



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 08:11 AM BST

PDB ID : 1LOD  
Title : INTERACTION OF A LEGUME LECTIN WITH TWO COMPONENTS OF  
THE BACTERIAL CELL WALL  
Authors : Bourne, Y.; Cambillau, C.  
Deposited on : 1993-01-27  
Resolution : 2.05 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 : 2.13.1  
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

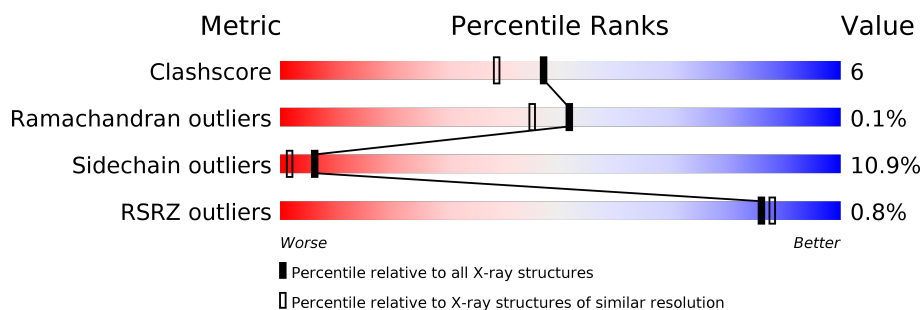
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	181	<div> <div>76%</div> <div>14%</div> <div>8%</div> <div>..</div> </div>
1	C	181	<div> <div>75%</div> <div>18%</div> <div>6%</div> <div>..</div> </div>
1	E	181	<div> <div>2%</div> <div>69%</div> <div>23%</div> <div>7%</div> <div>..</div> </div>
1	G	181	<div> <div>77%</div> <div>18%</div> <div>..</div> </div>
2	B	52	<div> <div>73%</div> <div>13%</div> <div>10%</div> </div>
2	D	52	<div> <div>81%</div> <div>10%</div> <div>10%</div> </div>
2	F	52	<div> <div>58%</div> <div>27%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	52	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MUR	E	690	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7490 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 LEGUME ISOLECTIN I (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	C	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	E	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	G	180	Total	C	N	O	0	0	0
			1397	890	230	277			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	LYS	conflict	UNP P04122
C	153	ALA	LYS	conflict	UNP P04122
E	153	ALA	LYS	conflict	UNP P04122
G	153	ALA	LYS	conflict	UNP P04122

- Molecule 2 is a protein called LEGUME ISOLECTIN I (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	0	0
			381	251	58	72			
2	D	47	Total	C	N	O	0	0	0
			376	248	58	70			
2	F	47	Total	C	N	O	0	0	0
			381	251	58	72			
2	H	47	Total	C	N	O	0	0	0
			376	248	58	70			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	TYR	PHE	conflict	UNP P12306
D	41	TYR	PHE	conflict	UNP P12306
F	41	TYR	PHE	conflict	UNP P12306
H	41	TYR	PHE	conflict	UNP P12306

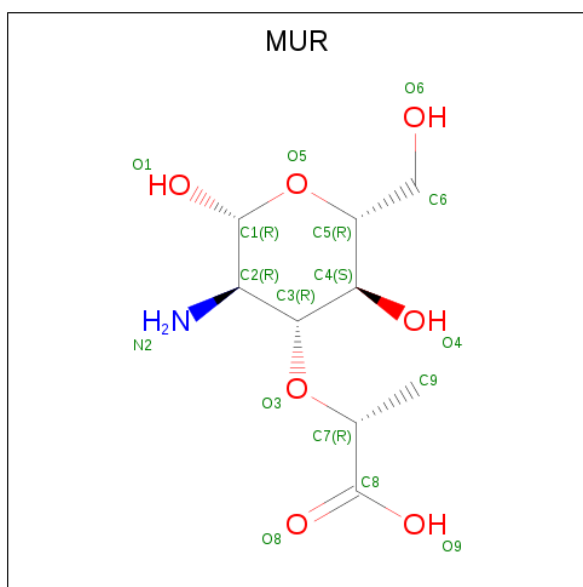
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mn 1 1	0	0
4	A	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0
4	E	1	Total Mn 1 1	0	0

- Molecule 5 is beta-muramic acid (three-letter code: MUR) (formula: C<sub>9</sub>H<sub>17</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	1	7		
5	C	1	Total	C	N	O	0	0
			17	9	1	7		
5	E	1	Total	C	N	O	0	0
			17	9	1	7		
5	G	1	Total	C	N	O	0	0
			17	9	1	7		

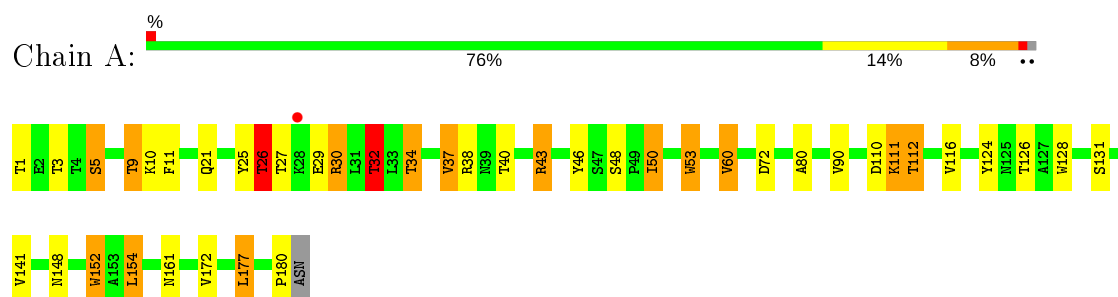
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O	0	0
			79	79		
6	B	14	Total	O	0	0
			14	14		
6	C	59	Total	O	0	0
			59	59		
6	D	11	Total	O	0	0
			11	11		
6	E	57	Total	O	0	0
			57	57		
6	F	12	Total	O	0	0
			12	12		
6	G	71	Total	O	0	0
			71	71		
6	H	9	Total	O	0	0
			9	9		

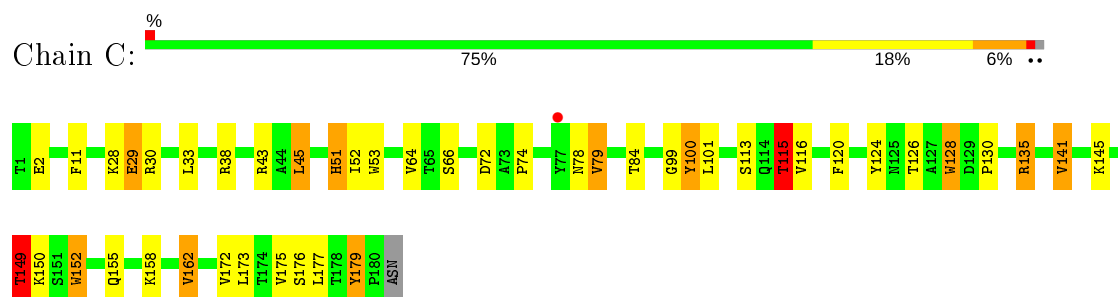
### 3 Residue-property plots [i](#)

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.

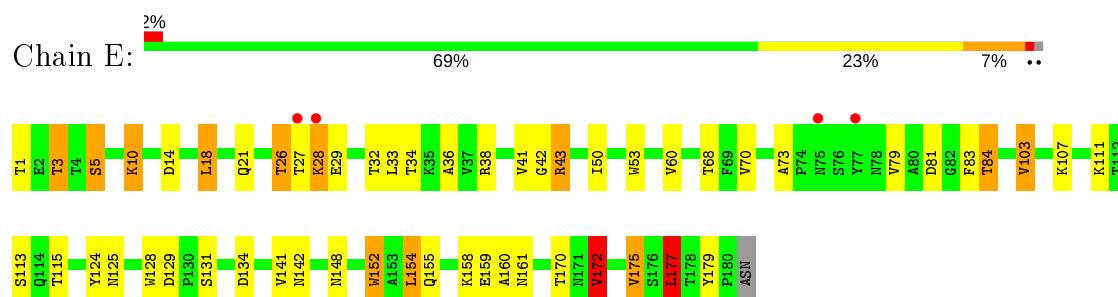
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



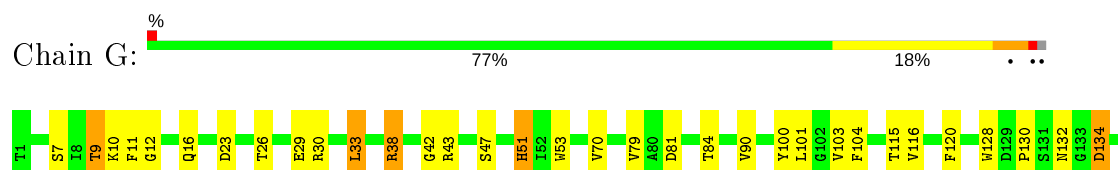
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

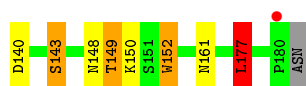


- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

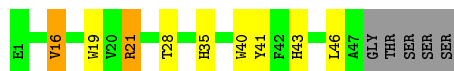


- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

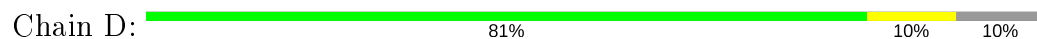




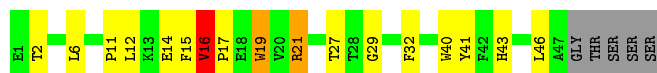
- Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



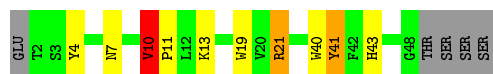
- Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



- Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



- Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.40Å 139.80Å 62.70Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.05 6.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.05) 95.4 (6.00-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.16 (at 2.05Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.197 , (Not available) 0.182 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.48 , 116.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: CA, MN, MUR

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	0.91	1/1431 (0.1%)	1.70	28/1954 (1.4%)
1	C	0.86	2/1431 (0.1%)	1.60	21/1954 (1.1%)
1	E	0.89	0/1431	1.64	24/1954 (1.2%)
1	G	0.90	0/1431	1.59	19/1954 (1.0%)
2	B	1.02	0/394	1.86	10/539 (1.9%)
2	D	1.00	0/389	1.63	6/532 (1.1%)
2	F	0.96	0/394	1.99	12/539 (2.2%)
2	H	1.08	1/389 (0.3%)	1.70	8/532 (1.5%)
All	All	0.92	4/7290 (0.1%)	1.67	128/9958 (1.3%)

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	G	0	1
2	H	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	10	VAL	CA-CB	6.39	1.68	1.54
1	C	141	VAL	CA-CB	6.22	1.67	1.54
1	A	141	VAL	CA-CB	6.11	1.67	1.54
1	C	115	THR	CA-CB	5.13	1.66	1.53

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	21	ARG	NE-CZ-NH1	18.05	129.33	120.30
2	F	21	ARG	NE-CZ-NH2	-17.62	111.49	120.30
2	B	21	ARG	NE-CZ-NH2	-13.50	113.55	120.30
2	B	21	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	A	38	ARG	NE-CZ-NH1	12.52	126.56	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	38	ARG	Sidechain
2	H	41	TYR	Sidechain

## 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	1397	0	1346	20	0
1	C	1397	0	1346	20	0
1	E	1397	0	1346	19	0
1	G	1397	0	1346	15	0
2	B	381	0	357	8	0
2	D	376	0	351	2	0
2	F	381	0	357	12	0
2	H	376	0	351	6	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	17	0	16	2	0
5	C	17	0	16	6	0
5	E	17	0	16	1	0
5	G	17	0	16	1	0
6	A	79	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	0	0	0
6	C	59	0	0	1	0
6	D	11	0	0	1	0
6	E	57	0	0	0	0
6	F	12	0	0	1	0
6	G	71	0	0	2	0
6	H	9	0	0	1	0
All	All	7490	0	6864	87	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 6.

The worst 5 of 87 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:21:GLN:HE22	1:A:43:ARG:HH21	1.34	0.72
1:E:21:GLN:HE22	1:E:43:ARG:HH21	1.39	0.69
1:A:110:ASP:OD1	1:A:112:THR:HB	1.96	0.66
5:G:920:MUR:C8	5:G:920:MUR:N2	2.60	0.65
1:A:124:TYR:CE2	1:A:126:THR:HG22	2.32	0.64

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	178/181 (98%)	175 (98%)	3 (2%)	0	100	100
1	C	178/181 (98%)	169 (95%)	9 (5%)	0	100	100
1	E	178/181 (98%)	170 (96%)	7 (4%)	1 (1%)	25	15
1	G	178/181 (98%)	172 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	D	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	F	45/52 (86%)	44 (98%)	1 (2%)	0	100	100
2	H	45/52 (86%)	44 (98%)	1 (2%)	0	100	100
All	All	892/932 (96%)	860 (96%)	31 (4%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	28	LYS

### 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	154/155 (99%)	136 (88%)	18 (12%)	5	1
1	C	154/155 (99%)	134 (87%)	20 (13%)	4	1
1	E	154/155 (99%)	130 (84%)	24 (16%)	2	0
1	G	154/155 (99%)	138 (90%)	16 (10%)	7	2
2	B	40/44 (91%)	38 (95%)	2 (5%)	24	16
2	D	39/44 (89%)	39 (100%)	0	100	100
2	F	40/44 (91%)	37 (92%)	3 (8%)	13	6
2	H	39/44 (89%)	38 (97%)	1 (3%)	46	39
All	All	774/796 (97%)	690 (89%)	84 (11%)	6	2

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	162	VAL
1	E	50	ILE
1	G	116	VAL

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Mol	Chain	Res	Type
1	C	176	SER
1	E	10	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	171	ASN
1	E	148	ASN
1	G	171	ASN
1	E	21	GLN
1	E	78	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 12 ligands modelled in this entry, 8 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	$\# Z  > 2$
5	MUR	A	230	-	14,17,17	3.77	3 (21%)	19,24,24	3.38	11 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MUR	G	920	-	14,17,17	2.57	2 (14%)	19,24,24	1.97	5 (26%)
5	MUR	C	460	-	14,17,17	2.31	2 (14%)	19,24,24	2.18	6 (31%)
5	MUR	E	690	-	14,17,17	2.21	2 (14%)	19,24,24	2.16	5 (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
5	MUR	A	230	-	-	0/6/30/30	0/1/1/1
5	MUR	E	690	-	1/1/7/7	4/6/30/30	0/1/1/1
5	MUR	G	920	-	-	1/6/30/30	0/1/1/1
5	MUR	C	460	-	-	1/6/30/30	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	230	MUR	C1-C2	-11.03	1.40	1.52
5	A	230	MUR	C2-N2	-7.55	1.35	1.47
5	G	920	MUR	C1-C2	-7.18	1.44	1.52
5	C	460	MUR	C1-C2	-6.00	1.46	1.52
5	C	460	MUR	C2-N2	-5.54	1.38	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	230	MUR	C4-C3-C2	-7.22	97.11	111.37
5	E	690	MUR	C4-C3-C2	-6.11	99.31	111.37
5	C	460	MUR	C9-C7-C8	-5.93	105.68	113.35
5	A	230	MUR	O5-C1-C2	-5.57	103.00	109.51
5	A	230	MUR	C9-C7-C8	-5.51	106.22	113.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	690	MUR	C7

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	920	MUR	C8-C7-O3-C3
5	E	690	MUR	O5-C5-C6-O6
5	E	690	MUR	C4-C5-C6-O6
5	E	690	MUR	C8-C7-O3-C3
5	E	690	MUR	C9-C7-O3-C3

There are no ring outliers.

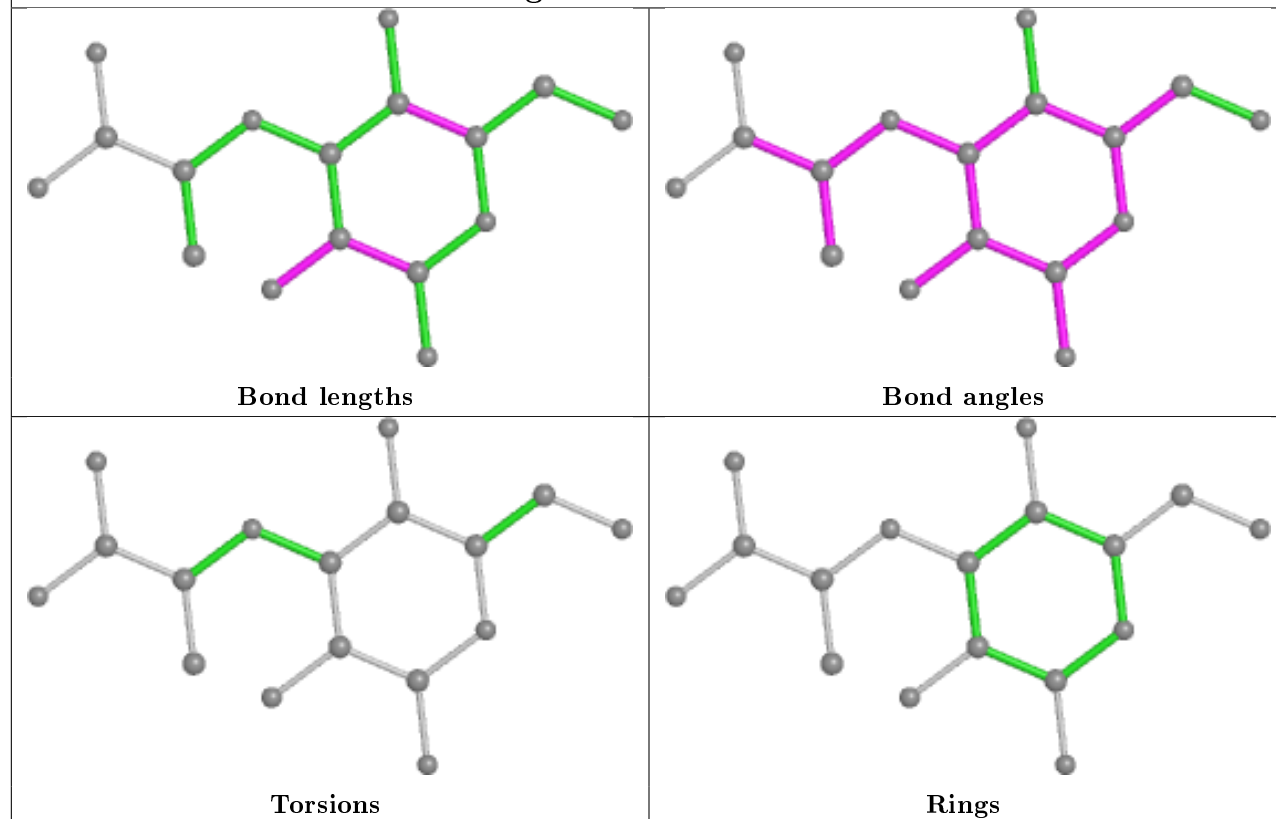
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	230	MUR	2	0
5	G	920	MUR	1	0
5	C	460	MUR	6	0
5	E	690	MUR	1	0

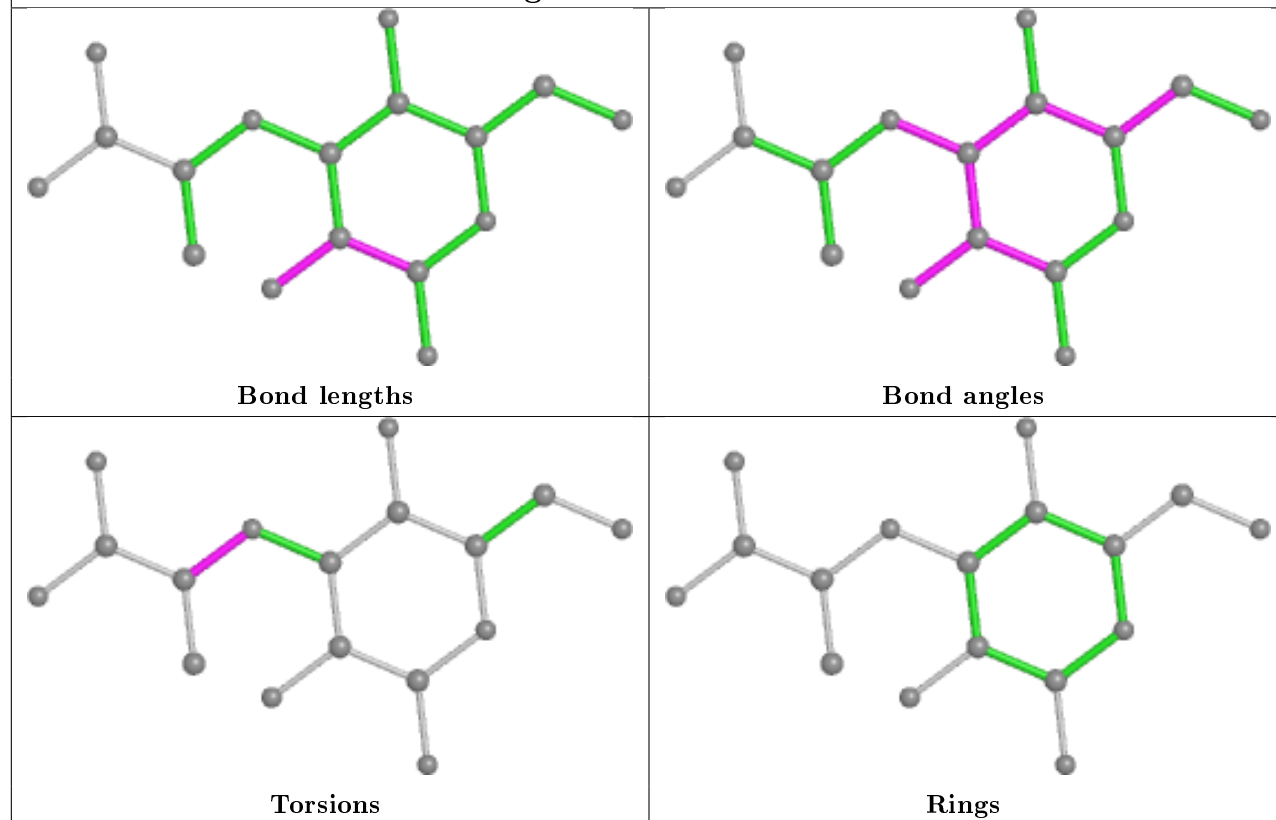
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



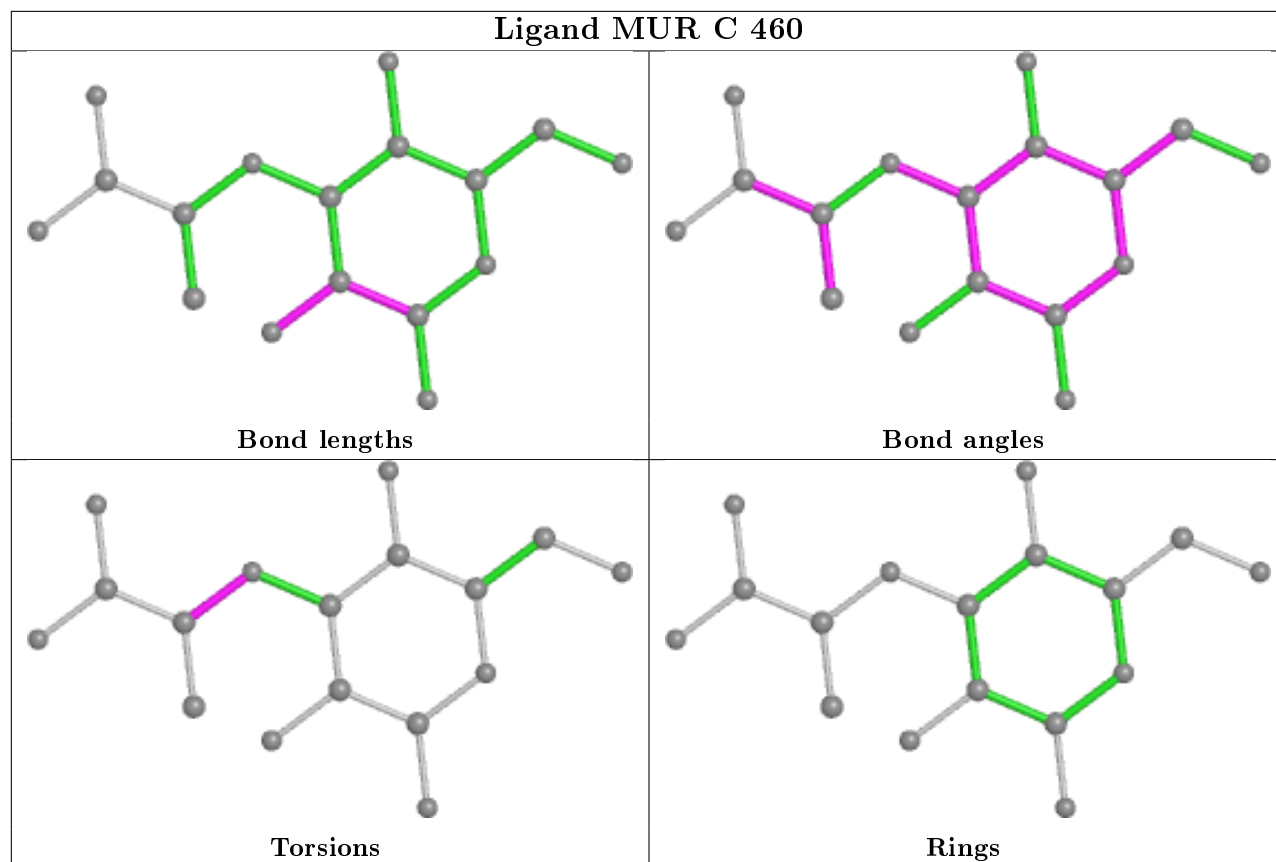
## Ligand MUR A 230



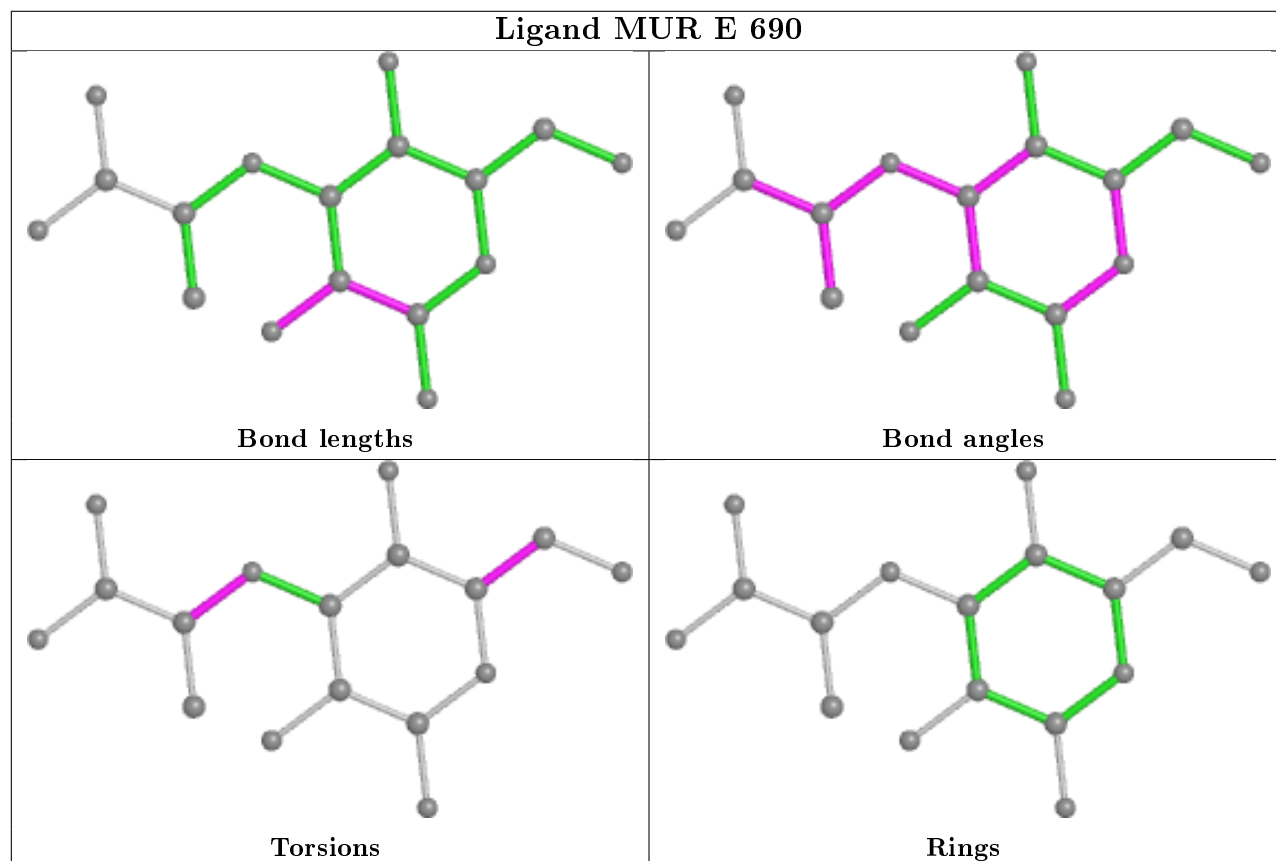
## Ligand MUR G 920



## Ligand MUR C 460



## Ligand MUR E 690



## 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	180/181 (99%)	-0.73	1 (0%) 89 91	10, 17, 31, 47	0
1	C	180/181 (99%)	-0.34	1 (0%) 89 91	14, 26, 43, 51	0
1	E	180/181 (99%)	-0.38	4 (2%) 62 66	12, 23, 42, 54	0
1	G	180/181 (99%)	-0.54	1 (0%) 89 91	12, 21, 35, 44	0
2	B	47/52 (90%)	-0.79	0 100 100	9, 17, 29, 37	0
2	D	47/52 (90%)	-0.54	0 100 100	12, 22, 37, 48	0
2	F	47/52 (90%)	-0.57	0 100 100	11, 23, 35, 41	0
2	H	47/52 (90%)	-0.64	0 100 100	12, 20, 33, 41	0
All	All	908/932 (97%)	-0.52	7 (0%) 86 88	9, 22, 39, 54	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	77	TYR	3.7
1	C	77	TYR	3.3
1	E	75	ASN	2.5
1	G	180	PRO	2.5
1	E	27	THR	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands

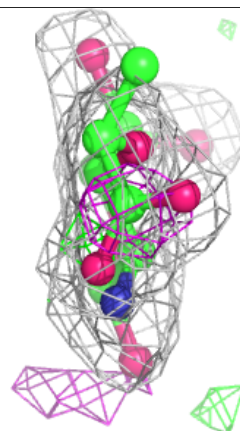
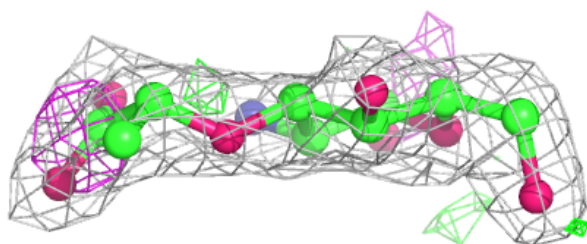
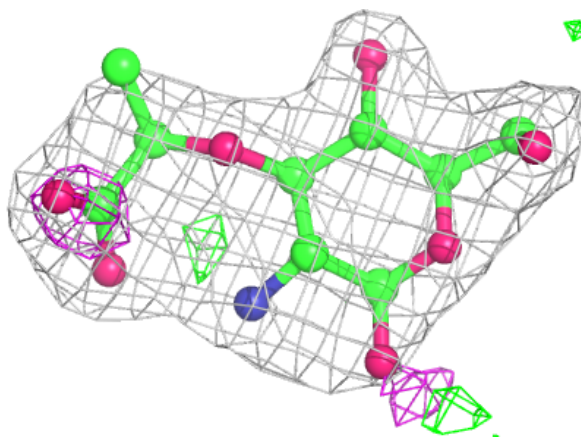
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	CA	C	458	1/1	0.43	0.17	44,44,44,44	0
4	MN	A	229	1/1	0.81	0.29	41,41,41,41	0
5	MUR	C	460	17/17	0.85	0.16	34,35,39,40	0
3	CA	E	688	1/1	0.86	0.12	29,29,29,29	0
5	MUR	G	920	17/17	0.88	0.14	21,24,31,35	0
5	MUR	E	690	17/17	0.88	0.17	29,34,38,39	0
3	CA	G	918	1/1	0.91	0.10	22,22,22,22	0
5	MUR	A	230	17/17	0.92	0.12	13,21,28,30	0
3	CA	A	228	1/1	0.95	0.18	28,28,28,28	0
4	MN	C	459	1/1	0.96	0.07	37,37,37,37	0
4	MN	E	689	1/1	0.98	0.07	16,16,16,16	0
4	MN	G	919	1/1	0.99	0.14	11,11,11,11	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.

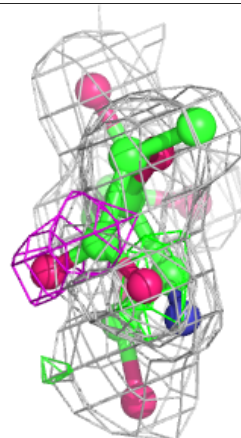
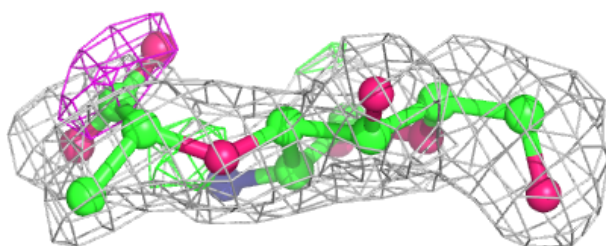
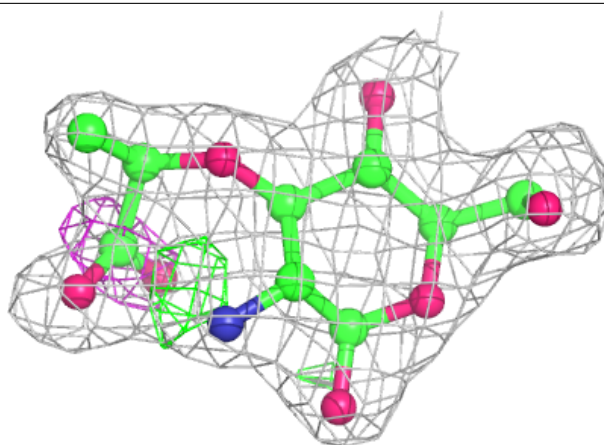
**Electron density around MUR C 460:**

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

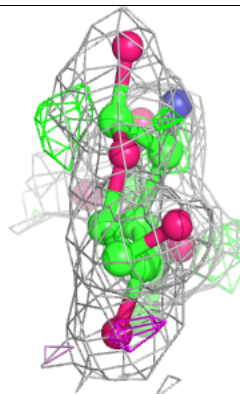
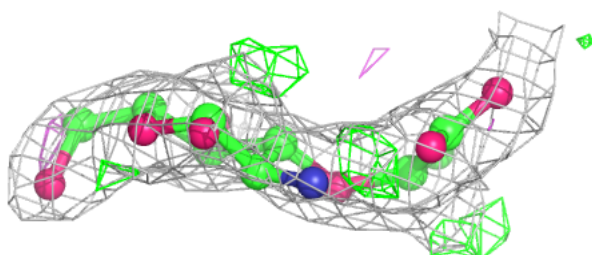
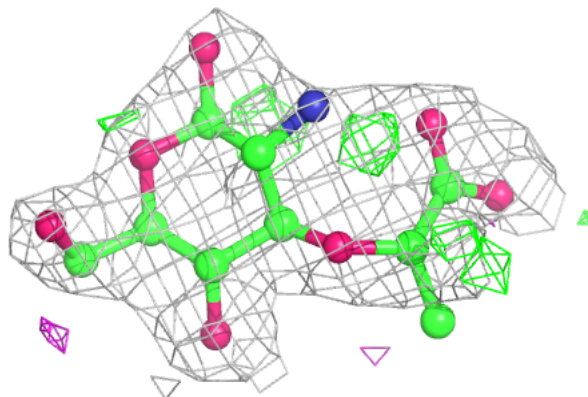


**Electron density around MUR G 920:**

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

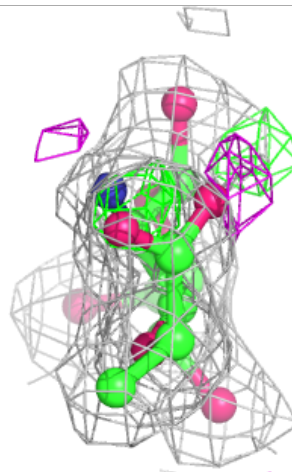
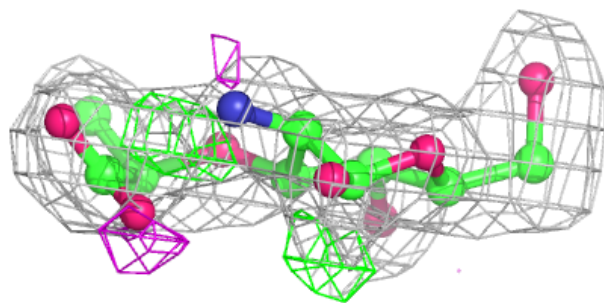
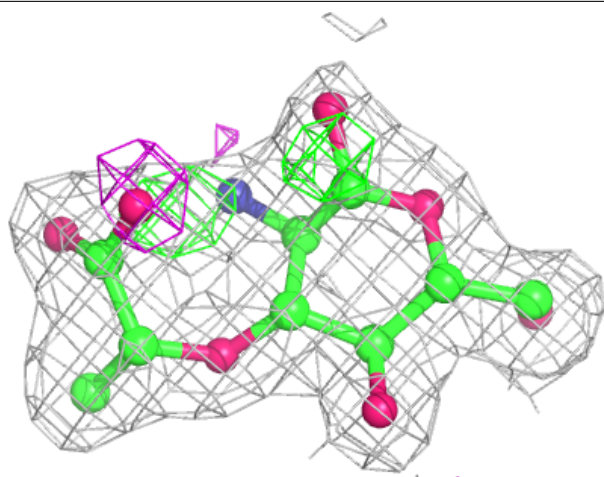
**Electron density around MUR E 690:**

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



**Electron density around MUR A 230:**

$2mF_o-DF_c$  (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.