wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 06:00 AM EDT

PDB ID	:	3LPP
Title	:	Crystal complex of N-terminal sucrase-isomaltase with kotalanol
Authors	:	Sim, L.; Rose, D.R.
Deposited on	:	2010-02-05
Resolution	:	2.15 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:

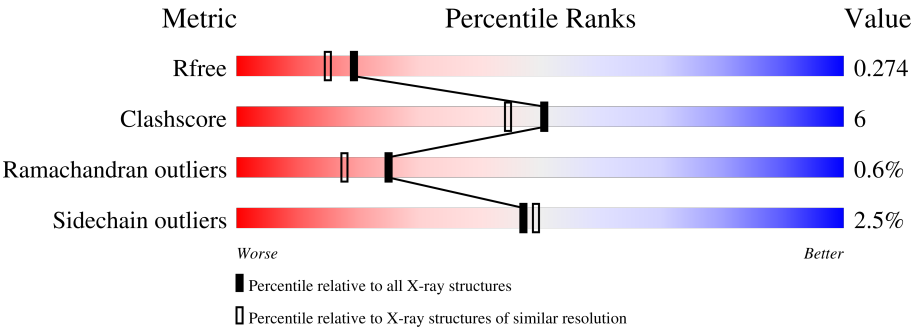
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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%

Mol	Chain	Length	Quality of chain
1	A	898	85% 11% • •
1	B	898	83% 13% • •
1	C	898	85% 12% • •
1	D	898	80% 14% • 5%
2	E	4	100%
2	H	4	25% 75%
3	F	2	100%

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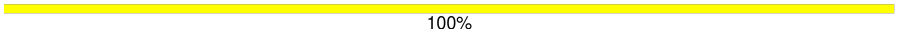
Mol	Chain	Length	Quality of chain
3	G	2	
3	I	2	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 30064 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 Sucrase-isomaltase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	0	0	0
			7035	4503	1183	1320	29			
1	B	869	Total	C	N	O	S	0	0	0
			7015	4491	1177	1318	29			
1	C	871	Total	C	N	O	S	0	0	0
			7029	4500	1180	1320	29			
1	D	853	Total	C	N	O	S	0	0	0
			6882	4416	1150	1289	27			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	expression tag	UNP P14410
A	2	SER	-	expression tag	UNP P14410
A	3	SER	-	expression tag	UNP P14410
A	4	HIS	-	expression tag	UNP P14410
A	5	HIS	-	expression tag	UNP P14410
A	6	HIS	-	expression tag	UNP P14410
A	7	HIS	-	expression tag	UNP P14410
A	8	HIS	-	expression tag	UNP P14410
A	9	HIS	-	expression tag	UNP P14410
A	10	GLY	-	expression tag	UNP P14410
A	11	GLU	-	expression tag	UNP P14410
A	12	PHE	-	expression tag	UNP P14410
A	13	ASP	-	expression tag	UNP P14410
A	14	ILE	-	expression tag	UNP P14410
A	15	PRO	-	expression tag	UNP P14410
A	16	THR	-	expression tag	UNP P14410
A	17	THR	-	expression tag	UNP P14410
A	18	GLU	-	expression tag	UNP P14410
A	19	ASN	-	expression tag	UNP P14410
A	20	LEU	-	expression tag	UNP P14410
A	21	TYR	-	expression tag	UNP P14410

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	PHE	-	expression tag	UNP P14410
A	23	GLN	-	expression tag	UNP P14410
A	24	SER	-	expression tag	UNP P14410
A	25	GLY	-	expression tag	UNP P14410
A	26	ILE	-	expression tag	UNP P14410
A	27	ARG	-	expression tag	UNP P14410
A	28	ARG	-	expression tag	UNP P14410
B	1	ARG	-	expression tag	UNP P14410
B	2	SER	-	expression tag	UNP P14410
B	3	SER	-	expression tag	UNP P14410
B	4	HIS	-	expression tag	UNP P14410
B	5	HIS	-	expression tag	UNP P14410
B	6	HIS	-	expression tag	UNP P14410
B	7	HIS	-	expression tag	UNP P14410
B	8	HIS	-	expression tag	UNP P14410
B	9	HIS	-	expression tag	UNP P14410
B	10	GLY	-	expression tag	UNP P14410
B	11	GLU	-	expression tag	UNP P14410
B	12	PHE	-	expression tag	UNP P14410
B	13	ASP	-	expression tag	UNP P14410
B	14	ILE	-	expression tag	UNP P14410
B	15	PRO	-	expression tag	UNP P14410
B	16	THR	-	expression tag	UNP P14410
B	17	THR	-	expression tag	UNP P14410
B	18	GLU	-	expression tag	UNP P14410
B	19	ASN	-	expression tag	UNP P14410
B	20	LEU	-	expression tag	UNP P14410
B	21	TYR	-	expression tag	UNP P14410
B	22	PHE	-	expression tag	UNP P14410
B	23	GLN	-	expression tag	UNP P14410
B	24	SER	-	expression tag	UNP P14410
B	25	GLY	-	expression tag	UNP P14410
B	26	ILE	-	expression tag	UNP P14410
B	27	ARG	-	expression tag	UNP P14410
B	28	ARG	-	expression tag	UNP P14410
C	1	ARG	-	expression tag	UNP P14410
C	2	SER	-	expression tag	UNP P14410
C	3	SER	-	expression tag	UNP P14410
C	4	HIS	-	expression tag	UNP P14410
C	5	HIS	-	expression tag	UNP P14410
C	6	HIS	-	expression tag	UNP P14410
C	7	HIS	-	expression tag	UNP P14410

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	HIS	-	expression tag	UNP P14410
C	9	HIS	-	expression tag	UNP P14410
C	10	GLY	-	expression tag	UNP P14410
C	11	GLU	-	expression tag	UNP P14410
C	12	PHE	-	expression tag	UNP P14410
C	13	ASP	-	expression tag	UNP P14410
C	14	ILE	-	expression tag	UNP P14410
C	15	PRO	-	expression tag	UNP P14410
C	16	THR	-	expression tag	UNP P14410
C	17	THR	-	expression tag	UNP P14410
C	18	GLU	-	expression tag	UNP P14410
C	19	ASN	-	expression tag	UNP P14410
C	20	LEU	-	expression tag	UNP P14410
C	21	TYR	-	expression tag	UNP P14410
C	22	PHE	-	expression tag	UNP P14410
C	23	GLN	-	expression tag	UNP P14410
C	24	SER	-	expression tag	UNP P14410
C	25	GLY	-	expression tag	UNP P14410
C	26	ILE	-	expression tag	UNP P14410
C	27	ARG	-	expression tag	UNP P14410
C	28	ARG	-	expression tag	UNP P14410
D	1	ARG	-	expression tag	UNP P14410
D	2	SER	-	expression tag	UNP P14410
D	3	SER	-	expression tag	UNP P14410
D	4	HIS	-	expression tag	UNP P14410
D	5	HIS	-	expression tag	UNP P14410
D	6	HIS	-	expression tag	UNP P14410
D	7	HIS	-	expression tag	UNP P14410
D	8	HIS	-	expression tag	UNP P14410
D	9	HIS	-	expression tag	UNP P14410
D	10	GLY	-	expression tag	UNP P14410
D	11	GLU	-	expression tag	UNP P14410
D	12	PHE	-	expression tag	UNP P14410
D	13	ASP	-	expression tag	UNP P14410
D	14	ILE	-	expression tag	UNP P14410
D	15	PRO	-	expression tag	UNP P14410
D	16	THR	-	expression tag	UNP P14410
D	17	THR	-	expression tag	UNP P14410
D	18	GLU	-	expression tag	UNP P14410
D	19	ASN	-	expression tag	UNP P14410
D	20	LEU	-	expression tag	UNP P14410
D	21	TYR	-	expression tag	UNP P14410

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	PHE	-	expression tag	UNP P14410
D	23	GLN	-	expression tag	UNP P14410
D	24	SER	-	expression tag	UNP P14410
D	25	GLY	-	expression tag	UNP P14410
D	26	ILE	-	expression tag	UNP P14410
D	27	ARG	-	expression tag	UNP P14410
D	28	ARG	-	expression tag	UNP P14410

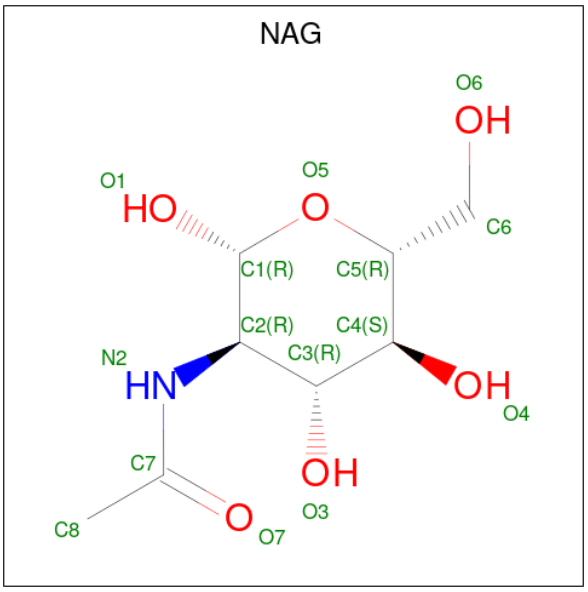
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

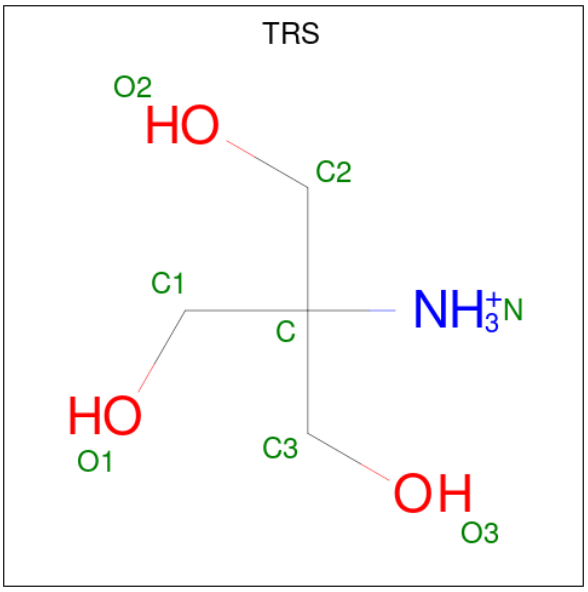
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



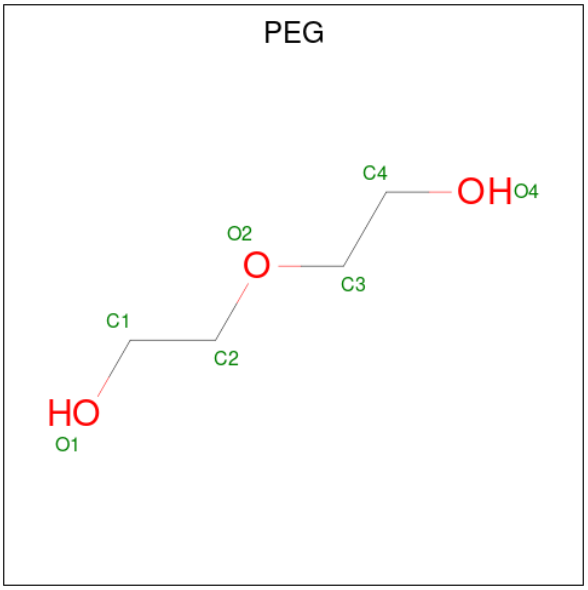
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 8 4 1 3	0	0
5	C	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

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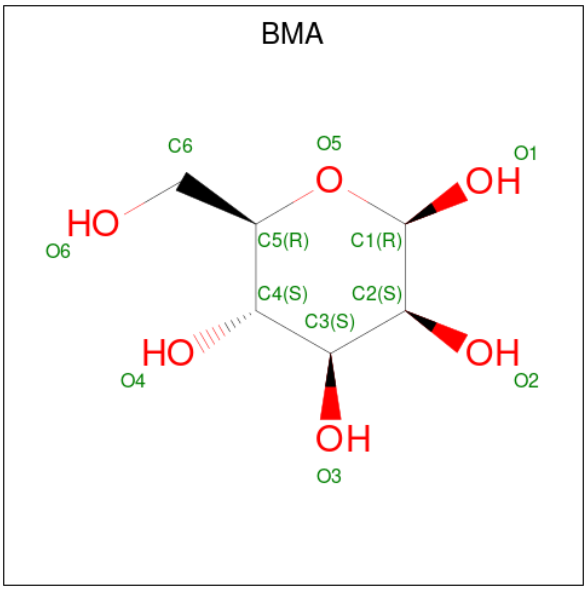
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

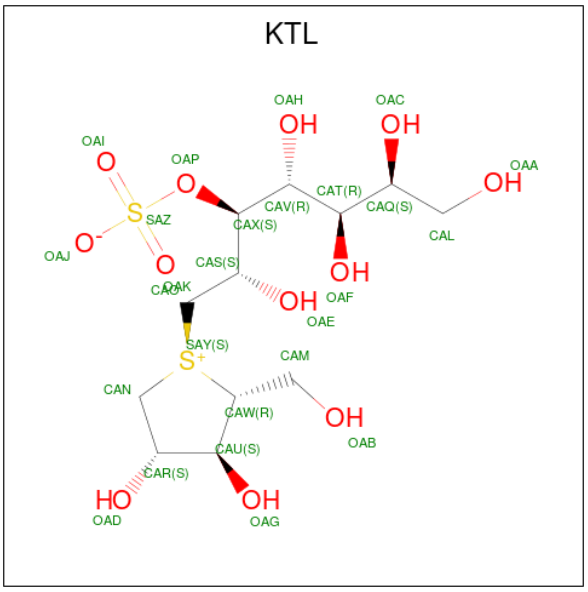
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 11 6 5	0	0

- Molecule 9 is (1S,2R,3R,4S)-1-{(1S)-2-[(2R,3S,4S)-3,4-dihydroxy-2-(hydroxymethyl)tetrahydrothiophenium-1-yl]-1-hydroxyethyl}-2,3,4,5-tetrahydroxypentyl sulfate (three-letter code: KTL) (formula: $C_{12}H_{24}O_{12}S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O	S	0	0
			26	12	12	2		
9	D	1	Total	C	O	S	0	0
			26	12	12	2		

- Molecule 10 is water.

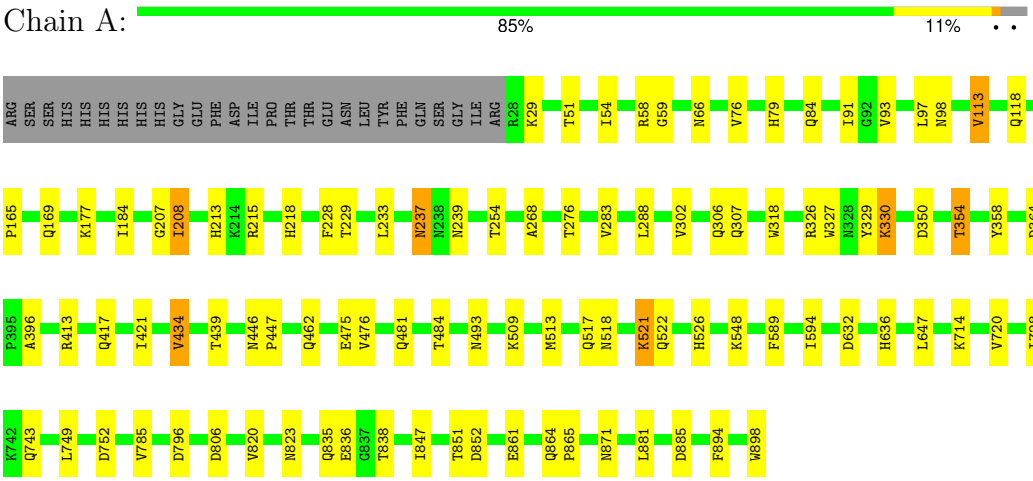
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	529	Total	O	0	0
			529	529		
10	B	514	Total	O	0	0
			514	514		
10	C	458	Total	O	0	0
			458	458		
10	D	226	Total	O	0	0
			226	226		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

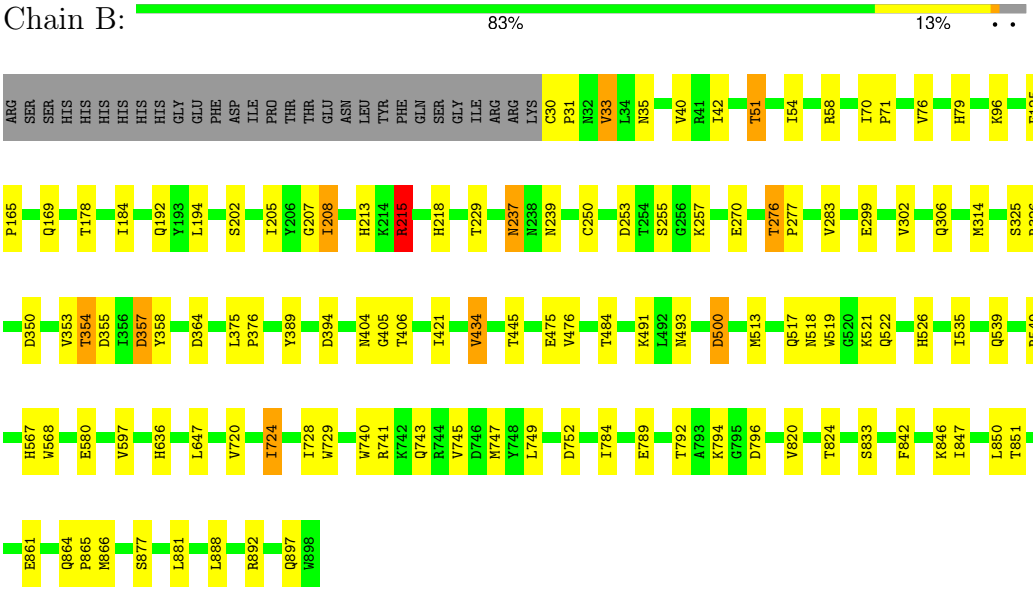
- Molecule 1: Sucrase-isomaltase

Chain A:



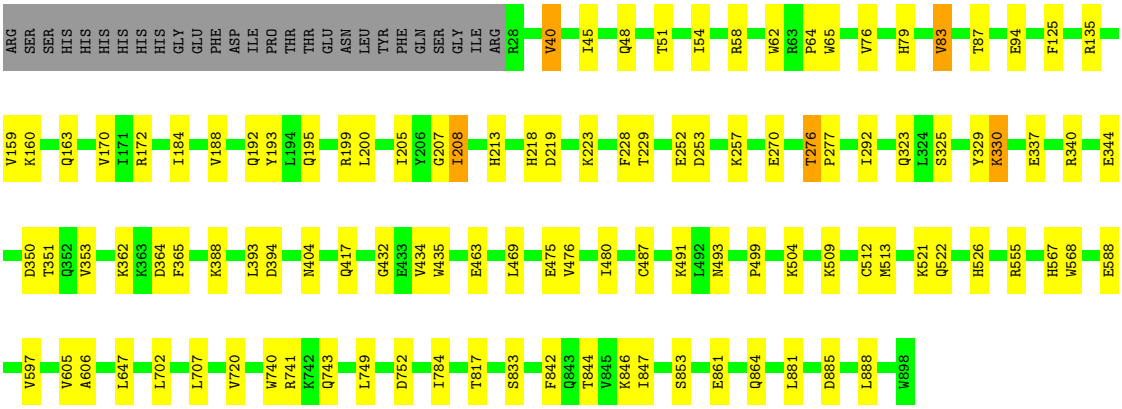
- Molecule 1: Sucrase-isomaltase

Chain B:



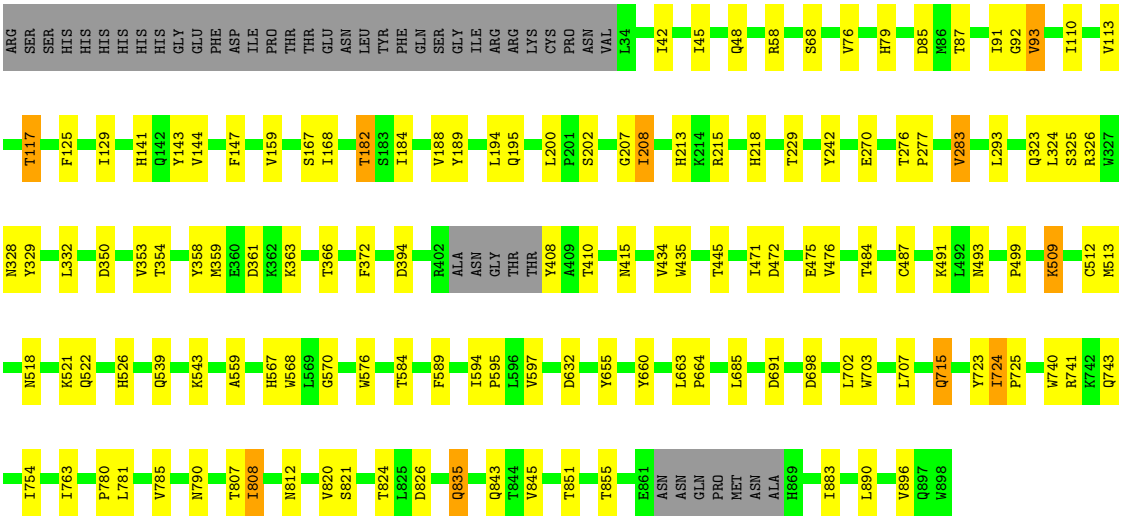
- Molecule 1: Sucrase-isomaltase

Chain C:



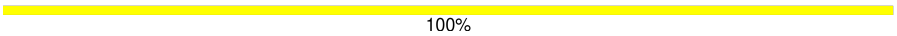
• Molecule 1: Sucrase-isomaltase

Chain D:



• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

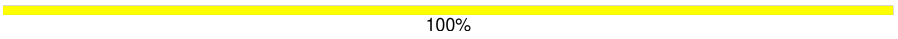


• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

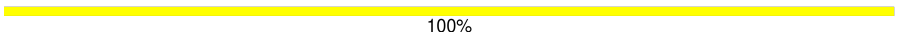


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.40Å 165.76Å 341.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.15 19.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.95-2.15) 94.8 (19.94-2.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.223 0.240 , 0.274	Depositor DCC
R_{free} test set	10150 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	30064	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: CL, MAN, BMA, TRS, KTL, NAG, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.59	0/7236	0.65	1/9868 (0.0%)
1	B	0.55	0/7216	0.64	1/9843 (0.0%)
1	C	0.55	0/7230	0.63	0/9861
1	D	0.44	0/7079	0.57	0/9653
All	All	0.54	0/28761	0.62	2/39225 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	233	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7035	0	6734	67	0
1	B	7015	0	6711	86	0
1	C	7029	0	6724	69	0
1	D	6882	0	6573	95	0
2	E	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	50	0	43	0	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
3	I	28	0	25	0	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0
4	C	42	0	39	0	0
5	A	8	0	12	0	0
5	C	8	0	12	0	0
6	A	7	0	10	0	0
6	B	7	0	10	3	0
6	C	7	0	10	3	0
6	D	7	0	10	0	0
7	A	1	0	0	0	0
8	B	11	0	10	1	0
9	B	26	0	24	0	0
9	D	26	0	24	2	0
10	A	529	0	0	9	0
10	B	514	0	0	11	0
10	C	458	0	0	12	0
10	D	226	0	0	9	0
All	All	30064	0	27103	316	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 316 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:C:487:CYS:HG	1:C:512:CYS:HG	1.05	1.01
1:B:741:ARG:H	1:B:743:GLN:HE21	1.13	0.93
1:C:741:ARG:H	1:C:743:GLN:HE21	1.13	0.88
1:C:51:THR:HG22	10:C:920:HOH:O	1.75	0.87
1:B:51:THR:HG21	10:C:1095:HOH:O	1.75	0.85

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	869/898 (97%)	831 (96%)	32 (4%)	6 (1%)	22	15
1	B	867/898 (96%)	825 (95%)	36 (4%)	6 (1%)	22	15
1	C	869/898 (97%)	825 (95%)	38 (4%)	6 (1%)	22	15
1	D	847/898 (94%)	800 (94%)	45 (5%)	2 (0%)	47	46
All	All	3452/3592 (96%)	3281 (95%)	151 (4%)	20 (1%)	25	18

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	B	276	THR
1	C	276	THR
1	D	276	THR
1	A	66	ASN

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	772/797 (97%)	756 (98%)	16 (2%)	53	57
1	B	770/797 (97%)	749 (97%)	21 (3%)	44	46
1	C	771/797 (97%)	759 (98%)	12 (2%)	62	67
1	D	751/797 (94%)	724 (96%)	27 (4%)	35	33
All	All	3064/3188 (96%)	2988 (98%)	76 (2%)	47	49

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	293	LEU
1	D	808	ILE
1	D	350	ASP
1	D	543	LYS
1	D	855	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	417	GLN
1	D	141	HIS
1	C	493	ASN
1	C	743	GLN
1	D	267	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)

14 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	NAG	E	1	1,2	14,14,15	0.65	0	17,19,21	0.99	1 (5%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	1.18	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	E	3	2	11,11,12	0.75	0	15,15,17	1.17	3 (20%)
2	MAN	E	4	2	11,11,12	0.56	0	15,15,17	0.95	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.57	0	17,19,21	1.20	1 (5%)
3	NAG	F	2	3	14,14,15	0.45	0	17,19,21	1.19	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.61	0	17,19,21	1.00	0
3	NAG	G	2	3	14,14,15	0.56	0	17,19,21	1.39	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.68	0	17,19,21	1.06	2 (11%)
2	NAG	H	2	2	14,14,15	0.49	0	17,19,21	1.49	1 (5%)
2	BMA	H	3	2	11,11,12	0.62	0	15,15,17	1.30	1 (6%)
2	MAN	H	4	2	11,11,12	0.65	0	15,15,17	0.77	0
3	NAG	I	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	2.32	3 (17%)
3	NAG	I	2	3	14,14,15	0.45	0	17,19,21	2.50	5 (29%)

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	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	C1-C2	2.05	1.55	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	2	NAG	C1-O5-C5	8.32	123.34	112.19
3	I	1	NAG	C1-O5-C5	7.76	122.58	112.19
2	H	2	NAG	C1-O5-C5	5.59	119.68	112.19
2	H	3	BMA	C1-O5-C5	3.98	117.52	112.19
3	F	2	NAG	C1-O5-C5	3.98	117.52	112.19

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6

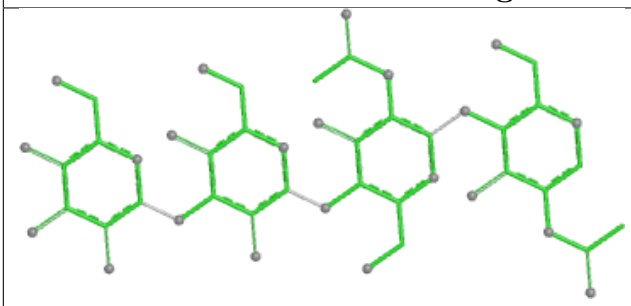
There are no ring outliers.

1 monomer is involved in 1 short contact:

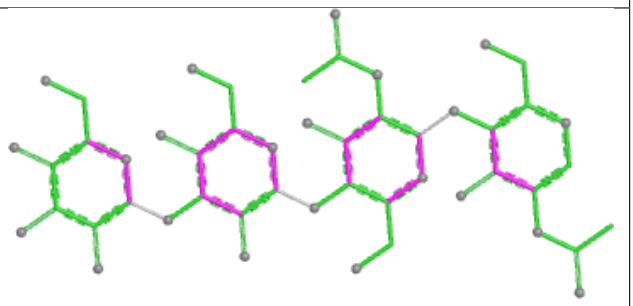
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0

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

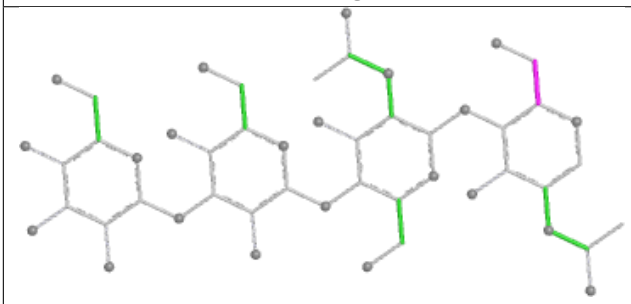
Oligosaccharide Chain E



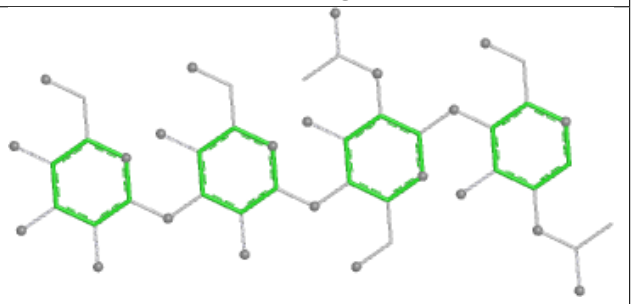
Bond lengths



Bond angles

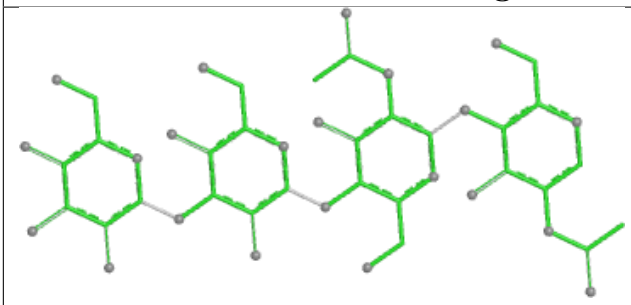


Torsions

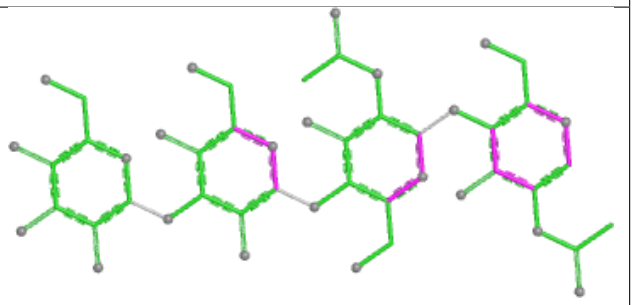


Rings

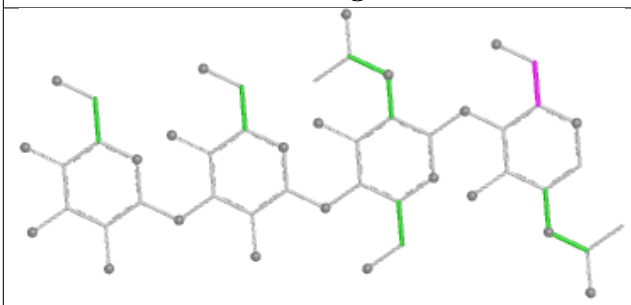
Oligosaccharide Chain H



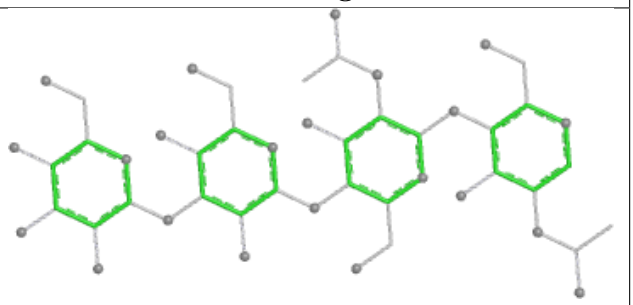
Bond lengths



Bond angles

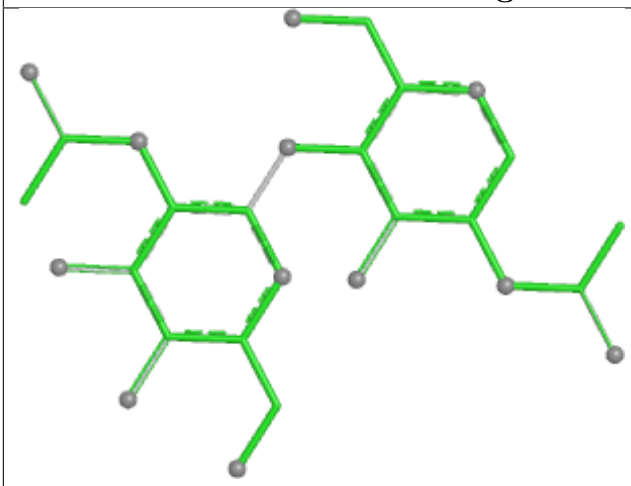


Torsions

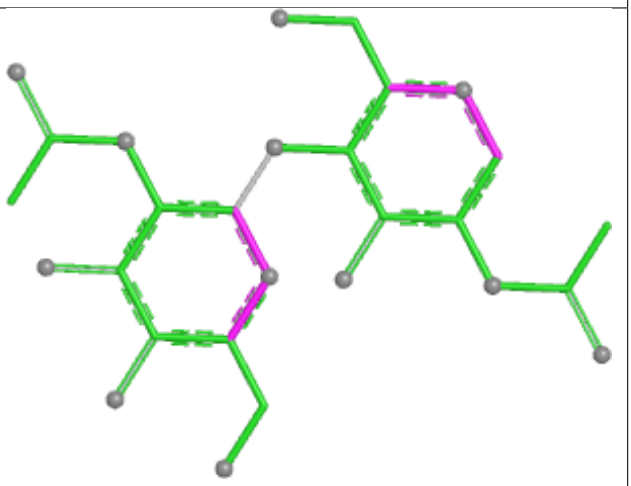


Rings

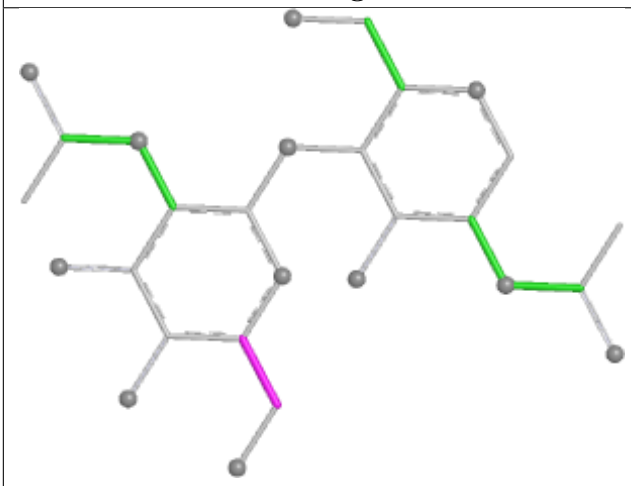
Oligosaccharide Chain F



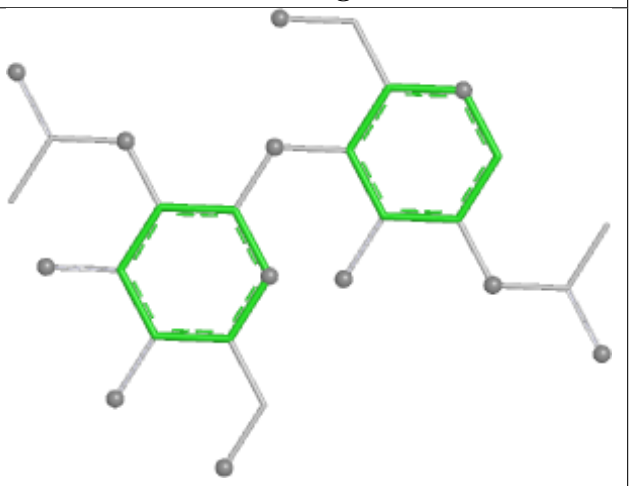
Bond lengths



Bond angles

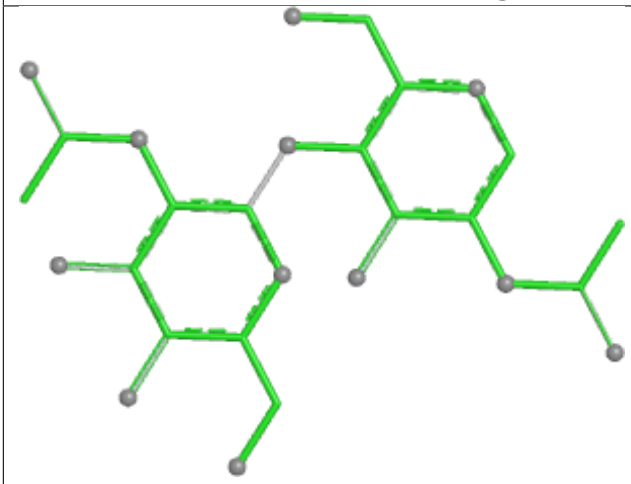


Torsions

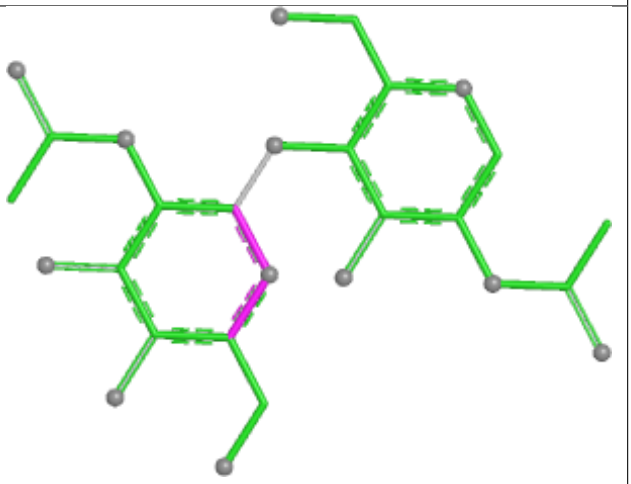


Rings

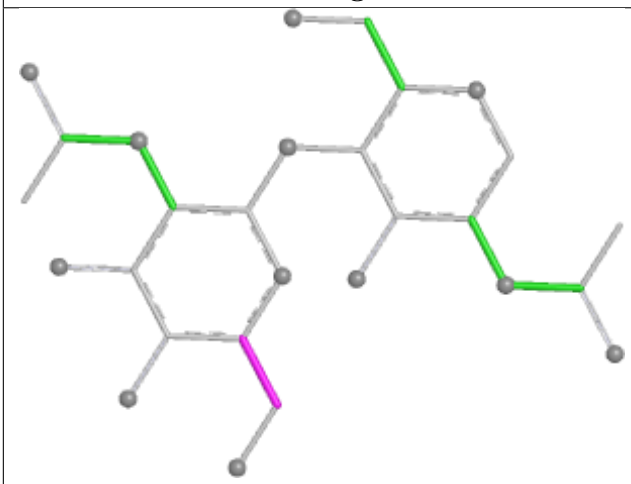
Oligosaccharide Chain G



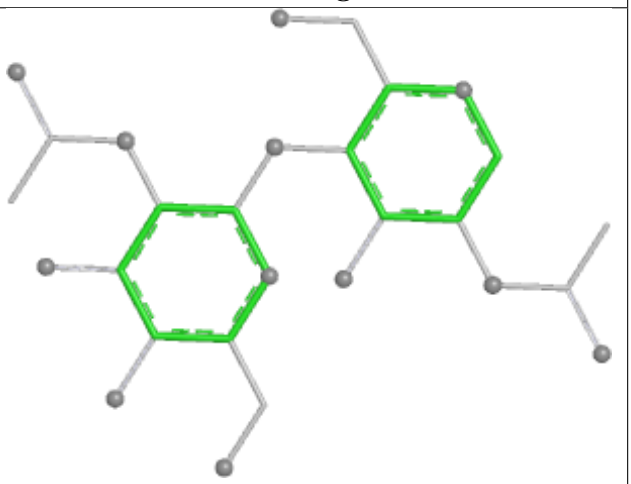
Bond lengths



Bond angles

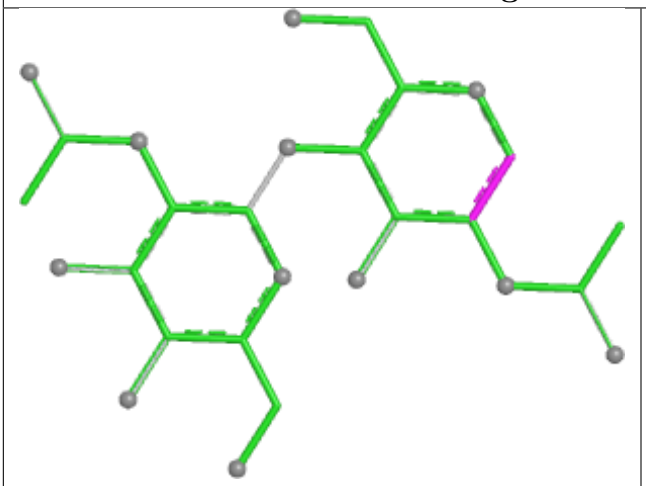


Torsions

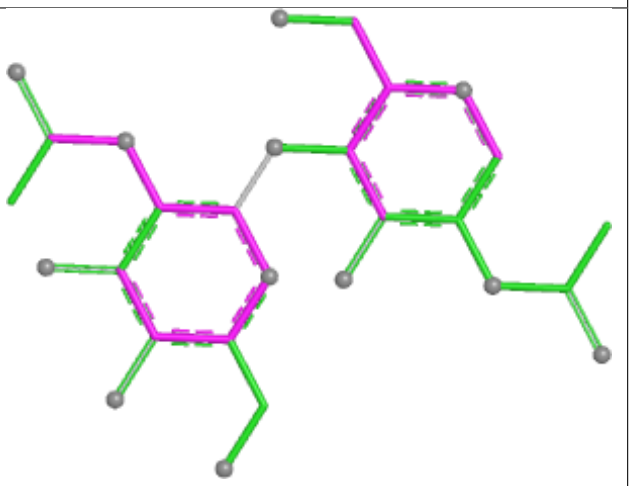


Rings

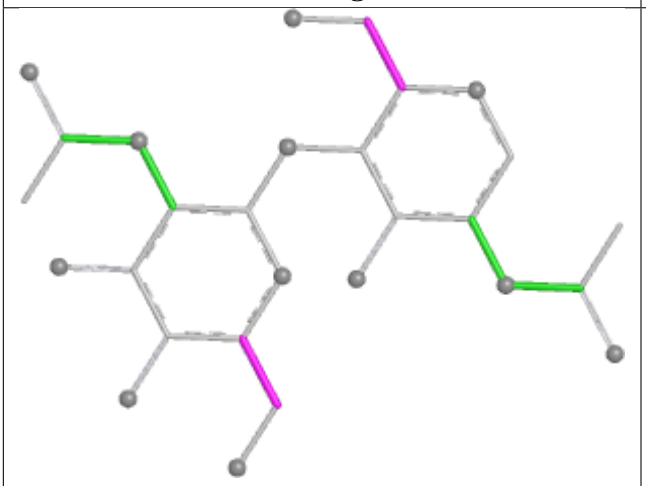
Oligosaccharide Chain I



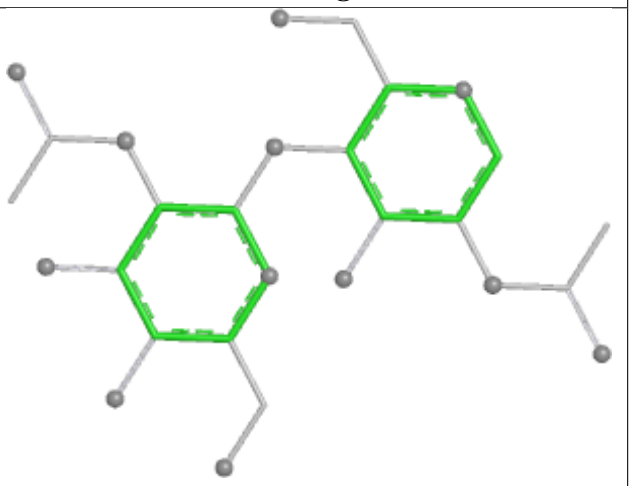
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\#\|Z\| > 2$
9	KTL	B	5001	-	21,26,26	1.77	1 (4%)	25,38,38	1.13	3 (12%)
4	NAG	B	2001	1	14,14,15	0.49	0	17,19,21	2.14	4 (23%)
4	NAG	C	4001	1	14,14,15	0.66	0	17,19,21	1.20	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PEG	A	7001	-	6,6,6	0.53	0	5,5,5	0.39	0
5	TRS	A	6001	-	7,7,7	0.48	0	9,9,9	1.05	1 (11%)
5	TRS	C	6001	-	7,7,7	0.33	0	9,9,9	0.45	0
4	NAG	A	4001	1	14,14,15	0.70	0	17,19,21	2.40	5 (29%)
6	PEG	B	7001	-	6,6,6	0.38	0	5,5,5	0.49	0
6	PEG	C	7001	-	6,6,6	0.46	0	5,5,5	0.25	0
4	NAG	C	2001	1	14,14,15	0.56	0	17,19,21	0.84	1 (5%)
9	KTL	D	5001	-	21,26,26	1.86	2 (9%)	25,38,38	0.97	2 (8%)
4	NAG	C	3001	1	14,14,15	0.48	0	17,19,21	1.28	1 (5%)
4	NAG	A	2001	1	14,14,15	0.56	0	17,19,21	2.00	1 (5%)
8	BMA	B	3003	-	11,11,12	0.47	0	15,15,17	0.60	0
6	PEG	D	7001	-	6,6,6	0.44	0	5,5,5	0.28	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
9	KTL	B	5001	-	-	6/28/45/45	0/1/1/1
4	NAG	B	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	C	4001	1	-	2/6/23/26	0/1/1/1
6	PEG	A	7001	-	-	2/4/4/4	-
5	TRS	A	6001	-	-	0/9/9/9	-
5	TRS	C	6001	-	-	0/9/9/9	-
4	NAG	A	4001	1	-	3/6/23/26	0/1/1/1
6	PEG	B	7001	-	-	3/4/4/4	-
6	PEG	C	7001	-	-	1/4/4/4	-
4	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
9	KTL	D	5001	-	-	12/28/45/45	0/1/1/1
4	NAG	C	3001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	4/6/23/26	0/1/1/1
8	BMA	B	3003	-	-	0/2/19/22	0/1/1/1
6	PEG	D	7001	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	5001	KTL	CAN-SAY	-7.84	1.66	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	5001	KTL	CAN-SAY	-7.09	1.67	1.82
9	D	5001	KTL	OAP-SAZ	2.40	1.64	1.57

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	NAG	C1-O5-C5	7.46	122.19	112.19
4	B	2001	NAG	C1-O5-C5	5.76	119.91	112.19
4	A	4001	NAG	C1-C2-N2	5.23	118.67	110.43
4	A	4001	NAG	C4-C3-C2	-4.99	103.71	111.02
4	A	4001	NAG	O5-C1-C2	-4.03	105.06	111.29

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4001	NAG	C1-C2-N2-C7
9	B	5001	KTL	OAB-CAM-CAW-CAU
9	B	5001	KTL	OAB-CAM-CAW-SAY
9	B	5001	KTL	OAF-CAT-CAV-CAX
9	D	5001	KTL	OAB-CAM-CAW-CAU

There are no ring outliers.

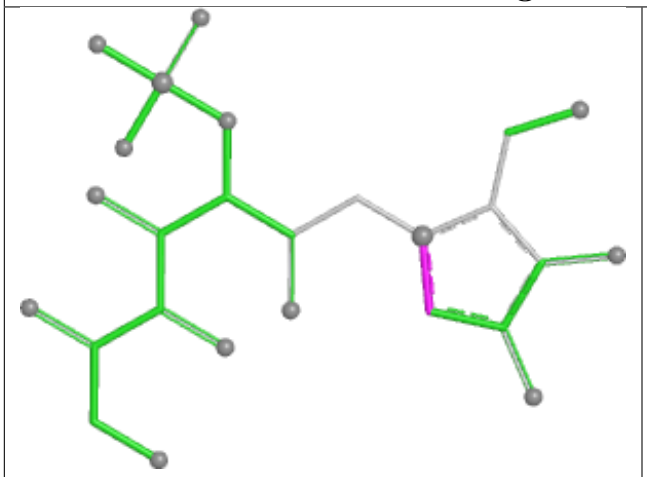
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	7001	PEG	3	0
6	C	7001	PEG	3	0
9	D	5001	KTL	2	0
8	B	3003	BMA	1	0

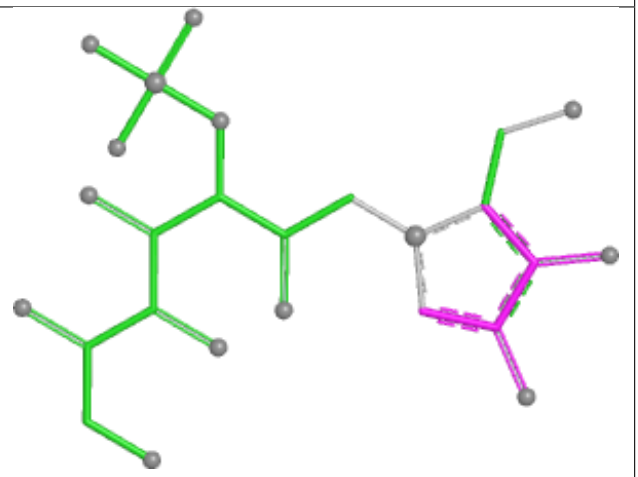
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

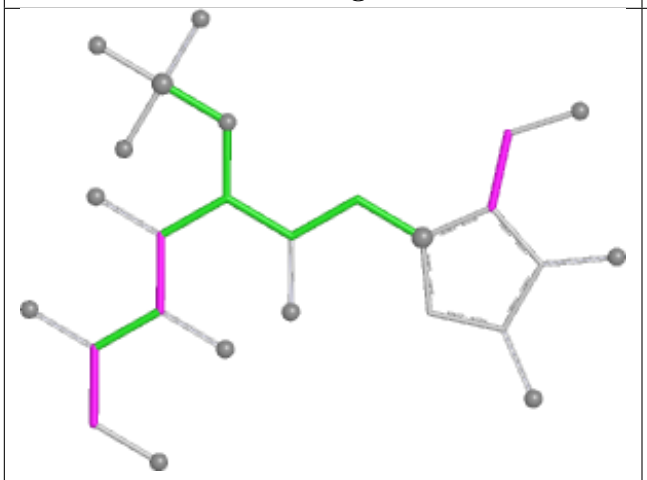
Ligand KTL B 5001



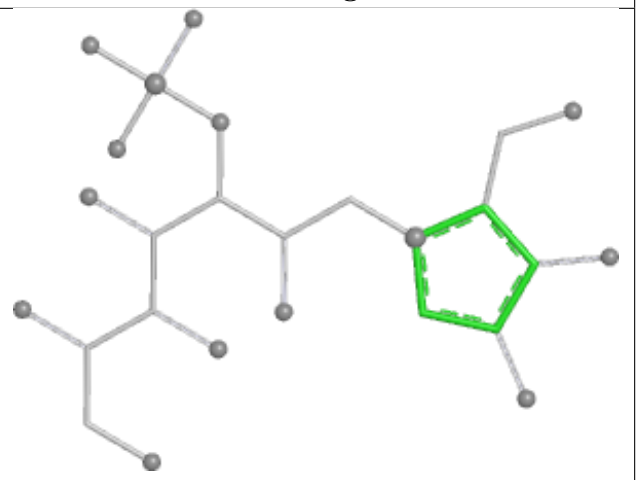
Bond lengths



Bond angles

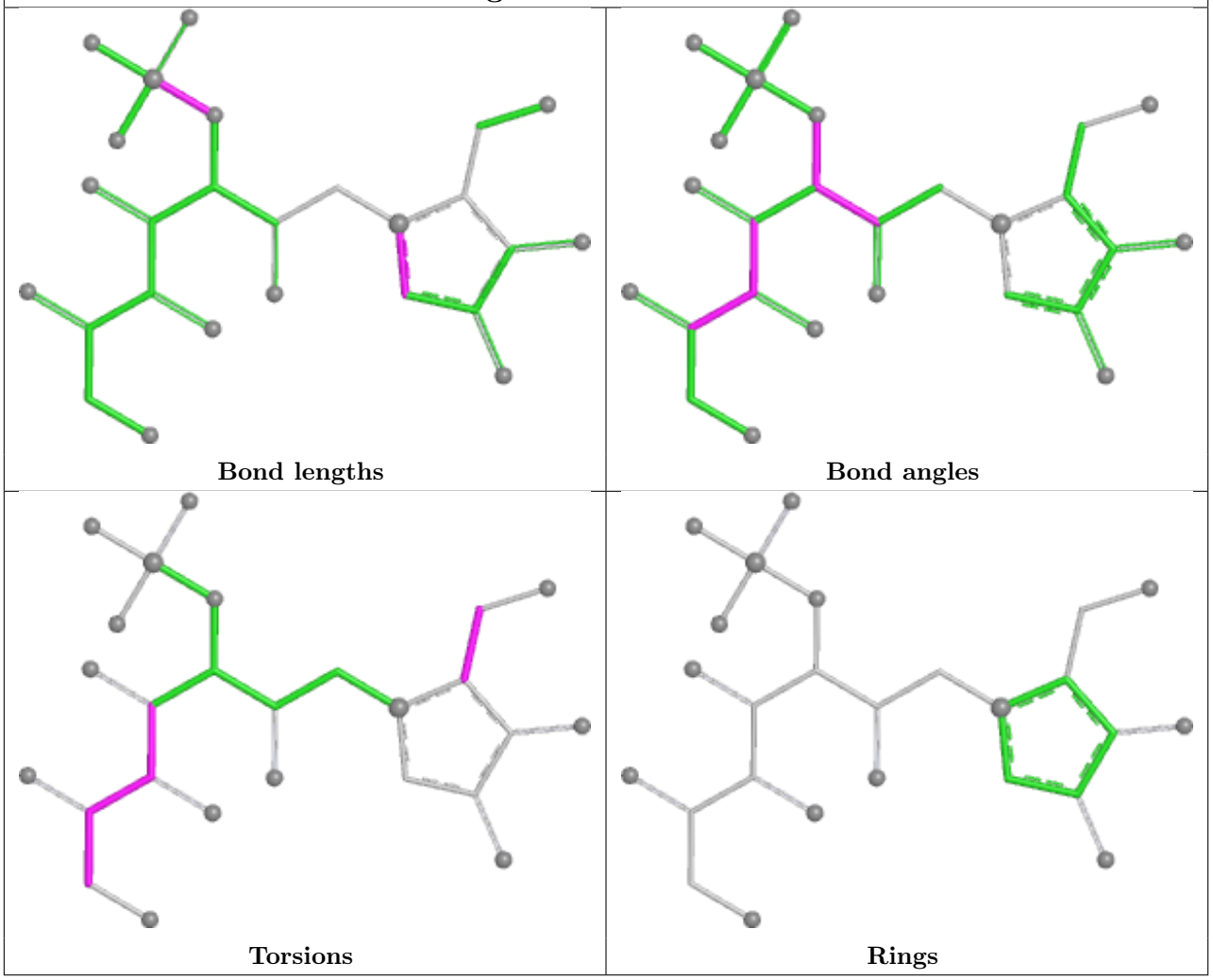


Torsions



Rings

Ligand KTL D 5001



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

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

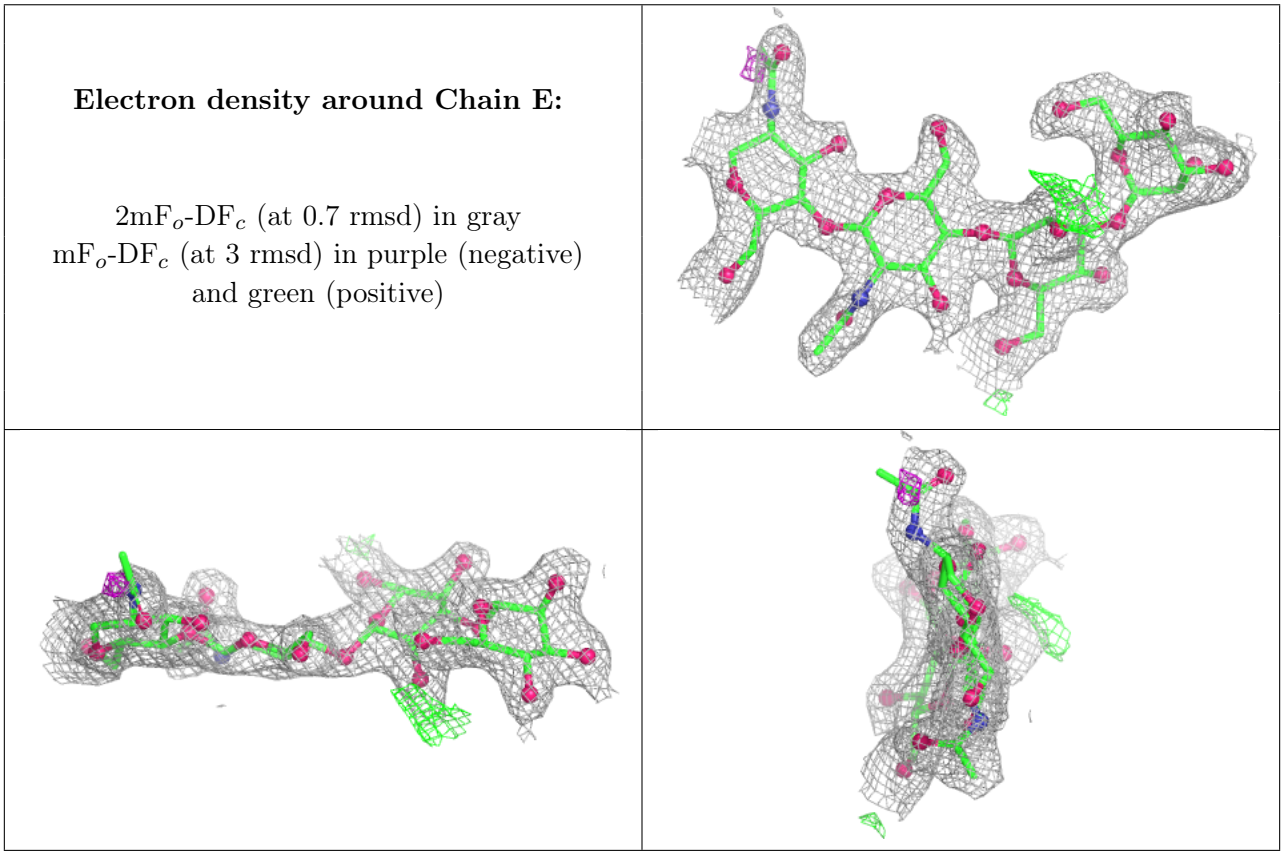
6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

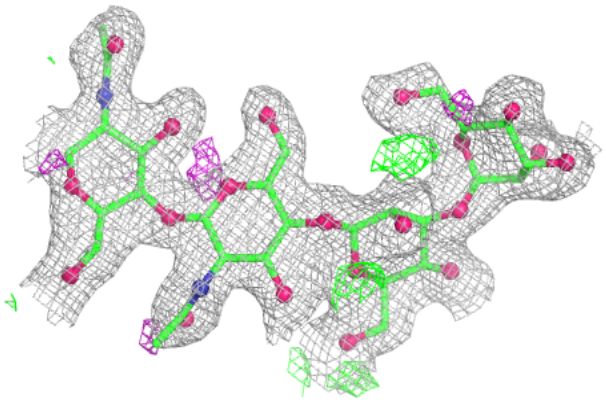
Unable to reproduce the depositors R factor - this section is therefore empty.

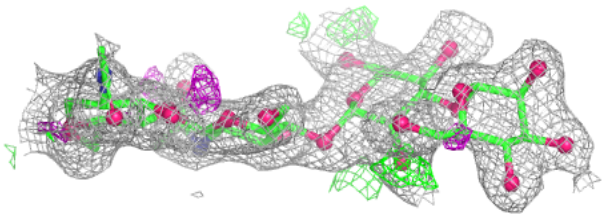
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

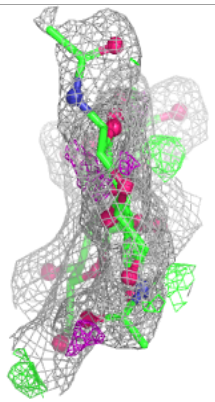


Electron density around Chain H:

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

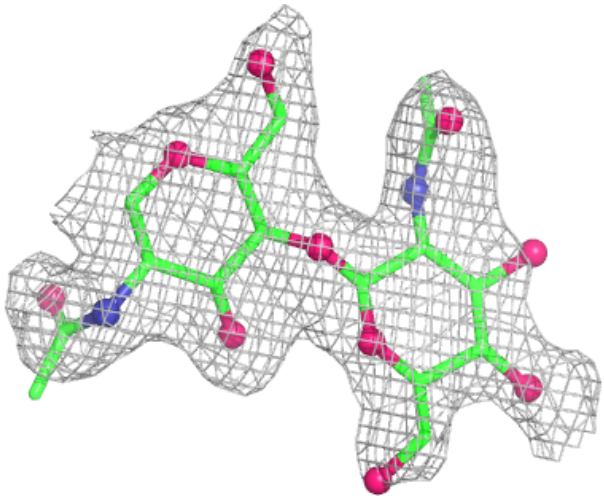


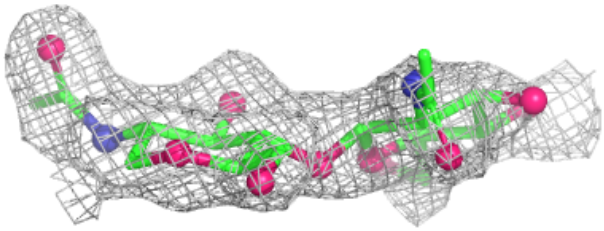


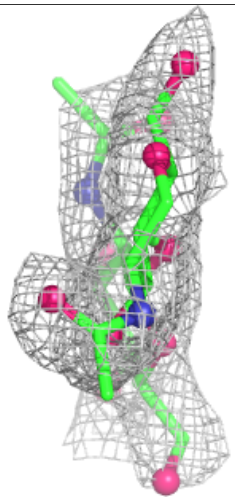


Electron density around Chain F:

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

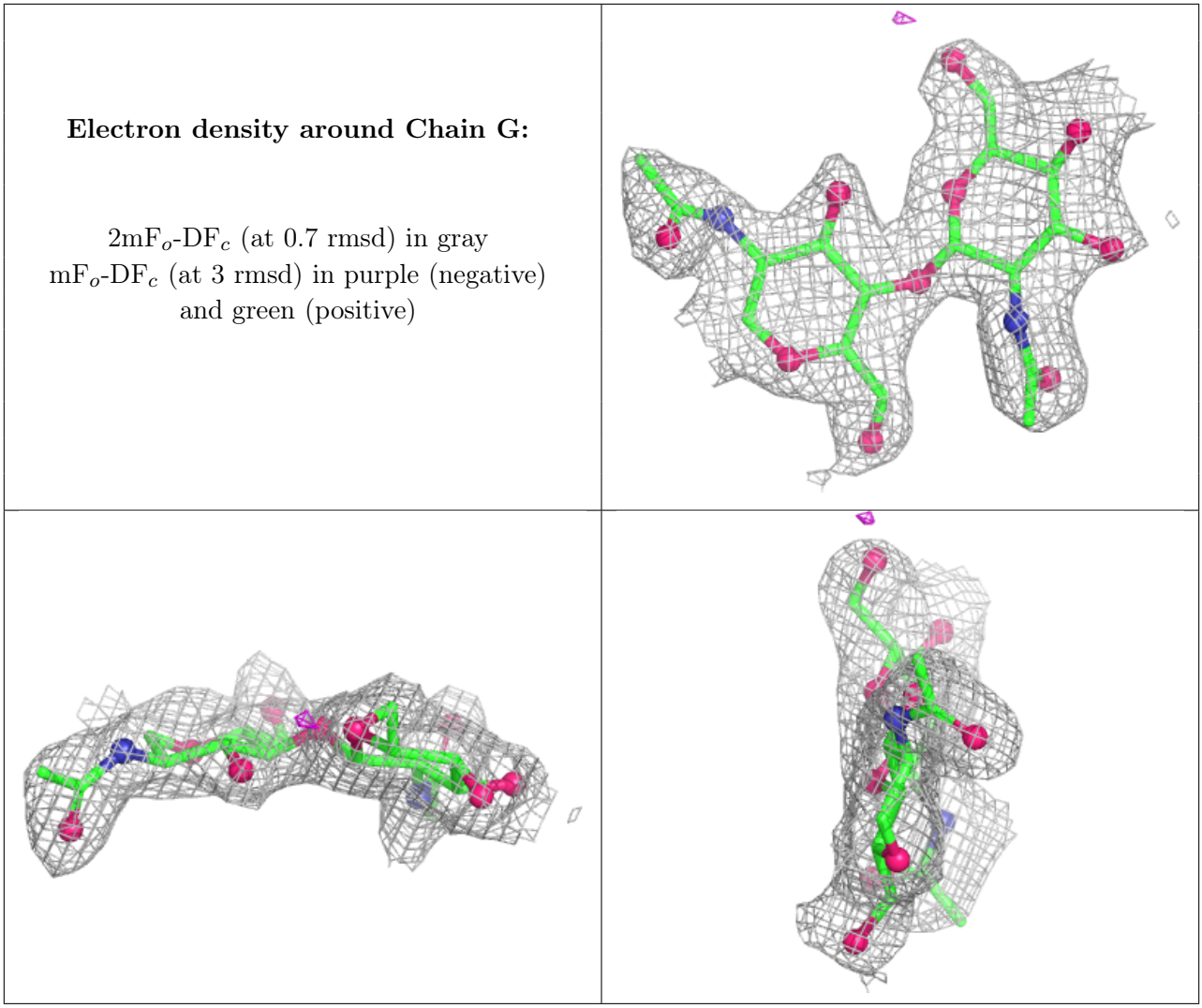






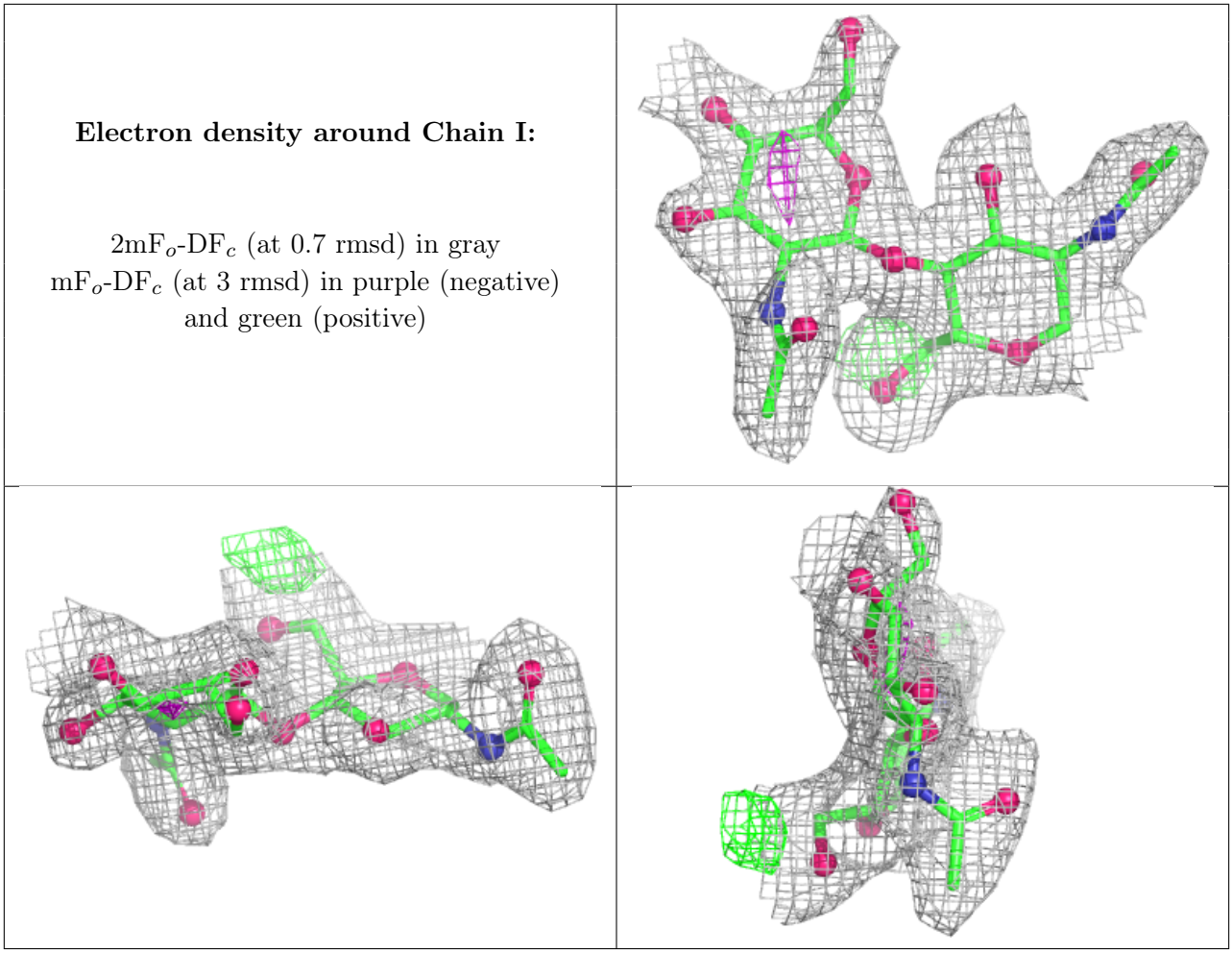
Electron density around Chain G:

$2mF_o$-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 I:

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



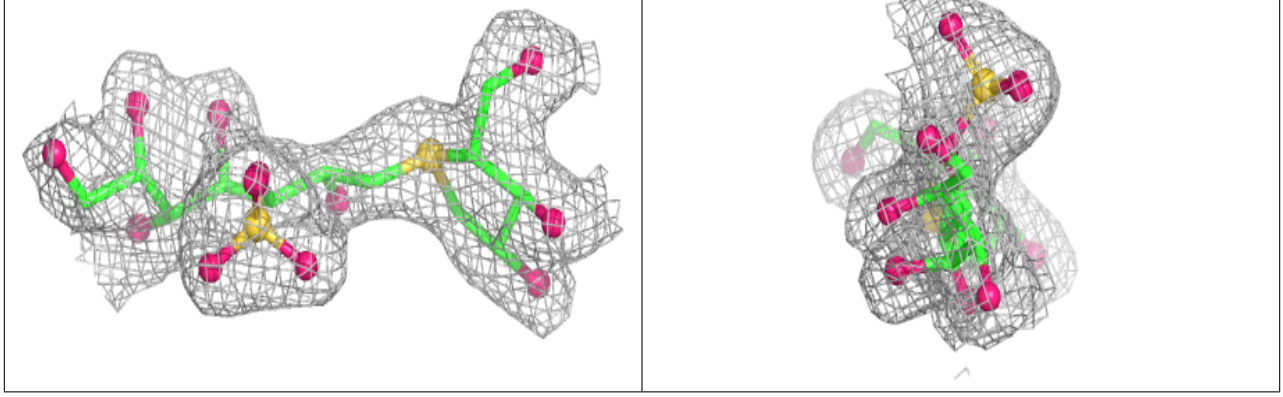
6.4 Ligands

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

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

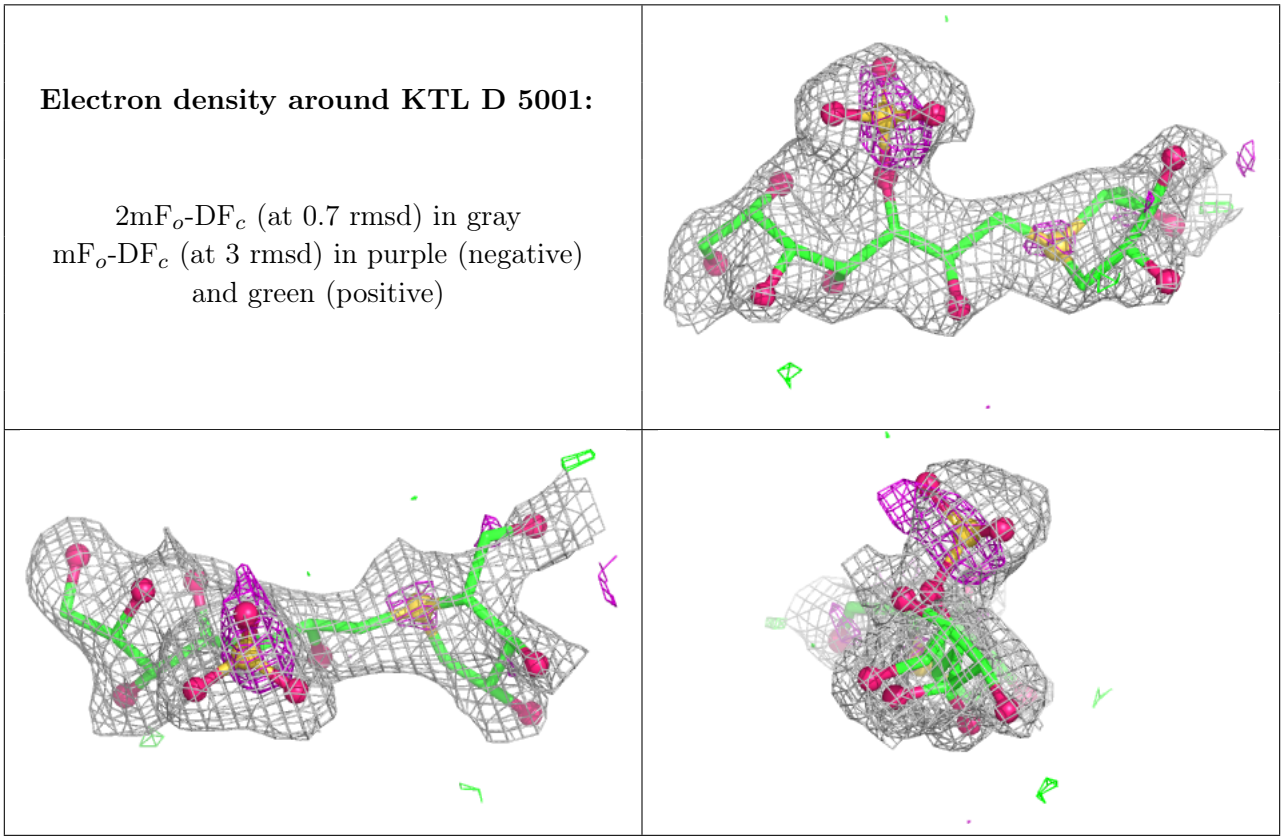
Electron density around KTL B 5001:

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



Electron density around KTL D 5001:

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



6.5 Other polymers (i)

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