



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 01:11 AM EDT

PDB ID : 7KYH  
Title : Botulism Neurotoxin Light Chain A app form  
Authors : Ortega, M.E.; Salzameda, N.T.  
Deposited on : 2020-12-07  
Resolution : 2.91 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>.

---

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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

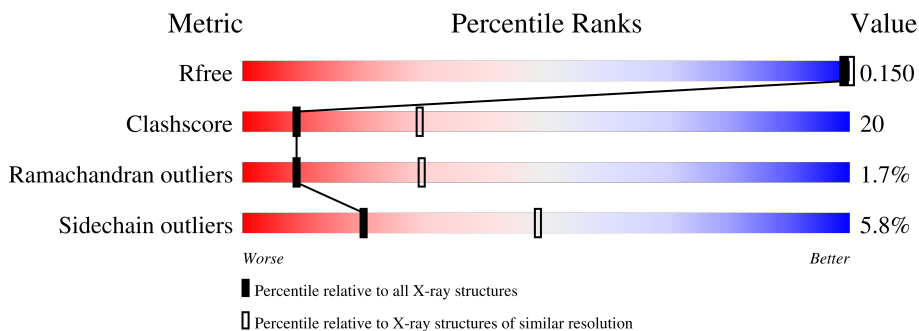
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	417	58% (green), 30% (yellow), 8% (grey), 0% (orange), 0% (red)
1	B	417	60% (green), 27% (yellow), 8% (grey), 5% (orange), 0% (red)
1	C	417	62% (green), 26% (yellow), 8% (grey), 0% (orange), 0% (red)
1	D	417	65% (green), 25% (yellow), 8% (grey), 0% (orange), 0% (red)

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12636 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 Bont/A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	3127	2020	512	588	7	0	0	0
1	B	385	3127	2020	512	588	7	0	0	0
1	C	385	3127	2020	512	588	7	0	0	0
1	D	385	3127	2020	512	588	7	0	0	0

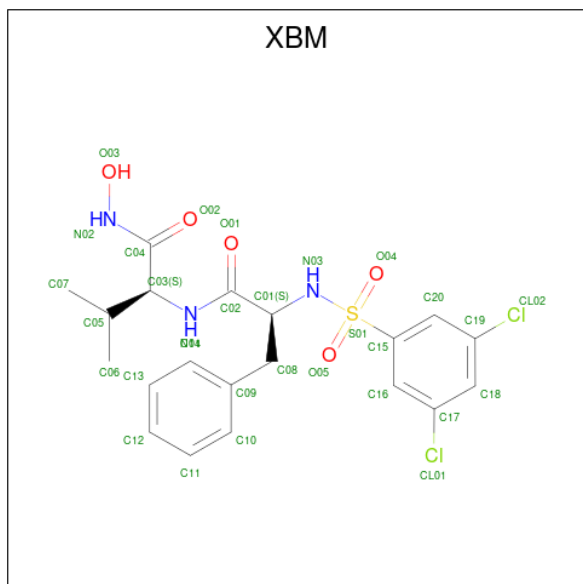
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	VAL	ALA	conflict	UNP C6K838
A	29	VAL	GLN	conflict	UNP C6K838
B	27	VAL	ALA	conflict	UNP C6K838
B	29	VAL	GLN	conflict	UNP C6K838
C	27	VAL	ALA	conflict	UNP C6K838
C	29	VAL	GLN	conflict	UNP C6K838
D	27	VAL	ALA	conflict	UNP C6K838
D	29	VAL	GLN	conflict	UNP C6K838

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

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

- Molecule 3 is N-[(3,5-dichlorophenyl)sulfonyl]-L-phenylalanyl-N-hydroxy-L-valinamide (three-letter code: XBM) (formula: C<sub>20</sub>H<sub>23</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).

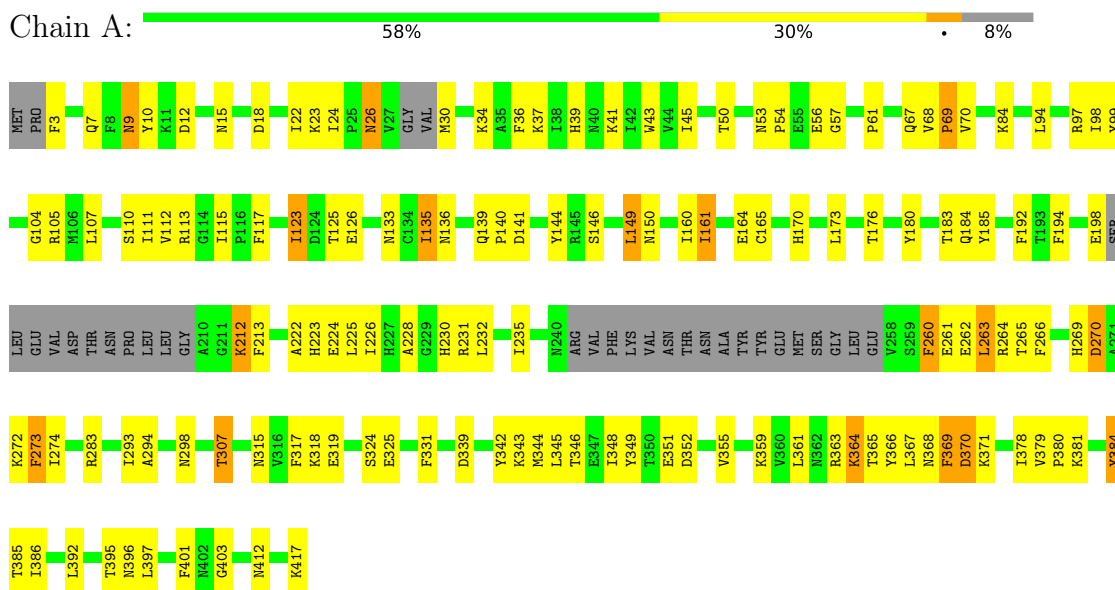


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
3	A	1	Total	C	Cl	N	O	S	0	0
			31	20	2	3	5	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			31	20	2	3	5	1		
3	C	1	Total	C	Cl	N	O	S	0	0
			31	20	2	3	5	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			31	20	2	3	5	1		

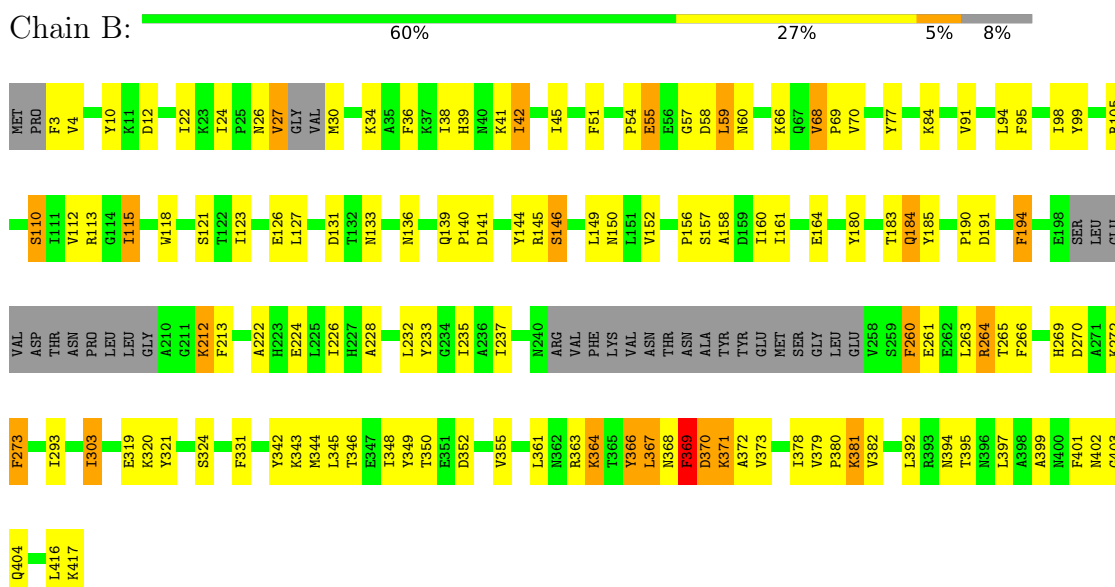
### 3 Residue-property plots [i](#)

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. 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.

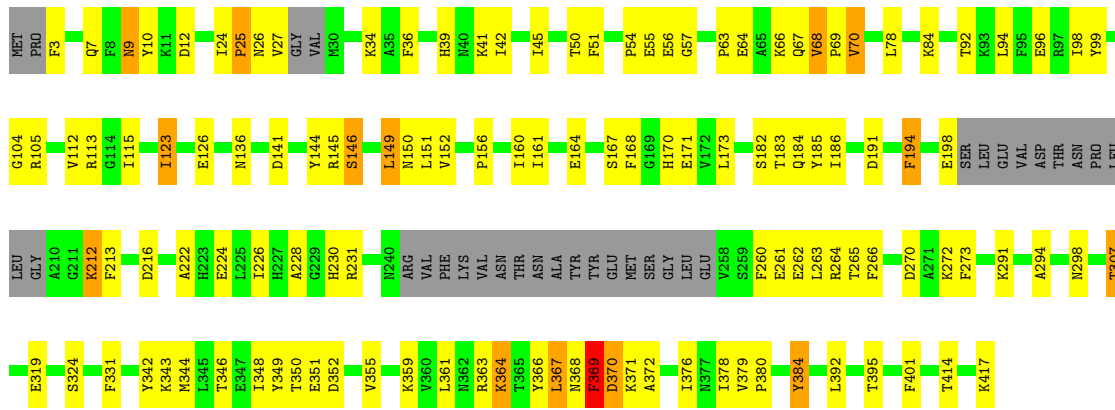
- Molecule 1: Bont/A1



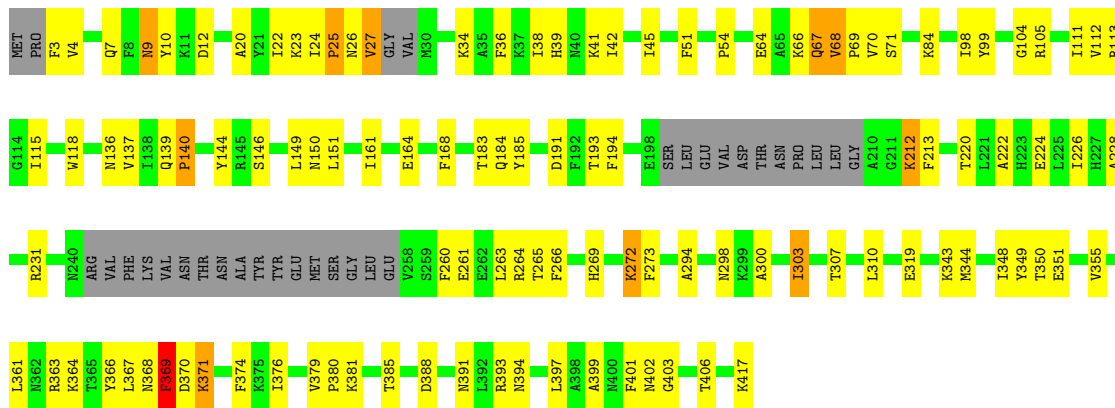
- Molecule 1: Bont/A1



• Molecule 1: Bont/A1



• Molecule 1: Bont/A1



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.31Å 84.05Å 99.72Å 103.78° 91.84° 108.67°	Depositor
Resolution (Å)	48.09 – 2.91 48.09 – 2.91	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.09-2.91) 89.5 (48.09-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.138 , 0.173 0.126 , 0.150	Depositor DCC
$R_{free}$ test set	2297 reflections (6.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtrriage
Anisotropy	0.685	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	12636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.13% 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: ZN, XBM

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	0.76	0/3199	0.97	0/4325
1	B	0.74	0/3199	0.97	0/4325
1	C	0.73	0/3199	0.96	0/4325
1	D	0.68	0/3199	0.84	0/4325
All	All	0.73	0/12796	0.94	0/17300

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	ASN	Peptide

### 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	3127	0	3084	140	0
1	B	3127	0	3084	152	0
1	C	3127	0	3084	158	0
1	D	3127	0	3084	121	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	A	31	0	0	4	0
3	B	31	0	0	2	0
3	C	31	0	0	3	0
3	D	31	0	0	4	0
All	All	12636	0	12336	506	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 20.

The worst 5 of 506 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:B:133:ASN:HA	1:B:183:THR:HG23	1.23	1.13
1:D:69:PRO:HG3	1:D:371:LYS:HA	1.32	1.11
1:A:69:PRO:HG3	1:A:371:LYS:HA	1.40	1.02
1:C:68:VAL:HG21	1:C:417:LYS:C	1.82	1.00
1:A:123:ILE:HD11	1:A:126:GLU:CB	1.97	0.95

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	377/417 (90%)	338 (90%)	32 (8%)	7 (2%)	<b>8</b> <b>27</b>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	377/417 (90%)	334 (89%)	35 (9%)	8 (2%)	7	24
1	C	377/417 (90%)	339 (90%)	32 (8%)	6 (2%)	9	31
1	D	377/417 (90%)	343 (91%)	29 (8%)	5 (1%)	12	36
All	All	1508/1668 (90%)	1354 (90%)	128 (8%)	26 (2%)	9	29

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	LYS
1	A	307	THR
1	A	369	PHE
1	B	59	LEU
1	B	212	LYS

### 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	346/374 (92%)	323 (93%)	23 (7%)	16	42
1	B	346/374 (92%)	326 (94%)	20 (6%)	20	48
1	C	346/374 (92%)	326 (94%)	20 (6%)	20	48
1	D	346/374 (92%)	329 (95%)	17 (5%)	25	56
All	All	1384/1496 (92%)	1304 (94%)	80 (6%)	20	48

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	343	LYS
1	D	260	PHE
1	C	364	LYS
1	D	27	VAL
1	D	307	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	269	HIS
1	D	409	ASN
1	D	412	ASN
1	D	394	ASN
1	B	412	ASN

### 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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z  > 2$
3	XBM	C	502	-	32,32,32	4.82	15 (46%)	44,45,45	3.59	21 (47%)
3	XBM	A	502	-	32,32,32	4.85	15 (46%)	44,45,45	3.98	23 (52%)
3	XBM	B	502	-	32,32,32	5.14	18 (56%)	44,45,45	3.78	18 (40%)
3	XBM	D	502	-	32,32,32	5.11	8 (25%)	44,45,45	2.79	15 (34%)

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
3	XBM	C	502	-	-	7/33/33/33	0/2/2/2
3	XBM	A	502	-	-	6/33/33/33	0/2/2/2
3	XBM	B	502	-	-	8/33/33/33	0/2/2/2
3	XBM	D	502	-	-	6/33/33/33	0/2/2/2

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	XBM	O05-S01	19.01	1.65	1.43
3	C	502	XBM	O05-S01	17.60	1.63	1.43
3	B	502	XBM	O05-S01	16.47	1.62	1.43
3	D	502	XBM	O04-S01	16.03	1.61	1.43
3	A	502	XBM	C04-N02	14.50	1.53	1.33

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	XBM	C17-C16-C15	11.99	128.98	118.23
3	B	502	XBM	O05-S01-C15	-11.37	93.96	107.97
3	C	502	XBM	O05-S01-C15	-10.81	94.65	107.97
3	D	502	XBM	O05-S01-C15	-9.99	95.66	107.97
3	B	502	XBM	C16-C15-S01	9.77	130.02	119.08

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

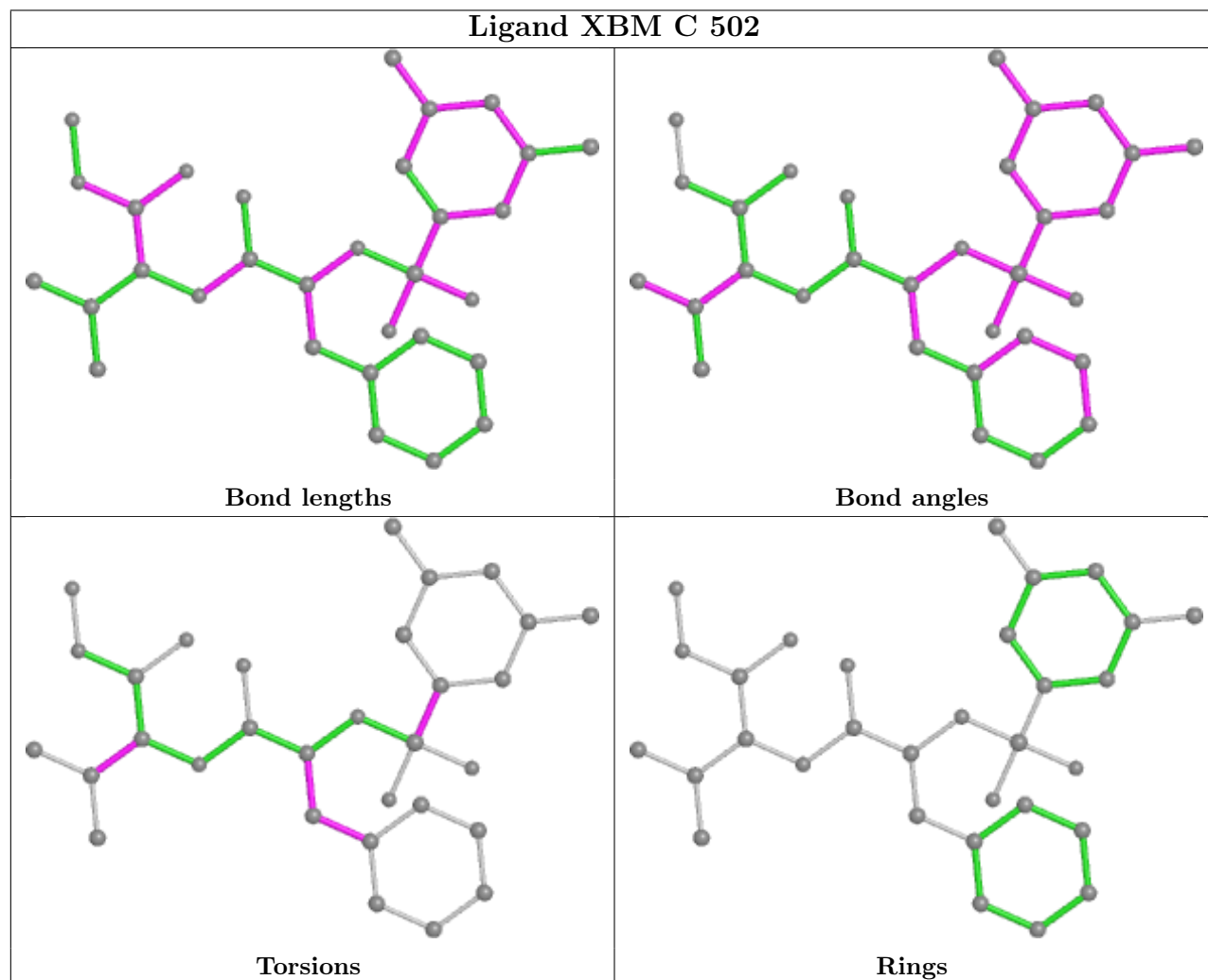
Mol	Chain	Res	Type	Atoms
3	A	502	XBM	N03-C01-C08-C09
3	B	502	XBM	N03-C01-C08-C09
3	C	502	XBM	N03-C01-C08-C09
3	D	502	XBM	N03-C01-C08-C09
3	A	502	XBM	C02-C01-C08-C09

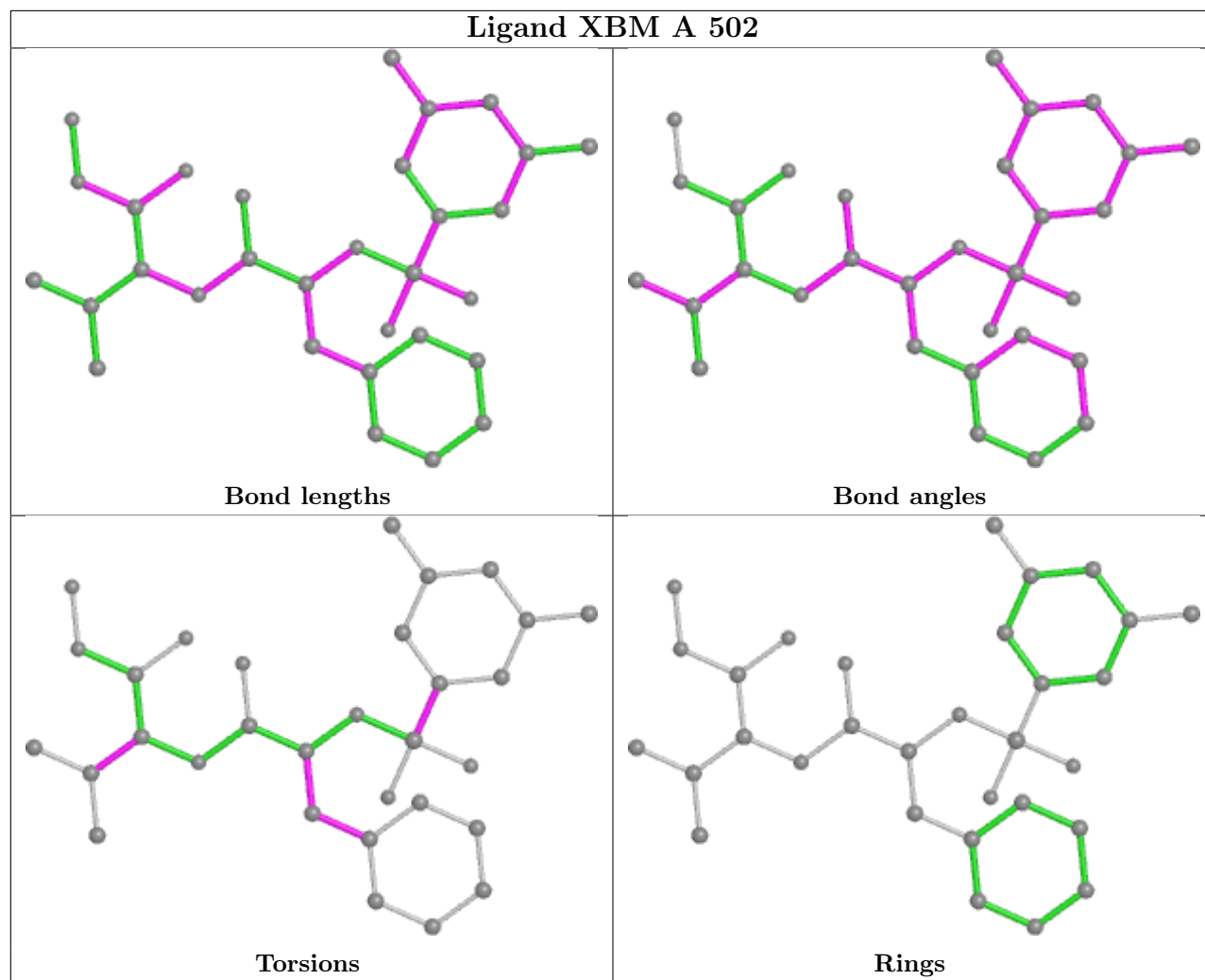
There are no ring outliers.

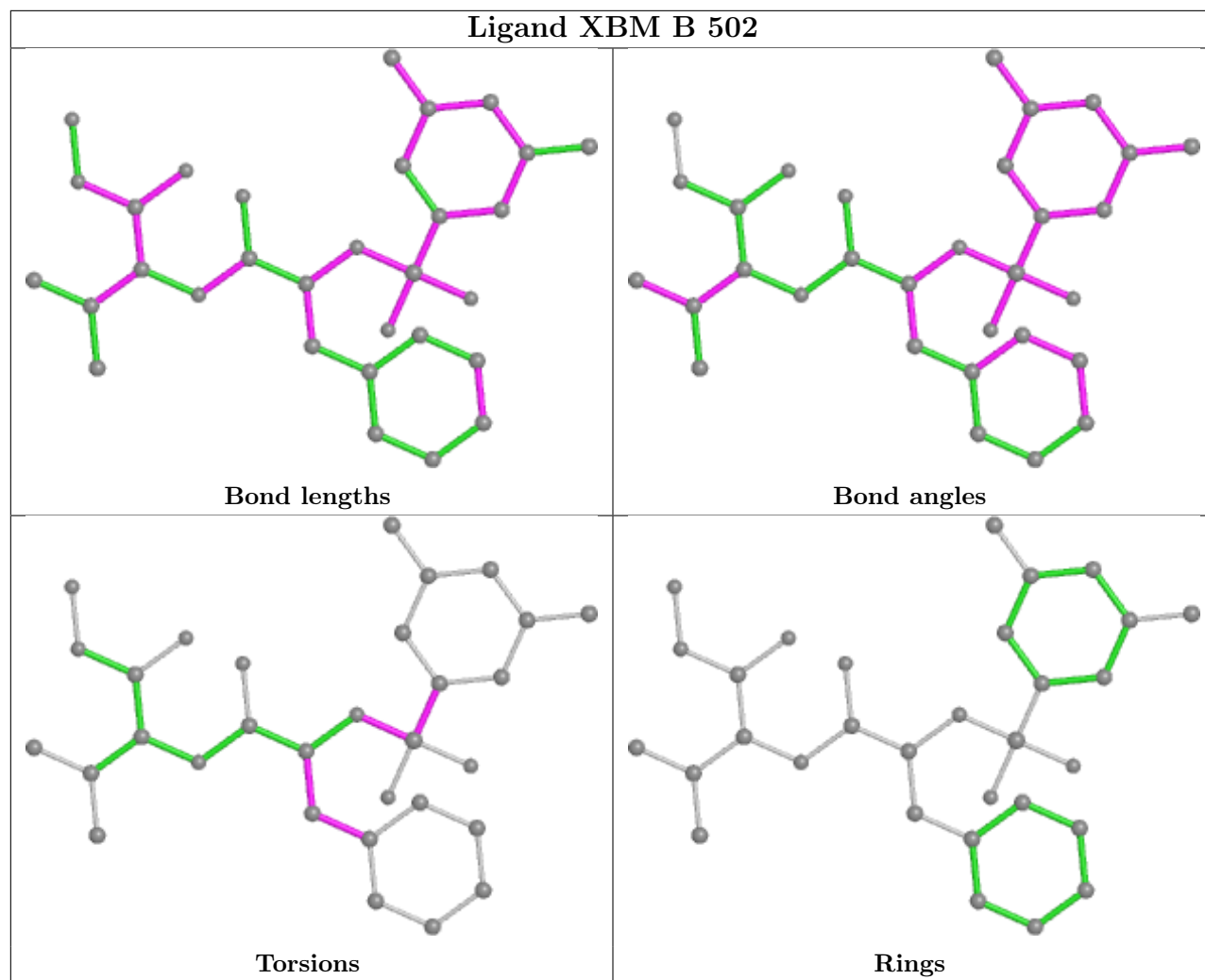
4 monomers are involved in 13 short contacts:

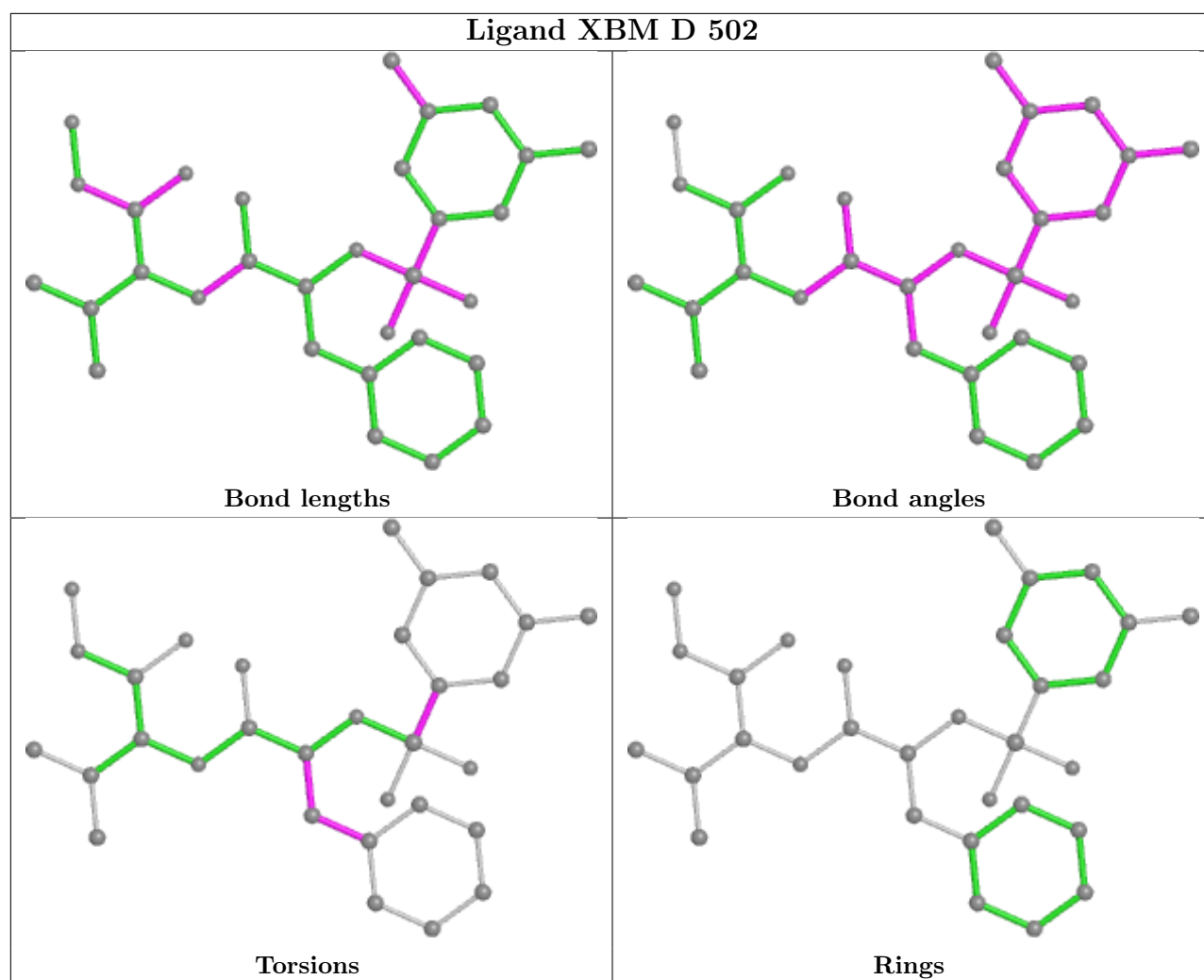
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	XBM	3	0
3	A	502	XBM	4	0
3	B	502	XBM	2	0
3	D	502	XBM	4	0

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](#)

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

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

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

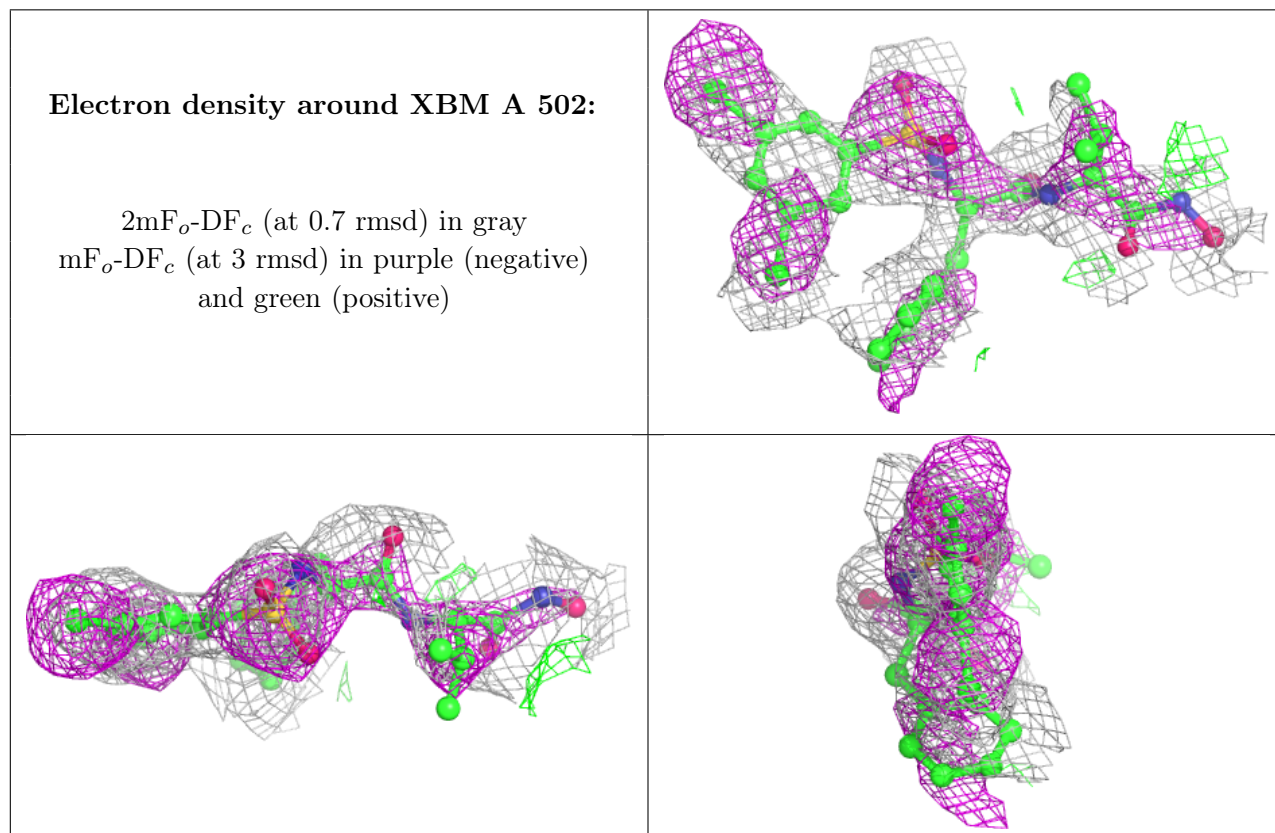
### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

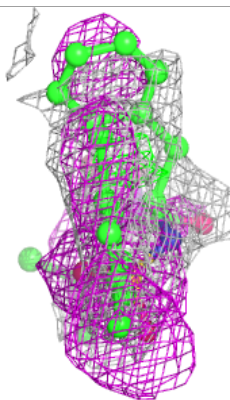
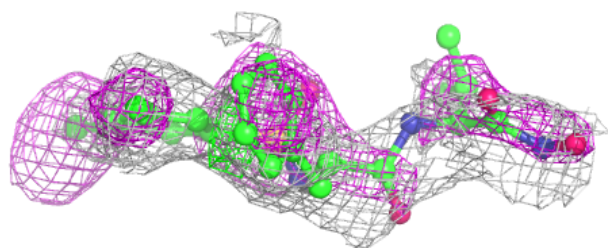
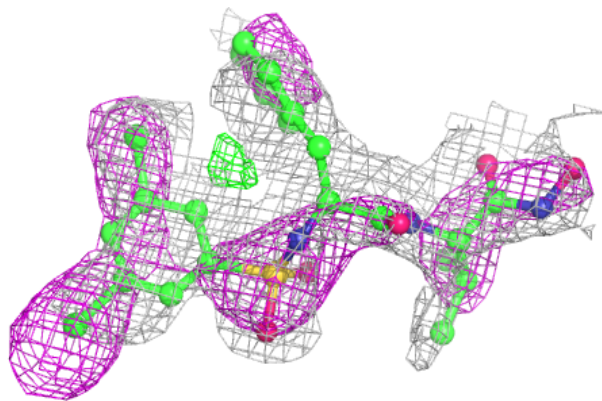
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

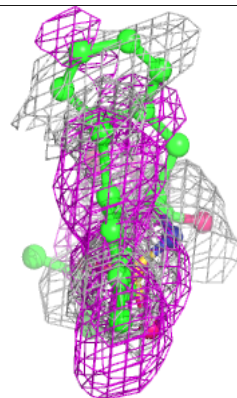
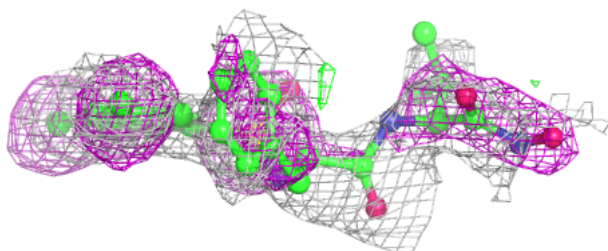
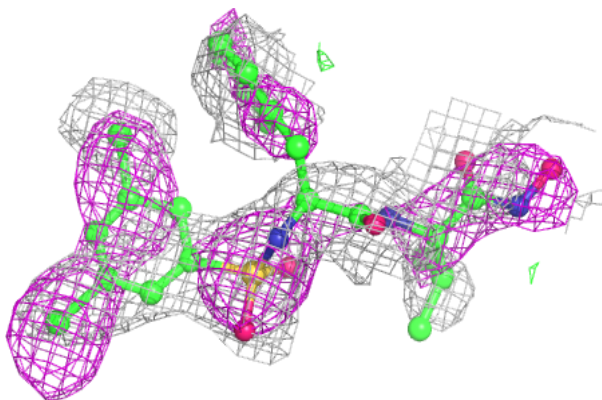


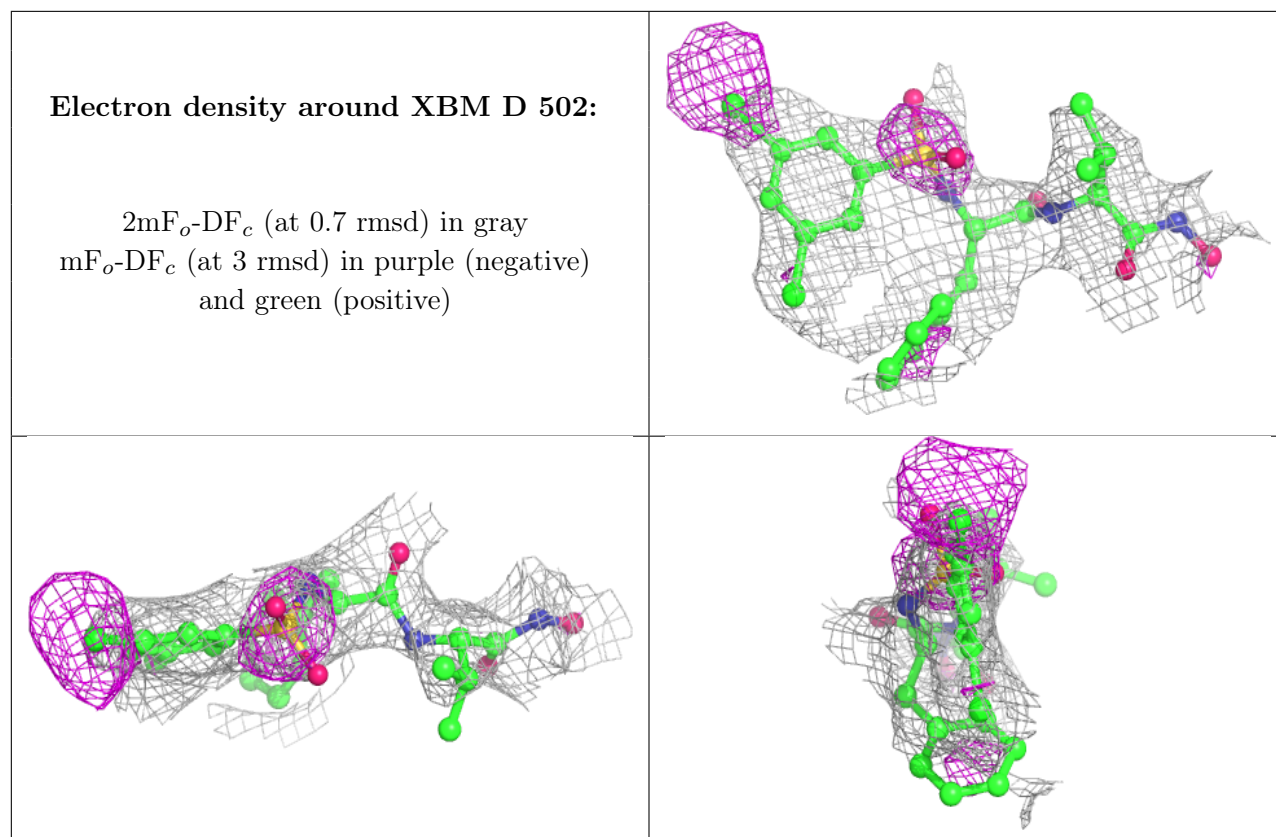
**Electron density around XBM B 502:**

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

**Electron density around XBM C 502:**

$2mF_o-DF_c$  (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 depositor's R factor - this section is therefore empty.