



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2022 – 11:39 pm GMT

PDB ID : 7B6W  
Title : Crystal structure of the human alpha1B adrenergic receptor in complex with inverse agonist (+)-cyclazosin  
Authors : Deluigi, M.; Morstein, L.; Hilge, M.; Schuster, M.; Merklinger, L.; Klipp, A.; Scott, D.J.; Plueckthun, A.  
Deposited on : 2020-12-08  
Resolution : 2.87 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.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

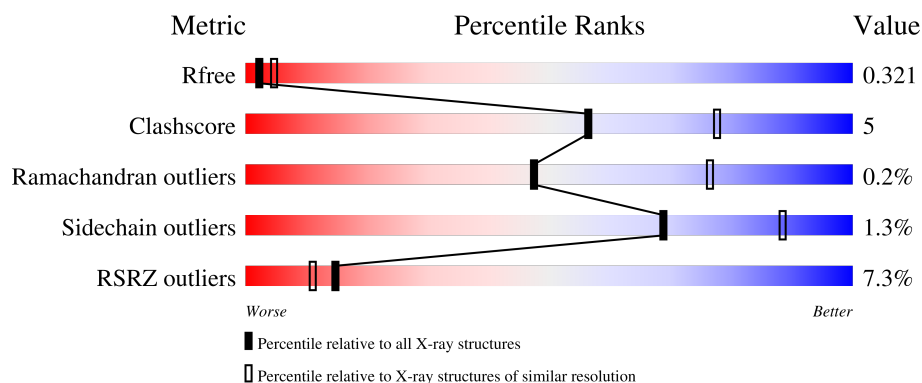
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.87 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))
$R_{free}$	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	AAA	459	

## 2 Entry composition [i](#)

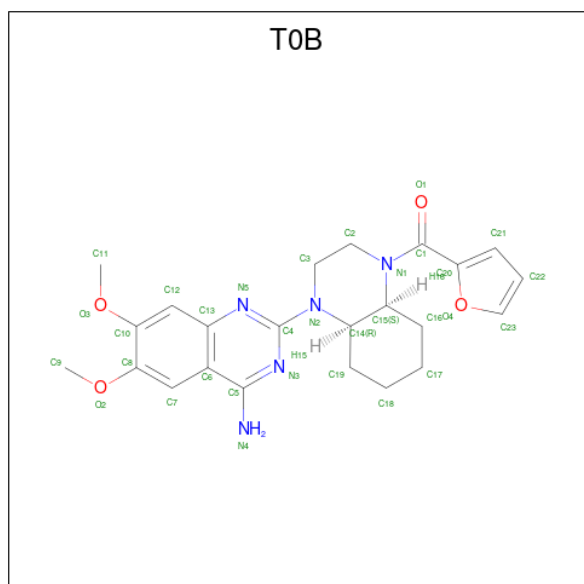
There are 2 unique types of molecules in this entry. The entry contains 6527 atoms, of which 3257 are hydrogens and 0 are deuteriums.

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 Alpha-1B adrenergic receptor,alpha1B adrenergic receptor,Alpha-1B adrenergic receptor,alpha1B adrenergic receptor,Alpha-1B adrenergic receptor,alpha1B adrenergic receptor,Alpha-1B adrenergic receptor,alpha1B adrenergic receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	438	Total	C	H	N	O	S	118	0	0
			6409	2100	3203	515	573	18			

- Molecule 2 is [(4 {a} {R}),8 {a} {S})-4-(4-azanyl-6,7-dimethoxy-quinazolin-2-yl)-2,3,4 {a} {a},5,6,7,8,8 {a}-octahydroquinoxalin-1-yl]-(furan-2-yl)methanone (three-letter code: T0B) (formula: C<sub>23</sub>H<sub>27</sub>N<sub>5</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

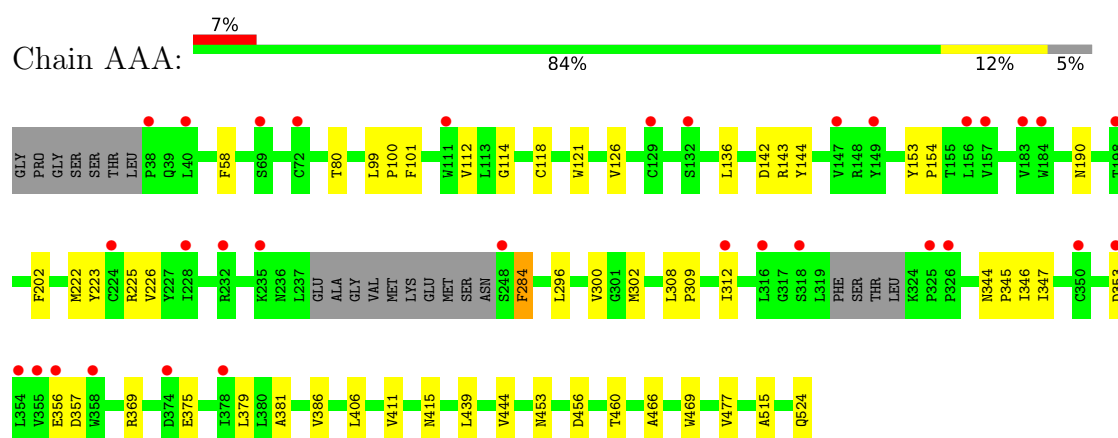


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O		0	1
			59	23	27	5	4			
2	AAA	1	Total	C	H	N	O		0	1
			59	23	27	5	4			

### 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: Alpha-1B adrenergic receptor,alpha1B adrenergic receptor,Alpha-1B adrenergic receptor,alpha1B adrenergic receptor,Alpha-1B adrenergic receptor,alpha1B adrenergic receptor,Alpha-1B adrenergic receptor,alpha1B adrenergic receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.88Å 76.42Å 151.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.73 – 2.87 28.71 – 2.87	Depositor EDS
% Data completeness (in resolution range)	79.3 (28.73-2.87) 79.4 (28.71-2.87)	Depositor EDS
$R_{merge}$	0.77	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.289 , 0.317 0.291 , 0.321	Depositor DCC
$R_{free}$ test set	743 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	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	0.81	EDS
Total number of atoms	6527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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: T0B

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	AAA	0.67	0/3278	0.73	0/4500

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	AAA	3206	3203	3104	30	4
2	AAA	64	54	0	4	0
All	All	3270	3257	3104	32	4

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 5.

All (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:AAA:466:ALA:O	1:AAA:469:TRP:O	2.14	0.66
1:AAA:309:PRO:O	1:AAA:312:ILE:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:344:ASN:HB2	1:AAA:345:PRO:HD3	1.89	0.53
1:AAA:126:VAL:HG22	2:AAA:601[A]:T0B:C8	2.39	0.52
1:AAA:353:ASP:HA	1:AAA:356:GLU:CB	2.40	0.52
1:AAA:80:THR:CG2	1:AAA:296:LEU:HD11	2.40	0.52
1:AAA:126:VAL:HG22	2:AAA:602[B]:T0B:C8	2.40	0.52
1:AAA:386:VAL:HG21	1:AAA:415:ASN:O	2.09	0.51
1:AAA:456:ASP:OD2	1:AAA:460:THR:OG1	2.29	0.50
1:AAA:439:LEU:HD11	1:AAA:477:VAL:HG21	1.93	0.50
1:AAA:144:TYR:CE1	1:AAA:225:ARG:HB3	2.47	0.49
1:AAA:99:LEU:N	1:AAA:100:PRO:CD	2.76	0.48
1:AAA:375:GLU:HG3	1:AAA:379:LEU:HD12	1.94	0.48
2:AAA:601[A]:T0B:C16	2:AAA:601[A]:T0B:O4	2.63	0.47
1:AAA:284:PHE:HD2	1:AAA:381:ALA:HA	1.79	0.47
1:AAA:406:LEU:HD11	1:AAA:444:VAL:HG21	1.96	0.46
1:AAA:112:VAL:HG23	1:AAA:112:VAL:O	2.16	0.45
1:AAA:114:GLY:HA2	1:AAA:118:CYS:HB2	1.97	0.45
1:AAA:456:ASP:CG	1:AAA:460:THR:HG1	2.20	0.45
1:AAA:80:THR:HG23	1:AAA:296:LEU:HD11	1.98	0.45
1:AAA:136:LEU:HD22	1:AAA:300:VAL:HG22	1.98	0.45
1:AAA:142:ASP:OD2	1:AAA:143:ARG:NH2	2.50	0.44
1:AAA:308:LEU:HB3	1:AAA:309:PRO:HD3	2.01	0.43
1:AAA:308:LEU:N	1:AAA:309:PRO:CD	2.82	0.43
1:AAA:101:PHE:CG	1:AAA:121:TRP:HB3	2.54	0.42
1:AAA:222:MET:O	1:AAA:226:VAL:HG23	2.20	0.41
1:AAA:302:MET:HG3	1:AAA:347:ILE:HD11	2.01	0.41
2:AAA:601[A]:T0B:O4	2:AAA:601[A]:T0B:C15	2.68	0.41
1:AAA:58:PHE:CD2	1:AAA:346:ILE:HD11	2.55	0.41
1:AAA:411:VAL:O	1:AAA:415:ASN:ND2	2.52	0.40
1:AAA:143:ARG:HD2	1:AAA:296:LEU:HD12	2.04	0.40
1:AAA:153:TYR:N	1:AAA:154:PRO:CD	2.85	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:369:ARG:HH21	1:AAA:515:ALA:HB1[3_655]	1.26	0.34
1:AAA:369:ARG:NH2	1:AAA:515:ALA:HB1[3_655]	1.45	0.15
1:AAA:190:ASN:O	1:AAA:453:ASN:O[4_455]	2.06	0.14
1:AAA:369:ARG:NH2	1:AAA:515:ALA:CB[3_655]	2.19	0.01

## 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	AAA	432/459 (94%)	407 (94%)	24 (6%)	1 (0%)	47 76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	357	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	AAA	316/381 (83%)	312 (99%)	4 (1%)	69 88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	202	PHE
1	AAA	223	TYR
1	AAA	284	PHE
1	AAA	524	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	T0B	AAA	602[B]	-	32,36,36	0.74	1 (3%)	36,52,52	0.90	1 (2%)
2	T0B	AAA	601[A]	-	32,36,36	0.78	2 (6%)	36,52,52	0.95	2 (5%)

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	T0B	AAA	602[B]	-	-	2/12/40/40	0/5/5/5
2	T0B	AAA	601[A]	-	-	0/12/40/40	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	601[A]	T0B	C20-C1	-2.32	1.46	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	602[B]	T0B	C4-N2	2.29	1.40	1.36
2	AAA	601[A]	T0B	C4-N2	2.28	1.40	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	602[B]	T0B	C19-C14-C15	2.46	115.90	110.23
2	AAA	601[A]	T0B	C19-C14-C15	2.33	115.58	110.23
2	AAA	601[A]	T0B	C20-C1-N1	2.31	122.42	119.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

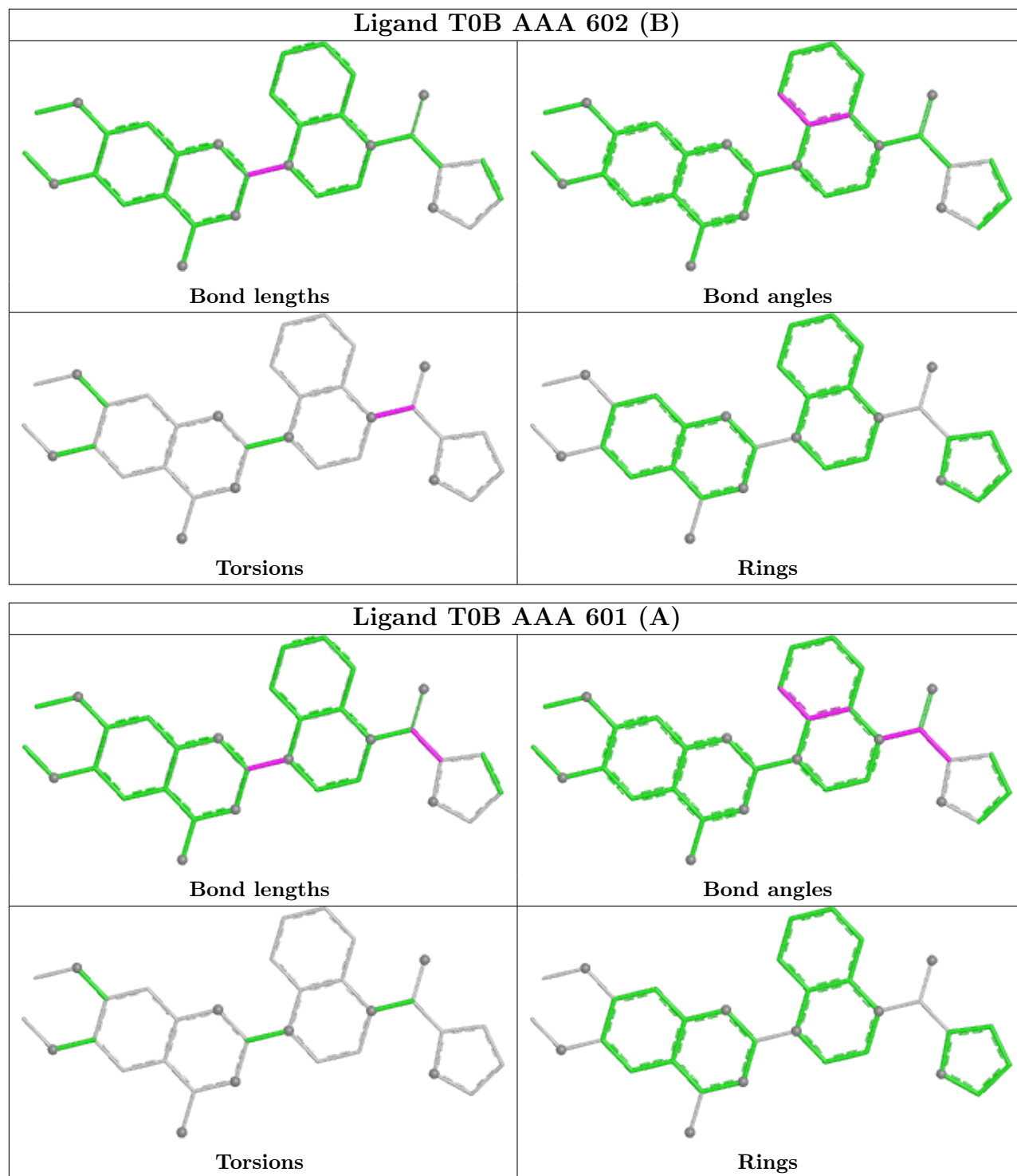
Mol	Chain	Res	Type	Atoms
2	AAA	602[B]	T0B	O1-C1-N1-C15
2	AAA	602[B]	T0B	C20-C1-N1-C15

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	602[B]	T0B	1	0
2	AAA	601[A]	T0B	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AAA	438/459 (95%)	0.37	32 (7%) 15 11	11, 29, 60, 78	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	38	PRO	4.3
1	AAA	354	LEU	4.2
1	AAA	228	ILE	4.1
1	AAA	355	VAL	3.6
1	AAA	232	ARG	3.6
1	AAA	353	ASP	3.5
1	AAA	350	CYS	3.4
1	AAA	72	CYS	3.3
1	AAA	184	TRP	3.3
1	AAA	378	ILE	3.3
1	AAA	111	TRP	3.2
1	AAA	132	SER	3.1
1	AAA	183	VAL	3.0
1	AAA	198	THR	2.8
1	AAA	325	PRO	2.7
1	AAA	235	LYS	2.6
1	AAA	129	CYS	2.6
1	AAA	40	LEU	2.5
1	AAA	356	GLU	2.4
1	AAA	248	SER	2.3
1	AAA	358	TRP	2.3
1	AAA	374	ASP	2.3
1	AAA	156	LEU	2.3
1	AAA	326	PRO	2.3
1	AAA	224	CYS	2.2
1	AAA	147	VAL	2.1
1	AAA	318	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	157	VAL	2.1
1	AAA	316	LEU	2.0
1	AAA	312	ILE	2.0
1	AAA	149	TYR	2.0
1	AAA	69	SER	2.0

## 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](#)

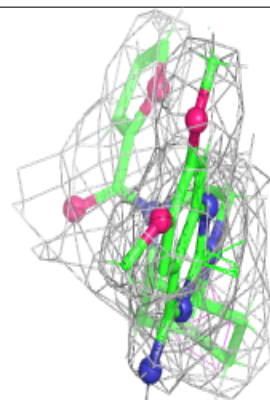
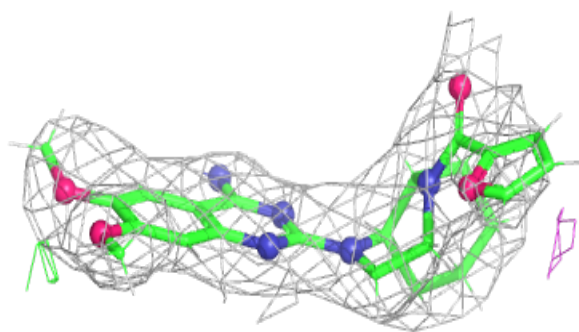
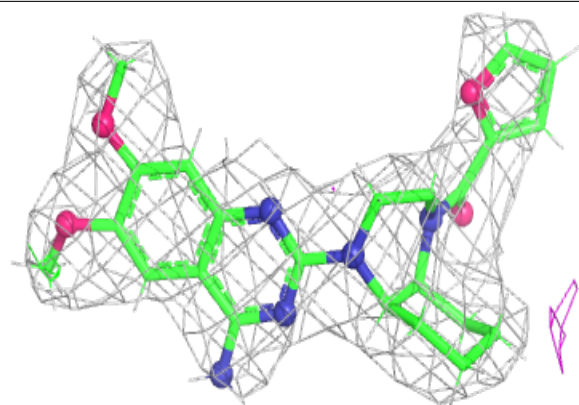
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	T0B	AAA	602[B]	32/32	0.90	0.21	28,31,34,34	59
2	T0B	AAA	601[A]	32/32	0.91	0.20	29,32,35,35	59

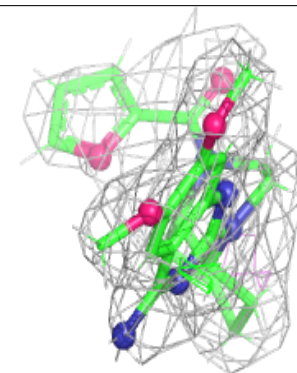
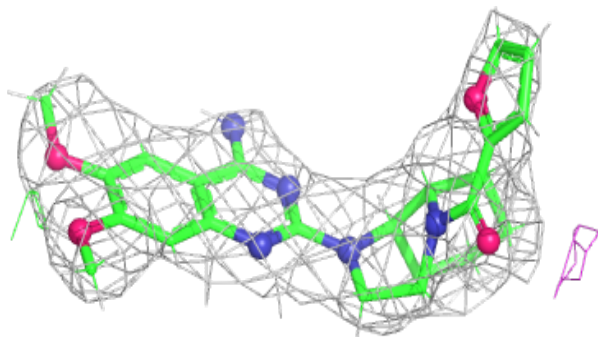
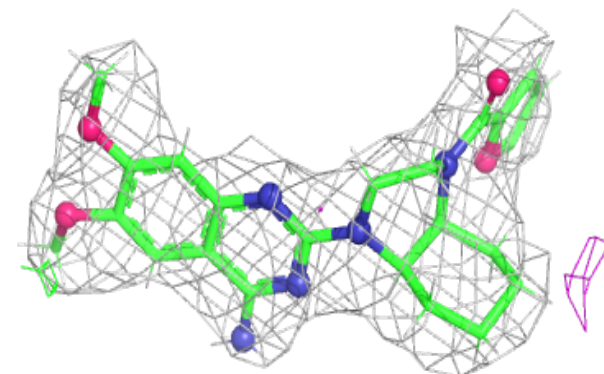
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around T0B AAA 602 (B):**

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

**Electron density around T0B AAA 601 (A):**

$2mF_o-DF_c$  (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.