



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 07:54 am BST

PDB ID : 6JN5  
Title : Serine Beta-Lactamase KPC-2 in Complex with Dual MBL/SBL Inhibitor MS23  
Authors : Li, G.-B.; Liu, S.  
Deposited on : 2019-03-13  
Resolution : 1.97 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

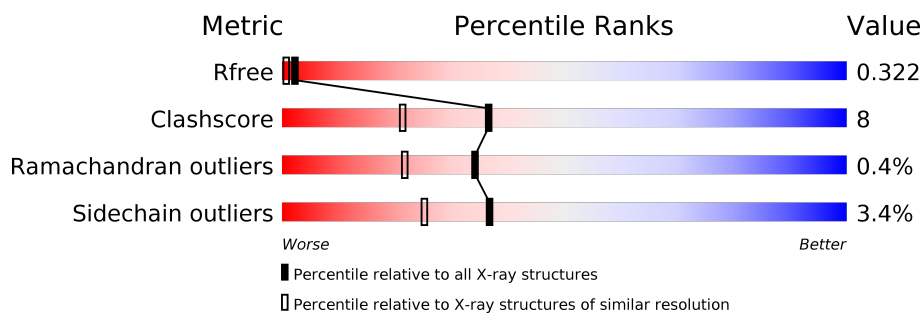
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)

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 on 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	264	84% 15%
1	B	264	82% 15% ..
1	C	264	82% 17% .
1	D	264	78% 19% ..

## 2 Entry composition [i](#)

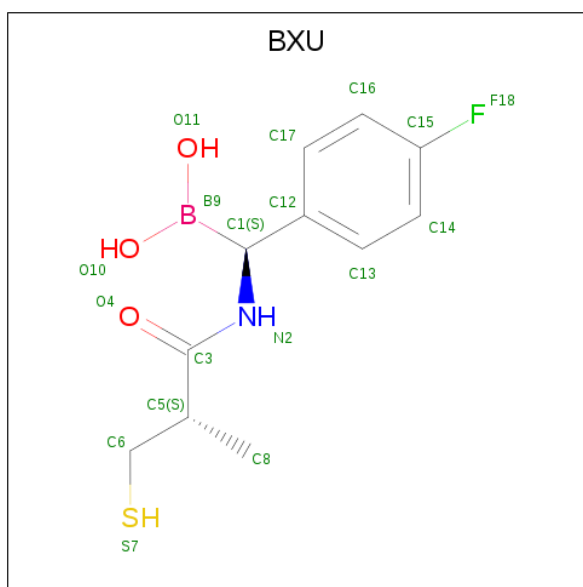
There are 3 unique types of molecules in this entry. The entry contains 8101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-Lactamase KPC-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	1
			1968	1239	346	378	5			
1	B	261	Total	C	N	O	S	0	0	1
			1945	1225	342	373	5			
1	C	264	Total	C	N	O	S	0	0	1
			1968	1239	346	378	5			
1	D	260	Total	C	N	O	S	0	0	1
			1938	1220	341	372	5			

- Molecule 2 is [(S)-(4-fluorophenyl)-[(2S)-2-methyl-3-sulfanyl-propanoyl]amino]methyl]boronic acid (three-letter code: BXU) (formula: C<sub>11</sub>H<sub>15</sub>BFNO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	F	N	O	S
			18	1	11	1	1	3	1
2	B	1	Total	B	C	F	N	O	S
			18	1	11	1	1	3	1

*Continued on next page...*

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	C	1	Total	B	C	F	N	O	S	0	0
			18	1	11	1	1	3	1		
2	D	1	Total	B	C	F	N	O	S	0	0
			18	1	11	1	1	3	1		

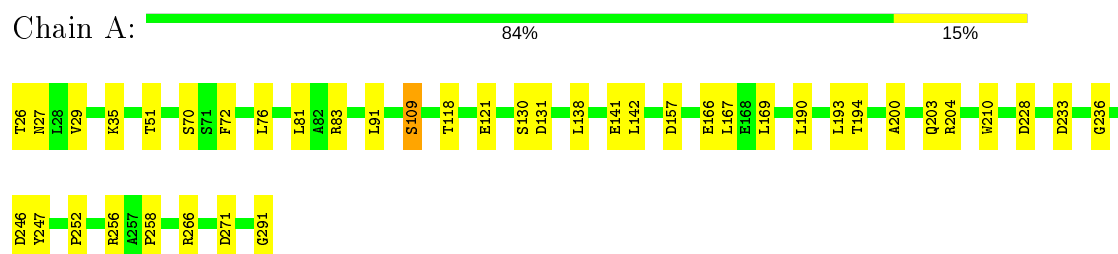
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	74	Total	O	0	0
			74	74		
3	C	39	Total	O	0	0
			39	39		
3	D	25	Total	O	0	0
			25	25		

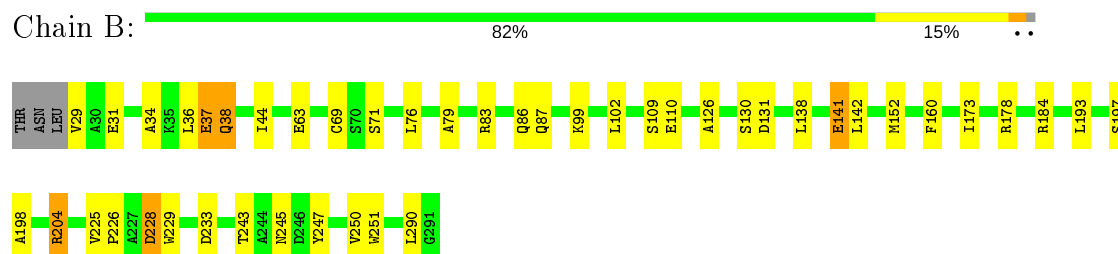
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

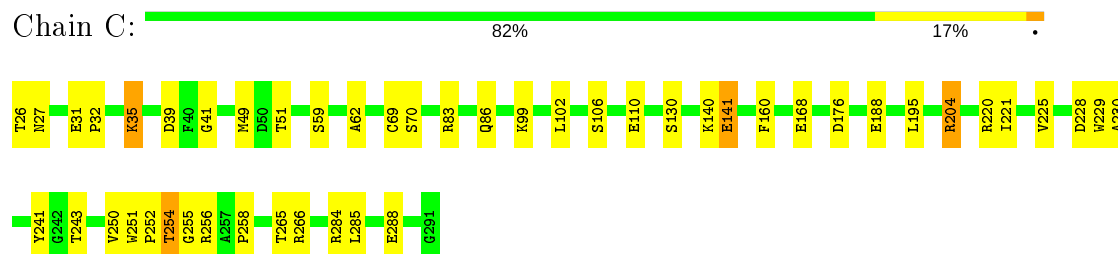
#### • Molecule 1: Serine Beta-Lactamase KPC-2



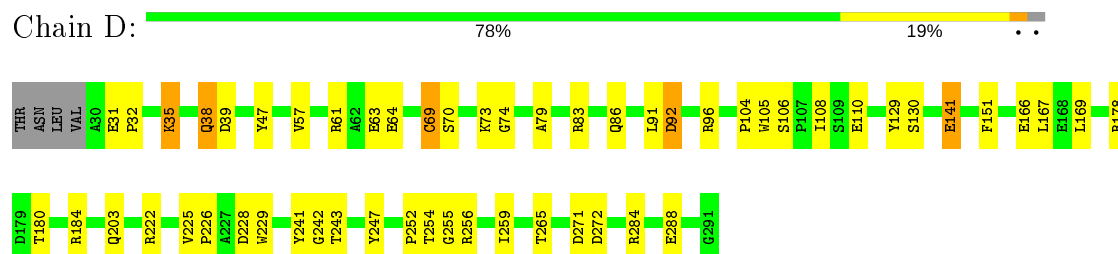
#### • Molecule 1: Serine Beta-Lactamase KPC-2



#### • Molecule 1: Serine Beta-Lactamase KPC-2



#### • Molecule 1: Serine Beta-Lactamase KPC-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.76 Å 164.76 Å 94.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.56 – 1.97 47.56 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.56-1.97) 73.2 (47.56-1.70)	Depositor EDS
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 1.70 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.275 , 0.316 0.282 , 0.322	Depositor DCC
$R_{free}$ test set	2004 reflections (1.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 19.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.390 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BXU

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	0.71	0/2008	0.77	1/2736 (0.0%)
1	B	0.76	2/1985 (0.1%)	0.82	3/2704 (0.1%)
1	C	0.68	1/2008 (0.0%)	0.79	2/2736 (0.1%)
1	D	0.61	0/1978	0.68	0/2694
All	All	0.69	3/7979 (0.0%)	0.77	6/10870 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	GLU	CB-CG	-6.19	1.40	1.52
1	B	251	TRP	CB-CG	-6.04	1.39	1.50
1	C	69	CYS	CB-SG	5.13	1.91	1.82

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	204	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	204	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	157	ASP	CB-CG-OD1	5.72	123.45	118.30
1	C	176	ASP	CB-CG-OD1	5.36	123.13	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1968	0	1949	30	0
1	B	1945	0	1925	29	0
1	C	1968	0	1948	31	1
1	D	1938	0	1915	40	1
2	A	18	0	0	2	0
2	B	18	0	0	0	0
2	C	18	0	0	3	0
2	D	18	0	0	3	0
3	A	72	0	0	7	0
3	B	74	0	0	2	1
3	C	39	0	0	5	0
3	D	25	0	0	3	0
All	All	8101	0	7737	123	2

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 123 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:D:70:SER:OG	2:D:301:BXU:O11	1.55	1.23
1:D:73:LYS:NZ	2:D:301:BXU:O11	2.04	0.91
1:B:83:ARG:NH2	1:B:141:GLU:O	2.02	0.91
1:D:31:GLU:OE2	3:D:401:HOH:O	1.93	0.86
1:A:26:THR:N	3:A:401:HOH:O	2.09	0.83

All (2) 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)
3:B:446:HOH:O	3:B:467:HOH:O[2_565]	2.04	0.16
1:C:195:LEU:O	1:D:96:ARG:NH2[6_557]	2.17	0.03



## 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	262/264 (99%)	251 (96%)	11 (4%)	0	100	100
1	B	259/264 (98%)	254 (98%)	5 (2%)	0	100	100
1	C	262/264 (99%)	250 (95%)	10 (4%)	2 (1%)	19	9
1	D	258/264 (98%)	249 (96%)	7 (3%)	2 (1%)	19	9
All	All	1041/1056 (99%)	1004 (96%)	33 (3%)	4 (0%)	34	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	254	THR
1	C	255	GLY
1	D	255	GLY
1	D	69	CYS

### 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	199/199 (100%)	193 (97%)	6 (3%)	41	29
1	B	196/199 (98%)	189 (96%)	7 (4%)	35	23
1	C	199/199 (100%)	194 (98%)	5 (2%)	47	39
1	D	195/199 (98%)	186 (95%)	9 (5%)	27	14
All	All	789/796 (99%)	762 (97%)	27 (3%)	37	25

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	228	ASP
1	C	130	SER
1	D	141	GLU
1	C	35	LYS
1	A	228	ASP

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	BXU	C	301	-	15,18,18	1.66	2 (13%)	15,24,24	2.19	5 (33%)
2	BXU	A	301	-	15,18,18	1.74	3 (20%)	15,24,24	2.97	6 (40%)
2	BXU	D	301	-	15,18,18	1.73	3 (20%)	15,24,24	2.10	6 (40%)
2	BXU	B	301	-	15,18,18	1.97	3 (20%)	15,24,24	3.60	4 (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	BXU	C	301	-	-	3/13/18/18	0/1/1/1
2	BXU	A	301	-	-	5/13/18/18	0/1/1/1
2	BXU	D	301	-	-	6/13/18/18	0/1/1/1
2	BXU	B	301	-	-	5/13/18/18	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)
2	D	301	BXU	C3-N2	5.05	1.45	1.34
2	A	301	BXU	C3-N2	5.02	1.45	1.34
2	C	301	BXU	C3-N2	5.00	1.45	1.34
2	B	301	BXU	C1-N2	-4.92	1.40	1.47
2	B	301	BXU	O4-C3	-3.81	1.15	1.23

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	BXU	C5-C3-N2	9.83	126.96	116.42
2	B	301	BXU	O4-C3-N2	-8.06	108.01	122.93
2	A	301	BXU	C5-C3-N2	7.75	124.73	116.42
2	D	301	BXU	C5-C3-N2	5.60	122.42	116.42
2	A	301	BXU	C5-C6-S7	-5.08	107.28	114.05

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

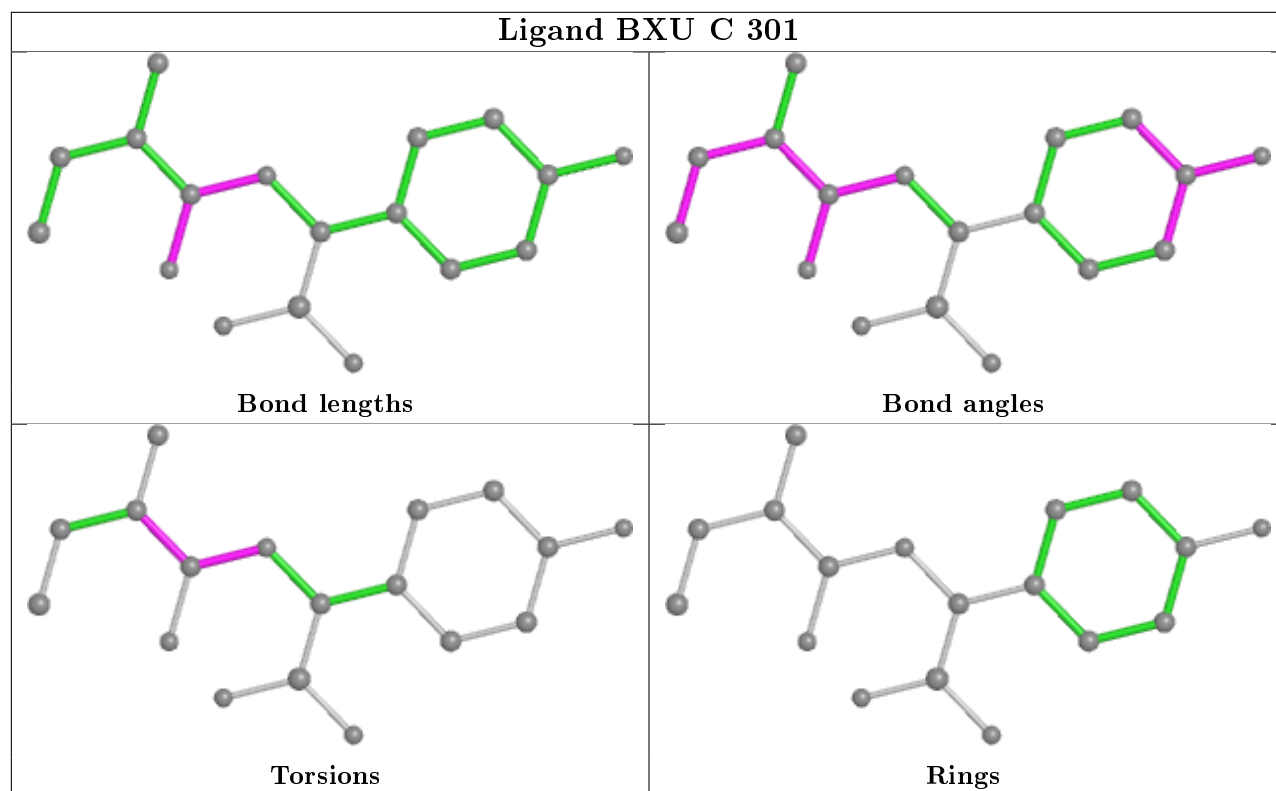
Mol	Chain	Res	Type	Atoms
2	C	301	BXU	O4-C3-N2-C1
2	A	301	BXU	O4-C3-N2-C1
2	D	301	BXU	O4-C3-N2-C1
2	B	301	BXU	O4-C3-N2-C1
2	B	301	BXU	C8-C5-C6-S7

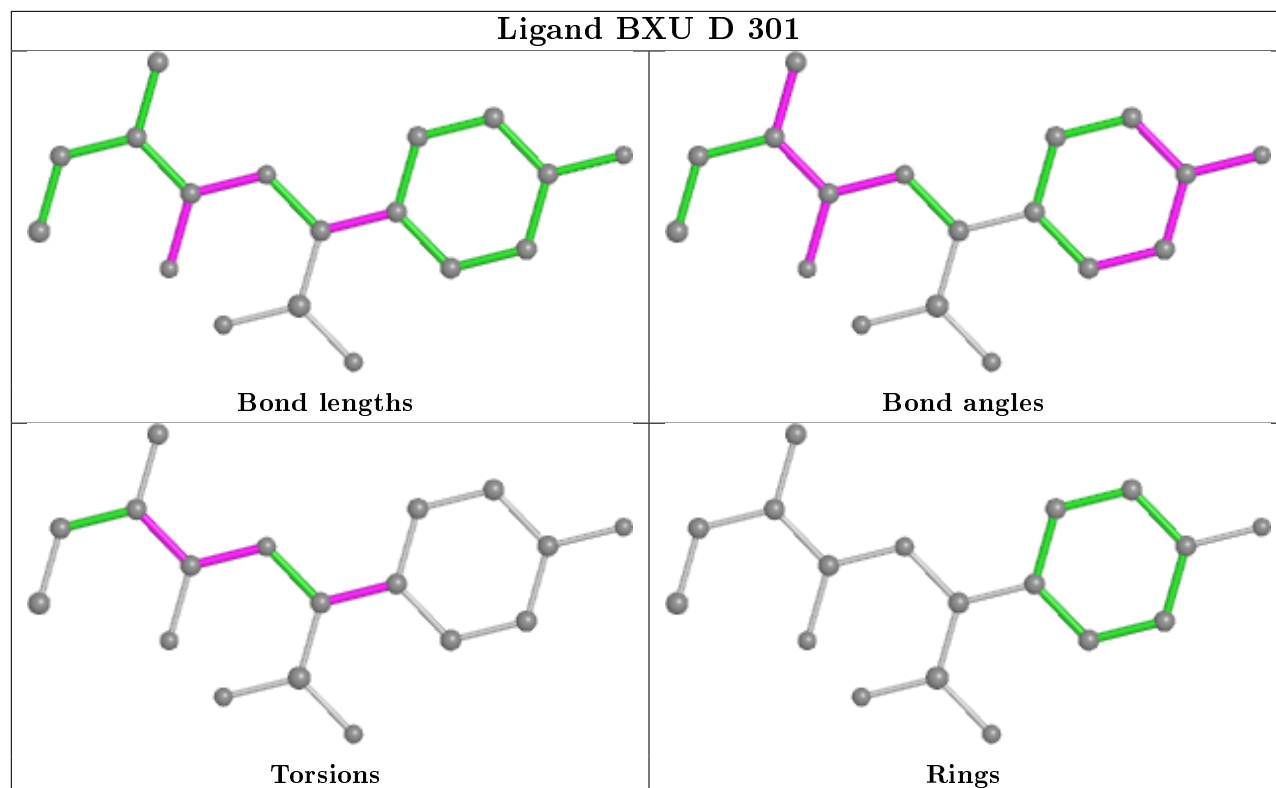
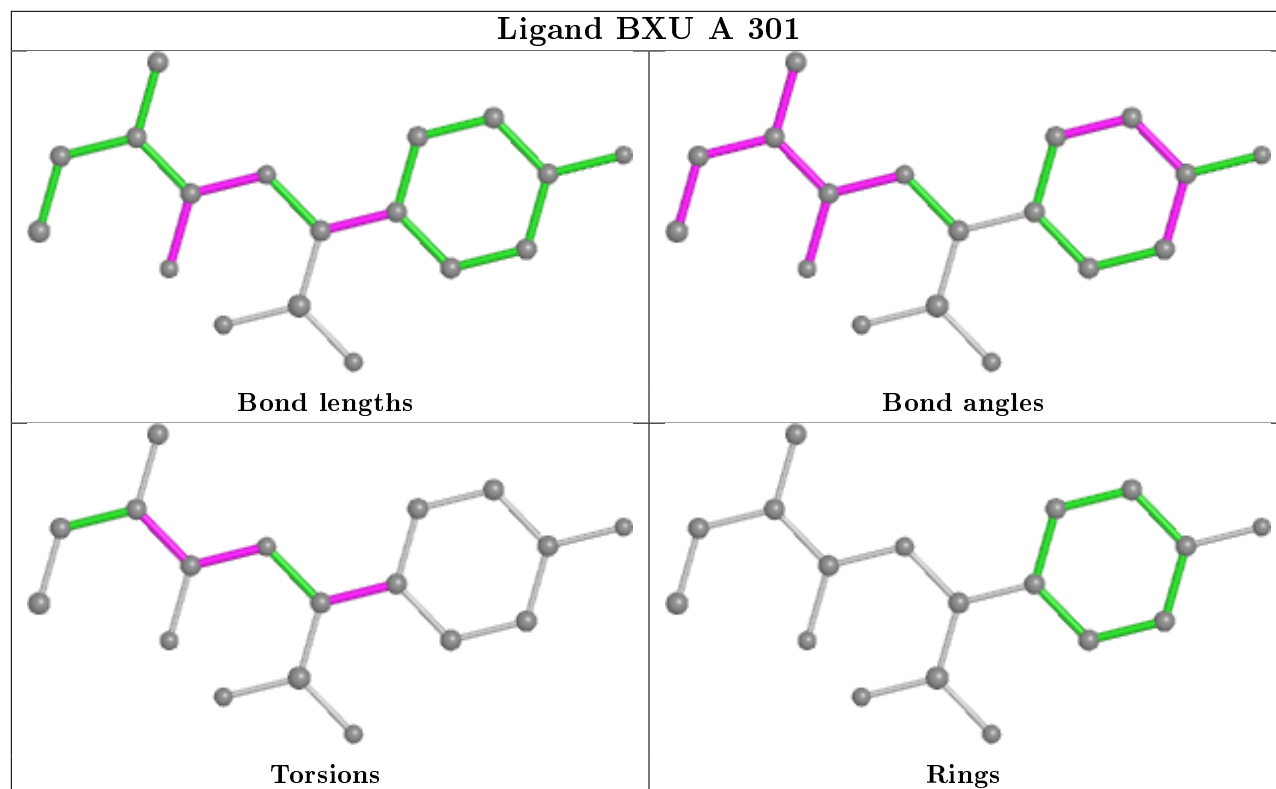
There are no ring outliers.

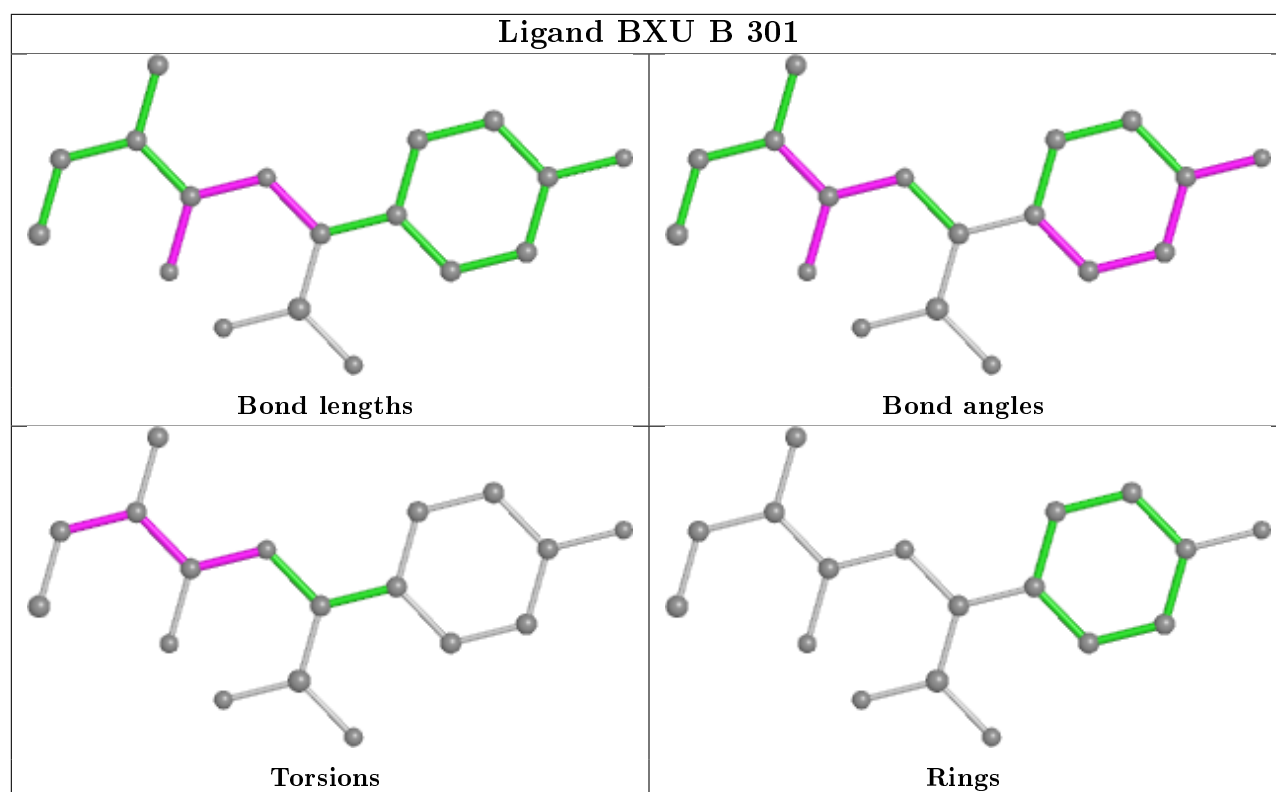
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	BXU	3	0
2	A	301	BXU	2	0
2	D	301	BXU	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 [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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

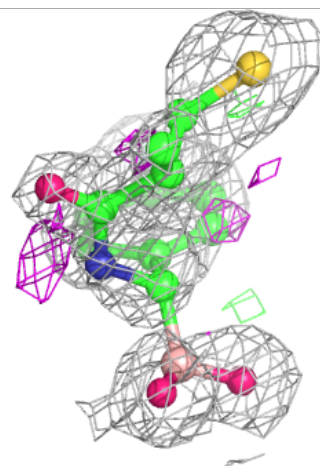
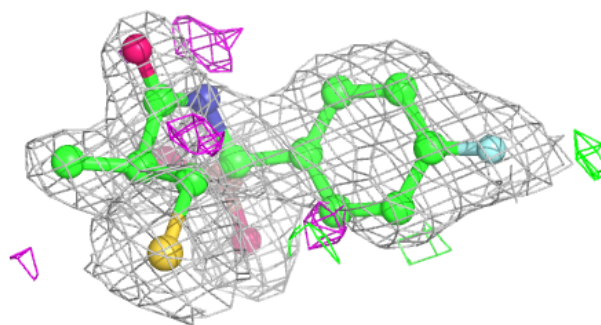
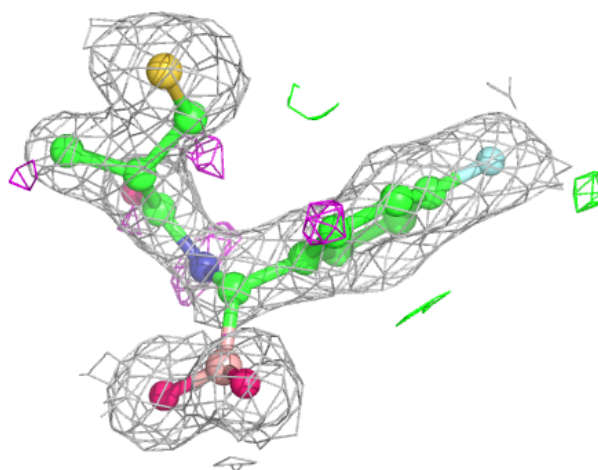
### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 BXU C 301:**

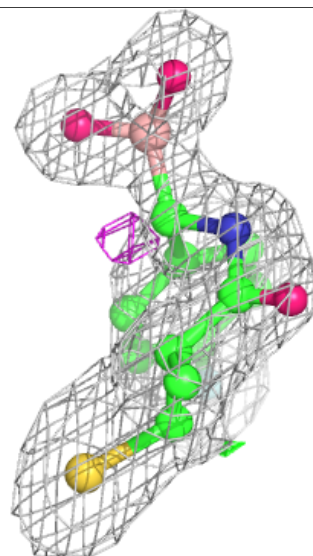
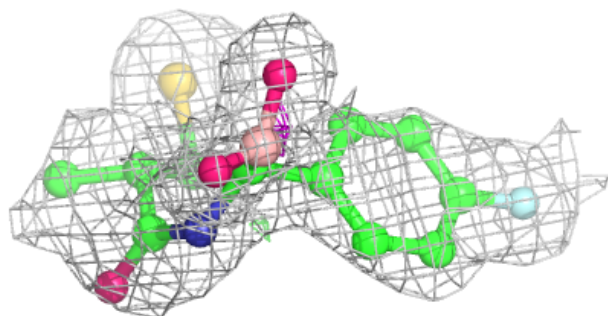
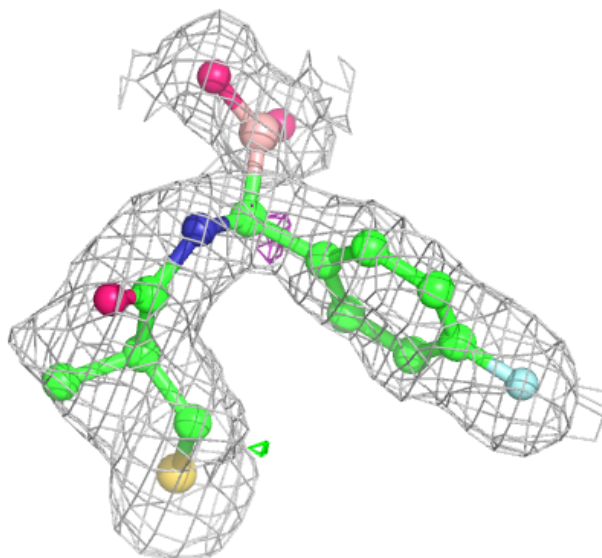
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





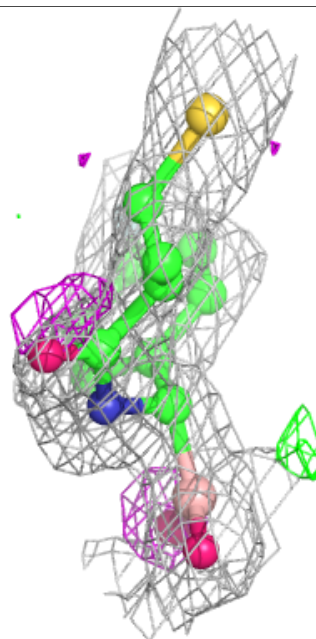
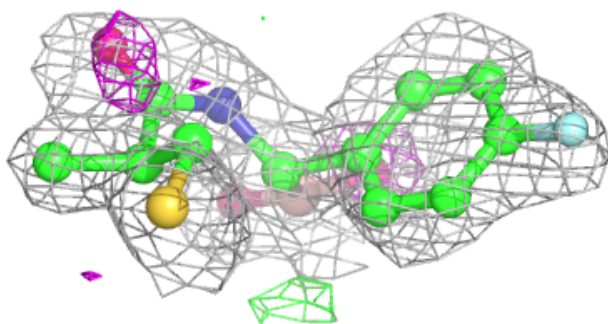
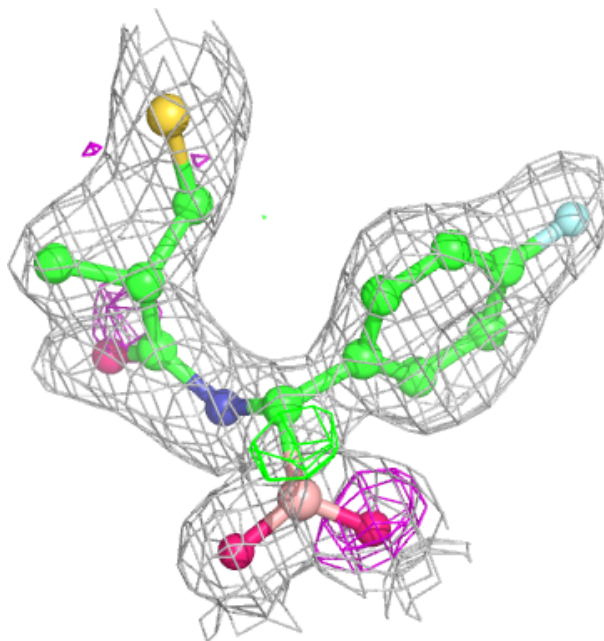
**Electron density around BXU A 301:**

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



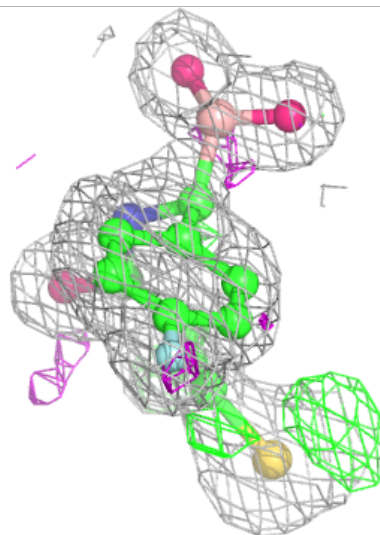
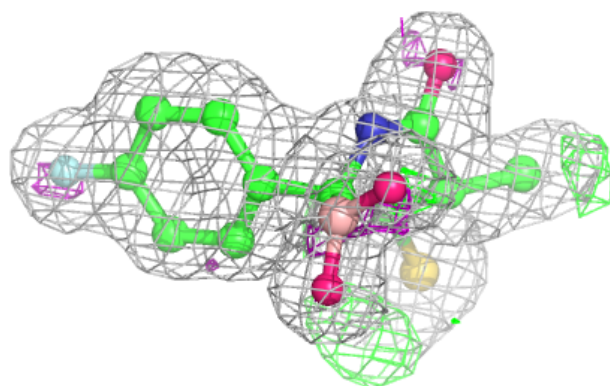
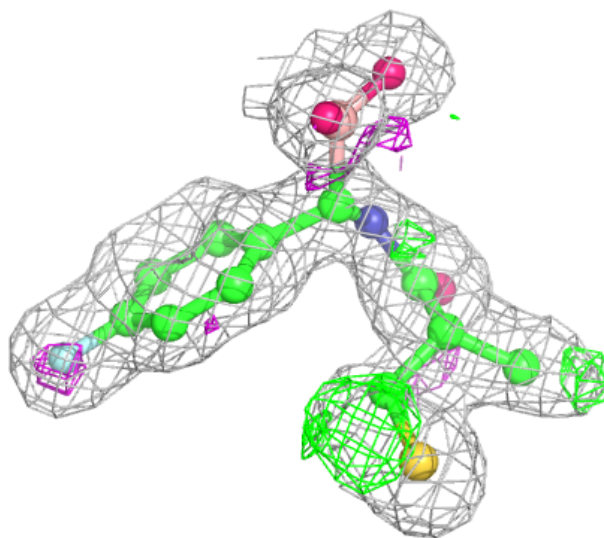
**Electron density around BXU D 301:**

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



**Electron density around BXU B 301:**

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

**6.5 Other polymers** [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.