



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 20, 2024 – 04:01 pm GMT

PDB ID : 7PE5  
Title : Crystal structure of Lymnaea stagnalis Acetylcholine-binding protein (Ls-AChBP) Q55R/M114V double mutant complexed with Triflumezopyrim  
Authors : Montgomery, M.G.  
Deposited on : 2021-08-09  
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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

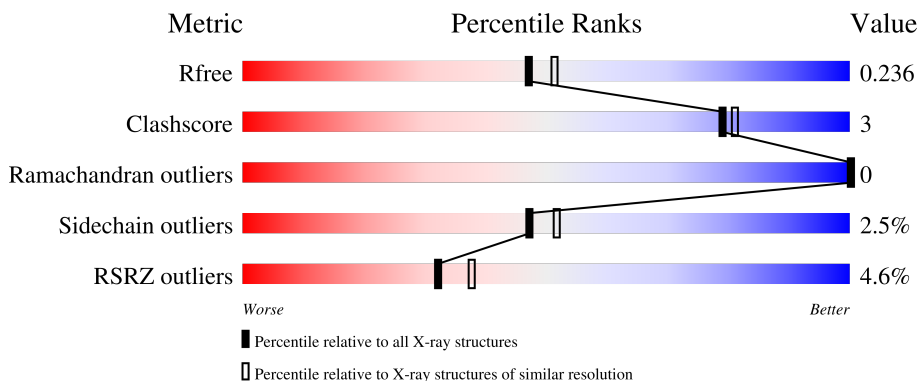
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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	AaA	210	 7% 92% 6%
1	BaB	210	 8% 91% 6%
1	CaC	210	 2% 91% 6%
1	DaD	210	 2% 93% 5%
1	EaE	210	 3% 93% 5%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8135 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AaA	201	Total 1608	C 1007	N 279	O 318	S 4	0	0	0
1	BaB	198	Total 1584	C 995	N 273	O 312	S 4	0	0	0
1	CaC	198	Total 1585	C 995	N 273	O 313	S 4	0	0	0
1	DaD	199	Total 1600	C 1004	N 277	O 315	S 4	0	1	0
1	EaE	200	Total 1600	C 1003	N 275	O 318	S 4	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

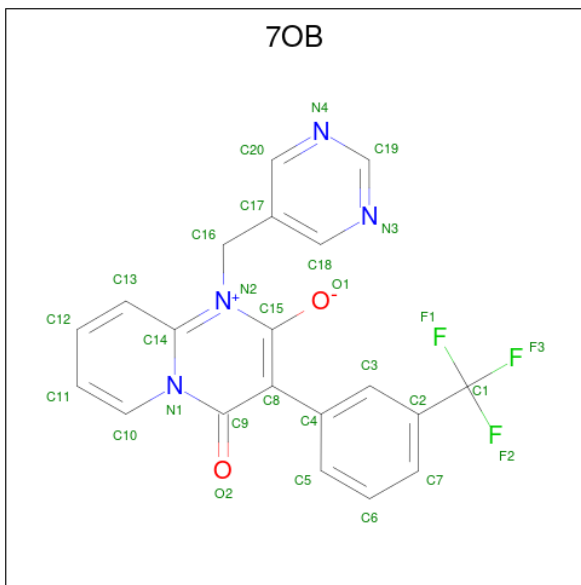
Chain	Residue	Modelled	Actual	Comment	Reference
AaA	1	ALA	-	expression tag	UNP P58154
AaA	55	ARG	GLN	engineered mutation	UNP P58154
AaA	66	ASP	ASN	engineered mutation	UNP P58154
AaA	114	VAL	MET	engineered mutation	UNP P58154
BaB	1	ALA	-	expression tag	UNP P58154
BaB	55	ARG	GLN	engineered mutation	UNP P58154
BaB	66	ASP	ASN	engineered mutation	UNP P58154
BaB	114	VAL	MET	engineered mutation	UNP P58154
CaC	1	ALA	-	expression tag	UNP P58154
CaC	55	ARG	GLN	engineered mutation	UNP P58154
CaC	66	ASP	ASN	engineered mutation	UNP P58154
CaC	114	VAL	MET	engineered mutation	UNP P58154
DaD	1	ALA	-	expression tag	UNP P58154
DaD	55	ARG	GLN	engineered mutation	UNP P58154
DaD	66	ASP	ASN	engineered mutation	UNP P58154
DaD	114	VAL	MET	engineered mutation	UNP P58154
EaE	1	ALA	-	expression tag	UNP P58154
EaE	55	ARG	GLN	engineered mutation	UNP P58154
EaE	66	ASP	ASN	engineered mutation	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
EaE	114	VAL	MET	engineered mutation	UNP P58154

- Molecule 2 is 4-oxidanylidene-1-(pyrimidin-5-ylmethyl)-3-[3-(trifluoromethyl)phenyl]pyridin-2-olate (three-letter code: 7OB) (formula:  $C_{20}H_{13}F_3N_4O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
2	BaB	1	Total	C	F	N	O	0	0
			29	20	3	4	2		
2	CaC	1	Total	C	F	N	O	0	0
			29	20	3	4	2		
2	DaD	1	Total	C	F	N	O	0	0
			29	20	3	4	2		
2	DaD	1	Total	C	F	N	O	0	0
			29	20	3	4	2		
2	EaE	1	Total	C	F	N	O	0	0
			29	20	3	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	AaA	2	Total	O	0	0
			2	2		
3	BaB	3	Total	O	0	0
			3	3		
3	CaC	2	Total	O	0	0
			2	2		

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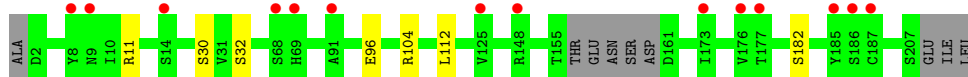
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	DaD	4	Total	0	0
			O		
3	EaE	2	Total	0	0
			O		

### 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.

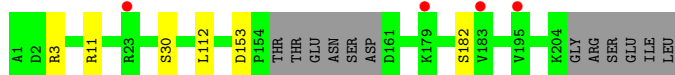
- Molecule 1: Acetylcholine-binding protein



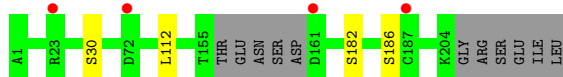
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.08Å 74.08Å 348.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.18 – 2.10 63.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (63.18-2.10) 99.5 (63.10-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.206 , 0.229 0.214 , 0.236	Depositor DCC
$R_{free}$ test set	3232 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtrriage
Anisotropy	0.604	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.072 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: 7OB

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	0.81	1/1643 (0.1%)	0.98	1/2240 (0.0%)
1	BaB	0.77	0/1619	0.93	0/2209
1	CaC	0.81	0/1620	1.00	2/2210 (0.1%)
1	DaD	0.84	0/1638	0.98	0/2234
1	EaE	0.85	0/1635	0.97	0/2231
All	All	0.82	1/8155 (0.0%)	0.97	3/11124 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AaA	96	GLU	CD-OE1	5.08	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AaA	104	ARG	CG-CD-NE	-10.74	89.25	111.80
1	CaC	11	ARG	CG-CD-NE	-9.44	91.97	111.80
1	CaC	3	ARG	CG-CD-NE	-5.52	100.20	111.80

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	1608	0	1559	0	0
1	BaB	1584	0	1542	0	0
1	CaC	1585	0	1539	0	0
1	DaD	1600	0	1559	0	0
1	EaE	1600	0	1550	0	0
2	BaB	29	0	0	0	0
2	CaC	29	0	0	0	0
2	DaD	58	0	0	0	0
2	EaE	29	0	0	0	0
3	AaA	2	0	0	0	0
3	BaB	3	0	0	0	0
3	CaC	2	0	0	0	0
3	DaD	4	0	0	0	0
3	EaE	2	0	0	0	0
All	All	8135	0	7749	0	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 3.

There are no clashes within the asymmetric unit.

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	AaA	197/210 (94%)	194 (98%)	3 (2%)	0	100	100
1	BaB	194/210 (92%)	193 (100%)	1 (0%)	0	100	100
1	CaC	194/210 (92%)	193 (100%)	1 (0%)	0	100	100
1	DaD	196/210 (93%)	195 (100%)	1 (0%)	0	100	100
1	EaE	196/210 (93%)	195 (100%)	1 (0%)	0	100	100
All	All	977/1050 (93%)	970 (99%)	7 (1%)	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	AaA	187/195 (96%)	182 (97%)	5 (3%)	44	48
1	BaB	184/195 (94%)	178 (97%)	6 (3%)	38	40
1	CaC	184/195 (94%)	180 (98%)	4 (2%)	52	57
1	DaD	186/195 (95%)	182 (98%)	4 (2%)	52	57
1	EaE	186/195 (95%)	182 (98%)	4 (2%)	52	57
All	All	927/975 (95%)	904 (98%)	23 (2%)	47	52

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CaC	182	SER
1	DaD	182	SER
1	DaD	112	LEU
1	DaD	186	SER
1	BaB	30	SER

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	7OB	EaE	301	-	29,32,32	1.32	3 (10%)	33,47,47	0.96	0
2	7OB	DaD	302	-	29,32,32	1.39	5 (17%)	33,47,47	0.82	0
2	7OB	BaB	301	-	29,32,32	1.25	5 (17%)	33,47,47	1.10	1 (3%)
2	7OB	CaC	301	-	29,32,32	1.24	3 (10%)	33,47,47	1.05	1 (3%)
2	7OB	DaD	301	-	29,32,32	1.52	4 (13%)	33,47,47	0.91	1 (3%)

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	7OB	EaE	301	-	-	0/12/14/14	0/4/4/4
2	7OB	DaD	302	-	-	0/12/14/14	0/4/4/4
2	7OB	BaB	301	-	-	0/12/14/14	0/4/4/4
2	7OB	CaC	301	-	-	0/12/14/14	0/4/4/4
2	7OB	DaD	301	-	-	0/12/14/14	0/4/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DaD	301	7OB	O1-C15	-4.82	1.16	1.30
2	EaE	301	7OB	O1-C15	-3.85	1.19	1.30
2	DaD	301	7OB	C8-C9	-3.65	1.34	1.44
2	BaB	301	7OB	O1-C15	-3.52	1.20	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CaC	301	7OB	O1-C15	-3.30	1.21	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CaC	301	7OB	O2-C9-C8	3.08	130.81	124.77
2	BaB	301	7OB	O2-C9-C8	2.19	129.06	124.77
2	DaD	301	7OB	C6-C7-C2	-2.01	118.65	120.76

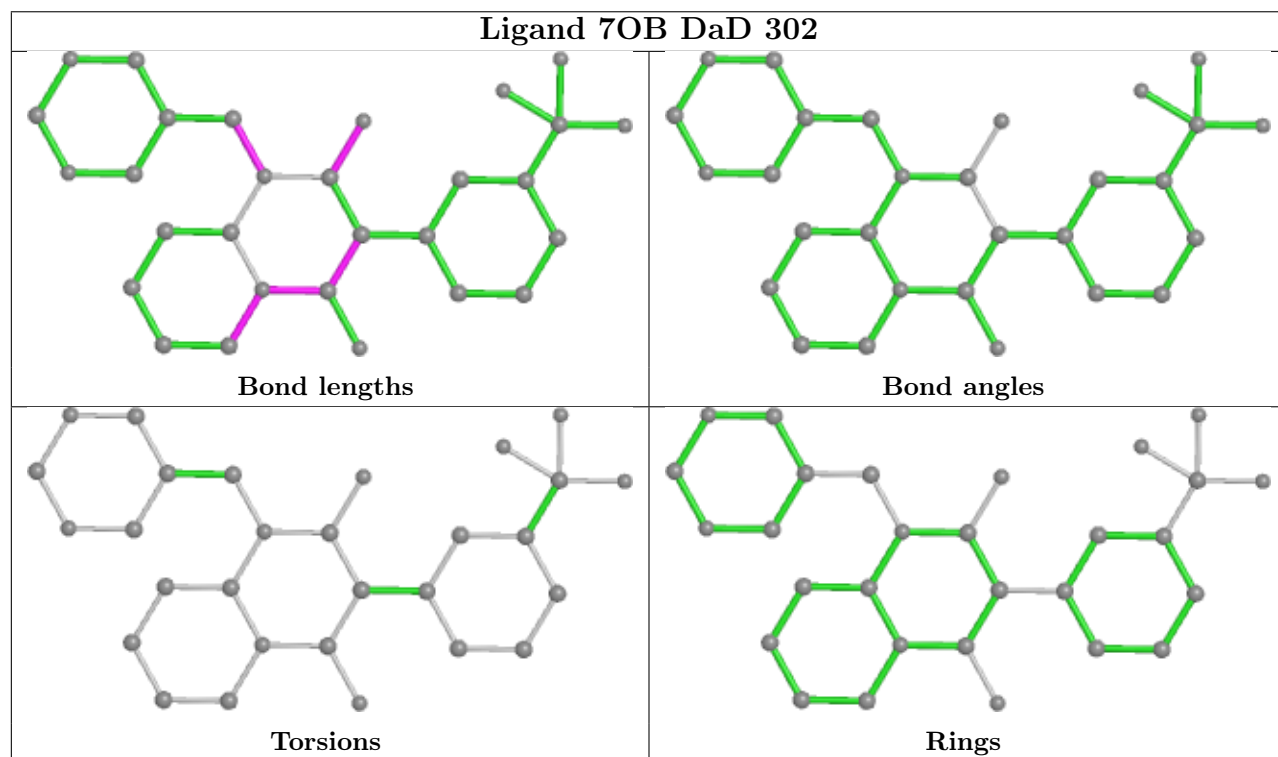
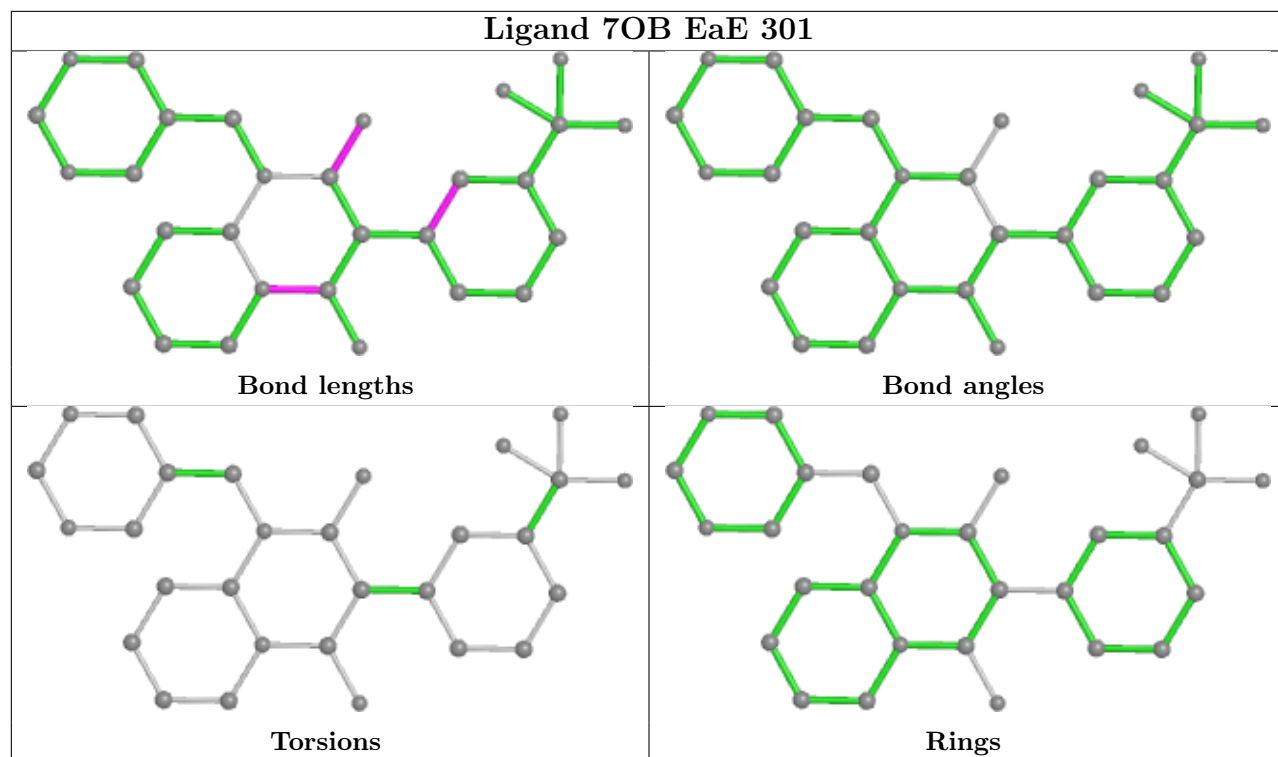
There are no chirality outliers.

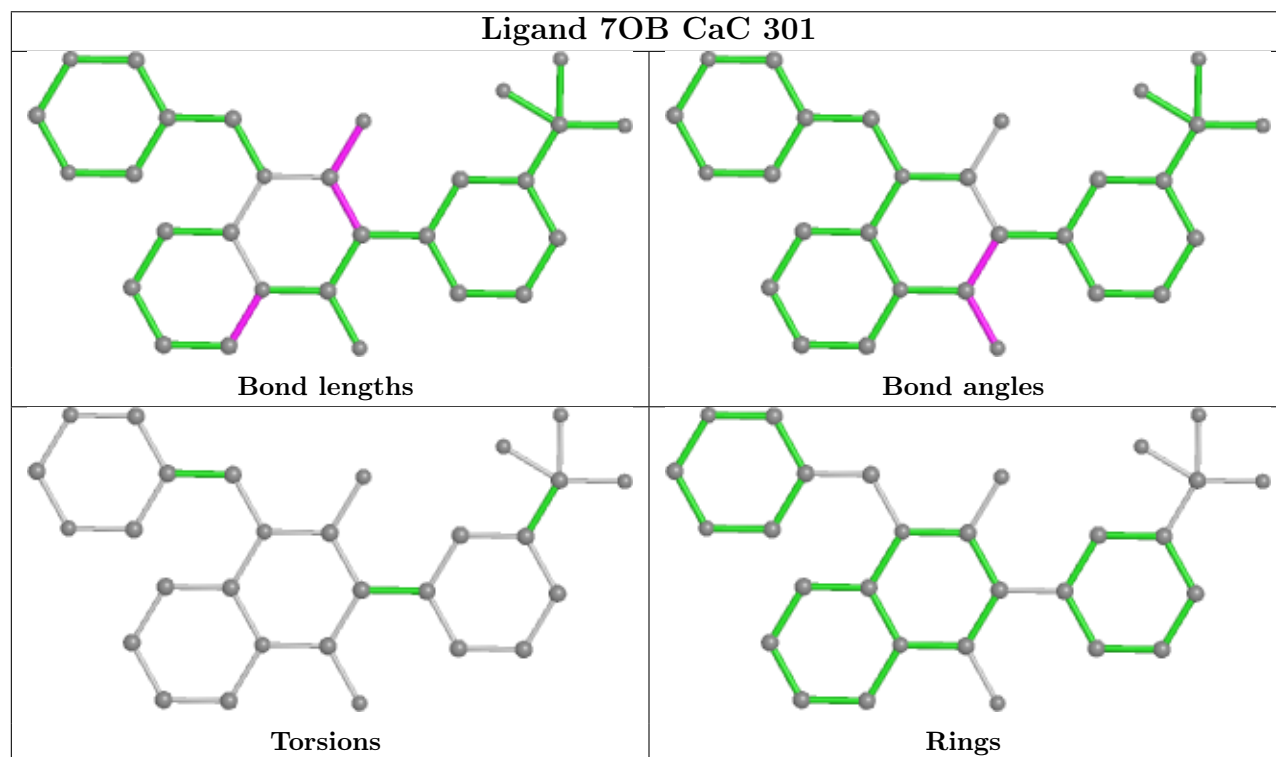
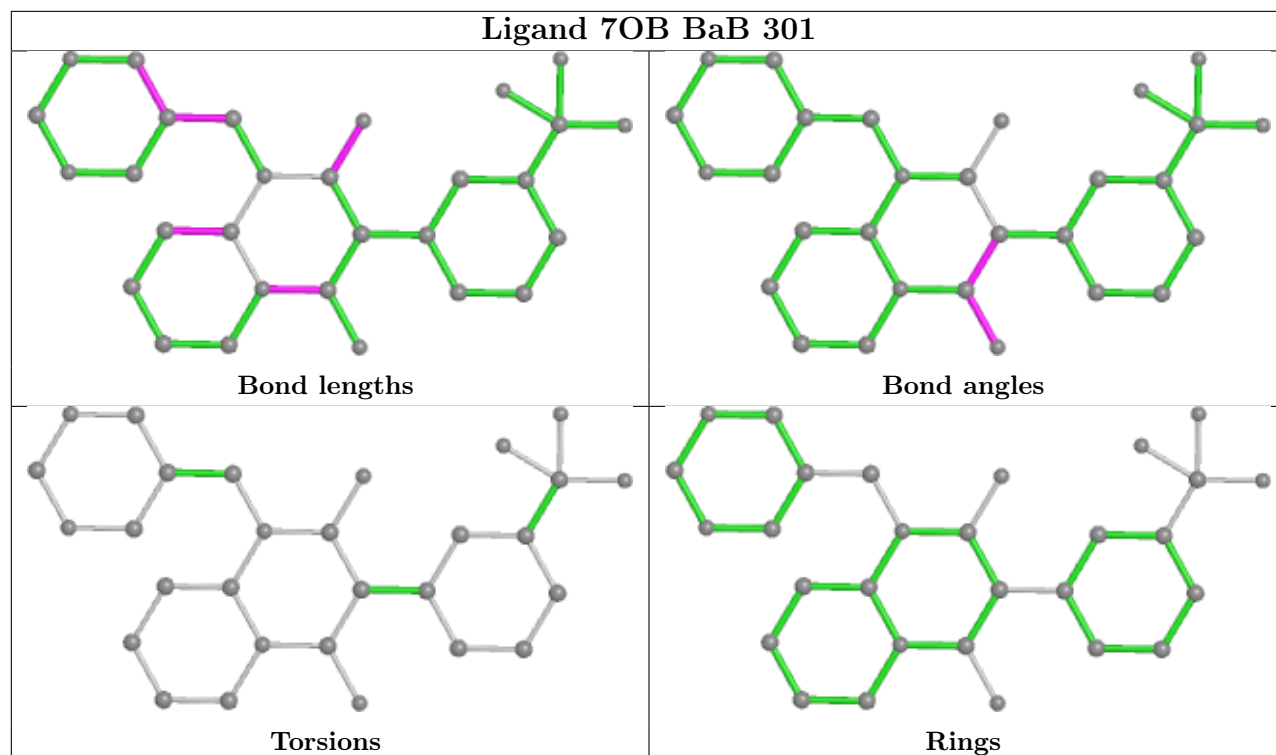
There are no torsion outliers.

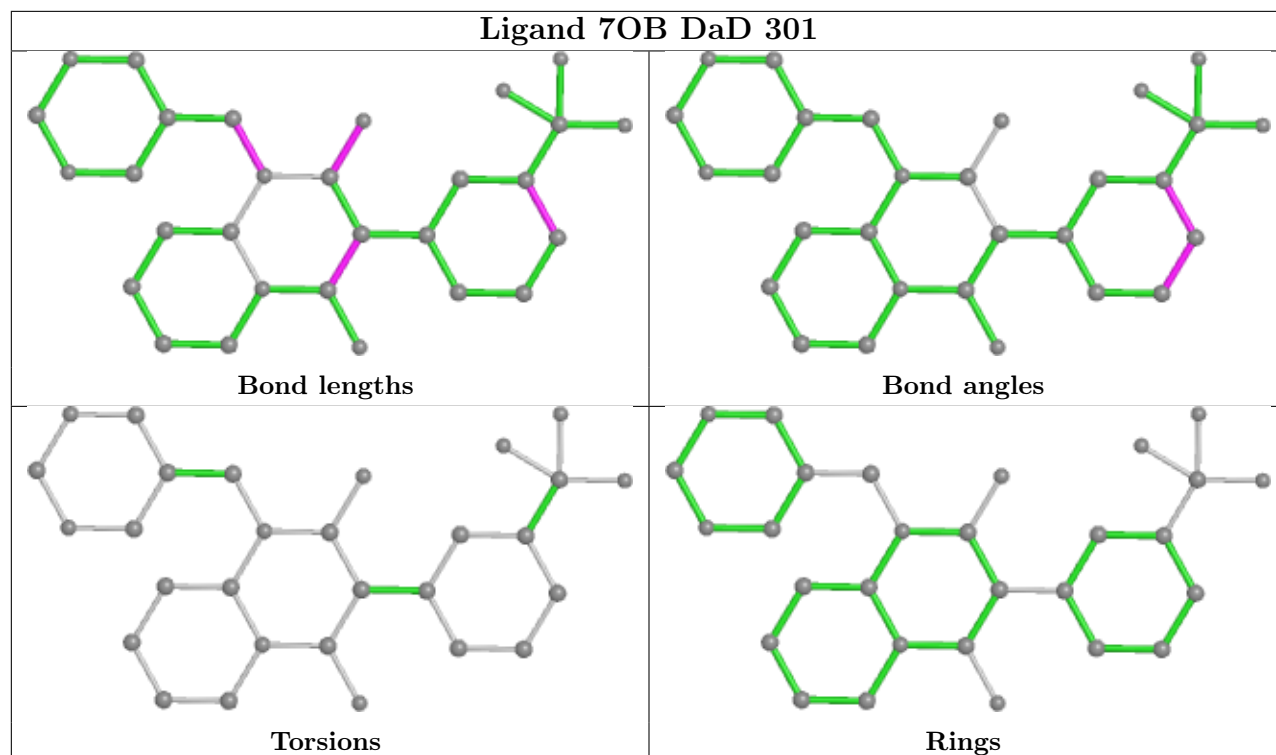
There are no ring outliers.

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 [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, 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	201/210 (95%)	0.58	14 (6%) 16 20	50, 76, 108, 139	0
1	BaB	198/210 (94%)	0.77	17 (8%) 10 13	52, 79, 115, 138	0
1	CaC	198/210 (94%)	0.39	4 (2%) 65 69	41, 63, 101, 115	0
1	DaD	199/210 (94%)	0.26	4 (2%) 65 69	37, 56, 96, 113	0
1	EaE	200/210 (95%)	0.38	7 (3%) 44 50	39, 59, 105, 149	0
All	All	996/1050 (94%)	0.47	46 (4%) 32 38	37, 67, 106, 149	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EaE	186	SER	5.8
1	AaA	69	HIS	5.6
1	BaB	23	ARG	5.4
1	EaE	185	TYR	5.4
1	EaE	187	CYS	5.1

### 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](#)

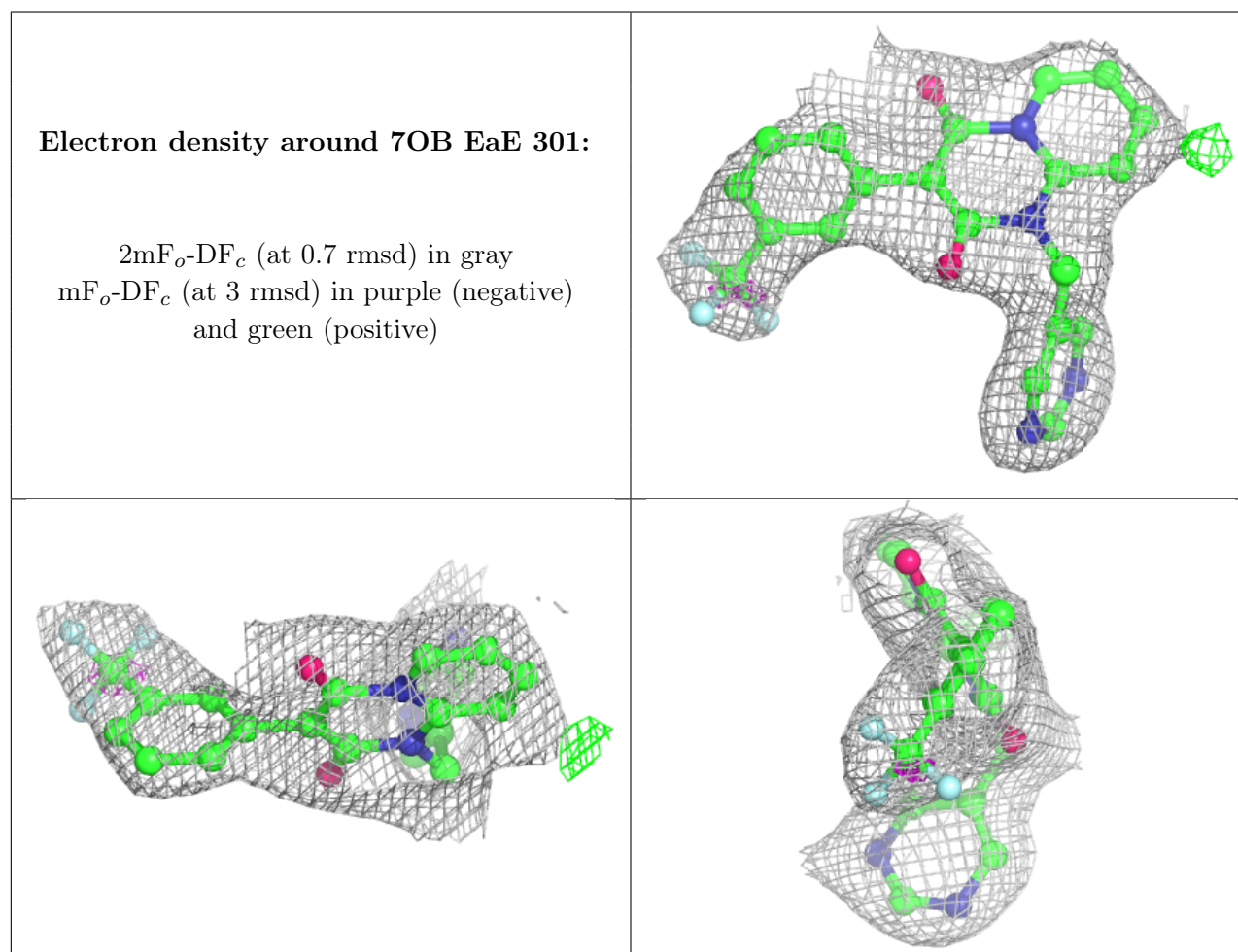
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

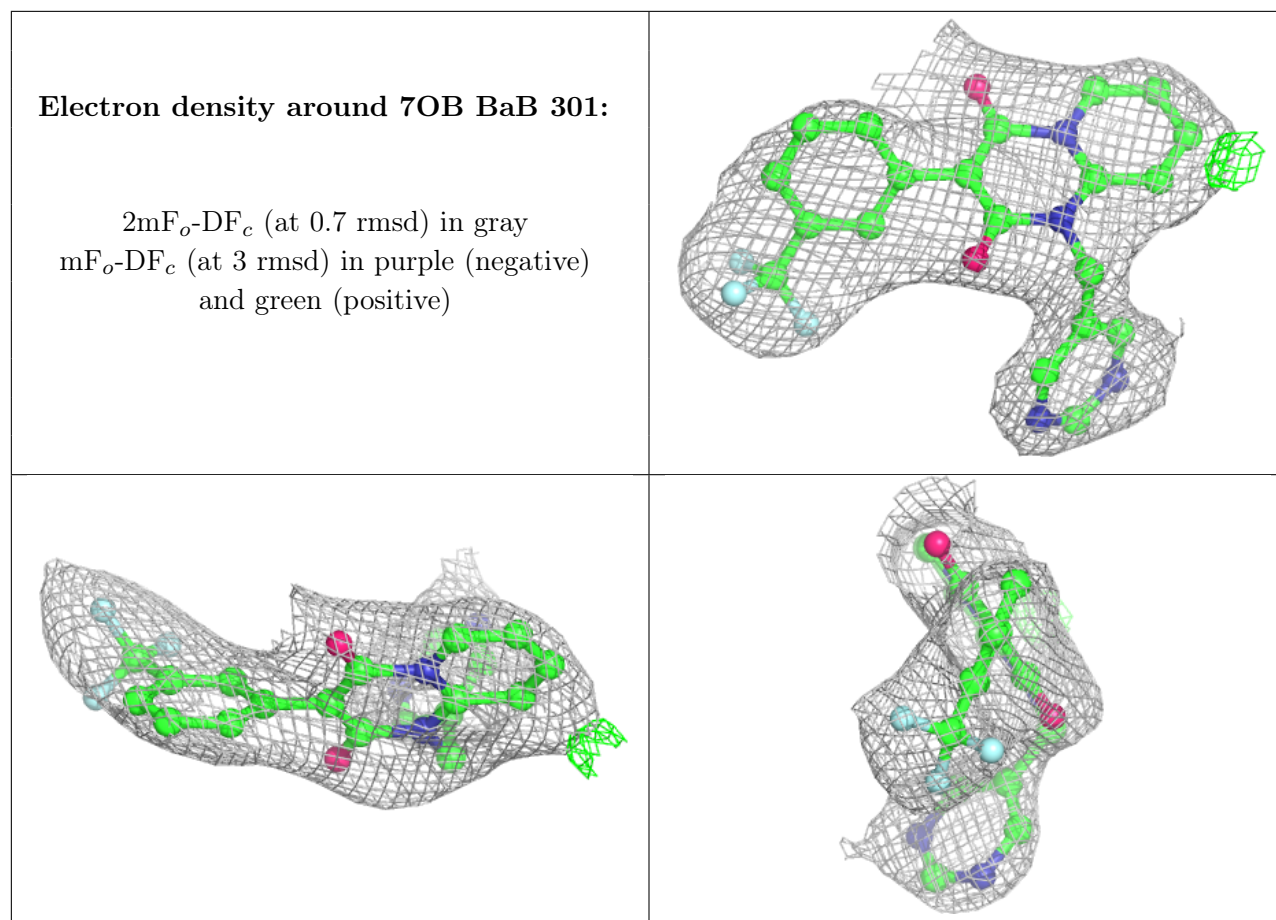


median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	7OB	EaE	301	29/29	0.92	0.15	65,74,100,104	0
2	7OB	BaB	301	29/29	0.95	0.15	67,78,98,100	0
2	7OB	CaC	301	29/29	0.96	0.13	59,64,89,100	0
2	7OB	DaD	302	29/29	0.97	0.12	49,53,79,82	0
2	7OB	DaD	301	29/29	0.98	0.12	46,51,75,80	0

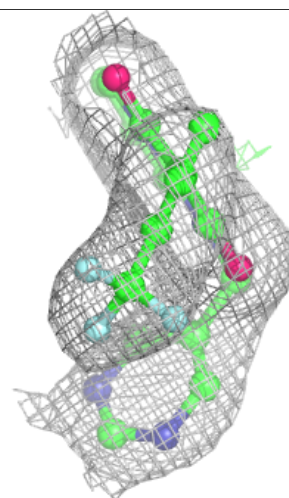
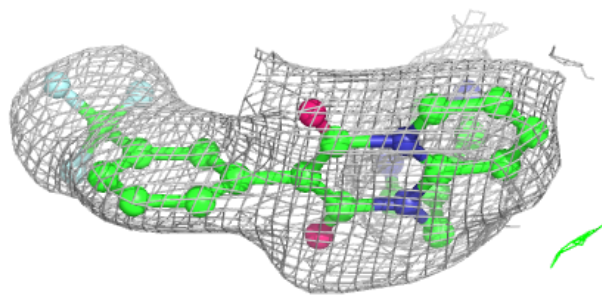
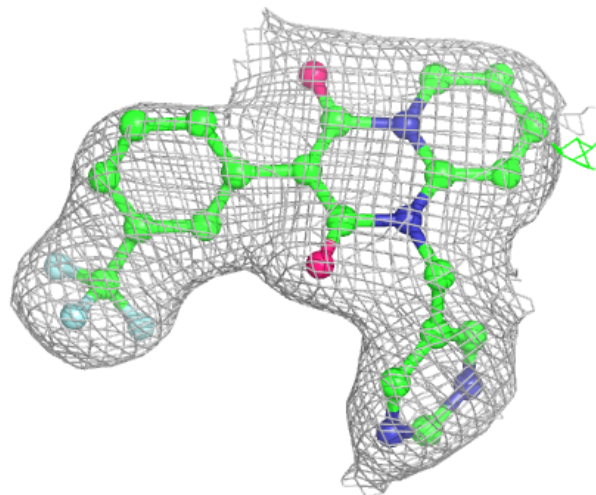
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





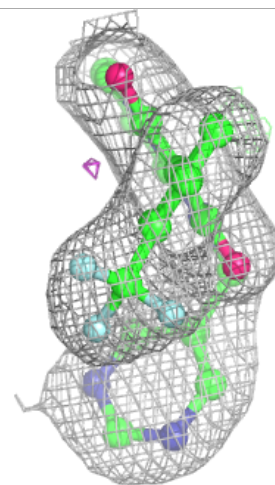
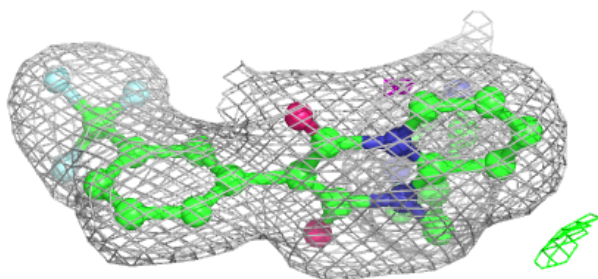
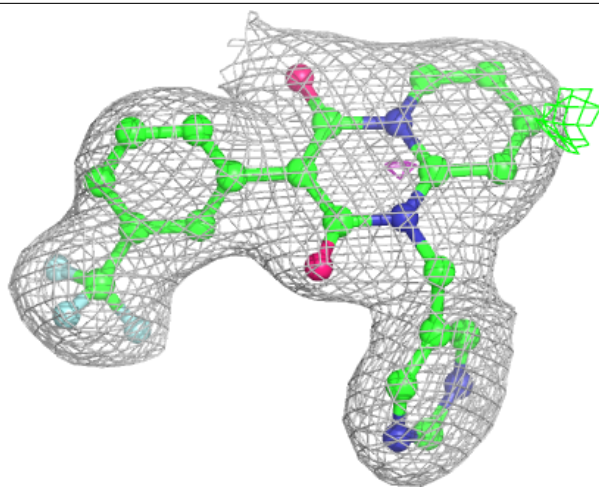
**Electron density around 7OB CaC 301:**

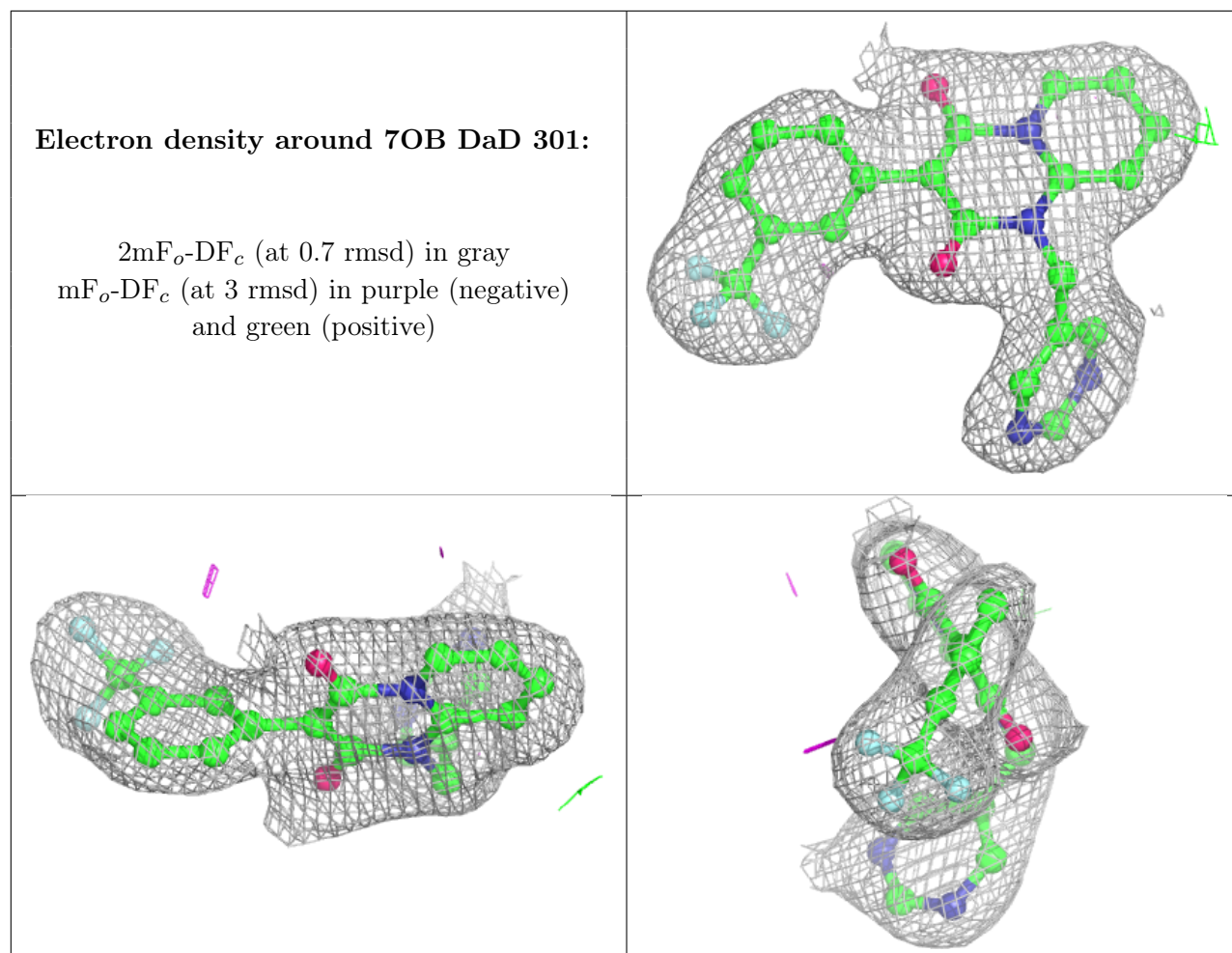
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 7OB DaD 302:**

$2mF_o-DF_c$  (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.