



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:42 PM UTC

PDB ID : 3LPP / pdb_00003lpp
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

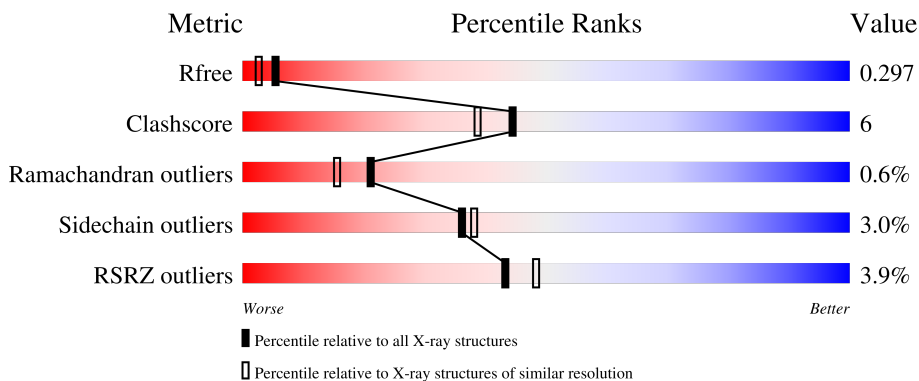
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.




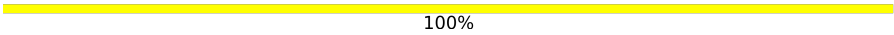

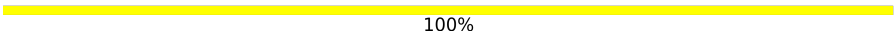
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 $\leq 5\%$. 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	898	 3% 84% 12% ..
1	B	898	 3% 82% 13% ..
1	C	898	 3% 84% 13% ..
1	D	898	 6% 79% 14% . 5%
2	E	4	 100%

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Mol	Chain	Length	Quality of chain
2	H	4	 25% 75%
3	F	2	 100%
3	G	2	 50% 50%
3	I	2	 100%

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

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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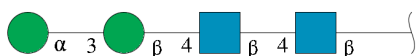
Chain	Residue	Modelled	Actual	Comment	Reference
C	8	HIS	-	expression tag	UNP P14410
C	9	HIS	-	expression tag	UNP P14410
C	10	GLY	-	expression tag	UNP P14410
C	11	GLU	-	expression tag	UNP P14410
C	12	PHE	-	expression tag	UNP P14410
C	13	ASP	-	expression tag	UNP P14410
C	14	ILE	-	expression tag	UNP P14410
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
			Total	C	N	O			
2	E	4	50	28	2	20	0	0	0
2	H	4	50	28	2	20	0	0	0

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



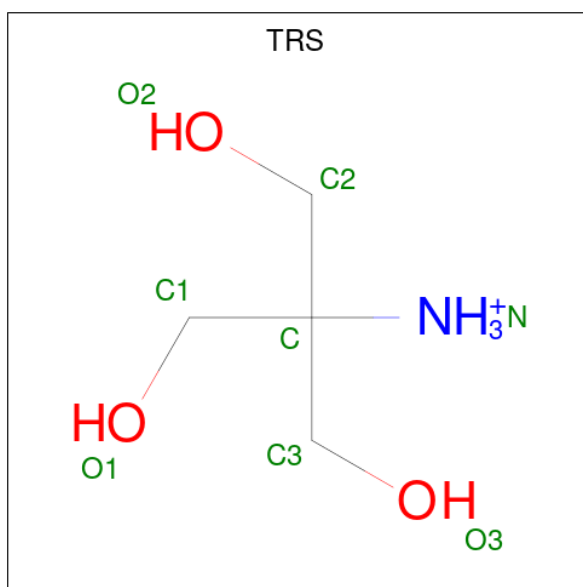
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0
3	I	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



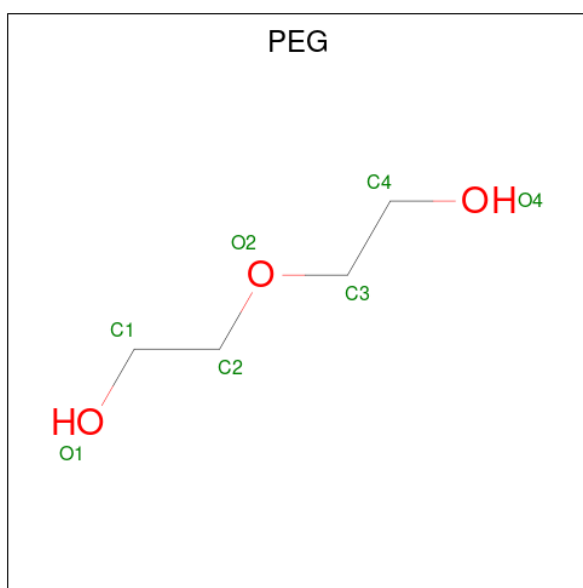
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total 14	8	1	5	0	0
4	A	1	Total 14	8	1	5	0	0
4	B	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0

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



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

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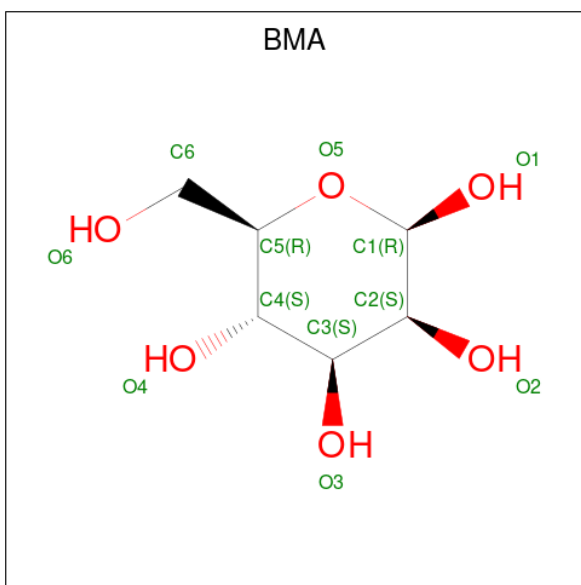
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is beta-D-mannopyranose (CCD ID: BMA) (formula: C₆H₁₂O₆).



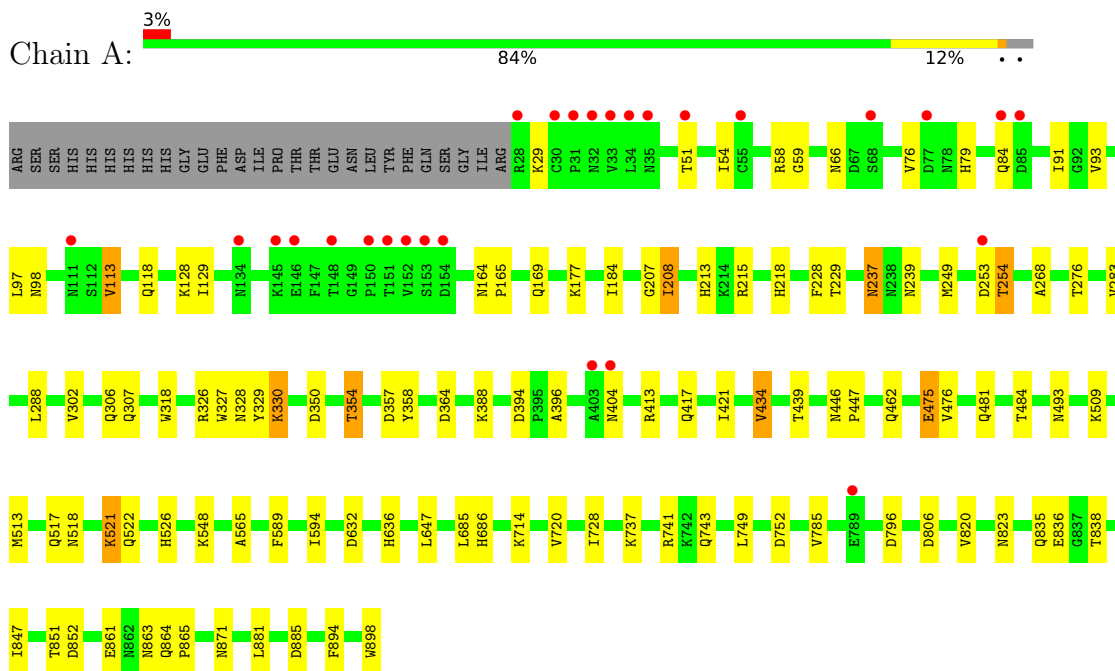
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
8	B	1	Total	C	O	0	0
			11	6	5		

- 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 (CCD ID: KTL) (formula: C₁₂H₂₄O₁₂S₂).

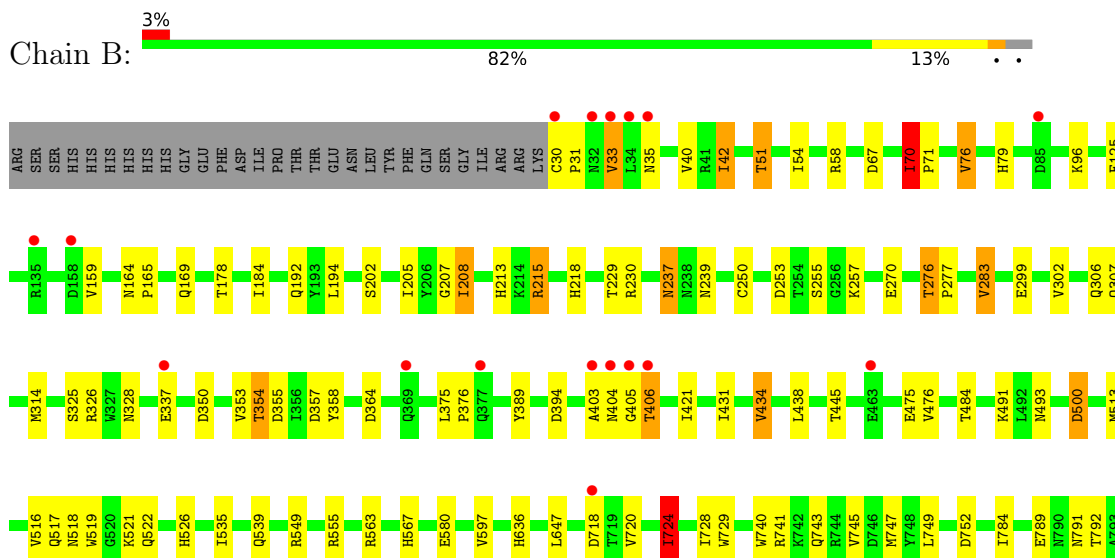
3 Residue-property plots [i](#)

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: Sucrase-isomaltase

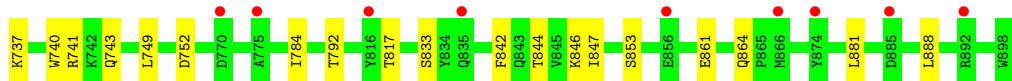
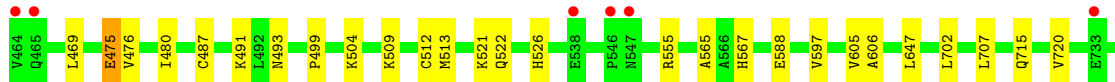
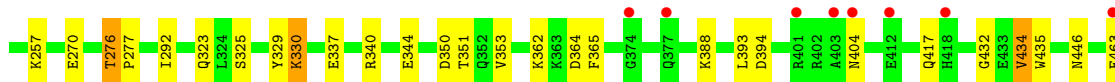
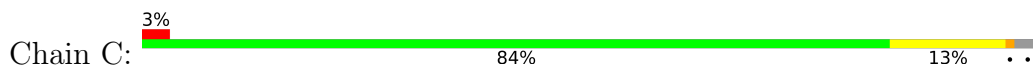


- Molecule 1: Sucrase-isomaltase

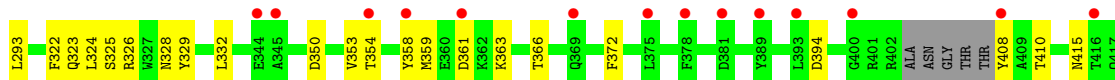
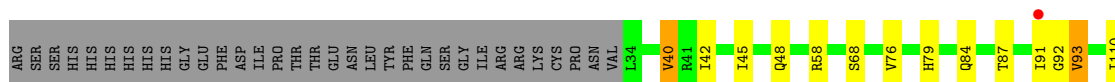
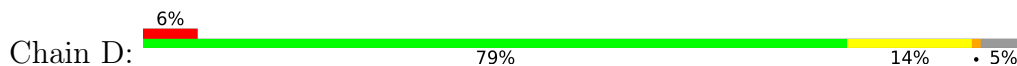




• Molecule 1: Sucrase-isomaltase



• Molecule 1: Sucrase-isomaltase





- 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: 100%



- 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: 25% 75%



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

Chain F: 100%



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

Chain G: 50% 50%



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

Chain I: 100%



4 Data and refinement statistics

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 19.95 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.95-2.15) 94.7 (19.95-2.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.15Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.223 (Not available) , 0.297	Depositor DCC
R_{free} test set	10150 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtrriage
Anisotropy	0.357	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, TRS, KTL, PEG, NAG, CL, MAN

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	0.71	0/7236	0.85	3/9868 (0.0%)
1	B	0.67	1/7216 (0.0%)	0.87	8/9843 (0.1%)
1	C	0.66	0/7230	0.83	5/9861 (0.1%)
1	D	0.54	0/7079	0.82	5/9653 (0.1%)
All	All	0.65	1/28761 (0.0%)	0.84	21/39225 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	VAL	CA-CB	5.15	1.61	1.54

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	GLU	N-CA-C	6.70	118.67	111.36
1	B	862	ASN	CB-CA-C	-6.27	108.70	117.23
1	D	718	ASP	N-CA-C	-6.05	106.44	113.88
1	B	718	ASP	N-CA-C	-5.90	106.41	113.97
1	B	70	ILE	CB-CA-C	5.87	116.40	110.94

There are no chirality outliers.

There are no planarity outliers.

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	7035	0	6734	73	0
1	B	7015	0	6711	90	0
1	C	7029	0	6724	71	0
1	D	6882	0	6573	97	0
2	E	50	0	43	0	0
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	1	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	330	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 330 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	1.14	0.94
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%)	18	13
1	B	867/898 (96%)	825 (95%)	36 (4%)	6 (1%)	18	13
1	C	869/898 (97%)	825 (95%)	38 (4%)	6 (1%)	18	13
1	D	847/898 (94%)	800 (94%)	45 (5%)	2 (0%)	43	44
All	All	3452/3592 (96%)	3281 (95%)	151 (4%)	20 (1%)	21	15

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%)	754 (98%)	18 (2%)	44	49
1	B	770/797 (97%)	744 (97%)	26 (3%)	32	33
1	C	771/797 (97%)	753 (98%)	18 (2%)	44	49
1	D	751/797 (94%)	721 (96%)	30 (4%)	28	27
All	All	3064/3188 (96%)	2972 (97%)	92 (3%)	36	38

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	737	LYS
1	D	283	VAL
1	C	817	THR
1	D	87	THR
1	D	415	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	493	ASN
1	D	119	ASN
1	C	526	HIS
1	C	823	ASN
1	D	192	GLN

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	2,1	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	2,1	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	2,1	-	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	2,1	-	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(°)	Ideal(°)
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:

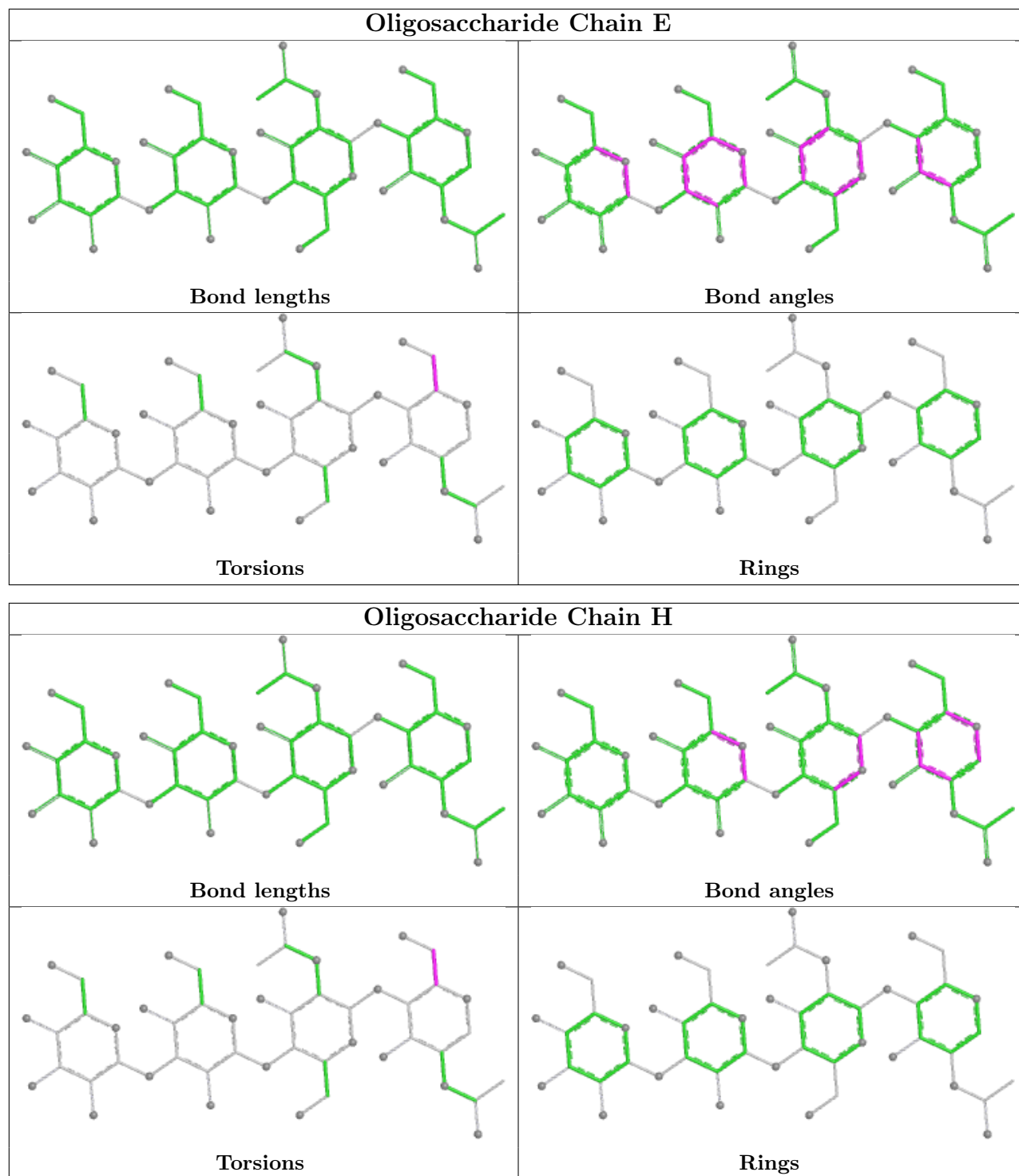
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6

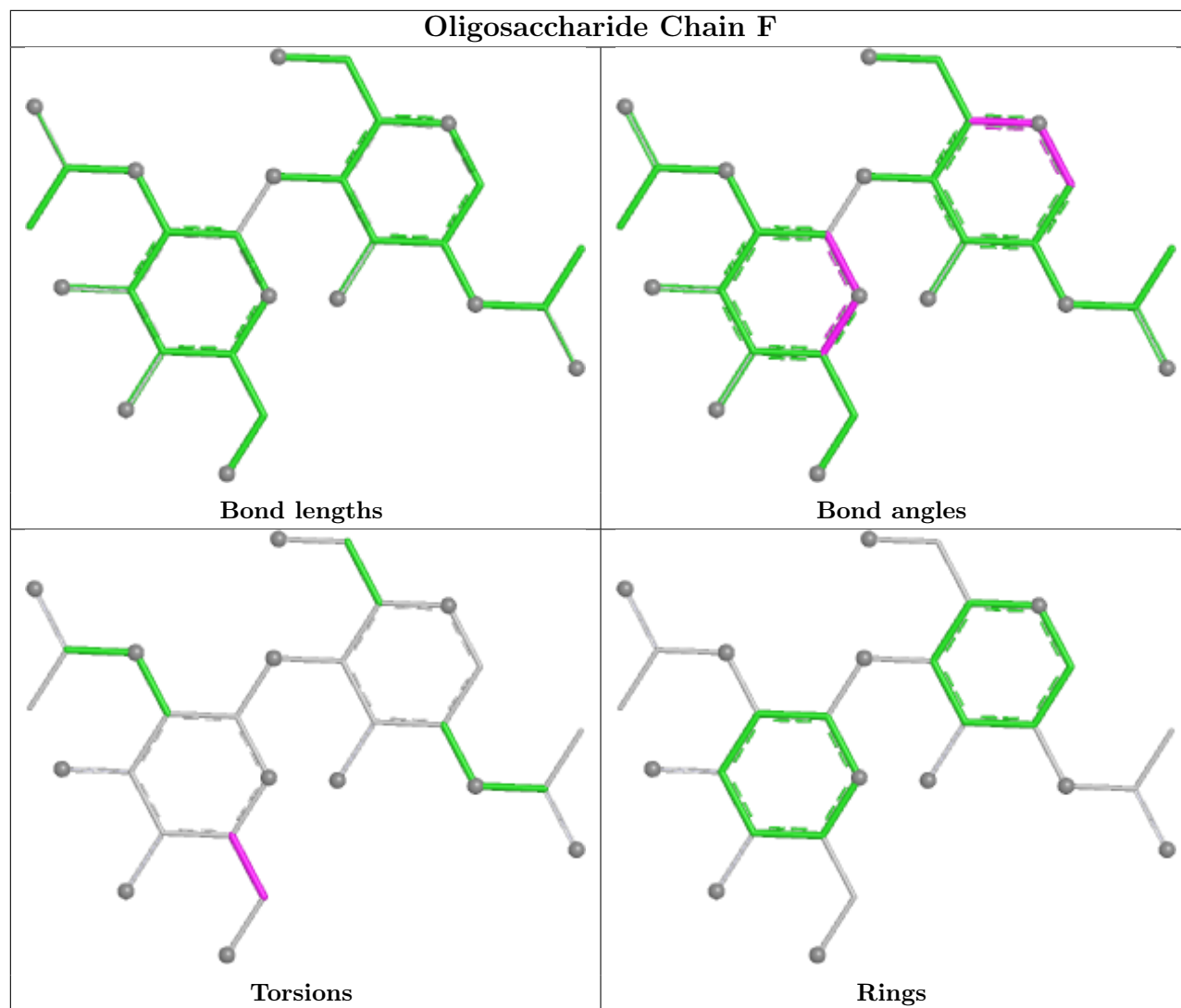
There are no ring outliers.

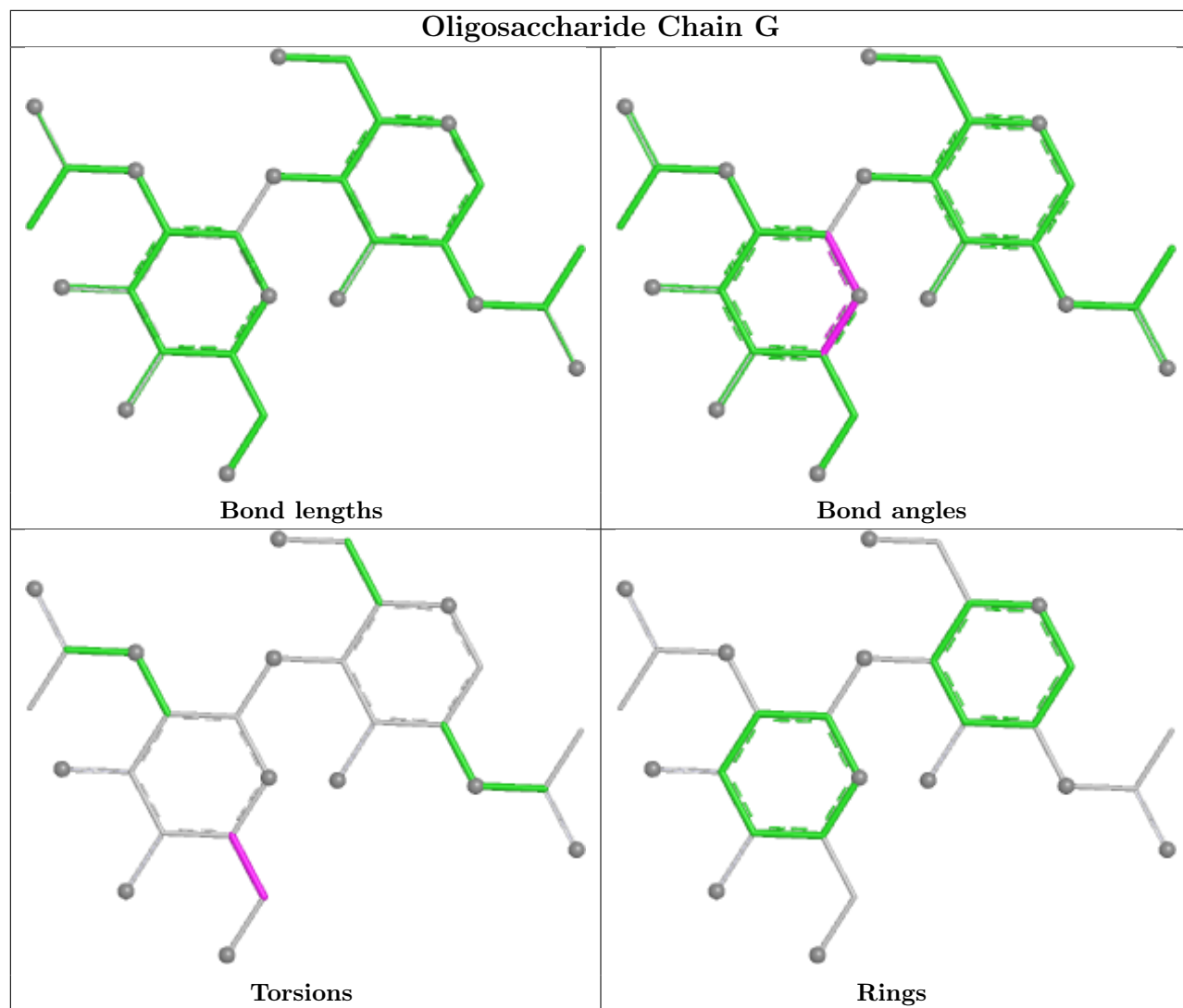
1 monomer is involved in 1 short contact:

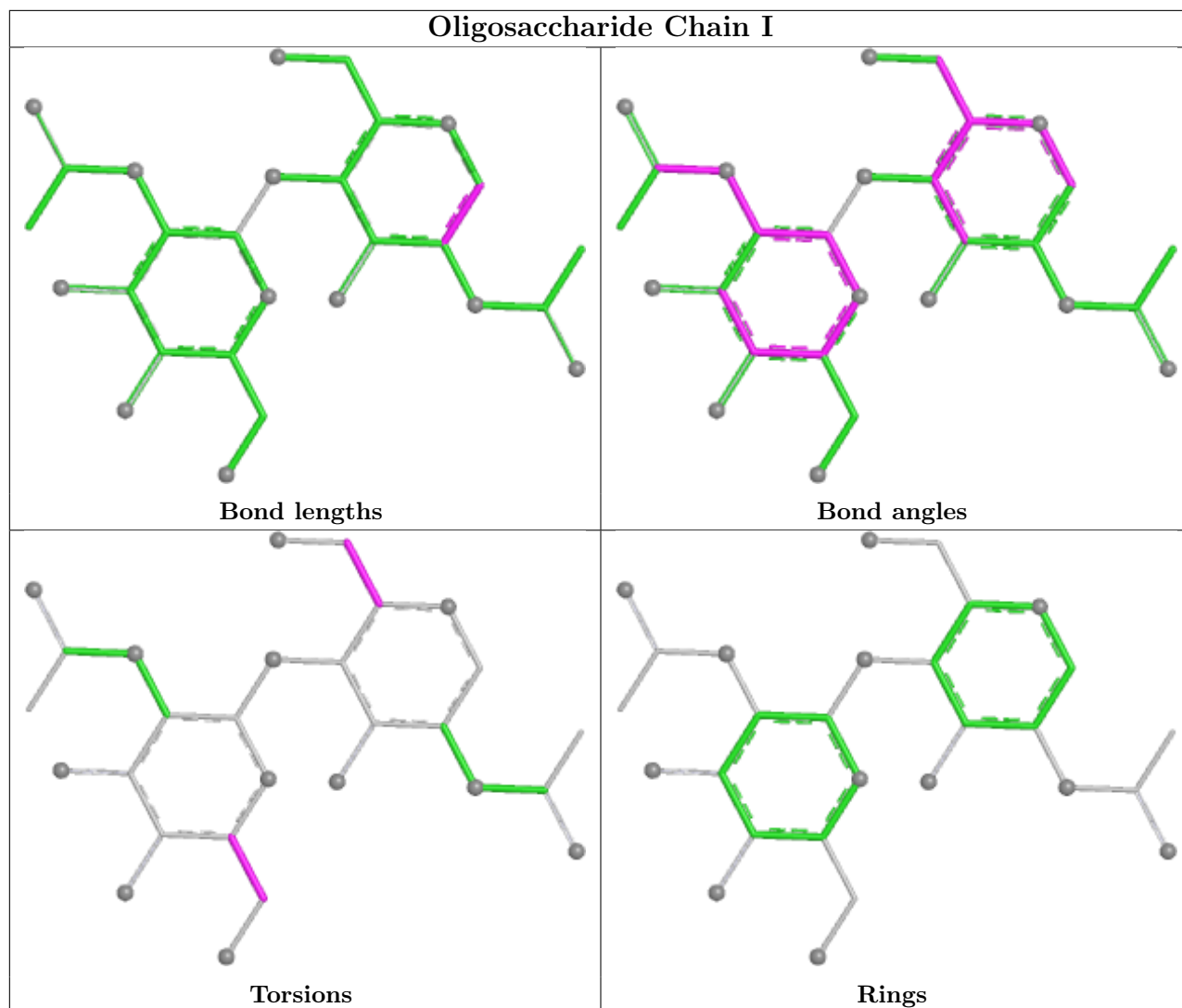
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0

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









5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	NAG	B	2001	1	14,14,15	0.49	0	17,19,21	2.14	4 (23%)
4	NAG	C	3001	1	14,14,15	0.48	0	17,19,21	1.28	1 (5%)
6	PEG	C	7001	-	6,6,6	0.46	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	2001	1	14,14,15	0.56	0	17,19,21	0.84	1 (5%)
5	TRS	C	6001	-	7,7,7	0.33	0	9,9,9	0.45	0
6	PEG	A	7001	-	6,6,6	0.53	0	5,5,5	0.39	0
6	PEG	B	7001	-	6,6,6	0.38	0	5,5,5	0.49	0
6	PEG	D	7001	-	6,6,6	0.44	0	5,5,5	0.28	0
4	NAG	A	4001	1	14,14,15	0.70	0	17,19,21	2.40	5 (29%)
9	KTL	B	5001	-	21,26,26	1.77	1 (4%)	25,38,38	1.13	3 (12%)
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
5	TRS	A	6001	-	7,7,7	0.48	0	9,9,9	1.05	1 (11%)
4	NAG	C	4001	1	14,14,15	0.66	0	17,19,21	1.20	1 (5%)
9	KTL	D	5001	-	21,26,26	1.86	2 (9%)	25,38,38	0.97	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	C	3001	1	-	0/6/23/26	0/1/1/1
6	PEG	C	7001	-	-	1/4/4/4	-
4	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
5	TRS	C	6001	-	-	0/9/9/9	-
6	PEG	A	7001	-	-	2/4/4/4	-
6	PEG	B	7001	-	-	3/4/4/4	-
6	PEG	D	7001	-	-	1/4/4/4	-
4	NAG	A	4001	1	-	3/6/23/26	0/1/1/1
9	KTL	B	5001	-	-	6/28/45/45	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
5	TRS	A	6001	-	-	0/9/9/9	-
4	NAG	C	4001	1	-	2/6/23/26	0/1/1/1
9	KTL	D	5001	-	-	12/28/45/45	0/1/1/1

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(°)	Ideal(°)
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

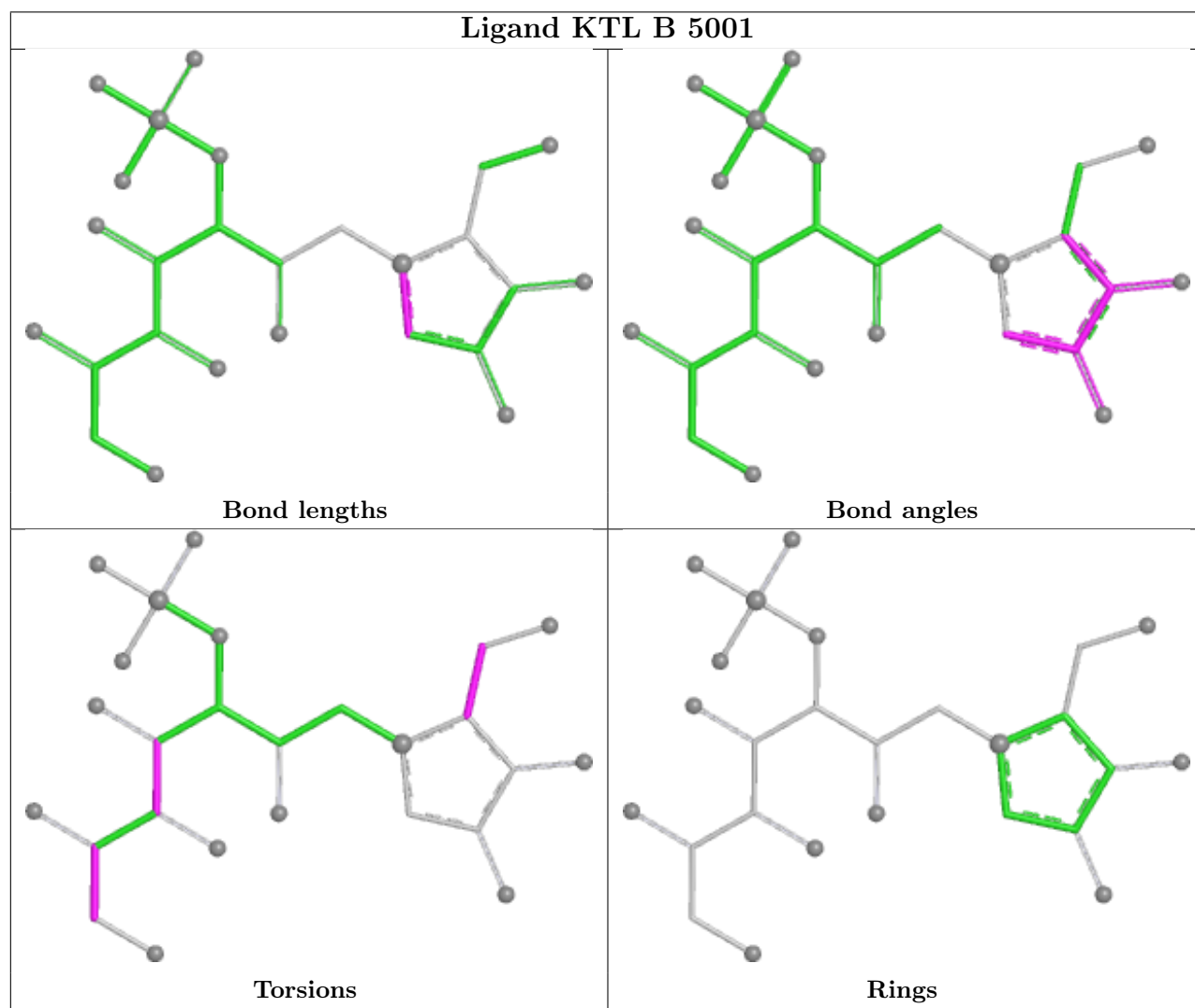
There are no ring outliers.

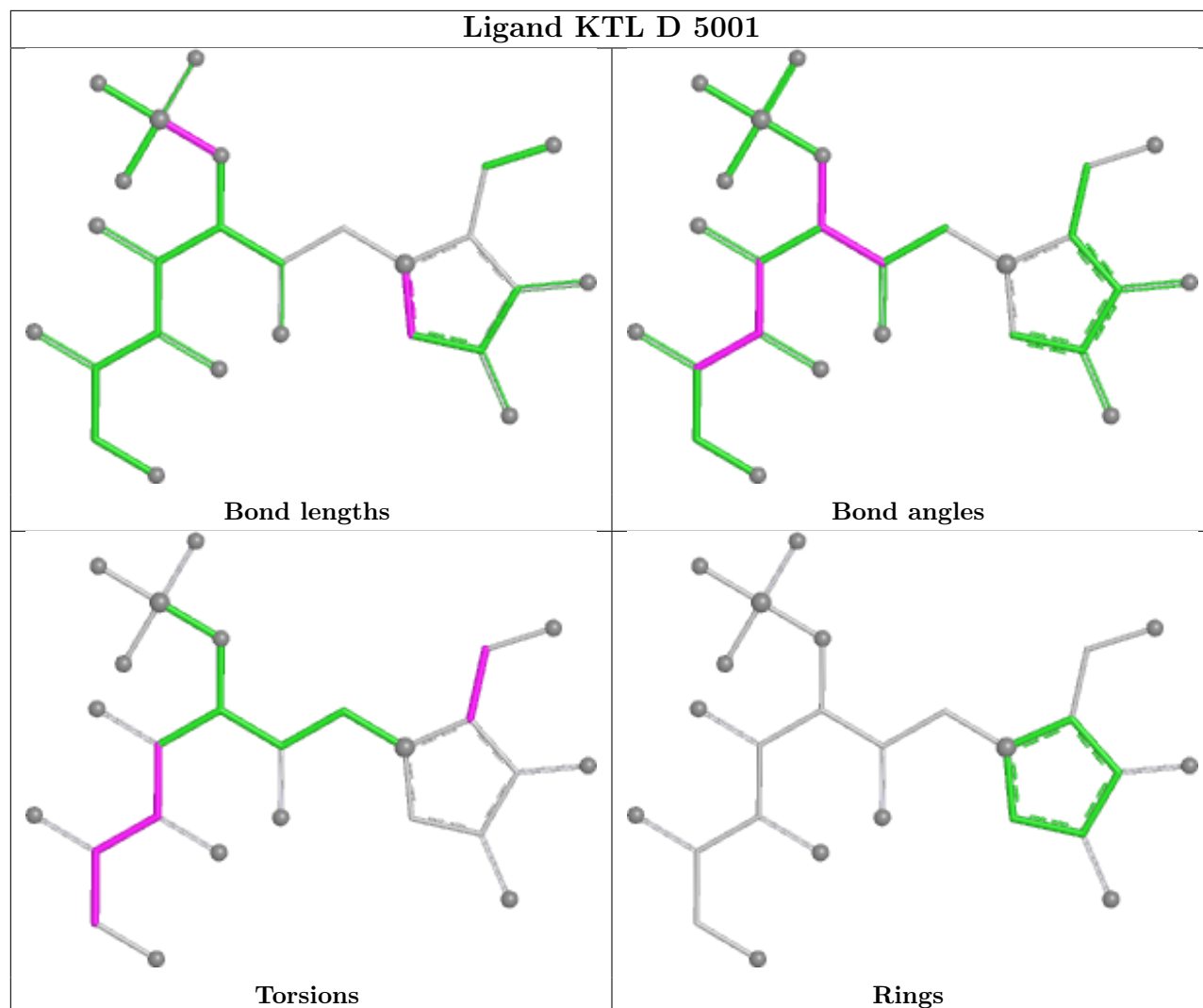
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	7001	PEG	3	0
6	B	7001	PEG	3	0
9	B	5001	KTL	1	0
8	B	3003	BMA	1	0
9	D	5001	KTL	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	871/898 (96%)	0.15	27 (3%) 51 55	4, 10, 19, 36	0
1	B	869/898 (96%)	0.19	28 (3%) 50 54	3, 11, 20, 37	0
1	C	871/898 (96%)	0.27	28 (3%) 50 54	5, 11, 21, 30	0
1	D	853/898 (94%)	0.79	53 (6%) 26 30	3, 11, 20, 27	0
All	All	3464/3592 (96%)	0.35	136 (3%) 43 48	3, 11, 20, 37	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	865	PRO	4.8
1	B	403	ALA	4.8
1	D	150	PRO	4.5
1	A	148	THR	4.3
1	B	32	ASN	4.3

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

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

6.3 Carbohydrates [i](#)

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, 95th 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.

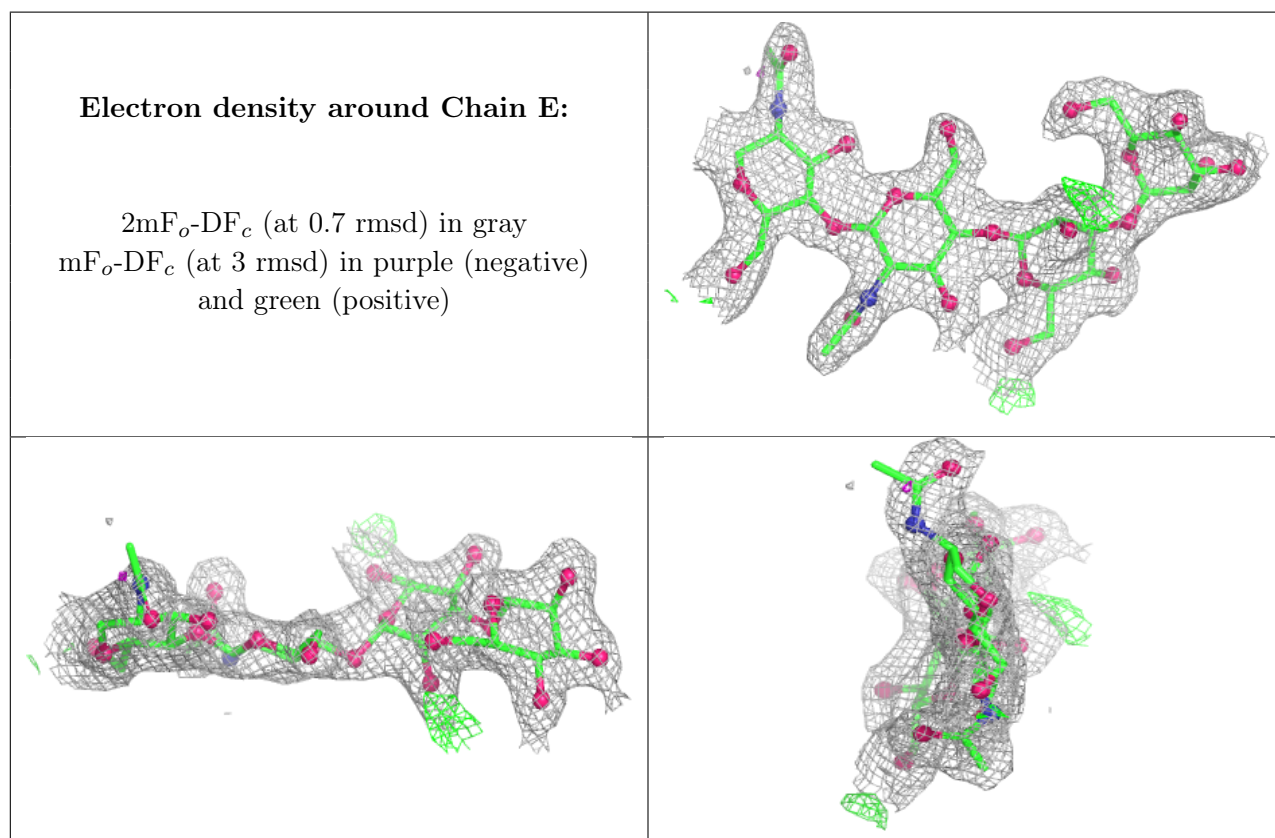
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	I	2	14/15	0.75	0.11	24,27,31,32	0
2	NAG	H	1	14/15	0.80	0.10	14,16,17,19	0

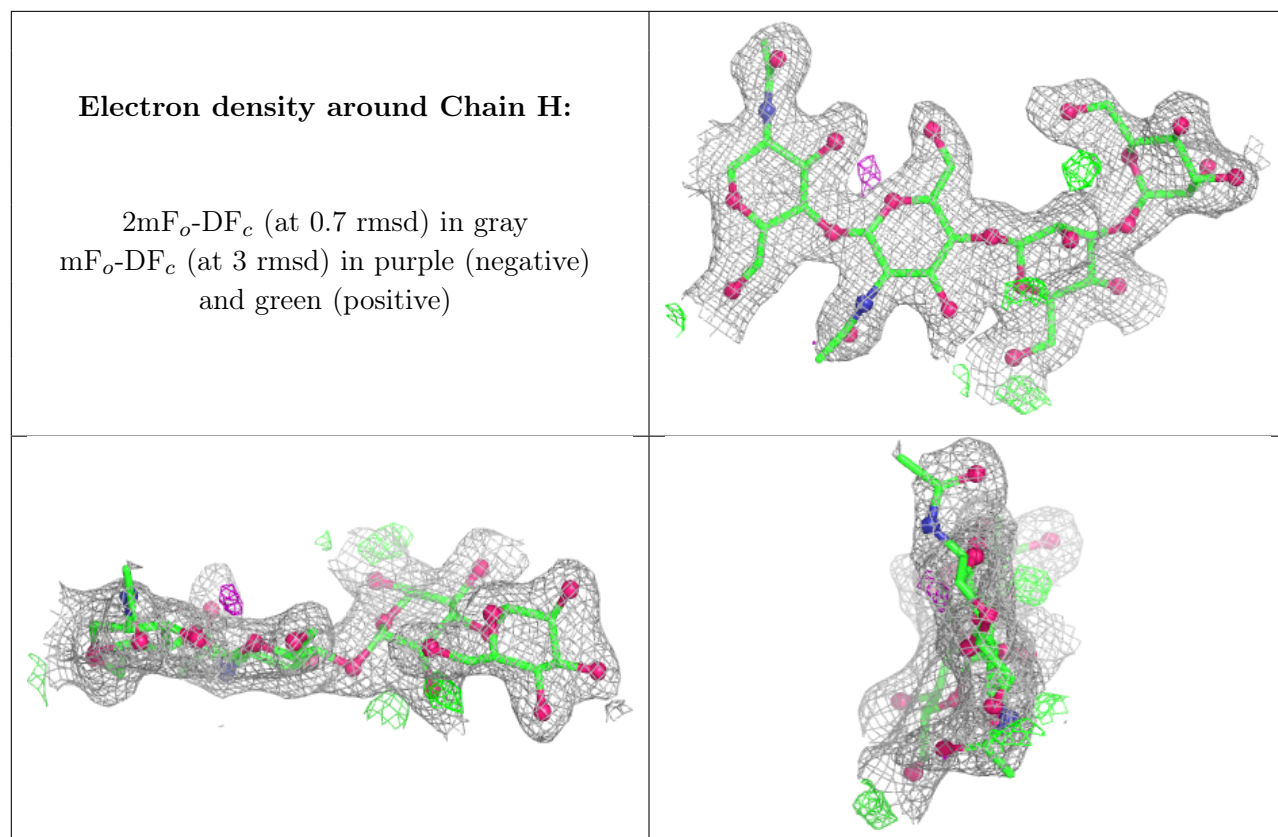
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	E	1	14/15	0.83	0.10	16,20,24,25	0
3	NAG	F	2	14/15	0.85	0.10	24,27,29,30	0
3	NAG	G	2	14/15	0.86	0.10	25,27,28,29	0
3	NAG	I	1	14/15	0.88	0.08	4,14,19,23	0
2	BMA	H	3	11/12	0.88	0.08	14,16,20,23	0
2	NAG	E	2	14/15	0.89	0.08	12,13,18,20	0
2	MAN	H	4	11/12	0.89	0.08	11,13,16,16	0
2	NAG	H	2	14/15	0.91	0.07	12,15,18,21	0
2	BMA	E	3	11/12	0.91	0.07	15,17,18,20	0
3	NAG	G	1	14/15	0.91	0.07	19,20,22,24	0
3	NAG	F	1	14/15	0.92	0.08	9,13,15,18	0
2	MAN	E	4	11/12	0.93	0.06	15,17,18,19	0

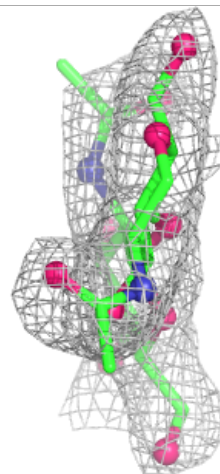
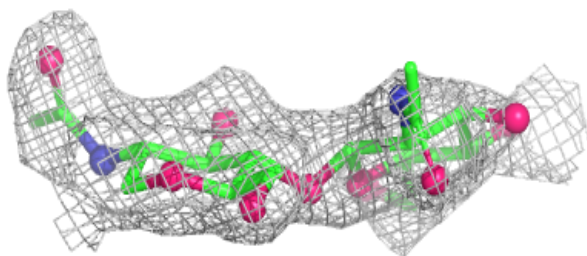
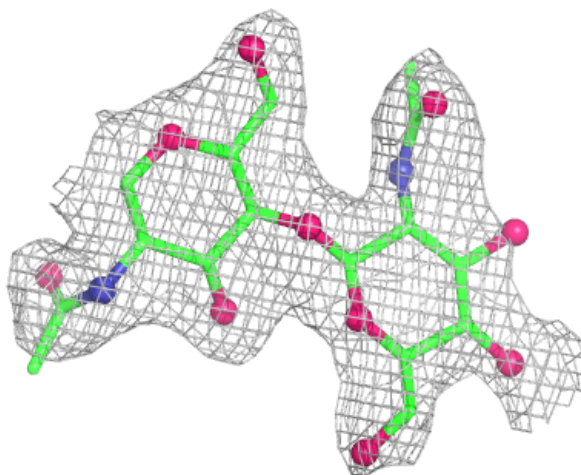
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





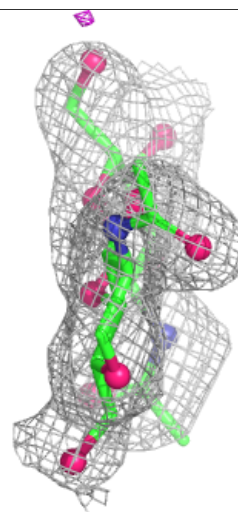
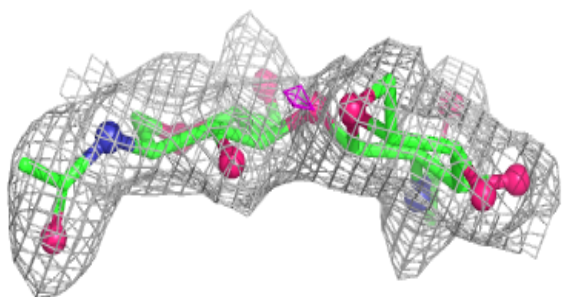
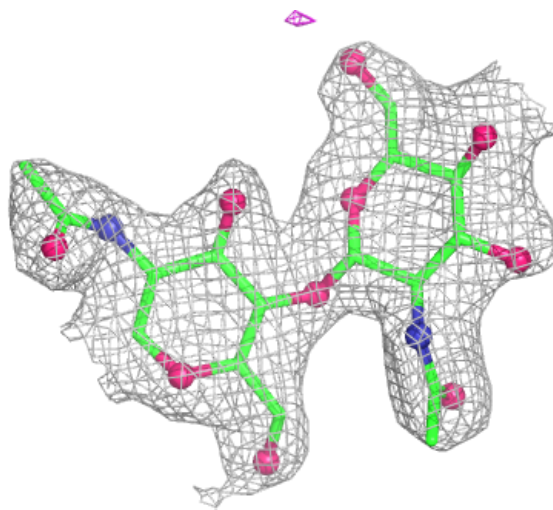
Electron density around Chain F:

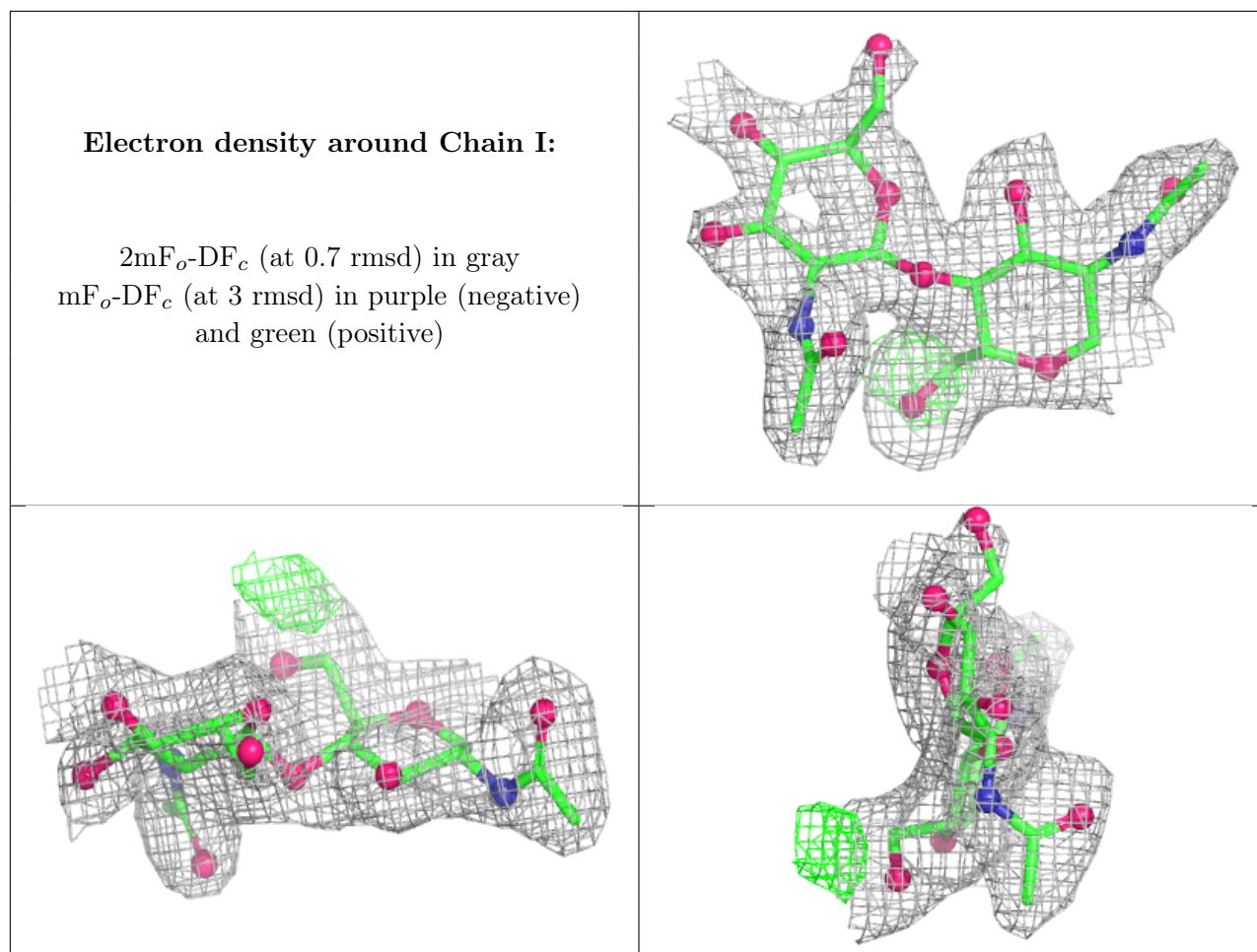
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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, 95th 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.

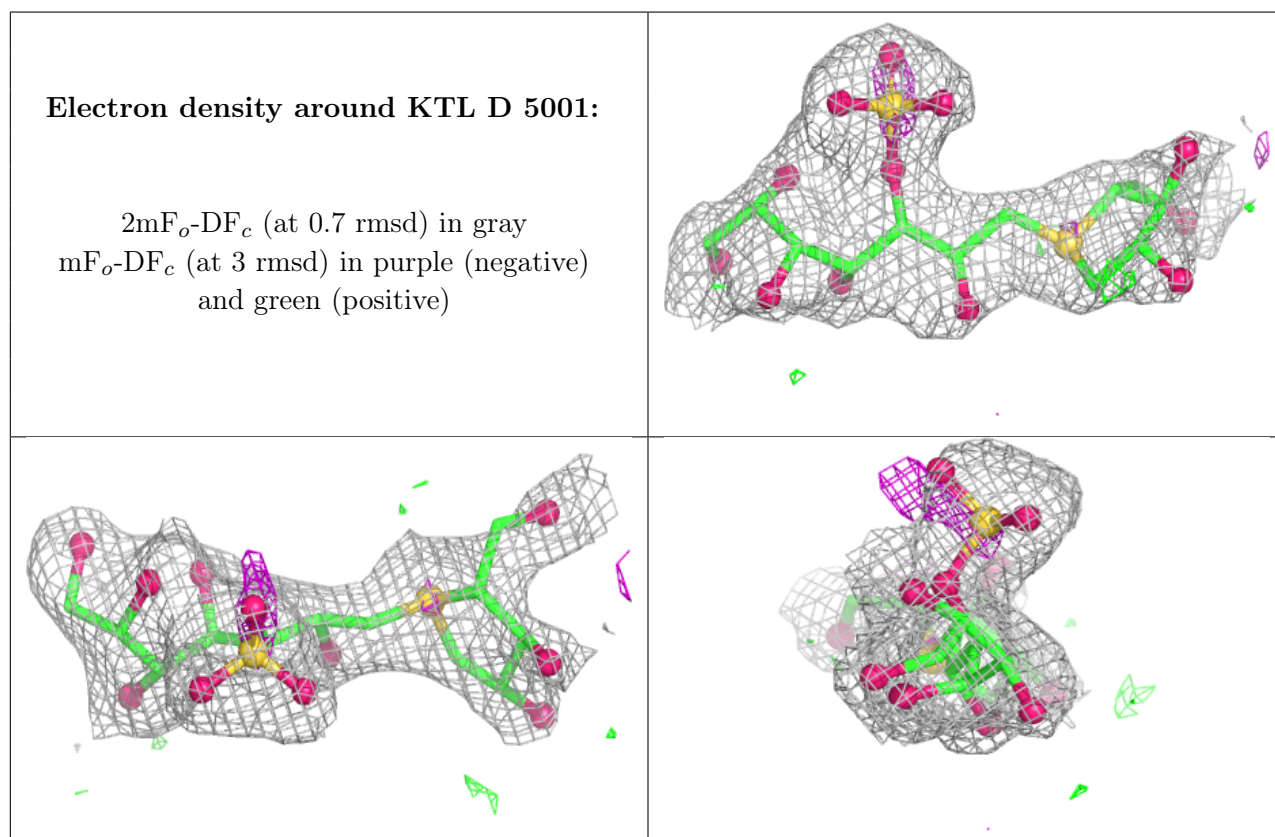
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	BMA	B	3003	11/12	0.62	0.19	61,62,63,63	0
4	NAG	A	2001	14/15	0.68	0.12	31,33,34,34	0
4	NAG	C	4001	14/15	0.73	0.12	35,40,41,42	0
4	NAG	A	4001	14/15	0.80	0.10	24,27,28,30	0
4	NAG	C	3001	14/15	0.80	0.10	22,25,26,27	0
6	PEG	D	7001	7/7	0.82	0.12	37,37,38,38	0
6	PEG	A	7001	7/7	0.85	0.13	21,22,25,25	0
6	PEG	C	7001	7/7	0.85	0.12	18,22,25,27	0
6	PEG	B	7001	7/7	0.87	0.13	20,20,21,22	0
5	TRS	A	6001	8/8	0.87	0.11	10,12,13,15	0
5	TRS	C	6001	8/8	0.87	0.09	20,20,20,21	0

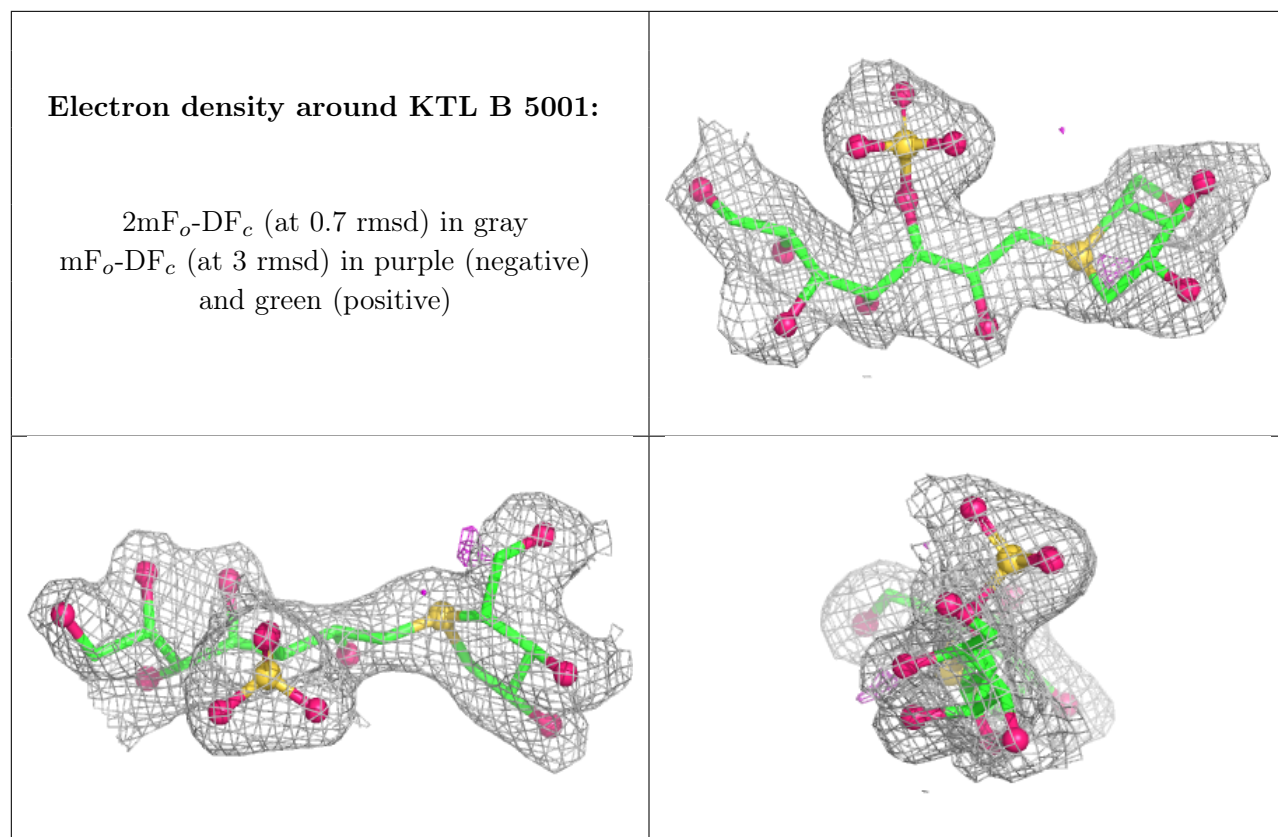
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	C	2001	14/15	0.87	0.08	16,22,26,27	0
9	KTL	D	5001	26/26	0.88	0.10	20,24,26,27	0
4	NAG	B	2001	14/15	0.89	0.08	9,16,18,21	0
9	KTL	B	5001	26/26	0.93	0.08	10,18,23,25	0
7	CL	A	8001	1/1	0.96	0.09	3,3,3,3	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.