wwPDB X-ray Structure Validation Summary Report (i)

Oct 27, 2026 – 03:14 pm GMT

PDB ID	:	33BU / pdb_000033bu
Title	:	Streptomyces sp. TLI_171 GH5_7 Mannanase, WT, product bound
Authors	:	Bloch, Y.
Deposited on	:	2026-08-06
Resolution	:	1.12 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

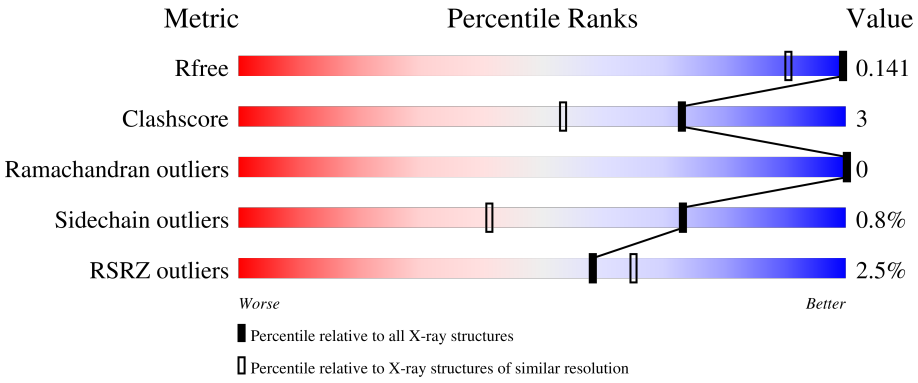
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

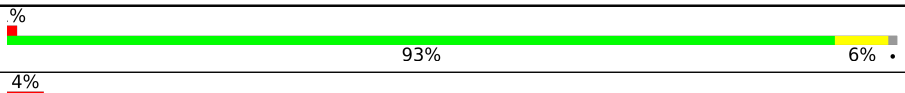
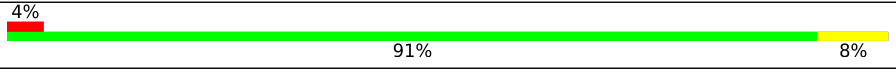
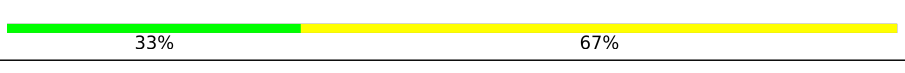
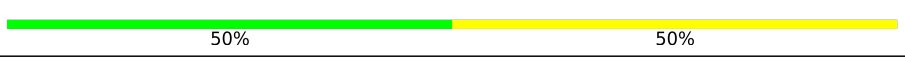
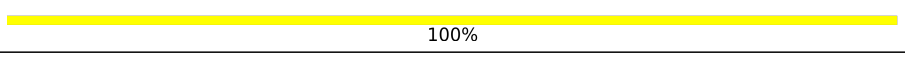
The reported resolution of this entry is 1.12 Å.

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}	180053	1985 (1.14-1.10)
Clashscore	190562	2021 (1.14-1.10)
Ramachandran outliers	187476	1978 (1.14-1.10)
Sidechain outliers	187428	1974 (1.14-1.10)
RSRZ outliers	180081	1984 (1.14-1.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	383	
1	B	383	
2	C	3	
3	D	2	
4	E	2	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13829 atoms, of which 6241 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 mannan endo-1,4-beta-mannosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	381	Total	C	H	N	O	S	79	46	0
			6301	2029	3072	588	600	12			
1	B	383	Total	C	H	N	O	S	84	35	0
			6233	2004	3039	583	596	11			

There are 45 discrepancies between the modelled and reference sequences:

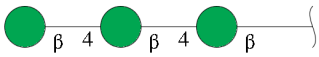
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLN	-	expression tag	UNP A0ABN2XY41
A	43	SER	-	expression tag	UNP A0ABN2XY41
A	44	ARG	-	expression tag	UNP A0ABN2XY41
A	45	SER	ALA	conflict	UNP A0ABN2XY41
A	50	GLY	ARG	conflict	UNP A0ABN2XY41
A	53	GLN	GLU	conflict	UNP A0ABN2XY41
A	59	ARG	GLU	conflict	UNP A0ABN2XY41
A	76	PRO	HIS	conflict	UNP A0ABN2XY41
A	94	ILE	VAL	conflict	UNP A0ABN2XY41
A	103	GLY	ASP	conflict	UNP A0ABN2XY41
A	105	HIS	ARG	conflict	UNP A0ABN2XY41
A	112	THR	PRO	conflict	UNP A0ABN2XY41
A	113	GLU	LYS	conflict	UNP A0ABN2XY41
A	115	TYR	PHE	conflict	UNP A0ABN2XY41
A	116	ARG	SER	conflict	UNP A0ABN2XY41
A	130	HIS	GLN	conflict	UNP A0ABN2XY41
A	158	THR	SER	conflict	UNP A0ABN2XY41
A	164	PRO	ALA	conflict	UNP A0ABN2XY41
A	172	ALA	THR	conflict	UNP A0ABN2XY41
A	192	GLU	LYS	conflict	UNP A0ABN2XY41
A	196	ARG	GLN	conflict	UNP A0ABN2XY41
A	201	TYR	HIS	conflict	UNP A0ABN2XY41
A	207	CYS	ALA	conflict	UNP A0ABN2XY41
A	254	ILE	VAL	conflict	UNP A0ABN2XY41
A	263	PRO	ALA	conflict	UNP A0ABN2XY41

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Chain	Residue	Modelled	Actual	Comment	Reference
A	264	ASN	ASP	conflict	UNP A0ABN2XY41
A	279	GLN	LEU	conflict	UNP A0ABN2XY41
A	305	ASN	SER	conflict	UNP A0ABN2XY41
A	306	THR	LYS	conflict	UNP A0ABN2XY41
A	309	VAL	THR	conflict	UNP A0ABN2XY41
A	312	ALA	THR	conflict	UNP A0ABN2XY41
A	320	ASN	THR	conflict	UNP A0ABN2XY41
A	324	THR	ALA	conflict	UNP A0ABN2XY41
A	328	ARG	LYS	conflict	UNP A0ABN2XY41
A	342	LEU	ILE	conflict	UNP A0ABN2XY41
A	345	ALA	GLY	conflict	UNP A0ABN2XY41
A	365	SER	ALA	conflict	UNP A0ABN2XY41
A	367	THR	ALA	conflict	UNP A0ABN2XY41
A	368	GLY	SER	conflict	UNP A0ABN2XY41
A	396	ILE	VAL	conflict	UNP A0ABN2XY41
A	418	GLU	LYS	conflict	UNP A0ABN2XY41
A	421	THR	ALA	conflict	UNP A0ABN2XY41
A	422	ALA	SER	conflict	UNP A0ABN2XY41
A	423	ALA	SER	conflict	UNP A0ABN2XY41
A	424	GLY	-	expression tag	UNP A0ABN2XY41

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-beta-D-mannopyranose -(1-4)-beta-D-mannopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
2	C	3	74	20	37	17	0	1	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-alpha-D-mannopyranos e.



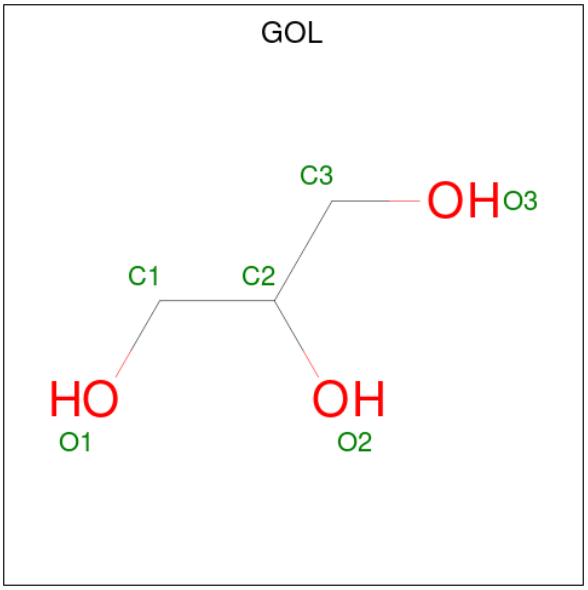
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
3	D	2	46	12	23	11	0	2	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-beta-D-mannopyranose.



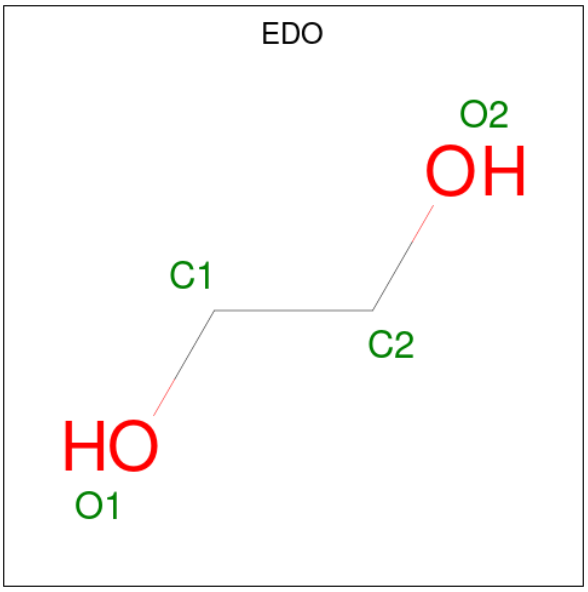
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	H	O	0	2	0
			42	12	20	10			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



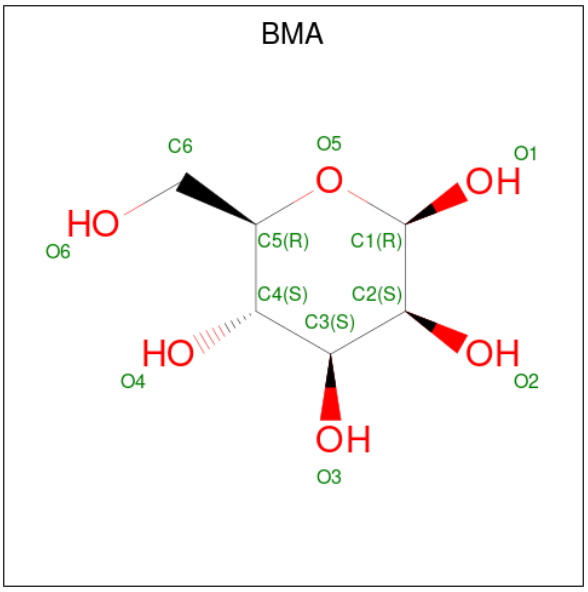
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	3	0
			14	3	8	3		
5	B	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	1
			20	4	12	4		

- Molecule 7 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	1
			23	6	11	6		
7	B	1	Total	C	H	O	0	1
			23	6	11	6		

- Molecule 8 is water.

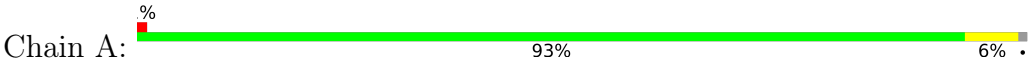
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	526	Total O 526 526	0	9
8	B	513	Total O 513 513	0	11

3 Residue-property plots

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: mannan endo-1,4-beta-mannosidase

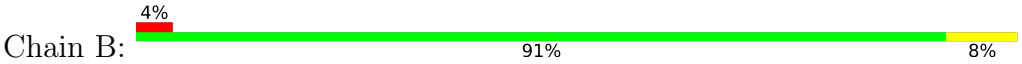
Chain A:

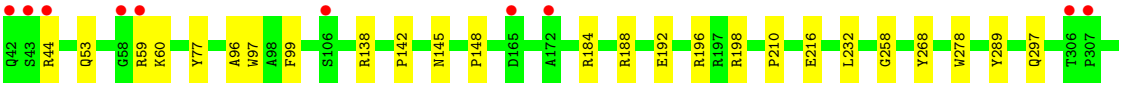


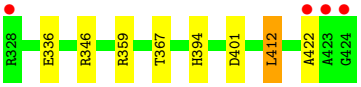


• Molecule 1: mannan endo-1,4-beta-mannosidase

Chain B:

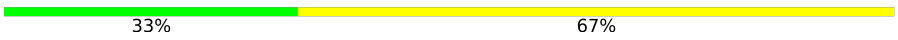






• Molecule 2: beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-beta-D-mannopyranose

Chain C:





• Molecule 3: beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose

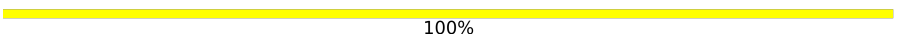
Chain D:





• Molecule 4: beta-D-mannopyranose-(1-4)-beta-D-mannopyranose

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	138.10Å 138.10Å 83.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.65 – 1.12 97.65 – 1.12	Depositor EDS
% Data completeness (in resolution range)	99.8 (97.65-1.12) 95.2 (97.65-1.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 1.13Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.148 , 0.160 0.131 , 0.141	Depositor DCC
R_{free} test set	2998 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	11.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	13829	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, BMA, GOL, EDO

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	0.77	0/3490	0.75	1/4747 (0.0%)
1	B	0.81	1/3413 (0.0%)	0.76	1/4642 (0.0%)
All	All	0.79	1/6903 (0.0%)	0.75	2/9389 (0.0%)

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	3
1	B	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	ALA	CA-CB	-6.87	1.41	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	401	ASP	CA-CB-CG	7.26	119.86	112.60
1	B	401	ASP	CA-CB-CG	6.59	119.19	112.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	407[A]	ARG	Sidechain
1	A	407[B]	ARG	Sidechain
1	B	184	ARG	Sidechain
1	B	198[A]	ARG	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	3229	3072	2899	17	0
1	B	3194	3039	2901	24	0
2	C	37	37	30	0	0
3	D	23	23	5	0	0
4	E	22	20	19	0	0
5	A	6	8	8	0	0
5	B	6	8	8	0	0
6	A	8	12	10	2	0
7	A	12	11	5	0	0
7	B	12	11	11	2	0
8	A	526	0	0	5	3
8	B	513	0	0	9	5
All	All	7588	6241	5896	41	5

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 3.

The worst 5 of 41 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:363:ASP:O	1:A:367[B]:THR:HG22	1.69	0.93
1:B:367[A]:THR:HG22	8:B:928:HOH:O	1.82	0.78
1:A:394:HIS:NE2	6:A:502[A]:EDO:H12	1.99	0.78
1:A:192[B]:GLU:OE1	8:A:601:HOH:O	2.03	0.77
1:B:188[B]:ARG:NH1	8:B:604:HOH:O	2.21	0.73

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1089:HOH:O	8:B:1089:HOH:O[7_555]	1.59	0.61
8:A:1004:HOH:O	8:B:837:HOH:O[7_556]	1.89	0.31
8:B:817:HOH:O	8:B:919:HOH:O[3_545]	2.02	0.18
8:A:958:HOH:O	8:B:983:HOH:O[4_556]	2.13	0.07
8:A:612:HOH:O	8:B:711:HOH:O[1_556]	2.16	0.04

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	425/383 (111%)	408 (96%)	17 (4%)	0	100	100
1	B	416/383 (109%)	403 (97%)	13 (3%)	0	100	100
All	All	841/766 (110%)	811 (96%)	30 (4%)	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	334/296 (113%)	331 (99%)	3 (1%)	70	38
1	B	327/296 (110%)	323 (99%)	4 (1%)	63	25
All	All	661/592 (112%)	654 (99%)	7 (1%)	73	29

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	TRP
1	B	232[A]	LEU
1	B	412	LEU
1	B	232[B]	LEU
1	A	232[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	105	HIS
1	B	130	HIS
1	B	305	ASN
1	B	394	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)

9 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BMA	C	1	2	12,12,12	0.78	0	17,17,17	0.54	0
2	BMA	C	2	2	11,11,12	1.13	1 (9%)	15,15,17	1.02	1 (6%)
2	BMA	C	3[A]	-	11,11,12	1.03	1 (9%)	15,15,17	0.51	0
2	BMA	C	3[B]	-	11,11,12	1.03	1 (9%)	15,15,17	0.52	0
3	MAN	D	1[B]	3	12,12,12	0.73	1 (8%)	17,17,17	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	E	1[A]	4	11,11,12	1.60	1 (9%)	15,15,17	0.85	1 (6%)
4	BMA	E	2[A]	4	11,11,12	1.01	1 (9%)	15,15,17	1.00	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
2	BMA	C	1	2	-	0/2/22/22	0/1/1/1
2	BMA	C	2	2	-	0/2/19/22	0/1/1/1
2	BMA	C	3[A]	-	-	0/2/19/22	0/1/1/1
2	BMA	C	3[B]	-	-	2/2/19/22	0/1/1/1
3	MAN	D	1[B]	3	-	2/2/22/22	0/1/1/1
4	BMA	E	1[A]	4	-	0/2/19/22	0/1/1/1
4	BMA	E	2[A]	4	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1[A]	BMA	C2-C3	-3.89	1.46	1.52
2	C	2	BMA	O5-C5	2.58	1.48	1.43
4	E	2[A]	BMA	O5-C5	2.57	1.48	1.43
3	D	1[B]	MAN	C3-C2	-2.21	1.46	1.52
2	C	3[A]	BMA	O4-C4	2.12	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	BMA	C1-C2-C3	3.13	113.51	109.67
4	E	1[A]	BMA	C1-C2-C3	2.30	112.50	109.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

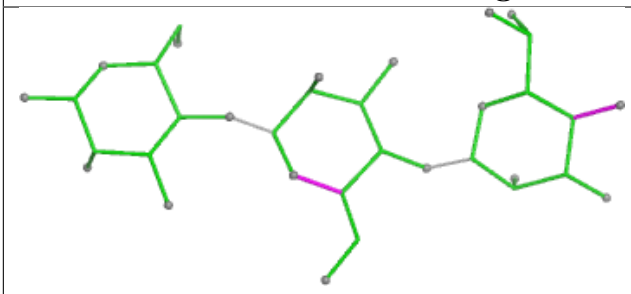
Mol	Chain	Res	Type	Atoms
3	D	1[B]	MAN	C4-C5-C6-O6
2	C	3[B]	BMA	O5-C5-C6-O6
2	C	3[B]	BMA	C4-C5-C6-O6
3	D	1[B]	MAN	O5-C5-C6-O6

There are no ring outliers.

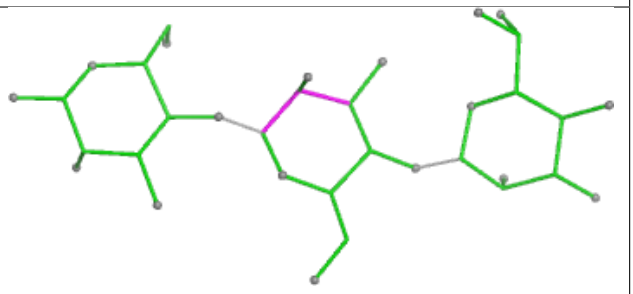
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

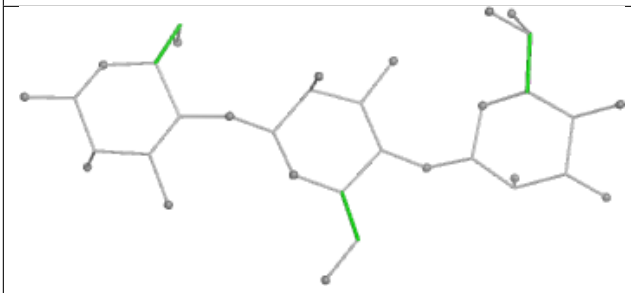
Oligosaccharide Chain C



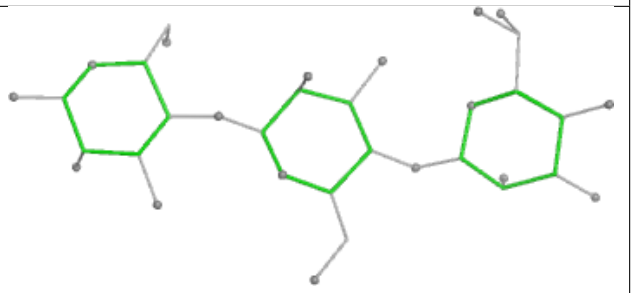
Bond lengths



Bond angles

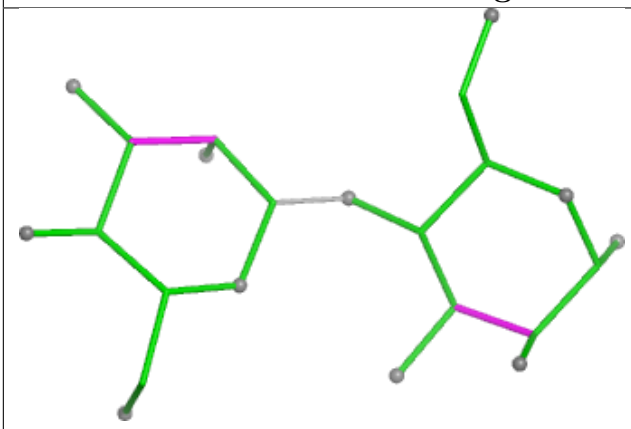


Torsions

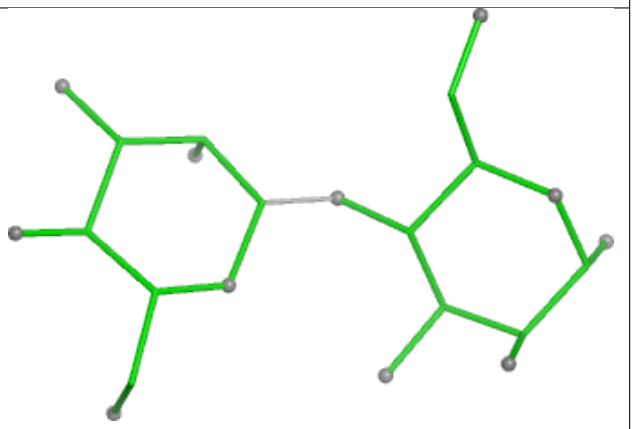


Rings

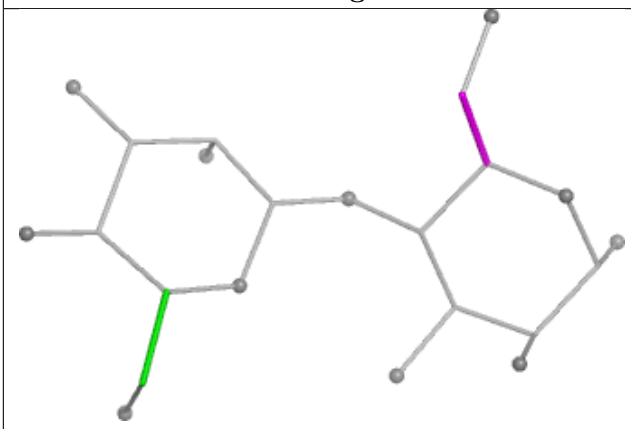
Oligosaccharide Chain D



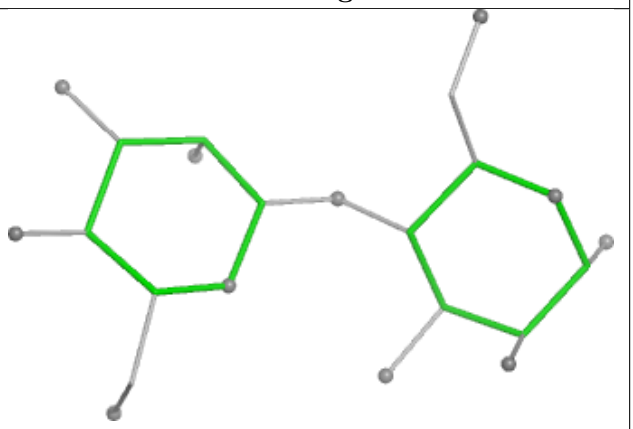
Bond lengths



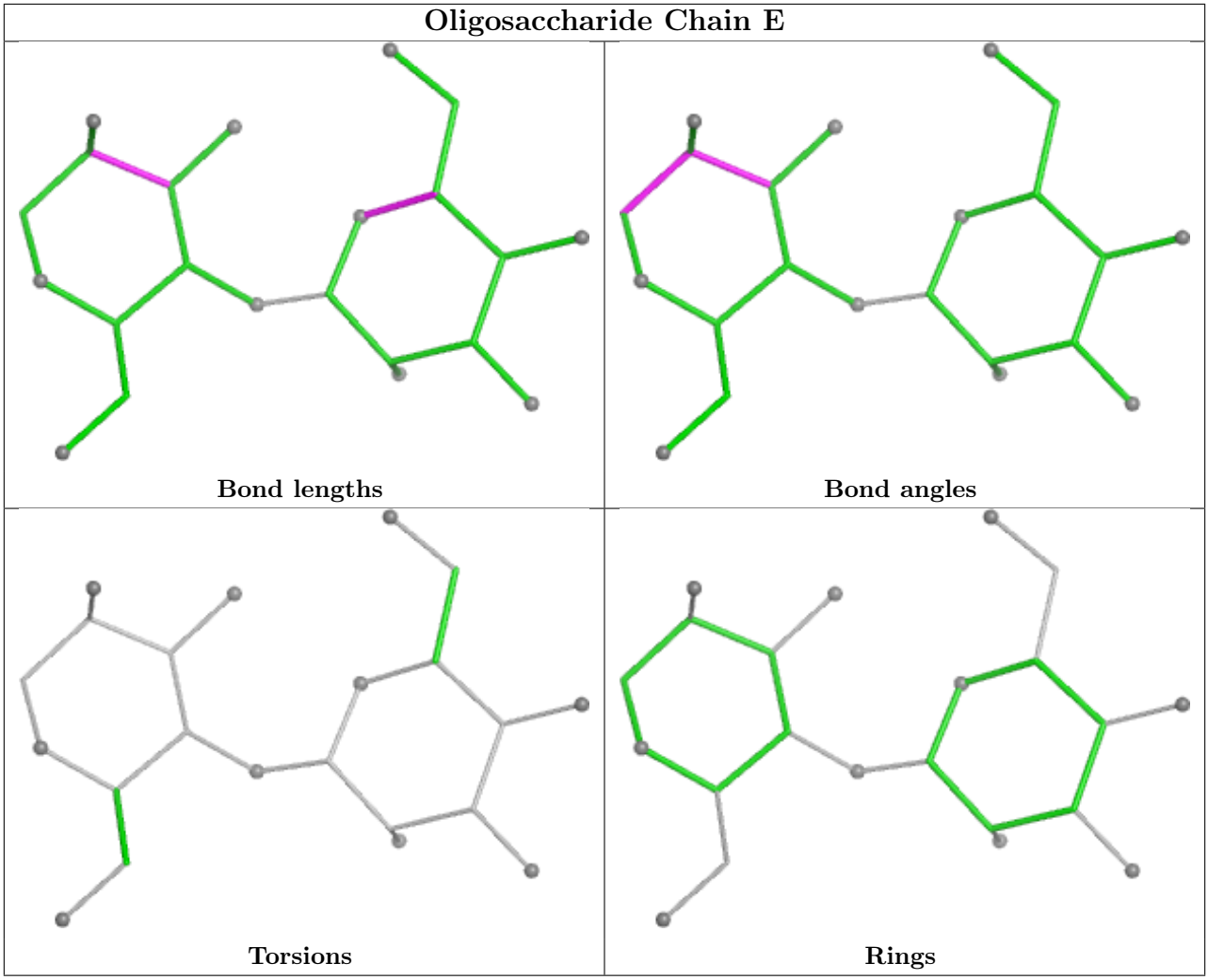
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	A	502[A]	-	3,3,3	0.88	0	2,2,2	0.06	0
7	BMA	B	502[A]	-	12,12,12	0.88	1 (8%)	17,17,17	0.44	0
5	GOL	B	501	-	5,5,5	0.23	0	5,5,5	0.40	0
5	GOL	A	501	-	5,5,5	0.29	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	A	503[A]	3	12,12,12	0.70	0	17,17,17	0.62	0
6	EDO	A	502[B]	-	3,3,3	0.95	0	2,2,2	0.30	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
6	EDO	A	502[A]	-	-	0/1/1/1	-
7	BMA	B	502[A]	-	-	0/2/22/22	0/1/1/1
5	GOL	B	501	-	-	2/4/4/4	-
5	GOL	A	501	-	-	2/4/4/4	-
7	BMA	A	503[A]	3	-	0/2/22/22	0/1/1/1
6	EDO	A	502[B]	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502[A]	BMA	C3-C2	-2.55	1.45	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	GOL	O1-C1-C2-C3
5	A	501	GOL	O1-C1-C2-C3
5	A	501	GOL	O1-C1-C2-O2
5	B	501	GOL	O1-C1-C2-O2

There are no ring outliers.

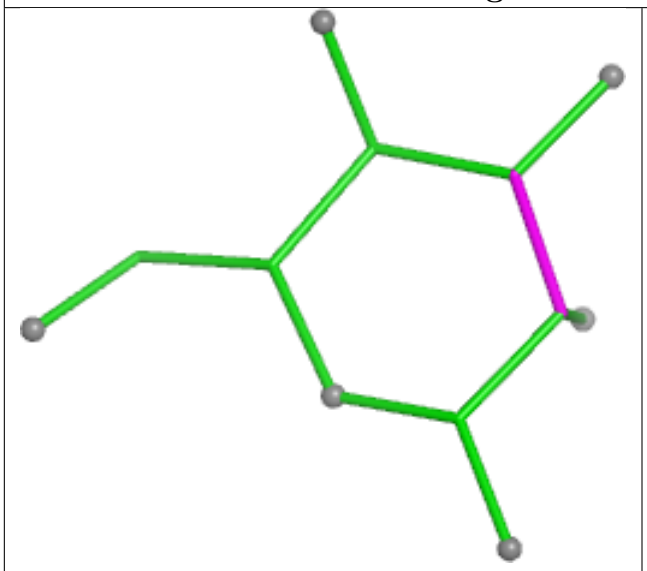
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502[A]	EDO	2	0
7	B	502[A]	BMA	2	0

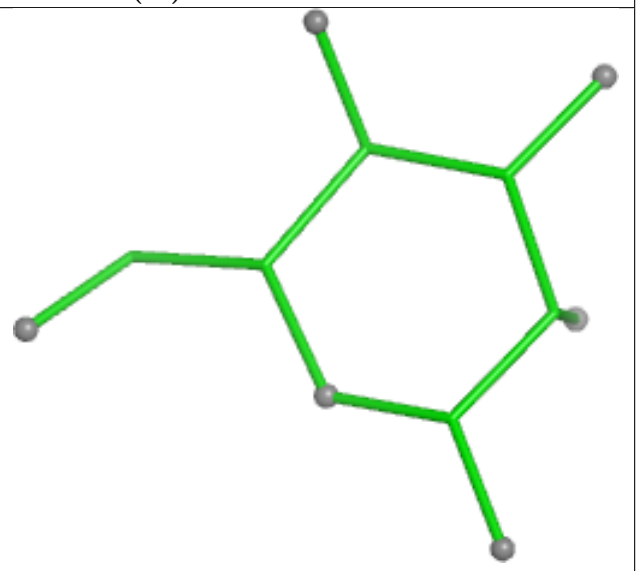
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

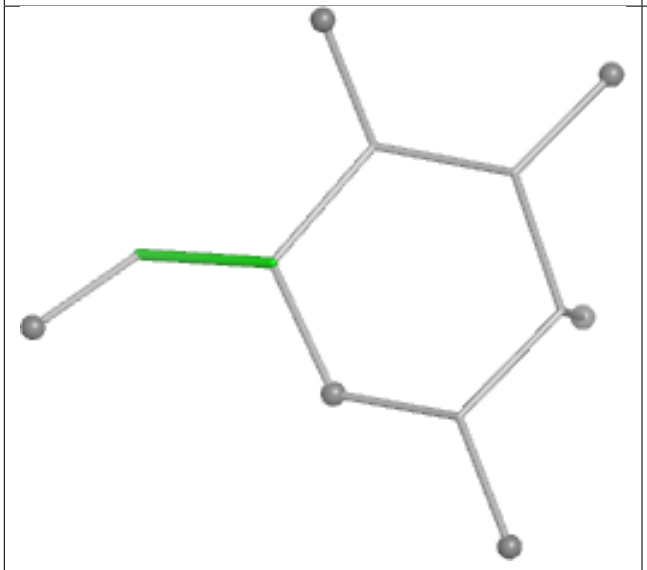
Ligand BMA B 502 (A)



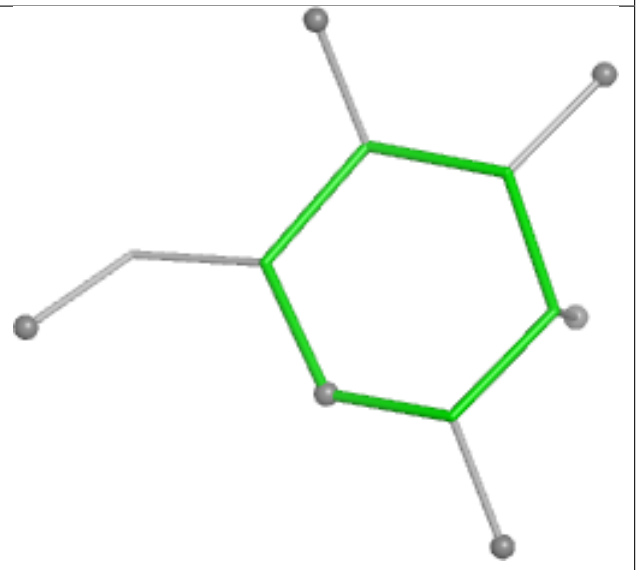
Bond lengths



Bond angles

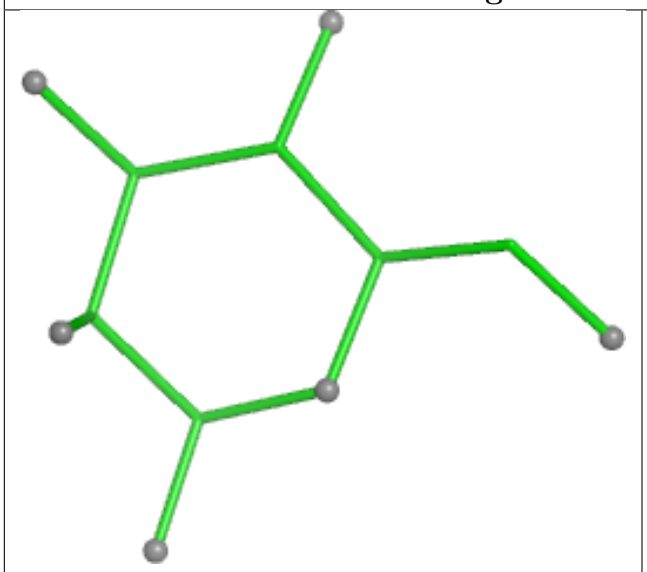


Torsions

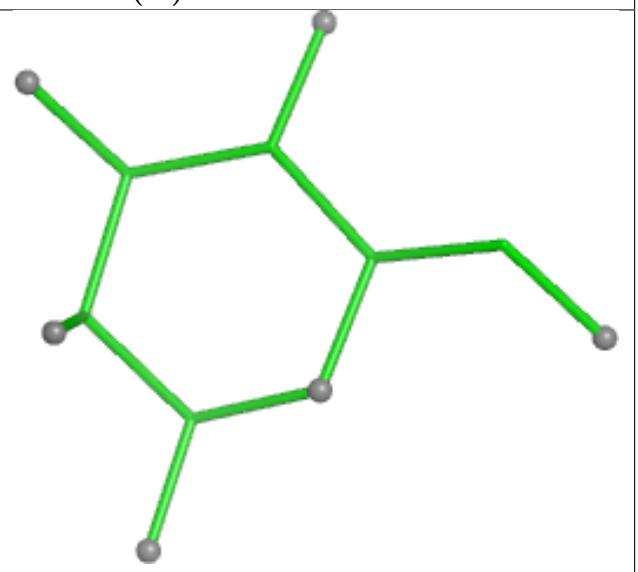


Rings

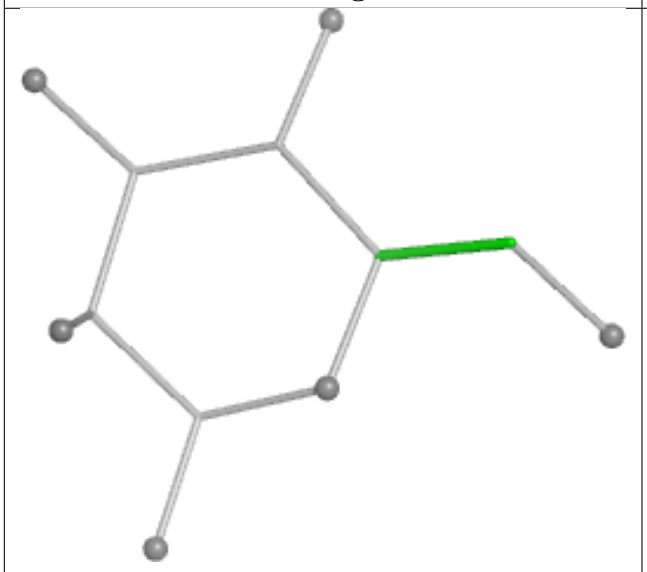
Ligand BMA A 503 (A)



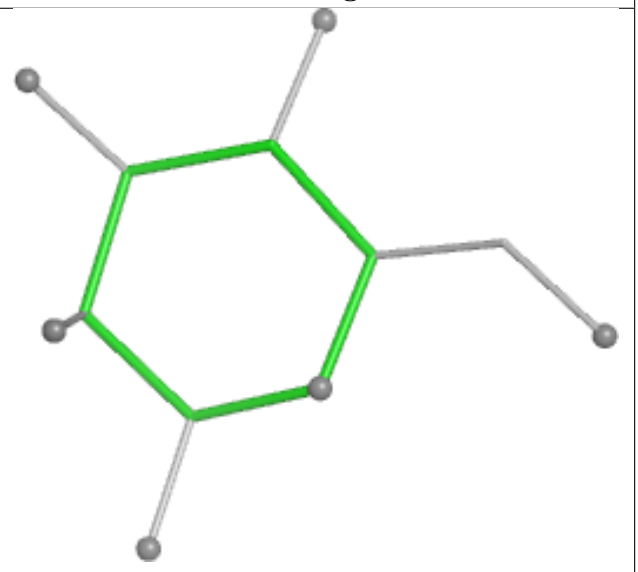
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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^2)	Q<0.9
1	A	381/383 (99%)	-0.28	5 (1%)	75	80	5, 12, 17, 37	27 (7%)
1	B	383/383 (100%)	-0.21	14 (3%)	45	51	5, 12, 19, 25	21 (5%)
All	All	764/766 (99%)	-0.24	19 (2%)	58	65	5, 12, 18, 37	48 (6%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	GLY	6.0
1	B	43	SER	5.2
1	B	423	ALA	4.5
1	B	307	PRO	4.3
1	B	59	ARG	4.2

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

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^{th} 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^2)	Q<0.9
4	BMA	E	1[A]	11/12	0.81	0.16	12,15,20,24	21
4	BMA	E	2[A]	11/12	0.87	0.13	12,14,19,19	21
3	BMA	D	2[B]	11/12	0.92	0.09	12,12,22,26	22
2	BMA	C	1	12/12	0.92	0.10	12,12,26,28	23
3	BMA	D	2[A]	11/12	0.92	0.09	12,12,22,26	22

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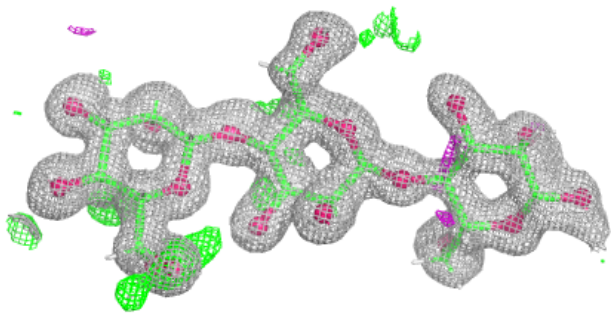
Continued from previous page...

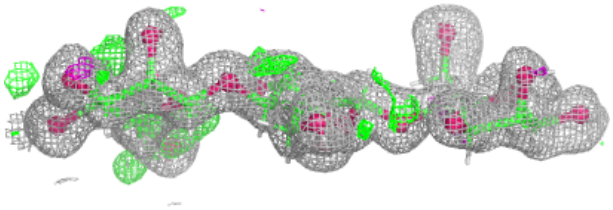
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	D	1[B]	12/12	0.94	0.08	12,12,15,16	23
2	BMA	C	3[B]	11/12	0.95	0.07	11,12,15,18	22
2	BMA	C	3[A]	11/12	0.95	0.07	9,12,15,15	22
2	BMA	C	2	11/12	0.96	0.07	11,12,14,17	21

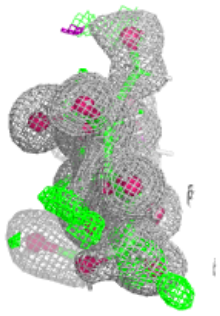
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

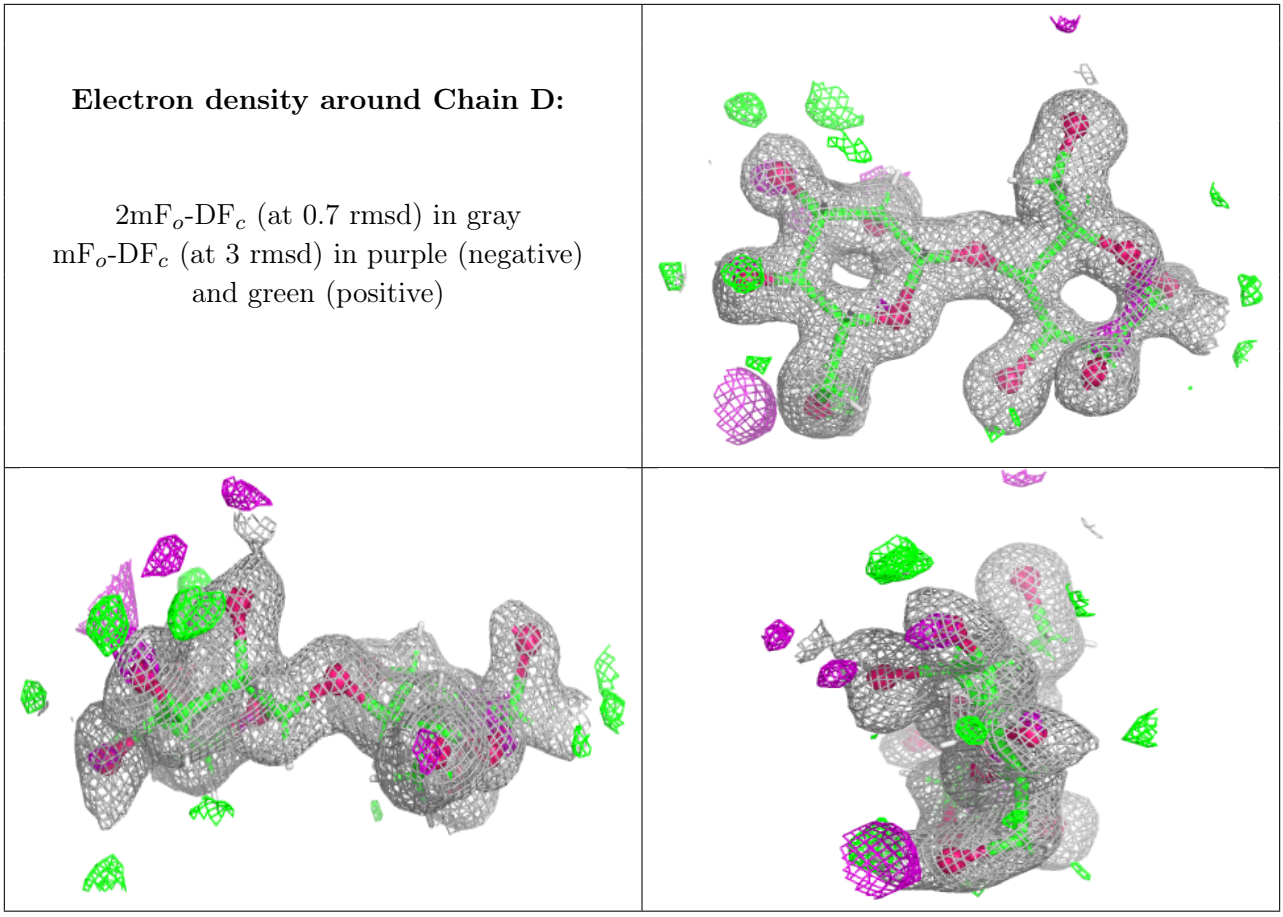






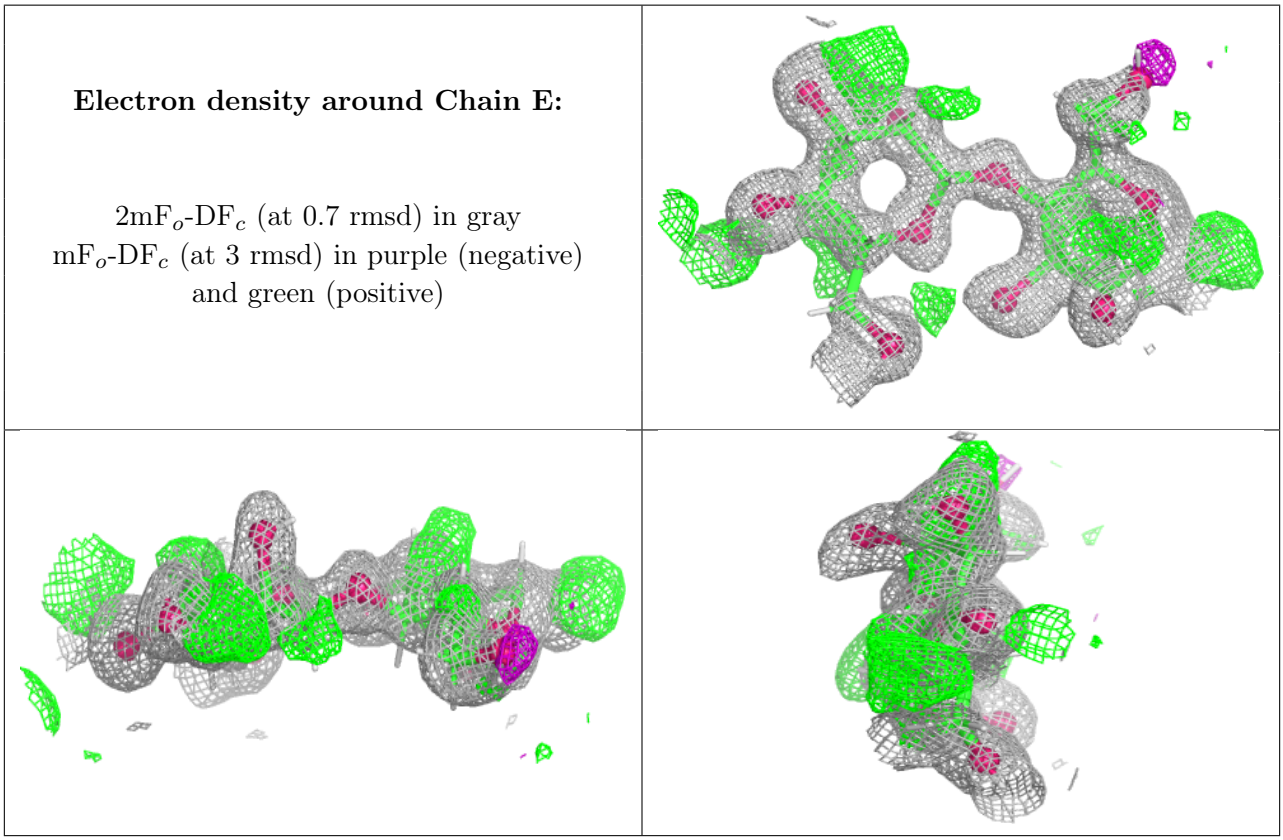
Electron density around Chain D:

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



Electron density around Chain E:

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



6.4 Ligands (i)

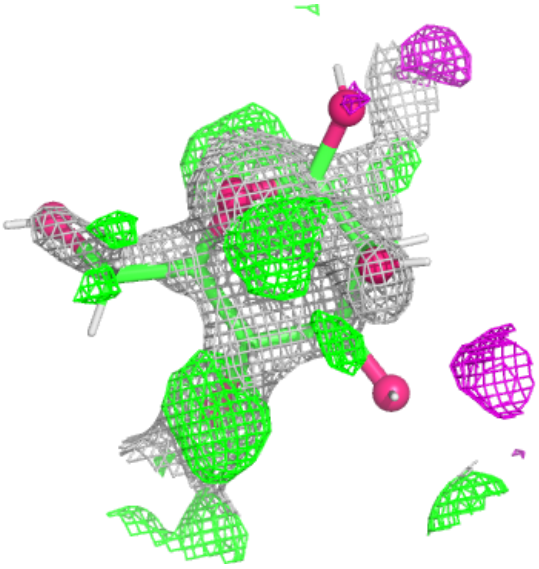
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

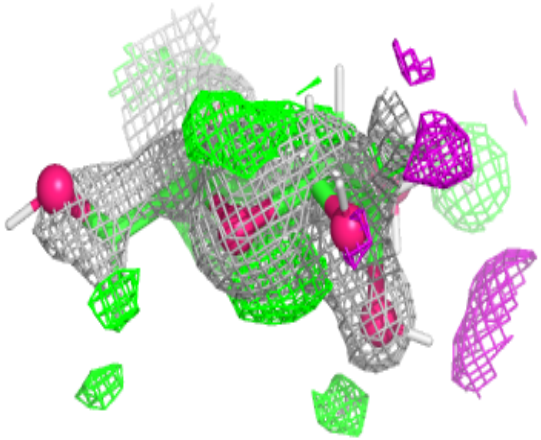
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	BMA	B	502[A]	12/12	0.66	0.34	12,20,26,33	23
6	EDO	A	502[B]	4/4	0.88	0.16	12,12,19,19	10
6	EDO	A	502[A]	4/4	0.88	0.16	12,12,21,22	10
5	GOL	B	501	6/6	0.90	0.09	12,24,29,32	3
5	GOL	A	501	6/6	0.90	0.10	12,12,27,28	3
7	BMA	A	503[A]	12/12	0.92	0.08	12,13,15,41	23

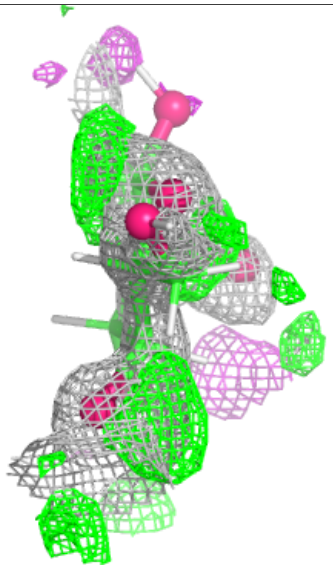
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BMA B 502 (A):

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

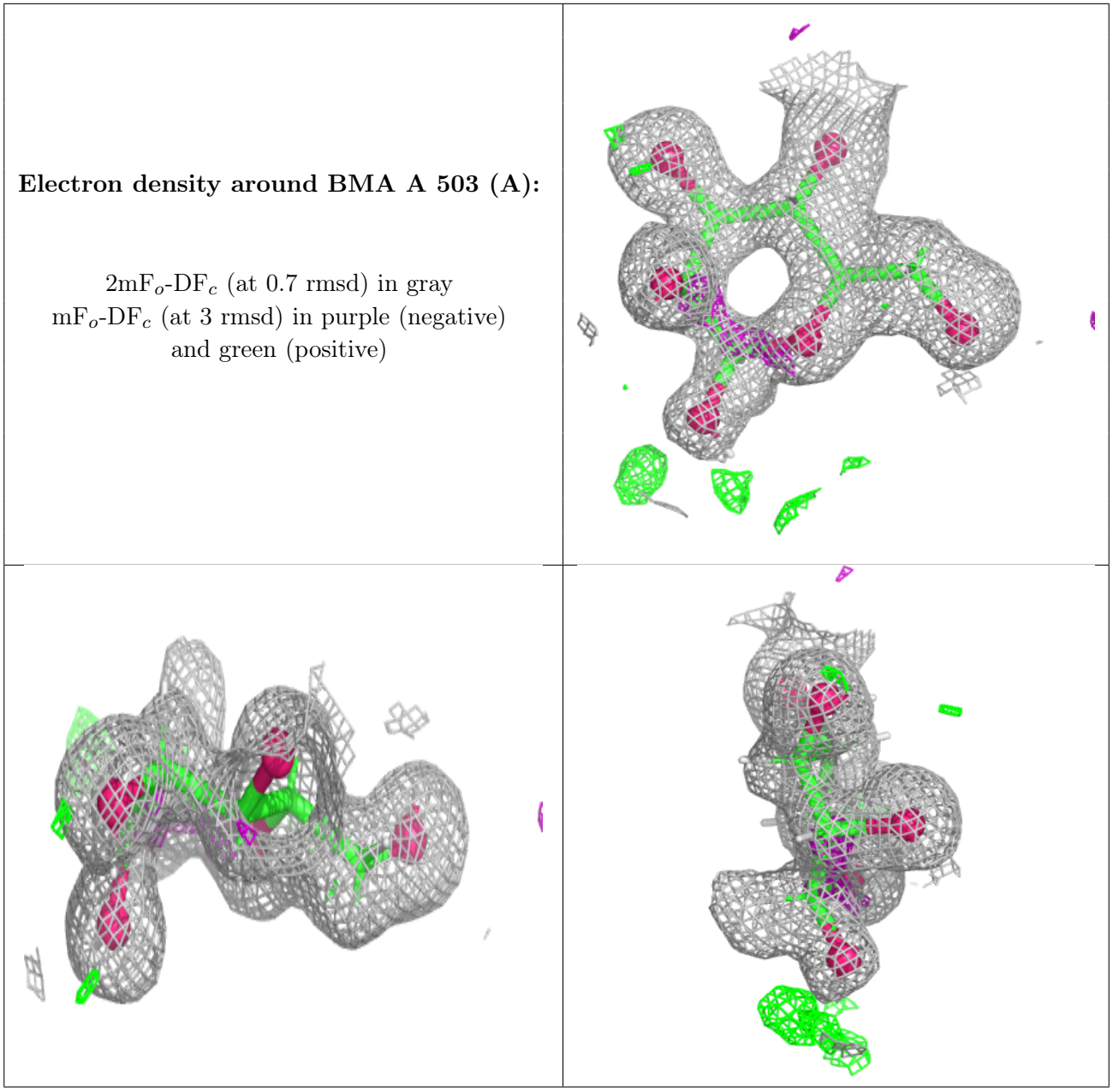






Electron density around BMA A 503 (A):

$2mF_o$-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.