



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:35 AM BST

PDB ID : 2JEC  
Title : crystal structure of recombinant DiocleA grandiflora lectin mutant E123A-H131N-K132Q complexed with 5-bromo-4-chloro-3-indolyl- $\alpha$ -D-mannose  
Authors : Nagano, C.S.; Sanz, L.; Cavada, B.S.; Calvete, J.J.  
Deposited on : 2007-01-16  
Resolution : 2.00 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.

---

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 : 2.13.1  
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) : 2.13.1

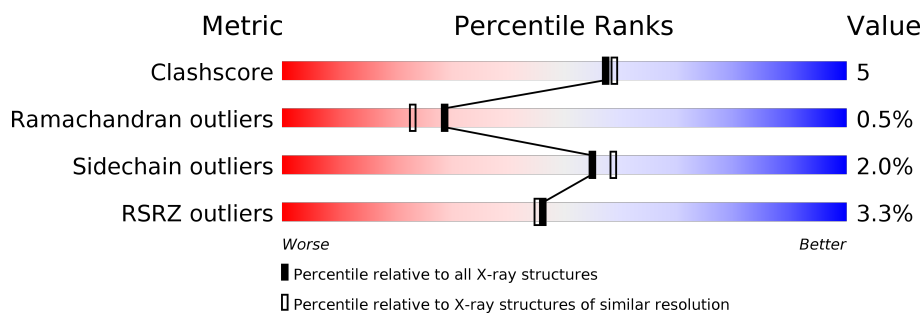
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	239	<div> <div> <div>0%</div> <div>92%</div> <div>8%</div> </div> </div>
1	B	239	<div> <div> <div>3%</div> <div>90%</div> <div>7%</div> </div> <div>•</div> </div>
1	C	239	<div> <div> <div>6%</div> <div>92%</div> <div>8%</div> </div> </div>
1	D	239	<div> <div> <div>3%</div> <div>90%</div> <div>9%</div> </div> <div>•</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8161 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 LECTIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	8	0
			1850	1172	308	369	1			
1	B	238	Total	C	N	O	S	0	2	0
			1818	1148	304	365	1			
1	C	238	Total	C	N	O	S	0	2	0
			1814	1145	301	366	2			
1	D	238	Total	C	N	O	S	0	4	0
			1835	1157	308	368	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP P08902
A	2	MET	-	expression tag	UNP P08902
A	125	ALA	GLU	engineered mutation	UNP P08902
A	133	ASN	HIS	engineered mutation	UNP P08902
A	134	GLN	LYS	engineered mutation	UNP P08902
A	157	GLN	GLU	conflict	UNP P08902
A	186	LYS	SER	conflict	UNP P08902
B	1	ALA	-	expression tag	UNP P08902
B	2	MET	-	expression tag	UNP P08902
B	125	ALA	GLU	engineered mutation	UNP P08902
B	133	ASN	HIS	engineered mutation	UNP P08902
B	134	GLN	LYS	engineered mutation	UNP P08902
B	157	GLN	GLU	conflict	UNP P08902
B	186	LYS	SER	conflict	UNP P08902
C	1	ALA	-	expression tag	UNP P08902
C	2	MET	-	expression tag	UNP P08902
C	125	ALA	GLU	engineered mutation	UNP P08902
C	133	ASN	HIS	engineered mutation	UNP P08902
C	134	GLN	LYS	engineered mutation	UNP P08902
C	157	GLN	GLU	conflict	UNP P08902
C	186	LYS	SER	conflict	UNP P08902

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ALA	-	expression tag	UNP P08902
D	2	MET	-	expression tag	UNP P08902
D	125	ALA	GLU	engineered mutation	UNP P08902
D	133	ASN	HIS	engineered mutation	UNP P08902
D	134	GLN	LYS	engineered mutation	UNP P08902
D	157	GLN	GLU	conflict	UNP P08902
D	186	LYS	SER	conflict	UNP P08902

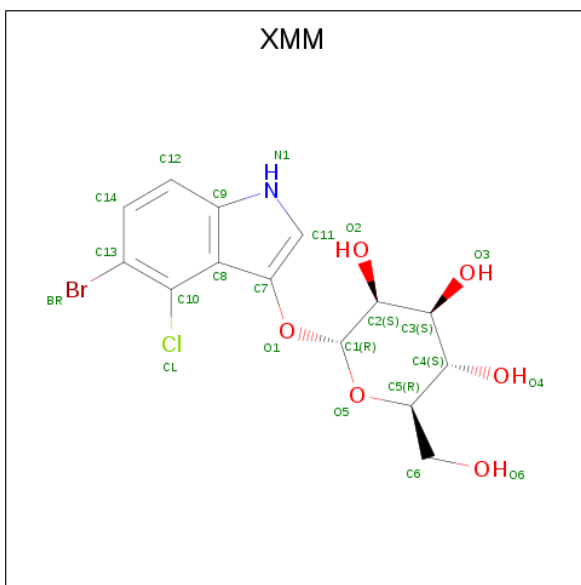
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mn 2 2	0	0
3	A	2	Total Mn 2 2	0	0
3	D	2	Total Mn 2 2	0	0
3	C	2	Total Mn 2 2	0	0

- Molecule 4 is 5-bromo-4-chloro-1H-indol-3-yl alpha-D-mannopyranoside (three-letter code: XMM) (formula: C<sub>14</sub>H<sub>15</sub>BrClNO<sub>6</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	Br	C	Cl	N	O	0	0
			23	1	14	1	1	6		
4	B	1	Total	Br	C	Cl	N	O	0	0
			23	1	14	1	1	6		
4	C	1	Total	Br	C	Cl	N	O	0	0
			23	1	14	1	1	6		
4	D	1	Total	Br	C	Cl	N	O	0	0
			23	1	14	1	1	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		
5	B	176	Total	O	0	0
			176	176		
5	C	162	Total	O	0	0
			162	162		
5	D	179	Total	O	0	0
			179	179		

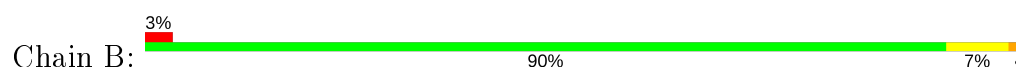
### 3 Residue-property plots [i](#)

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.

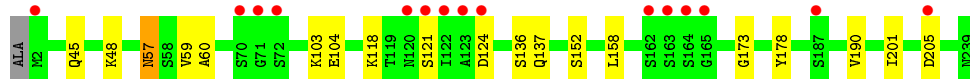
- Molecule 1: LECTIN ALPHA CHAIN



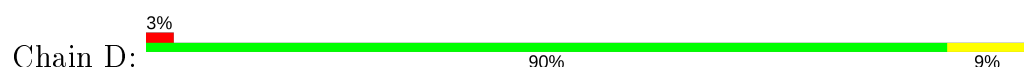
- Molecule 1: LECTIN ALPHA CHAIN



- Molecule 1: LECTIN ALPHA CHAIN



- Molecule 1: LECTIN ALPHA CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.19Å 84.55Å 176.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.04 – 2.00 28.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (88.04-2.00) 99.5 (28.10-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.11 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.179 , 0.230 0.181 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8161	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: XMM, CA, MN

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	0.73	0/1916	0.74	0/2612
1	B	0.67	0/1866	0.72	0/2545
1	C	0.69	0/1862	0.71	0/2540
1	D	0.66	0/1886	0.69	0/2571
All	All	0.69	0/7530	0.72	0/10268

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ILE	Peptide
1	A	133	ASN	Peptide

### 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	1850	0	1811	23	0
1	B	1818	0	1759	24	0
1	C	1814	0	1745	15	0
1	D	1835	0	1775	22	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	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	23	0	15	0	0
4	B	23	0	15	0	0
4	C	23	0	15	0	0
4	D	23	0	15	0	0
5	A	223	0	0	5	0
5	B	176	0	0	2	0
5	C	162	0	0	0	0
5	D	179	0	0	2	0
All	All	8161	0	7150	72	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 5.

All (72) 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:A:11[B]:LEU:HD23	1:A:27[B]:ILE:HG22	1.52	0.89
1:B:120:ASN:HD22	1:B:121:SER:H	1.17	0.84
1:A:11[B]:LEU:HD21	1:A:67:VAL:HG21	1.59	0.82
1:A:52:VAL:HG22	1:A:67:VAL:HG22	1.61	0.82
1:D:27:ILE:HD12	1:D:67:VAL:HG23	1.61	0.82
1:D:27:ILE:HD12	1:D:67:VAL:CG2	2.11	0.80
1:B:120:ASN:ND2	1:B:121:SER:H	1.80	0.79
1:A:45:GLN:NE2	1:A:72:SER:OG	2.19	0.75
1:A:134:GLN:HG2	5:A:2116:HOH:O	1.86	0.74
1:A:178:TYR:CE1	1:B:178:TYR:CE1	2.80	0.69
1:B:120:ASN:HD22	1:B:121:SER:N	1.90	0.69
1:D:52:VAL:HG22	1:D:67:VAL:HG22	1.72	0.69
1:A:126[B]:ASN:ND2	5:A:2122:HOH:O	2.28	0.65
1:A:72:SER:HB2	5:A:2083:HOH:O	1.95	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ASN:HD22	1:C:59:VAL:H	1.44	0.64
1:D:27:ILE:CD1	1:D:67:VAL:HG23	2.28	0.63
1:D:185:GLU:OE1	1:D:187:SER:OG	2.16	0.62
1:C:178:TYR:CE1	1:D:178:TYR:CE1	2.87	0.62
1:A:166:ASP:OD2	5:A:2152:HOH:O	2.16	0.61
1:D:158:LEU:O	1:D:173:GLY:HA3	2.01	0.61
1:B:120:ASN:ND2	1:B:121:SER:N	2.49	0.61
1:A:11[B]:LEU:HD23	1:A:27[B]:ILE:CG2	2.27	0.61
1:C:45:GLN:HB3	1:C:48:LYS:HD2	1.86	0.58
1:D:41:ARG:HD3	5:D:2044:HOH:O	2.03	0.58
1:C:137:GLN:H	1:C:137:GLN:CD	2.07	0.58
1:B:119:THR:OG1	1:B:120:ASN:N	2.36	0.57
1:A:27[A]:ILE:HD12	1:A:67:VAL:CG2	2.36	0.56
1:D:53[B]:HIS:CD2	1:D:196[B]:THR:HG22	2.41	0.55
1:D:57:ASN:HD22	1:D:59:VAL:H	1.54	0.54
1:A:118:LYS:HZ3	1:A:122:ILE:HA	1.74	0.53
1:A:178:TYR:CE1	1:B:178:TYR:HE1	2.24	0.53
1:C:103:LYS:HG2	1:C:205:ASP:OD2	2.09	0.52
1:A:27[A]:ILE:HD12	1:A:67:VAL:HG23	1.91	0.52
1:C:158:LEU:O	1:C:173:GLY:HA3	2.10	0.52
1:C:57:ASN:ND2	1:C:60:ALA:H	2.08	0.51
1:B:76:THR:HG23	1:C:59:VAL:HG13	1.92	0.50
1:A:178:TYR:HE1	1:B:178:TYR:CE1	2.30	0.50
1:A:126[B]:ASN:ND2	5:A:2123:HOH:O	2.44	0.49
1:B:158:LEU:O	1:B:173:GLY:HA3	2.11	0.49
1:D:53[B]:HIS:HD2	1:D:196[B]:THR:HG22	1.76	0.49
1:A:57:ASN:HD22	1:A:59:VAL:H	1.59	0.49
1:B:53[A]:HIS:HE1	5:B:2045:HOH:O	1.95	0.49
1:D:160:LYS:HB3	1:D:168:GLN:HG3	1.93	0.49
1:A:178:TYR:CD1	1:B:178:TYR:CE1	3.01	0.48
1:B:41:ARG:O	1:B:75:THR:HG21	2.14	0.48
1:C:178:TYR:CE1	1:D:178:TYR:HE1	2.29	0.47
1:D:53[B]:HIS:HD2	1:D:196[B]:THR:CG2	2.26	0.47
1:B:31:ILE:HG23	1:B:86:VAL:HG11	1.97	0.47
1:B:120:ASN:H	1:B:120:ASN:HD22	1.63	0.47
1:B:53[B]:HIS:CE1	1:C:118:LYS:HG2	2.49	0.47
1:A:11[B]:LEU:CD2	1:A:67:VAL:HG21	2.39	0.46
1:A:45:GLN:HE22	1:A:72:SER:HG	1.59	0.46
1:D:27:ILE:HD12	1:D:67:VAL:HG21	1.93	0.46
1:D:32:LYS:HD2	1:D:86:VAL:HG13	1.96	0.46
1:A:131:SER:O	1:B:126:ASN:HA	2.16	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:SER:HB2	1:C:137:GLN:NE2	2.30	0.45
1:B:120:ASN:C	1:B:121:SER:O	2.54	0.44
1:A:11[B]:LEU:HD21	1:A:67:VAL:CG2	2.41	0.44
1:C:57:ASN:HD21	1:C:60:ALA:H	1.64	0.44
1:D:41:ARG:O	1:D:75:THR:HG21	2.18	0.44
1:B:53[A]:HIS:CE1	5:B:2045:HOH:O	2.70	0.43
1:C:178:TYR:HE1	1:D:178:TYR:CE1	2.32	0.43
1:C:104:GLU:HB2	1:C:201:ILE:HG23	2.01	0.43
1:B:118:LYS:HE3	1:B:124:ASP:OD1	2.18	0.43
1:D:47:GLY:HA2	1:D:202:LYS:HG2	2.02	0.42
1:B:123:ALA:O	1:B:124:ASP:C	2.58	0.42
1:D:194[B]:ASP:OD2	5:D:2141:HOH:O	2.21	0.42
1:D:136:SER:O	1:D:150:THR:HG21	2.20	0.41
1:D:53[B]:HIS:CD2	1:D:196[B]:THR:CG2	3.02	0.41
1:B:117:LEU:HD21	1:B:185:GLU:HG2	2.03	0.41
1:B:64:SER:HB3	1:C:59:VAL:HG12	2.03	0.41
1:A:178:TYR:CD1	1:B:178:TYR:CD1	3.09	0.40

There are no symmetry-related clashes.

## 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	244/239 (102%)	238 (98%)	5 (2%)	1 (0%)	34	30
1	B	238/239 (100%)	227 (95%)	8 (3%)	3 (1%)	12	6
1	C	238/239 (100%)	229 (96%)	8 (3%)	1 (0%)	34	30
1	D	240/239 (100%)	228 (95%)	12 (5%)	0	100	100
All	All	960/956 (100%)	922 (96%)	33 (3%)	5 (0%)	29	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	ILE
1	B	124	ASP
1	A	122	ILE
1	B	121	SER
1	C	121	SER

### 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	210/204 (103%)	206 (98%)	4 (2%)	57	61
1	B	204/204 (100%)	199 (98%)	5 (2%)	47	49
1	C	203/204 (100%)	199 (98%)	4 (2%)	55	58
1	D	206/204 (101%)	203 (98%)	3 (2%)	65	69
All	All	823/816 (101%)	807 (98%)	16 (2%)	55	61

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	122	ILE
1	A	128	LEU
1	A	185	GLU
1	B	18	ASP
1	B	23	ASN
1	B	120	ASN
1	B	122	ILE
1	B	126	ASN
1	C	57	ASN
1	C	124	ASP
1	C	152	SER
1	C	190	VAL
1	D	120	ASN
1	D	136	SER
1	D	168	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	45	GLN
1	A	57	ASN
1	A	239	ASN
1	B	23	ASN
1	B	120	ASN
1	B	133	ASN
1	B	137	GLN
1	B	239	ASN
1	C	23	ASN
1	C	45	GLN
1	C	57	ASN
1	C	84	ASN
1	C	137	GLN
1	C	168	GLN
1	C	239	ASN
1	D	23	ASN
1	D	57	ASN
1	D	157	GLN
1	D	239	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 16 ligands modelled in this entry, 12 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
4	XMM	A	242	-	24,25,25	1.15	1 (4%)	26,37,37	0.96	0
4	XMM	B	242	-	24,25,25	1.08	1 (4%)	26,37,37	1.16	2 (7%)
4	XMM	C	242	-	24,25,25	1.11	1 (4%)	26,37,37	1.08	1 (3%)
4	XMM	D	242	-	24,25,25	1.04	1 (4%)	26,37,37	0.92	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
4	XMM	A	242	-	-	0/4/26/26	0/3/3/3
4	XMM	B	242	-	-	0/4/26/26	0/3/3/3
4	XMM	C	242	-	-	0/4/26/26	0/3/3/3
4	XMM	D	242	-	-	0/4/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	242	XMM	O1-C1	2.72	1.45	1.41
4	B	242	XMM	O1-C1	2.56	1.45	1.41
4	D	242	XMM	O1-C1	2.45	1.44	1.41
4	C	242	XMM	C12-C14	2.10	1.41	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	242	XMM	BR-C13-C10	-4.21	116.41	121.34
4	B	242	XMM	C1-O5-C5	2.47	118.54	113.69
4	D	242	XMM	O5-C1-O1	2.44	114.48	108.29
4	C	242	XMM	O5-C1-O1	2.30	114.14	108.29

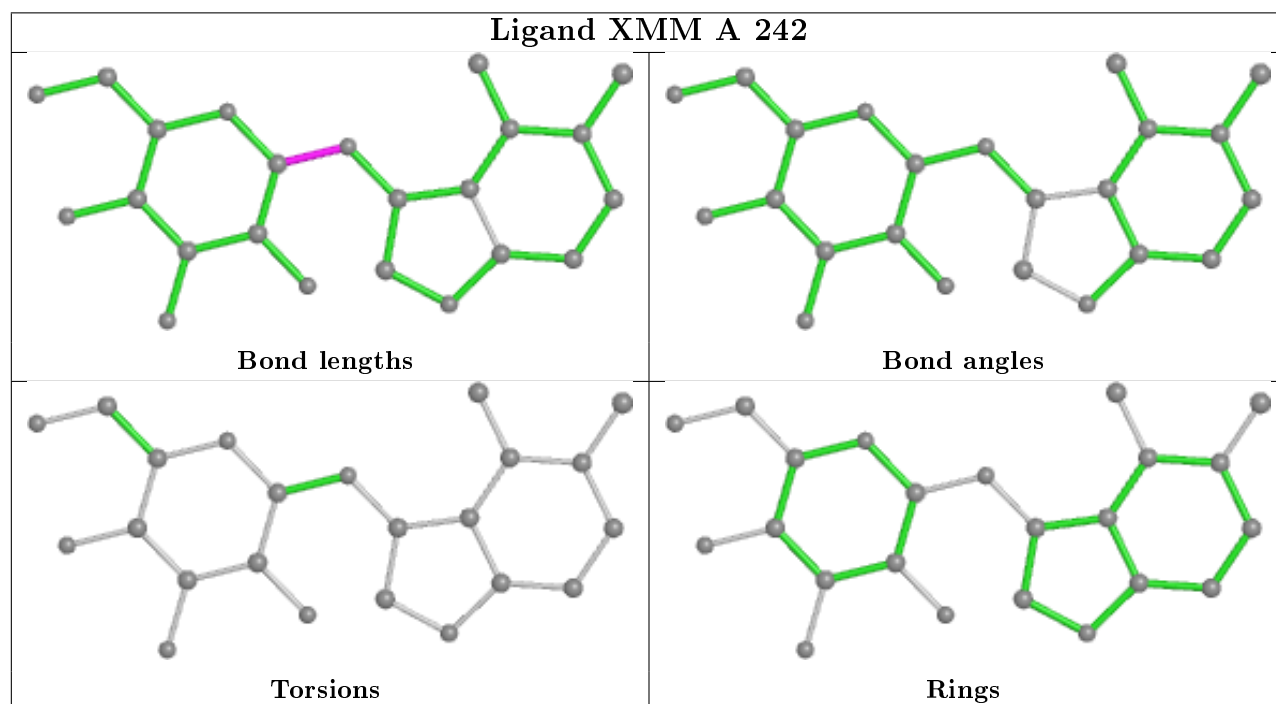
There are no chirality outliers.

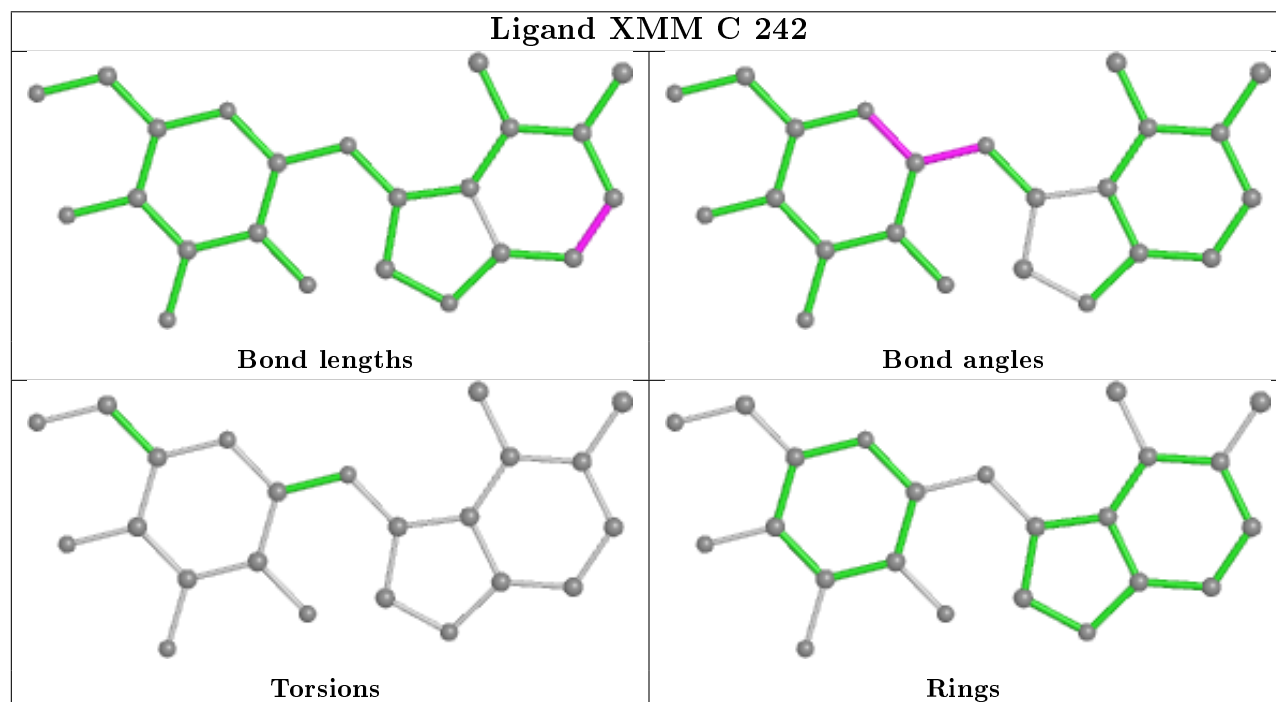
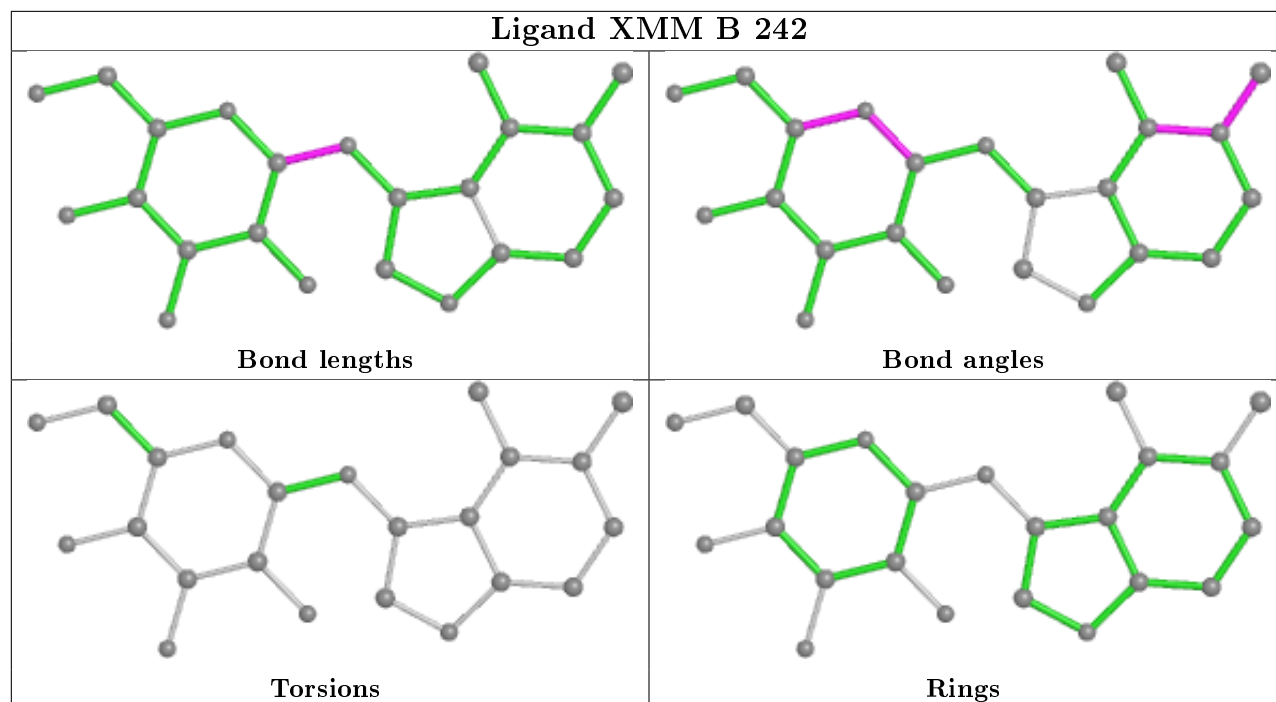
There are no torsion outliers.

There are no ring outliers.

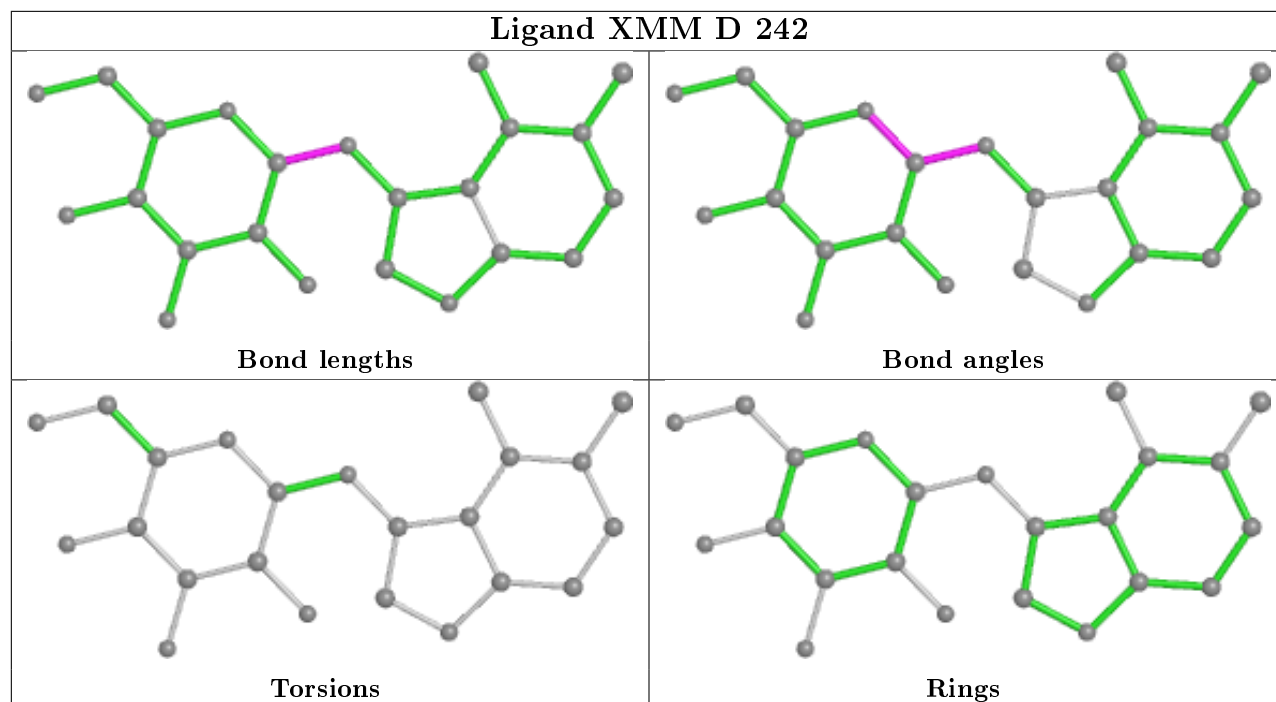
No monomer is involved in short contacts.

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	238/239 (99%)	-0.35	2 (0%) 86 85	6, 13, 29, 43	0
1	B	238/239 (99%)	-0.16	7 (2%) 51 50	9, 17, 30, 49	0
1	C	238/239 (99%)	0.05	15 (6%) 20 19	10, 19, 39, 45	0
1	D	238/239 (99%)	-0.06	7 (2%) 51 50	11, 18, 35, 40	0
All	All	952/956 (99%)	-0.13	31 (3%) 46 45	6, 17, 34, 49	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	ILE	6.8
1	C	122	ILE	6.4
1	B	122	ILE	5.6
1	B	120	ASN	5.4
1	A	122	ILE	5.1
1	B	121	SER	4.8
1	C	163	SER	4.5
1	D	2	MET	4.4
1	D	187	SER	4.0
1	B	123	ALA	3.8
1	C	70	SER	3.6
1	D	163	SER	3.4
1	C	2	MET	3.4
1	C	164	SER	3.2
1	C	120	ASN	3.1
1	C	123	ALA	3.1
1	C	72	SER	3.1
1	C	187	SER	3.1
1	D	206	ARG	3.0
1	C	71	GLY	3.0
1	A	71	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	124	ASP	2.6
1	C	165	GLY	2.6
1	D	120	ASN	2.5
1	C	121	SER	2.5
1	B	72	SER	2.4
1	B	124	ASP	2.3
1	D	212	ILE	2.3
1	C	205	ASP	2.3
1	B	212	ILE	2.3
1	C	162	SER	2.1

## 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
3	MN	B	243	1/1	0.68	0.26	43,43,43,43	1
4	XMM	C	242	23/23	0.88	0.15	17,23,43,47	0
3	MN	D	243	1/1	0.90	0.11	44,44,44,44	1
4	XMM	B	242	23/23	0.94	0.11	14,21,35,41	0
3	MN	C	243	1/1	0.95	0.23	43,43,43,43	1
3	MN	A	243	1/1	0.96	0.09	29,29,29,29	1
4	XMM	A	242	23/23	0.97	0.08	9,14,26,33	0
4	XMM	D	242	23/23	0.97	0.09	15,18,26,30	0
3	MN	D	241	1/1	0.99	0.08	12,12,12,12	0
2	CA	C	240	1/1	0.99	0.04	15,15,15,15	0
2	CA	A	240	1/1	0.99	0.04	8,8,8,8	0
2	CA	B	240	1/1	0.99	0.07	17,17,17,17	0
3	MN	B	241	1/1	1.00	0.07	16,16,16,16	0

*Continued on next page...*

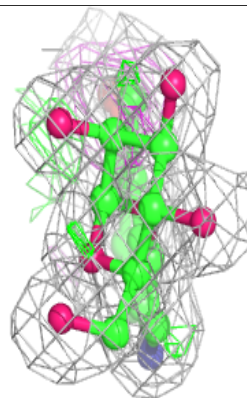
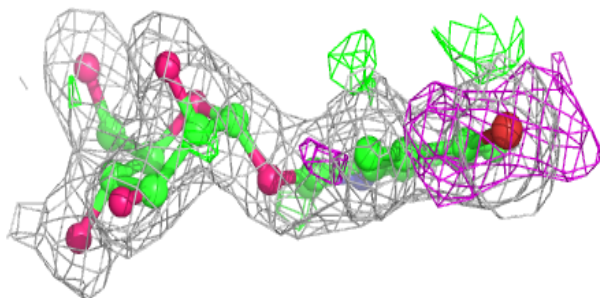
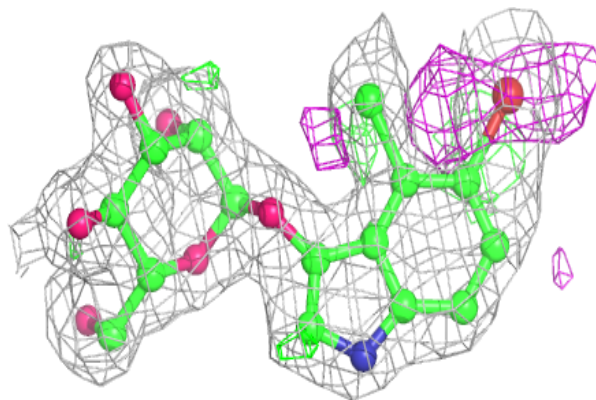
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	D	240	1/1	1.00	0.07	13,13,13,13	0
3	MN	A	241	1/1	1.00	0.08	9,9,9,9	0
3	MN	C	241	1/1	1.00	0.07	14,14,14,14	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.

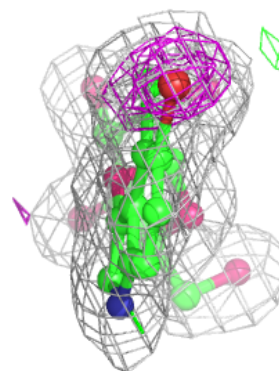
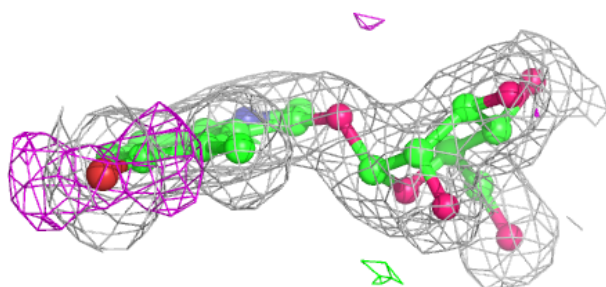
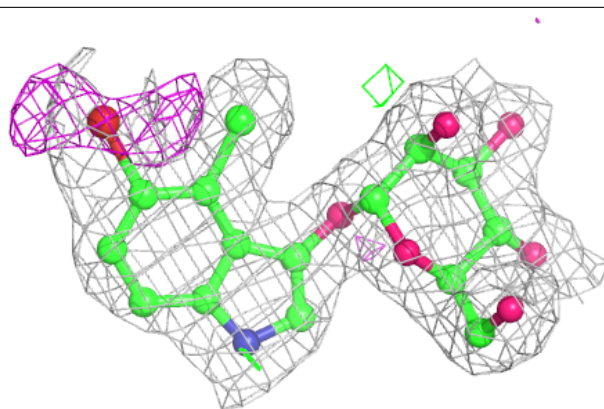
**Electron density around XMM C 242:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

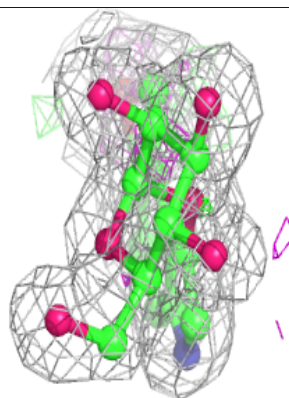
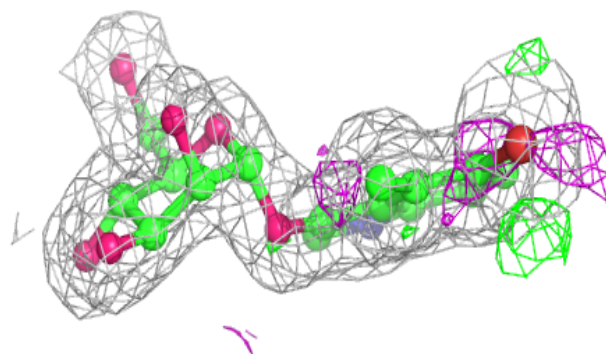
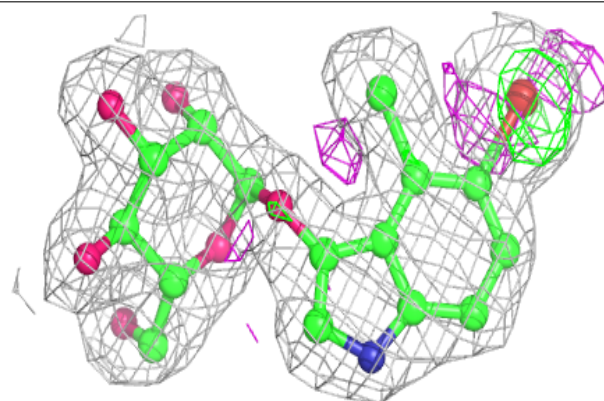


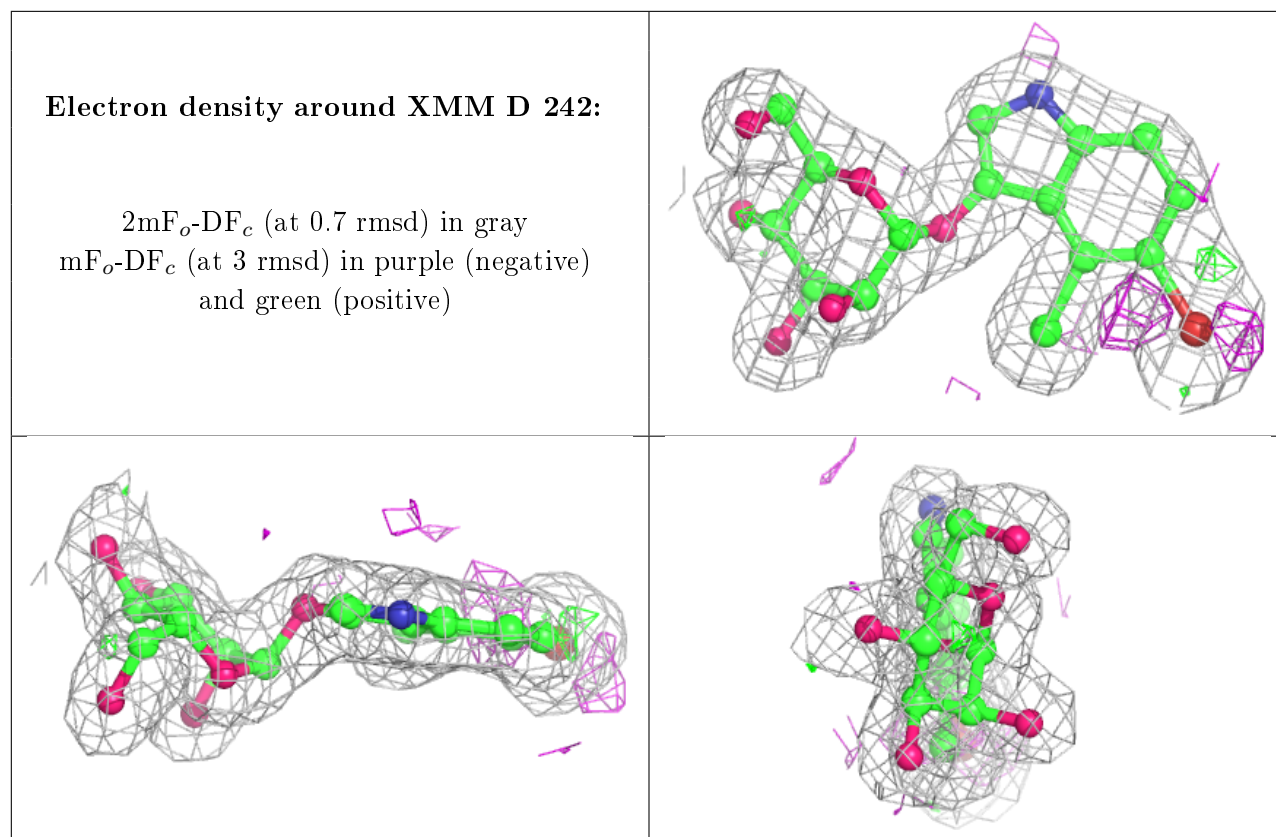
**Electron density around XMM B 242:**

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

**Electron density around XMM A 242:**

$2mF_o-DF_c$  (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.