0A0	2183	0	0	0	0
2	A	37	0	0	0	0
2	H0A0	37	0	0	0	0
3	A	60	0	0	1	0
3	H0A0	60	0	0	0	0
All	All	4614	0	2207	32	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 8.

The worst 5 of 32 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:174:LYS:HG2	1:A:179:ASN:HA	1.57	0.86
1:A:173:LEU:HD13	1:A:212:VAL:HG11	1.75	0.68
1:A:297:ASN:HD22	1:A:451:GLN:HE22	1.50	0.58
1:A:252:SER:HB2	1:A:259:CYS:HB2	1.88	0.56
1:A:176:VAL:HG11	1:A:205:VAL:HG22	1.91	0.52

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	274/304 (90%)	263 (96%)	11 (4%)	0	100	100
1	H0A0	266/304 (88%)	257 (97%)	8 (3%)	1 (0%)	30	29
All	All	540/608 (89%)	520 (96%)	19 (4%)	1 (0%)	44	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H0A0	181	ASP

### 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	242/260 (93%)	241 (100%)	1 (0%)	89	93
1	H0A0	236/260 (91%)	229 (97%)	7 (3%)	36	40
All	All	478/520 (92%)	470 (98%)	8 (2%)	56	63

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H0A0	448	LYS
1	H0A0	443	LYS
1	H0A0	251	PHE
1	H0A0	241	GLN
1	H0A0	253	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	166	HIS
1	A	190	ASN
1	A	442	ASN
1	A	451	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	TPO	A	345	1	8,10,11	1.11	0	10,14,16	1.92	1 (10%)
1	TPO	H0A0	345	1	8,10,11	1.09	0	10,14,16	1.95	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	A	346	1	8,9,10	1.62	1 (12%)	7,12,14	1.24	1 (14%)
1	TPO	A	342	1	8,10,11	1.12	0	10,14,16	2.09	2 (20%)
1	SEP	H0A0	346	1	8,9,10	1.62	1 (12%)	7,12,14	1.16	1 (14%)
1	TPO	H0A0	342	1	8,10,11	1.11	0	10,14,16	1.87	1 (10%)

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	TPO	A	345	1	-	3/9/11/13	-
1	TPO	H0A0	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	A	342	1	-	0/9/11/13	-
1	SEP	H0A0	346	1	-	2/6/8/10	-
1	TPO	H0A0	342	1	-	3/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	SEP	P-O1P	3.53	1.61	1.50
1	H0A0	346	SEP	P-O1P	3.53	1.61	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TPO	P-OG1-CB	-5.90	107.31	123.33
1	H0A0	342	TPO	P-OG1-CB	-5.46	108.48	123.33
1	H0A0	345	TPO	P-OG1-CB	-5.42	108.60	123.33
1	A	345	TPO	P-OG1-CB	-5.37	108.74	123.33
1	A	346	SEP	OG-CB-CA	2.55	110.62	108.14

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	H0A0	342	TPO	N-CA-CB-OG1
1	H0A0	342	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
1	H0A0	345	TPO	N-CA-CB-OG1
1	H0A0	346	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

## 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	A1BWX	H0A0	501	-	36,41,41	1.43	3 (8%)	49,63,63	1.30	5 (10%)
2	A1BWX	A	501	-	36,41,41	1.41	2 (5%)	49,63,63	1.28	6 (12%)

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	A1BWX	H0A0	501	-	-	5/23/47/47	0/6/5/5
2	A1BWX	A	501	-	-	6/23/47/47	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H0A0	501	A1BWX	C26-C25	6.25	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1BWX	C26-C25	6.13	1.48	1.39
2	H0A0	501	A1BWX	C07-N08	2.34	1.38	1.33
2	A	501	A1BWX	C07-N08	2.25	1.38	1.33
2	H0A0	501	A1BWX	C24-C22	2.09	1.42	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H0A0	501	A1BWX	C24-C25-C28	3.81	122.90	119.66
2	H0A0	501	A1BWX	C37-C19-C34	-3.62	105.45	108.84
2	A	501	A1BWX	C24-C25-C28	3.59	122.71	119.66
2	A	501	A1BWX	C37-C19-C34	-3.10	105.93	108.84
2	H0A0	501	A1BWX	C24-C25-C26	-2.43	116.00	118.13

There are no chirality outliers.

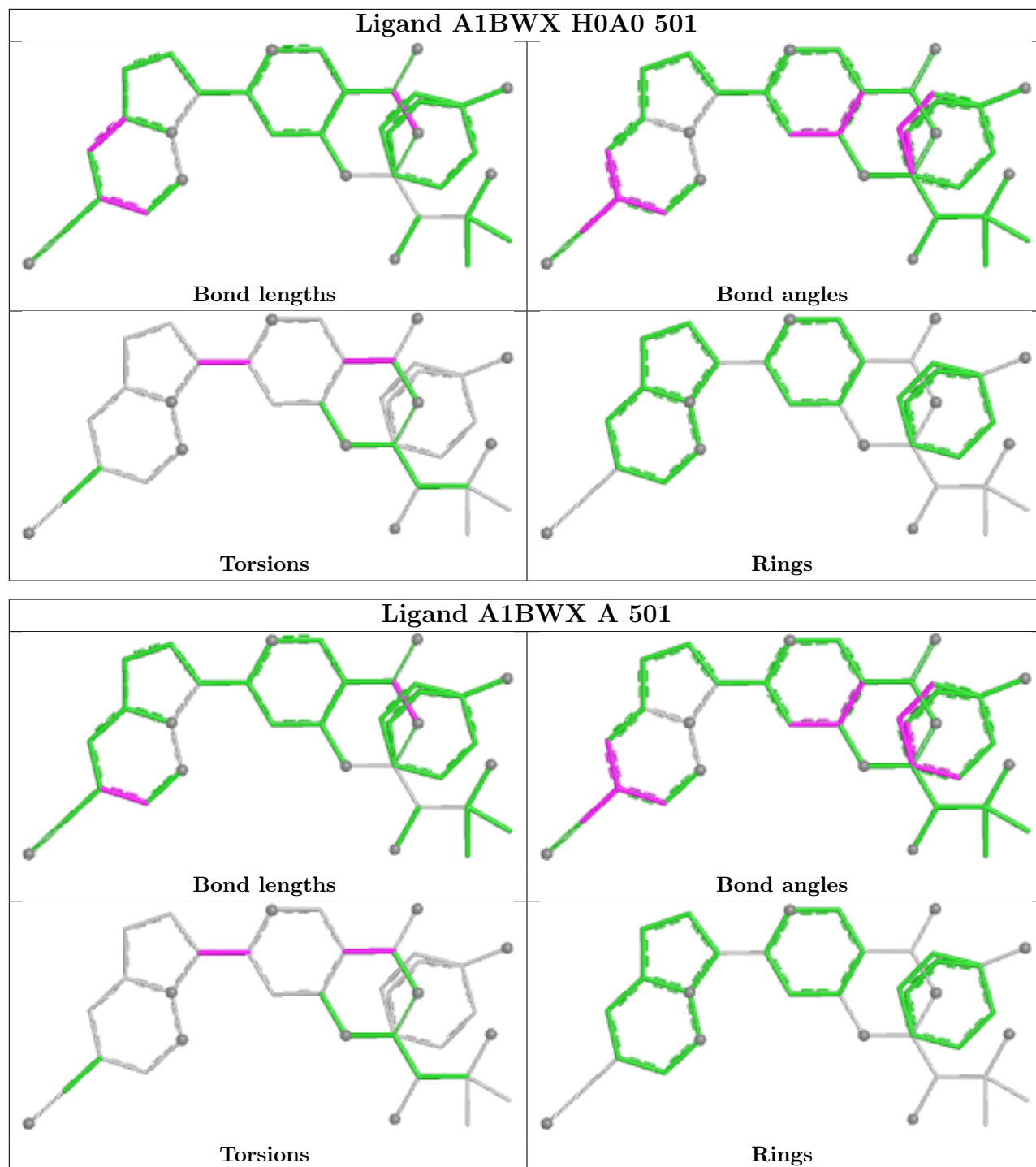
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1BWX	N03-C04-C11-C20
2	A	501	A1BWX	N03-C04-C11-N23
2	H0A0	501	A1BWX	C05-C04-C11-C20
2	H0A0	501	A1BWX	C05-C04-C11-N23
2	H0A0	501	A1BWX	N03-C04-C11-C20

There are no ring outliers.

No monomer is involved in short contacts.

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	281/304 (92%)	1.28	63 (22%) 3 3	29, 56, 92, 109	0
1	H0A0	274/304 (90%)	1.12	68 (24%) 2 2	23, 53, 114, 139	1 (0%)
All	All	555/608 (91%)	1.20	131 (23%) 2 2	23, 54, 107, 139	1 (0%)

The worst 5 of 131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	TYR	5.9
1	A	226	LEU	5.8
1	H0A0	221	ILE	5.8
1	A	176	VAL	5.8
1	A	195	GLY	5.7

### 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	A	346	10/11	0.54	0.15	73,84,101,106	0
1	TPO	A	342	11/12	0.67	0.17	65,82,89,107	0
1	SEP	H0A0	346	10/11	0.78	0.11	62,83,108,110	0
1	TPO	H0A0	342	11/12	0.81	0.15	61,74,83,85	0
1	TPO	H0A0	345	11/12	0.86	0.14	57,69,78,81	0
1	TPO	A	345	11/12	0.90	0.10	64,71,76,80	0

### 6.3 Carbohydrates [i](#)

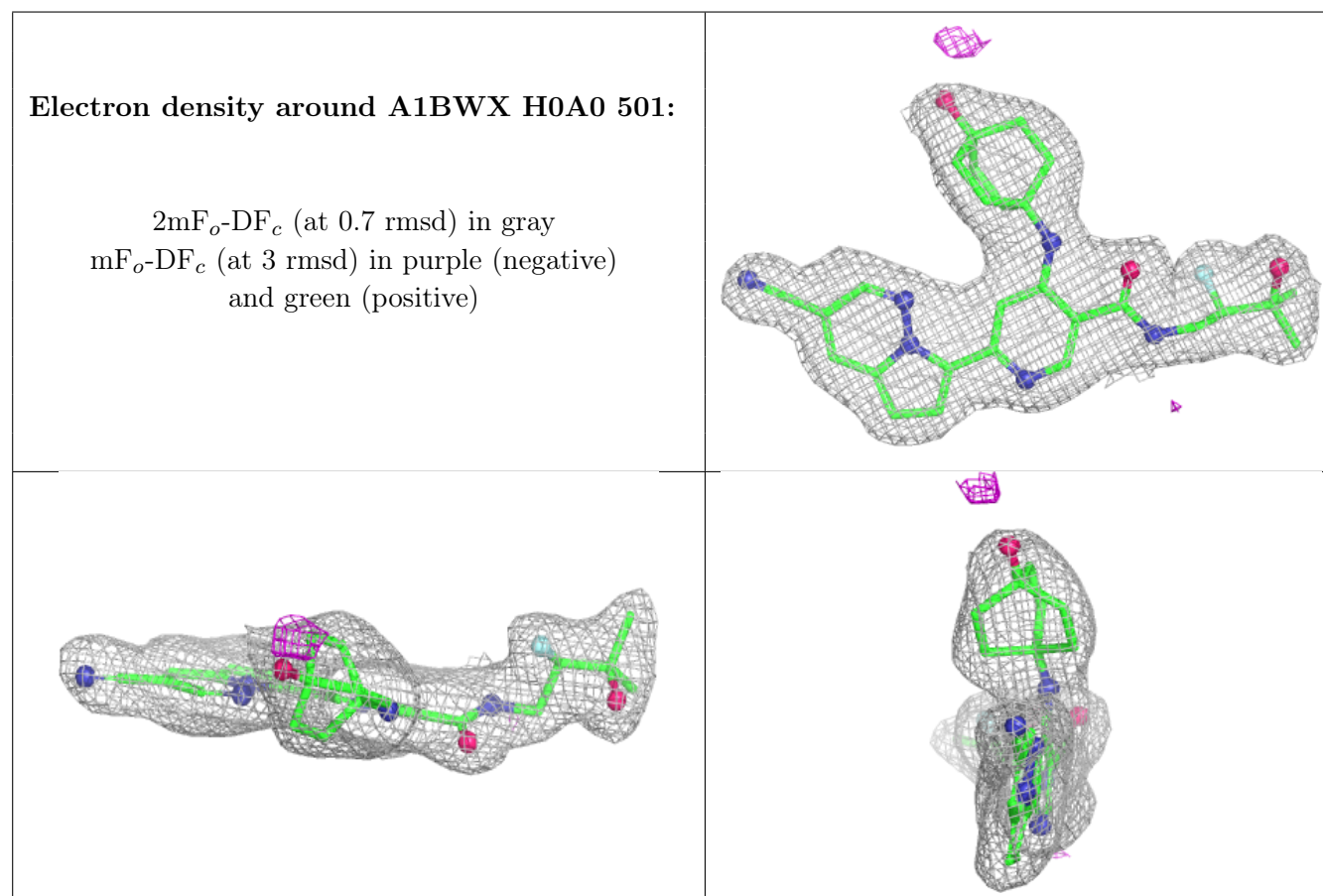
There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1BWX	H0A0	501	37/37	0.92	0.11	34,44,57,63	0
2	A1BWX	A	501	37/37	0.93	0.10	29,40,48,57	0

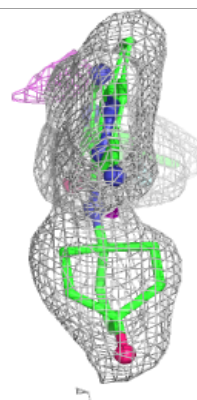
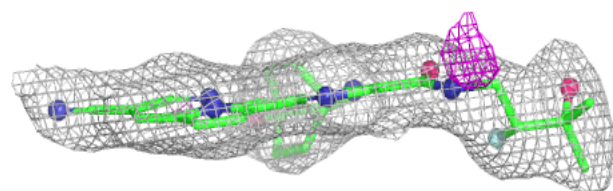
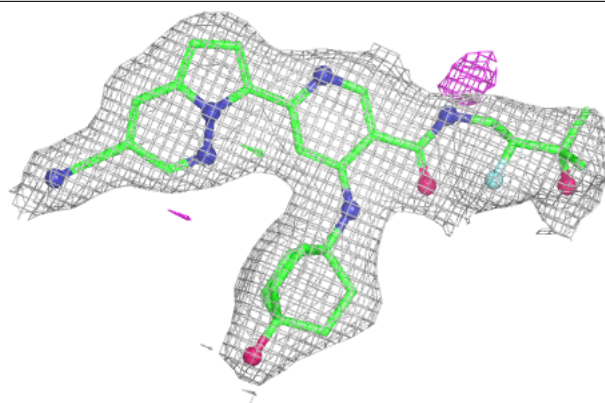
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





**Electron density around A1BWX A 501:**

$2mF_o-DF_c$  (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.