



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:21 am BST

PDB ID : 4MTZ  
Title : Structure of XIAP-BIR1 in complex with NF023  
Authors : Cossu, F.; Milani, M.; Grassi, S.; Mastrangelo, E.; Bolognesi, M.  
Deposited on : 2013-09-20  
Resolution : 2.10 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 : 1.8.5 (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

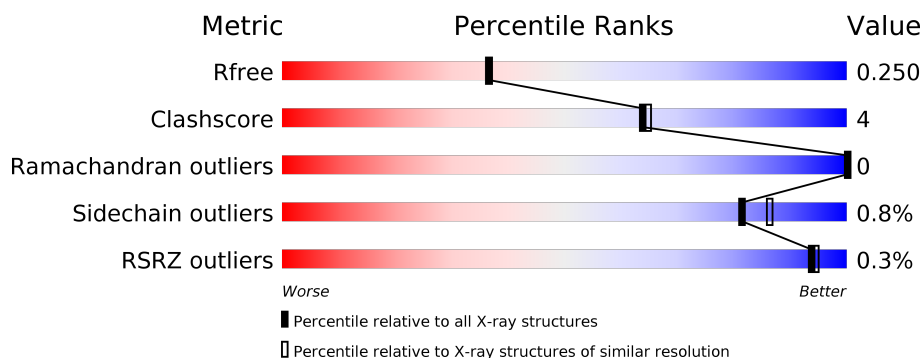
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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 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  $\leq 5\%$ . 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	111	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 68%; width: 30%; height: 10px; background-color: grey;"></div> <div style="position: absolute; bottom: 0; left: 68%; width: 30%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 68%; width: 30%; height: 10px; background-color: orange;"></div> <div style="position: absolute; bottom: 0; left: 68%; width: 30%; height: 10px; background-color: red;"></div> </div> <div>68% 30%</div> </div>
1	B	111	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 64%; width: 31%; height: 10px; background-color: grey;"></div> <div style="position: absolute; bottom: 0; left: 64%; width: 31%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 64%; width: 31%; height: 10px; background-color: orange;"></div> <div style="position: absolute; bottom: 0; left: 64%; width: 31%; height: 10px; background-color: red;"></div> </div> <div>64% 5% 31%</div> </div>
1	C	111	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 64%; width: 31%; height: 10px; background-color: grey;"></div> <div style="position: absolute; bottom: 0; left: 64%; width: 31%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 64%; width: 31%; height: 10px; background-color: orange;"></div> <div style="position: absolute; bottom: 0; left: 64%; width: 31%; height: 10px; background-color: red;"></div> </div> <div>64% 5% 31%</div> </div>
1	D	111	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 65%; width: 31%; height: 10px; background-color: grey;"></div> <div style="position: absolute; bottom: 0; left: 65%; width: 31%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 65%; width: 31%; height: 10px; background-color: orange;"></div> <div style="position: absolute; bottom: 0; left: 65%; width: 31%; height: 10px; background-color: red;"></div> </div> <div>65% 5% 31%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2737 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 E3 ubiquitin-protein ligase XIAP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	2	0
			628	397	114	113	4			
1	B	77	Total	C	N	O	S	0	0	0
			608	385	110	110	3			
1	C	77	Total	C	N	O	S	0	0	0
			608	385	110	110	3			
1	D	77	Total	C	N	O	S	0	1	0
			616	390	113	110	3			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P98170
A	-10	GLY	-	expression tag	UNP P98170
A	-9	SER	-	expression tag	UNP P98170
A	-8	SER	-	expression tag	UNP P98170
A	-7	HIS	-	expression tag	UNP P98170
A	-6	HIS	-	expression tag	UNP P98170
A	-5	HIS	-	expression tag	UNP P98170
A	-4	HIS	-	expression tag	UNP P98170
A	-3	HIS	-	expression tag	UNP P98170
A	-2	HIS	-	expression tag	UNP P98170
A	-1	SER	-	expression tag	UNP P98170
A	0	SER	-	expression tag	UNP P98170
A	1	GLY	-	expression tag	UNP P98170
A	2	LEU	-	expression tag	UNP P98170
A	3	VAL	-	expression tag	UNP P98170
A	4	PRO	-	expression tag	UNP P98170
A	5	GLN	-	expression tag	UNP P98170
A	6	GLY	-	expression tag	UNP P98170
A	7	SER	-	expression tag	UNP P98170
A	8	HIS	-	expression tag	UNP P98170
A	9	MET	-	expression tag	UNP P98170

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Chain	Residue	Modelled	Actual	Comment	Reference
B	989	MET	-	expression tag	UNP P98170
B	990	GLY	-	expression tag	UNP P98170
B	991	SER	-	expression tag	UNP P98170
B	992	SER	-	expression tag	UNP P98170
B	993	HIS	-	expression tag	UNP P98170
B	994	HIS	-	expression tag	UNP P98170
B	995	HIS	-	expression tag	UNP P98170
B	996	HIS	-	expression tag	UNP P98170
B	997	HIS	-	expression tag	UNP P98170
B	998	HIS	-	expression tag	UNP P98170
B	999	SER	-	expression tag	UNP P98170
B	1000	SER	-	expression tag	UNP P98170
B	1001	GLY	-	expression tag	UNP P98170
B	1002	LEU	-	expression tag	UNP P98170
B	1003	VAL	-	expression tag	UNP P98170
B	1004	PRO	-	expression tag	UNP P98170
B	1005	GLN	-	expression tag	UNP P98170
B	1006	GLY	-	expression tag	UNP P98170
B	1007	SER	-	expression tag	UNP P98170
B	1008	HIS	-	expression tag	UNP P98170
B	1009	MET	-	expression tag	UNP P98170
D	2989	MET	-	expression tag	UNP P98170
D	2990	GLY	-	expression tag	UNP P98170
D	2991	SER	-	expression tag	UNP P98170
D	2992	SER	-	expression tag	UNP P98170
D	2993	HIS	-	expression tag	UNP P98170
D	2994	HIS	-	expression tag	UNP P98170
D	2995	HIS	-	expression tag	UNP P98170
D	2996	HIS	-	expression tag	UNP P98170
D	2997	HIS	-	expression tag	UNP P98170
D	2998	HIS	-	expression tag	UNP P98170
D	2999	SER	-	expression tag	UNP P98170
D	3000	SER	-	expression tag	UNP P98170
D	3001	GLY	-	expression tag	UNP P98170
D	3002	LEU	-	expression tag	UNP P98170
D	3003	VAL	-	expression tag	UNP P98170
D	3004	PRO	-	expression tag	UNP P98170
D	3005	GLN	-	expression tag	UNP P98170
D	3006	GLY	-	expression tag	UNP P98170
D	3007	SER	-	expression tag	UNP P98170
D	3008	HIS	-	expression tag	UNP P98170
D	3009	MET	-	expression tag	UNP P98170

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2989	MET	-	expression tag	UNP P98170
C	2990	GLY	-	expression tag	UNP P98170
C	2991	SER	-	expression tag	UNP P98170
C	2992	SER	-	expression tag	UNP P98170
C	2993	HIS	-	expression tag	UNP P98170
C	2994	HIS	-	expression tag	UNP P98170
C	2995	HIS	-	expression tag	UNP P98170
C	2996	HIS	-	expression tag	UNP P98170
C	2997	HIS	-	expression tag	UNP P98170
C	2998	HIS	-	expression tag	UNP P98170
C	2999	SER	-	expression tag	UNP P98170
C	3000	SER	-	expression tag	UNP P98170
C	3001	GLY	-	expression tag	UNP P98170
C	3002	LEU	-	expression tag	UNP P98170
C	3003	VAL	-	expression tag	UNP P98170
C	3004	PRO	-	expression tag	UNP P98170
C	3005	GLN	-	expression tag	UNP P98170
C	3006	GLY	-	expression tag	UNP P98170
C	3007	SER	-	expression tag	UNP P98170
C	3008	HIS	-	expression tag	UNP P98170
C	3009	MET	-	expression tag	UNP P98170

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

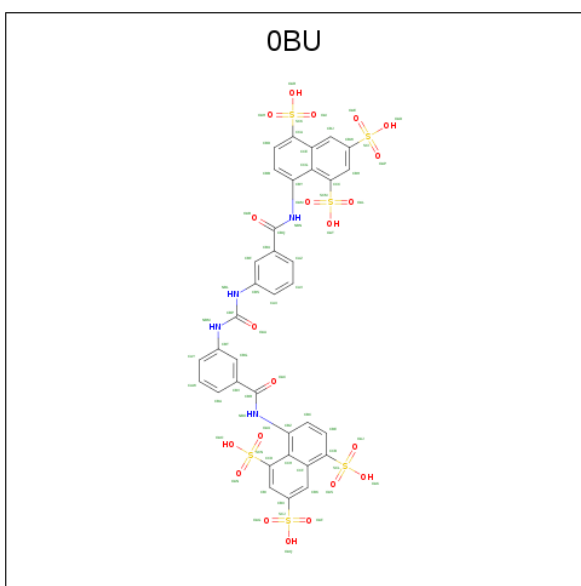
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 8-({3-[(3-[(4,6,8-trisulfonaphthalen-1-yl)carbamoyl]phenyl)carbamoyl]amino]benzoyl}amino)naphthalene-1,3,5-trisulfonic acid (three-letter code: 0BU) (formula:  $C_{35}H_{26}N_4O_{21}S_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			66	35	4	21	6		
4	D	1	Total	C	N	O	S	0	0
			66	35	4	21	6		

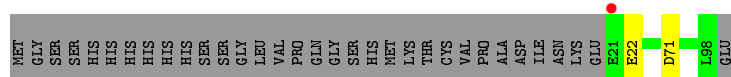
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total 36	O 36	0	0
5	B	25	Total 25	O 25	0	0
5	C	32	Total 32	O 32	0	0
5	D	43	Total 43	O 43	0	0

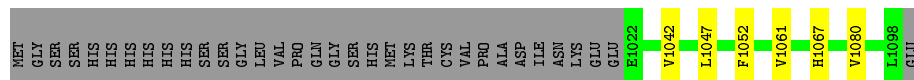
### 3 Residue-property plots [i](#)

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 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.

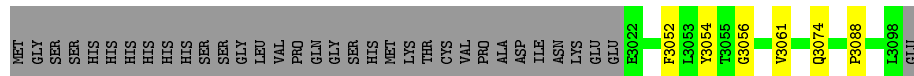
- Molecule 1: E3 ubiquitin-protein ligase XIAP



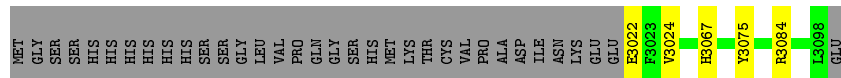
- Molecule 1: E3 ubiquitin-protein ligase XIAP



- Molecule 1: E3 ubiquitin-protein ligase XIAP



- Molecule 1: E3 ubiquitin-protein ligase XIAP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.85Å 76.21Å 71.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.19 – 2.10 71.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (71.19-2.10) 99.3 (71.19-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.190 , 0.242 0.199 , 0.250	Depositor DCC
$R_{free}$ test set	1175 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.126 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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 24.79 % 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 3.5861e-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: 0BU, ZN, SO4

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	0.59	0/651	0.71	0/878
1	B	0.55	0/625	0.69	0/844
1	C	0.50	0/625	0.69	0/844
1	D	0.53	0/636	0.72	0/858
All	All	0.54	0/2537	0.70	0/3424

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	628	0	591	0	0
1	B	608	0	568	4	0
1	C	608	0	568	4	0
1	D	616	0	581	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	66	0	26	5	0
4	D	66	0	26	5	0
5	A	36	0	0	0	0
5	B	25	0	0	1	0
5	C	32	0	0	0	0
5	D	43	0	0	3	0
All	All	2737	0	2360	21	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.

All (21) 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:3022:GLU:HG3	1:D:3024:VAL:HG23	1.77	0.64
4:D:3102:0BU:HBJ	4:D:3102:0BU:OAI	2.03	0.59
1:B:1067:HIS:HD2	5:D:3222:HOH:O	1.86	0.58
4:D:3102:0BU:SCM	4:D:3102:0BU:NBN	2.80	0.53
4:C:3102:0BU:NBO	4:C:3102:0BU:SCN	2.84	0.51
1:B:1080:VAL:HG23	5:B:1213:HOH:O	2.11	0.50
4:C:3102:0BU:NBN	4:C:3102:0BU:SCM	2.83	0.50
4:D:3102:0BU:SCN	4:D:3102:0BU:NBO	2.78	0.49
1:C:3074:GLN:HB3	1:D:3075:TYR:OH	2.13	0.49
1:D:3022:GLU:CG	1:D:3024:VAL:HG23	2.42	0.47
1:C:3088:PRO:HD2	4:C:3102:0BU:HBC	1.97	0.47
4:D:3102:0BU:OAC	4:D:3102:0BU:HBC	2.15	0.46
1:B:1052:PHE:HB3	1:B:1061:VAL:HB	1.98	0.46
1:D:3067:HIS:HD2	5:D:3212:HOH:O	2.01	0.44
1:C:3052:PHE:HB3	1:C:3061:VAL:HB	1.99	0.44
4:C:3102:0BU:HBJ	4:C:3102:0BU:OAI	2.19	0.43
1:C:3054:TYR:CE2	1:C:3056:GLY:HA2	2.53	0.42
1:B:1042:VAL:HG23	1:B:1047:LEU:HD11	2.01	0.42
1:D:3084[A]:ARG:NH1	5:D:3233:HOH:O	2.46	0.41
4:C:3102:0BU:OAB	4:C:3102:0BU:HBB	2.21	0.41
4:D:3102:0BU:NBO	4:D:3102:0BU:OAO	2.54	0.40

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	78/111 (70%)	77 (99%)	1 (1%)	0	100	100
1	B	75/111 (68%)	72 (96%)	3 (4%)	0	100	100
1	C	75/111 (68%)	73 (97%)	2 (3%)	0	100	100
1	D	76/111 (68%)	76 (100%)	0	0	100	100
All	All	304/444 (68%)	298 (98%)	6 (2%)	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	A	66/93 (71%)	64 (97%)	2 (3%)	41	44
1	B	63/93 (68%)	63 (100%)	0	100	100
1	C	63/93 (68%)	63 (100%)	0	100	100
1	D	64/93 (69%)	64 (100%)	0	100	100
All	All	256/372 (69%)	254 (99%)	2 (1%)	81	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	71	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1067	HIS
1	C	3035	ASN
1	D	3067	HIS

### 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](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z  > 2$
4	0BU	C	3102	-	67,71,71	1.61	11 (16%)	97,113,113	1.21	8 (8%)
4	0BU	D	3102	-	67,71,71	1.49	9 (13%)	97,113,113	1.10	6 (6%)
3	SO4	B	1102	-	4,4,4	0.44	0	6,6,6	0.20	0

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
4	0BU	C	3102	-	-	10/60/60/60	0/6/6/6
4	0BU	D	3102	-	-	14/60/60/60	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3102	0BU	CBV-CBR	-3.76	1.42	1.50
4	C	3102	0BU	CBU-CBQ	-3.72	1.42	1.50
4	D	3102	0BU	CBU-CBQ	-3.71	1.42	1.50
4	C	3102	0BU	CBT-NBM	-3.43	1.34	1.41
4	C	3102	0BU	CBX-SCJ	-3.41	1.70	1.77
4	D	3102	0BU	CBV-CBR	-3.37	1.43	1.50
4	C	3102	0BU	CBY-NBN	-2.86	1.33	1.41
4	D	3102	0BU	CBS-NBL	-2.83	1.35	1.41
4	C	3102	0BU	CBZ-NBO	-2.68	1.34	1.41
4	D	3102	0BU	CBT-NBM	-2.62	1.36	1.41
4	D	3102	0BU	CBY-NBN	-2.48	1.34	1.41
4	D	3102	0BU	CCA-CCE	-2.39	1.39	1.43
4	C	3102	0BU	OAL-SCM	2.37	1.55	1.43
4	D	3102	0BU	CBZ-NBO	-2.28	1.35	1.41
4	C	3102	0BU	CCA-CCE	-2.21	1.39	1.43
4	C	3102	0BU	CBS-NBL	-2.21	1.37	1.41
4	C	3102	0BU	CBW-SCI	-2.11	1.72	1.77
4	C	3102	0BU	CCC-CCG	-2.09	1.41	1.43
4	D	3102	0BU	OAF-SCJ	2.03	1.54	1.43
4	D	3102	0BU	CCB-CCF	-2.00	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3102	0BU	OAU-SCN-CCD	4.01	118.41	106.43
4	C	3102	0BU	CCD-CCH-CCF	3.48	119.62	116.34
4	D	3102	0BU	OAL-SCM-CCC	3.45	116.74	106.43
4	D	3102	0BU	CBV-CBG-CBT	3.27	124.85	120.44
4	C	3102	0BU	OAL-SCM-CCC	3.21	116.00	106.43
4	D	3102	0BU	CBA-CBV-CBG	-2.79	115.93	119.24
4	C	3102	0BU	CCB-CCF-CCH	2.60	122.17	118.01
4	D	3102	0BU	OAE-SCI-CBW	2.45	112.30	106.65
4	D	3102	0BU	CCA-CCE-CCG	2.35	121.78	118.01
4	C	3102	0BU	CBI-CCD-CCH	-2.25	118.48	121.25
4	C	3102	0BU	CBU-CBF-CBS	2.23	123.45	120.44
4	C	3102	0BU	CBZ-NBO-CBR	-2.21	122.09	128.64
4	D	3102	0BU	CAY-CBT-CBG	-2.09	117.17	119.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3102	0BU	CAX-CBS-CBF	-2.04	117.23	119.65

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3102	0BU	NBO-CBR-CBV-CBA
4	C	3102	0BU	NBO-CBR-CBV-CBA
4	C	3102	0BU	CBG-CBT-NBM-CBP
4	C	3102	0BU	NBO-CBR-CBV-CBG
4	D	3102	0BU	NBO-CBR-CBV-CBG
4	C	3102	0BU	OAC-CBR-CBV-CBA
4	D	3102	0BU	NBN-CBQ-CBU-CAZ
4	C	3102	0BU	CAY-CBT-NBM-CBP
4	D	3102	0BU	OAB-CBQ-CBU-CAZ
4	C	3102	0BU	OAC-CBR-CBV-CBG
4	D	3102	0BU	CCE-CCA-SCK-OAH
4	D	3102	0BU	CCE-CCA-SCK-OAI
4	D	3102	0BU	OAC-CBR-CBV-CBA
4	C	3102	0BU	NBN-CBQ-CBU-CAZ
4	C	3102	0BU	NBN-CBQ-CBU-CBF
4	D	3102	0BU	NBN-CBQ-CBU-CBF
4	D	3102	0BU	OAB-CBQ-CBU-CBF
4	D	3102	0BU	OAC-CBR-CBV-CBG
4	D	3102	0BU	CBD-CCA-SCK-OAR
4	D	3102	0BU	CCE-CCA-SCK-OAR
4	D	3102	0BU	CBF-CBS-NBL-CBP
4	C	3102	0BU	OAB-CBQ-CBU-CAZ
4	C	3102	0BU	OAB-CBQ-CBU-CBF
4	D	3102	0BU	CAX-CBS-NBL-CBP

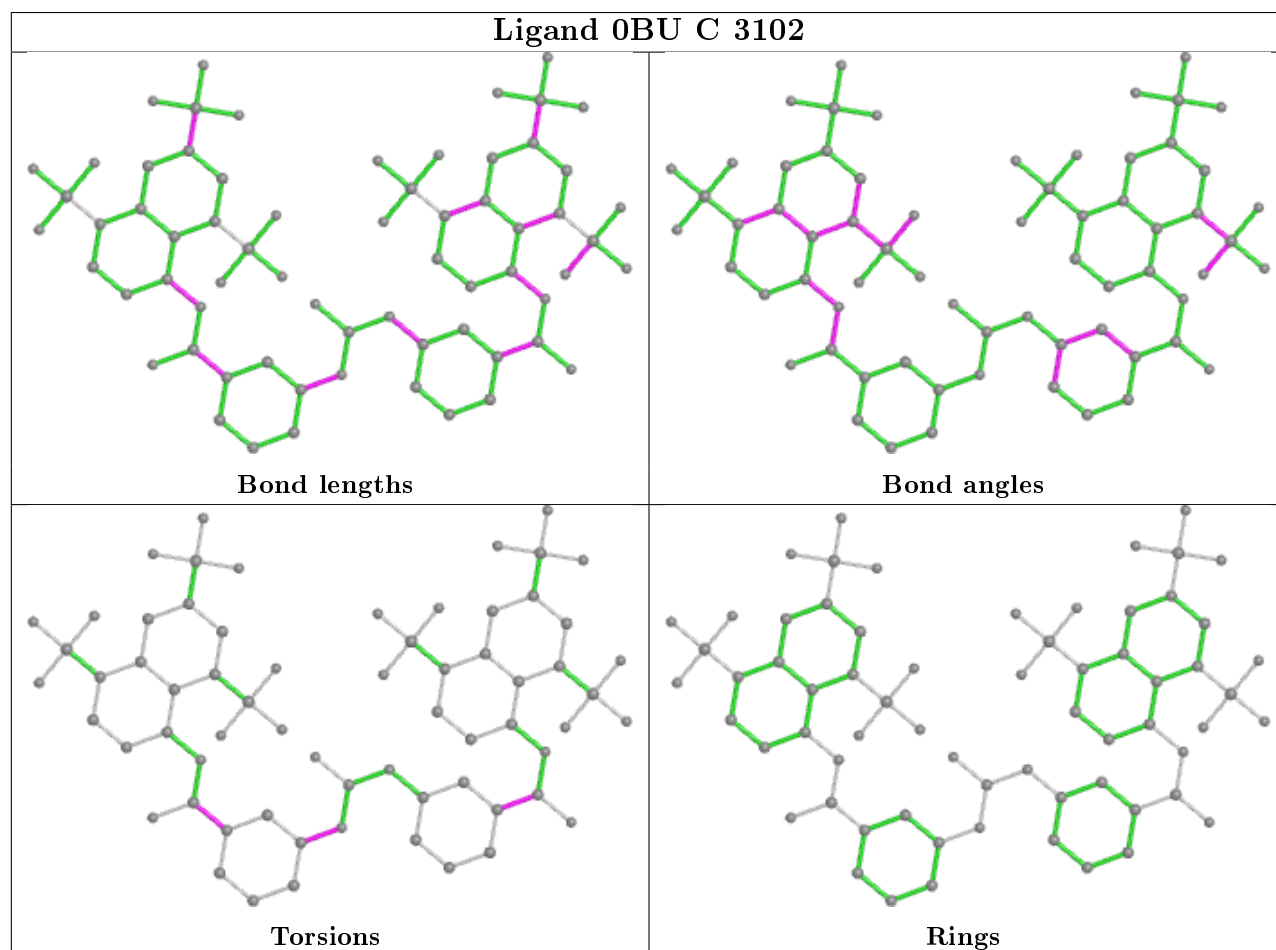
There are no ring outliers.

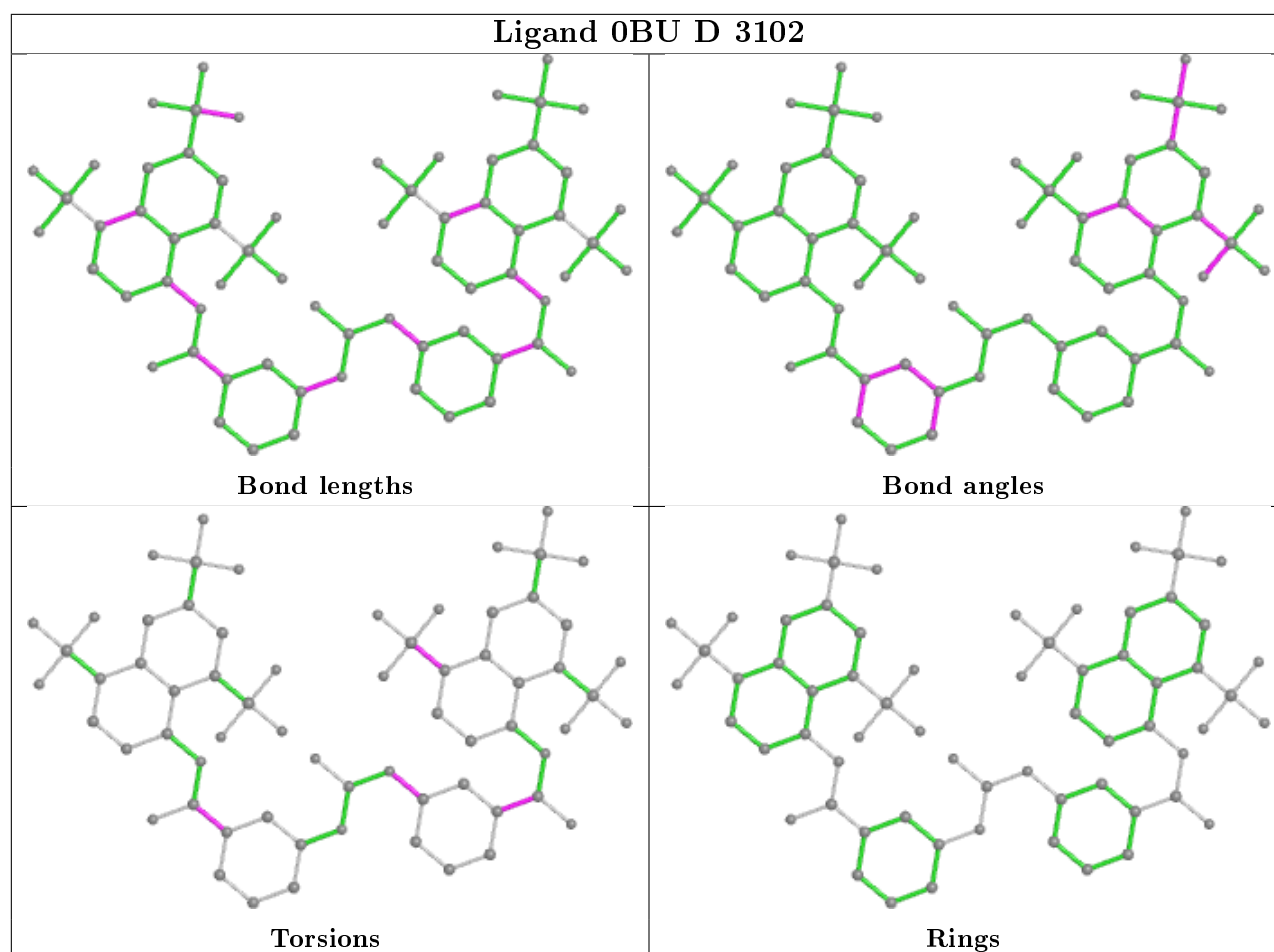
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3102	0BU	5	0
4	D	3102	0BU	5	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](#)

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	78/111 (70%)	-0.26	1 (1%) 77 80	21, 33, 56, 82	0
1	B	77/111 (69%)	-0.21	0 100 100	26, 37, 64, 73	0
1	C	77/111 (69%)	-0.17	0 100 100	26, 40, 66, 75	0
1	D	77/111 (69%)	-0.24	0 100 100	24, 35, 60, 67	0
All	All	309/444 (69%)	-0.22	1 (0%) 94 94	21, 37, 64, 82	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	GLU	3.1

### 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 carbohydrates 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.

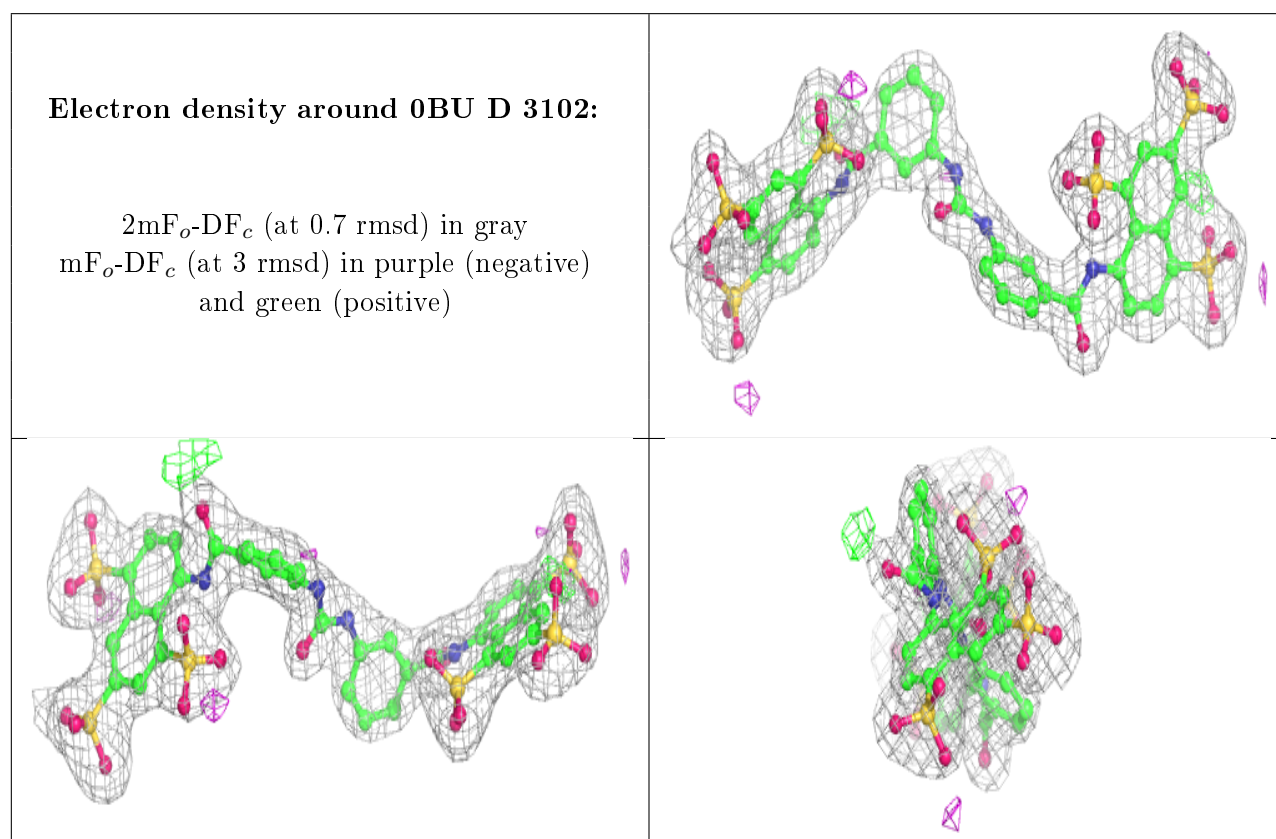
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	0BU	D	3102	66/66	0.96	0.10	29,43,59,69	0

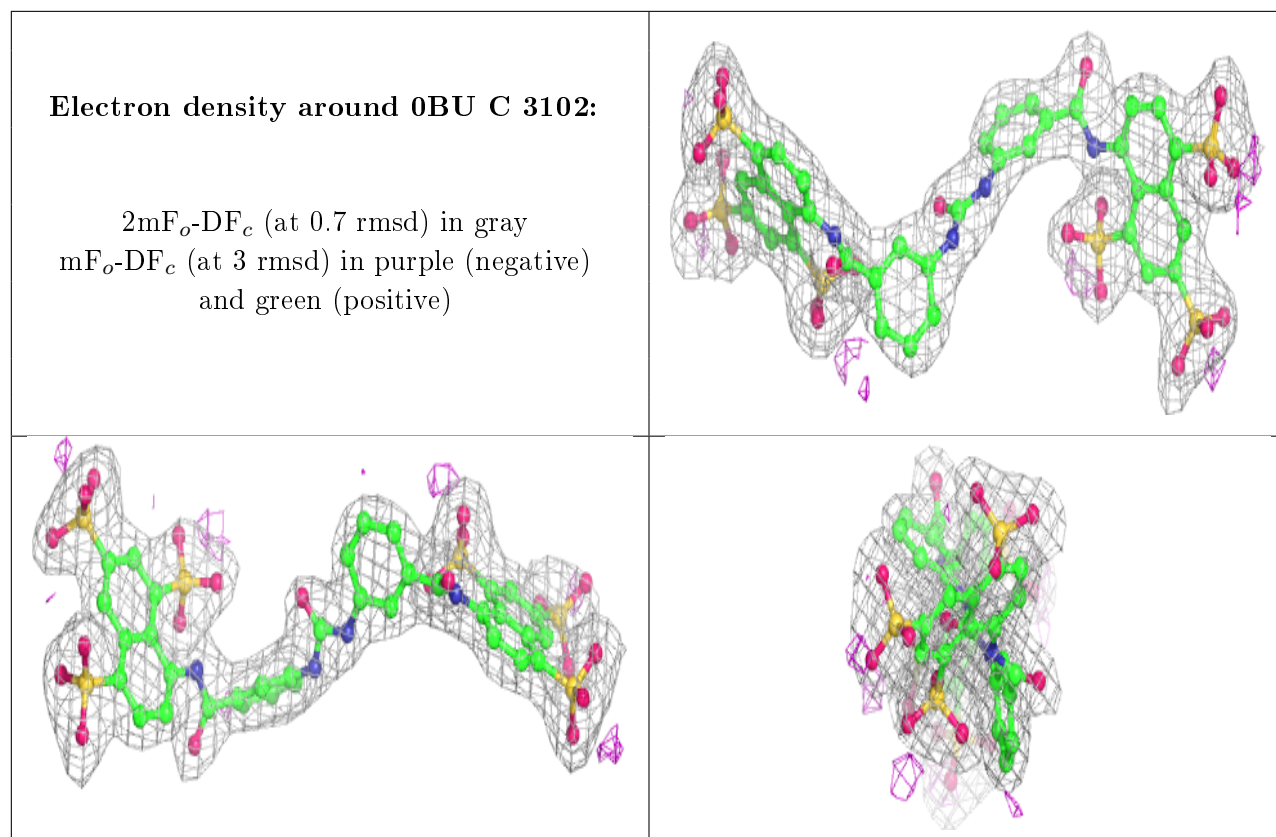
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	1102	5/5	0.96	0.10	57,63,86,97	0
4	0BU	C	3102	66/66	0.97	0.09	29,41,56,69	0
2	ZN	A	200	1/1	1.00	0.13	27,27,27,27	0
2	ZN	C	3101	1/1	1.00	0.12	30,30,30,30	0
2	ZN	D	3101	1/1	1.00	0.13	29,29,29,29	0
2	ZN	B	1101	1/1	1.00	0.11	27,27,27,27	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.