



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 10:27 PM UTC

PDB ID : 6TS2 / pdb_00006ts2
Title : Truncated version of Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) lacking domain TRXL2 (417-650).
Authors : Roversi, P.; Zitzmann, N.
Deposited on : 2019-12-19
Resolution : 5.74 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)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

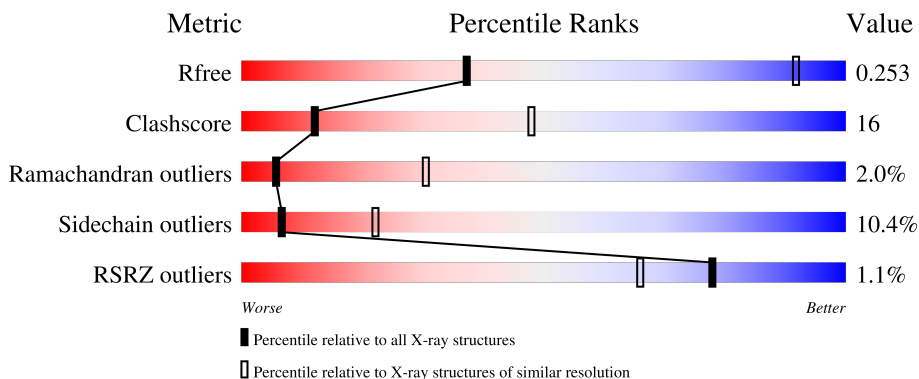
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.74 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.





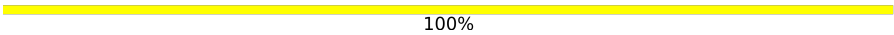
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (7.46-4.00)
Clashscore	190562	1171 (7.46-4.00)
Ramachandran outliers	187476	1005 (7.40-4.00)
Sidechain outliers	187428	1004 (7.50-3.98)
RSRZ outliers	180081	1103 (7.46-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1260	 2% 59% 25% 12%
1	B	1260	 2% 49% 32% 6% 11%
1	C	1260	 57% 26% 12%
1	D	1260	 2% 56% 28% 6% 11%
2	E	5	 60% 40%

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Mol	Chain	Length	Quality of chain
3	F	3	 33% 67%
3	H	3	 33% 67%
4	G	4	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 36079 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 UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1111	8882	5671	1509	1675	27	0	0	0
1	B	1120	8955	5718	1522	1688	27	0	0	0
1	C	1113	8898	5680	1512	1678	28	0	0	0
1	D	1123	8983	5735	1529	1691	28	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

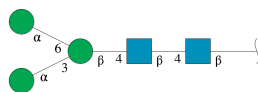
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58
B	21	GLU	-	expression tag	UNP G0SB58
B	22	THR	-	expression tag	UNP G0SB58
B	23	GLY	-	expression tag	UNP G0SB58
B	1506	GLY	-	expression tag	UNP G0SB58
B	1507	THR	-	expression tag	UNP G0SB58
B	1508	LYS	-	expression tag	UNP G0SB58
B	1509	HIS	-	expression tag	UNP G0SB58
B	1510	HIS	-	expression tag	UNP G0SB58

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1511	HIS	-	expression tag	UNP G0SB58
B	1512	HIS	-	expression tag	UNP G0SB58
B	1513	HIS	-	expression tag	UNP G0SB58
B	1514	HIS	-	expression tag	UNP G0SB58
C	21	GLU	-	expression tag	UNP G0SB58
C	22	THR	-	expression tag	UNP G0SB58
C	23	GLY	-	expression tag	UNP G0SB58
C	1506	GLY	-	expression tag	UNP G0SB58
C	1507	THR	-	expression tag	UNP G0SB58
C	1508	LYS	-	expression tag	UNP G0SB58
C	1509	HIS	-	expression tag	UNP G0SB58
C	1510	HIS	-	expression tag	UNP G0SB58
C	1511	HIS	-	expression tag	UNP G0SB58
C	1512	HIS	-	expression tag	UNP G0SB58
C	1513	HIS	-	expression tag	UNP G0SB58
C	1514	HIS	-	expression tag	UNP G0SB58
D	21	GLU	-	expression tag	UNP G0SB58
D	22	THR	-	expression tag	UNP G0SB58
D	23	GLY	-	expression tag	UNP G0SB58
D	1506	GLY	-	expression tag	UNP G0SB58
D	1507	THR	-	expression tag	UNP G0SB58
D	1508	LYS	-	expression tag	UNP G0SB58
D	1509	HIS	-	expression tag	UNP G0SB58
D	1510	HIS	-	expression tag	UNP G0SB58
D	1511	HIS	-	expression tag	UNP G0SB58
D	1512	HIS	-	expression tag	UNP G0SB58
D	1513	HIS	-	expression tag	UNP G0SB58
D	1514	HIS	-	expression tag	UNP G0SB58

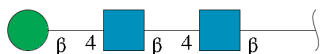
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	5	61	34	2	25	0	0	0

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

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



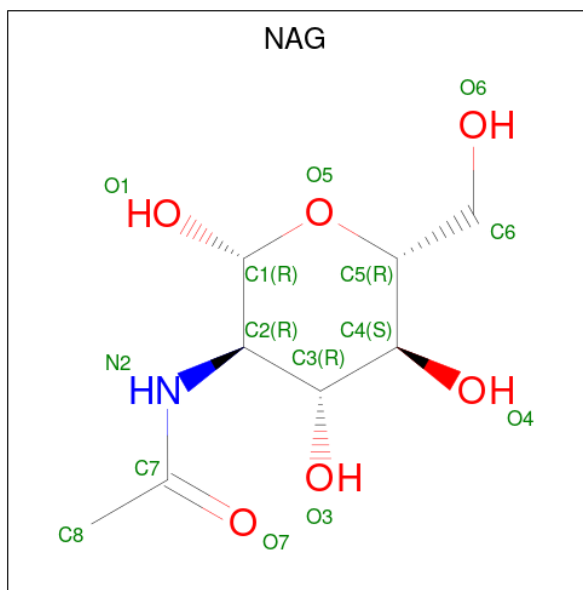
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	3	39	22	2	15	0	0	0
3	H	3	39	22	2	15	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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			
4	G	4	50	28	2	20	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

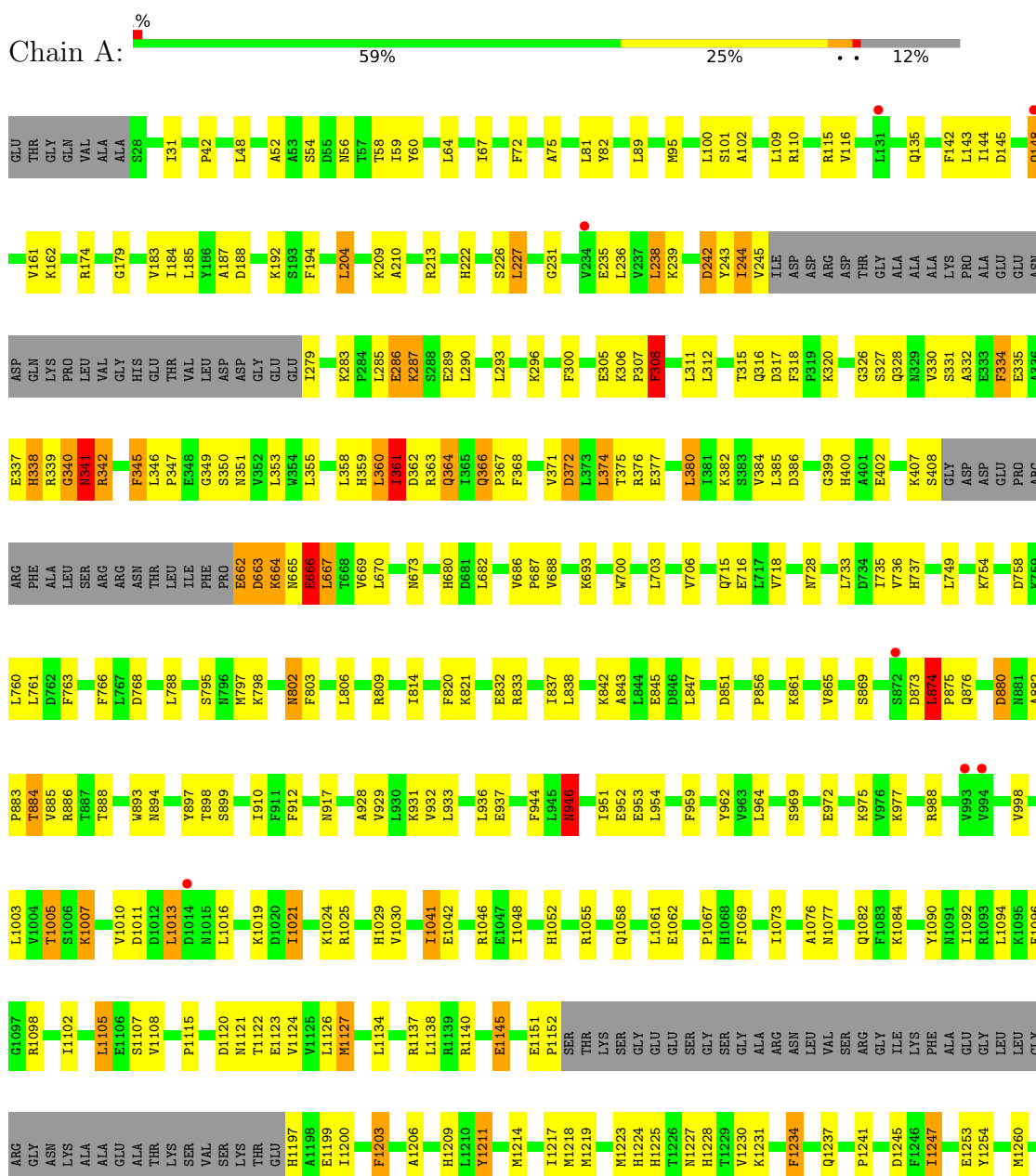
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

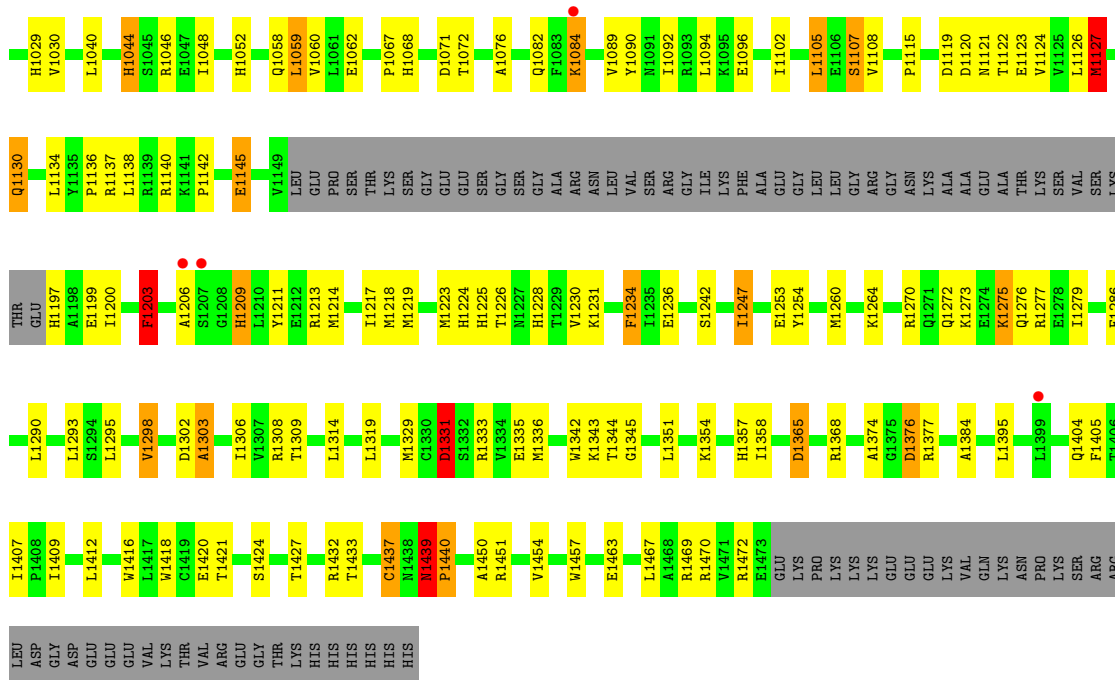
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

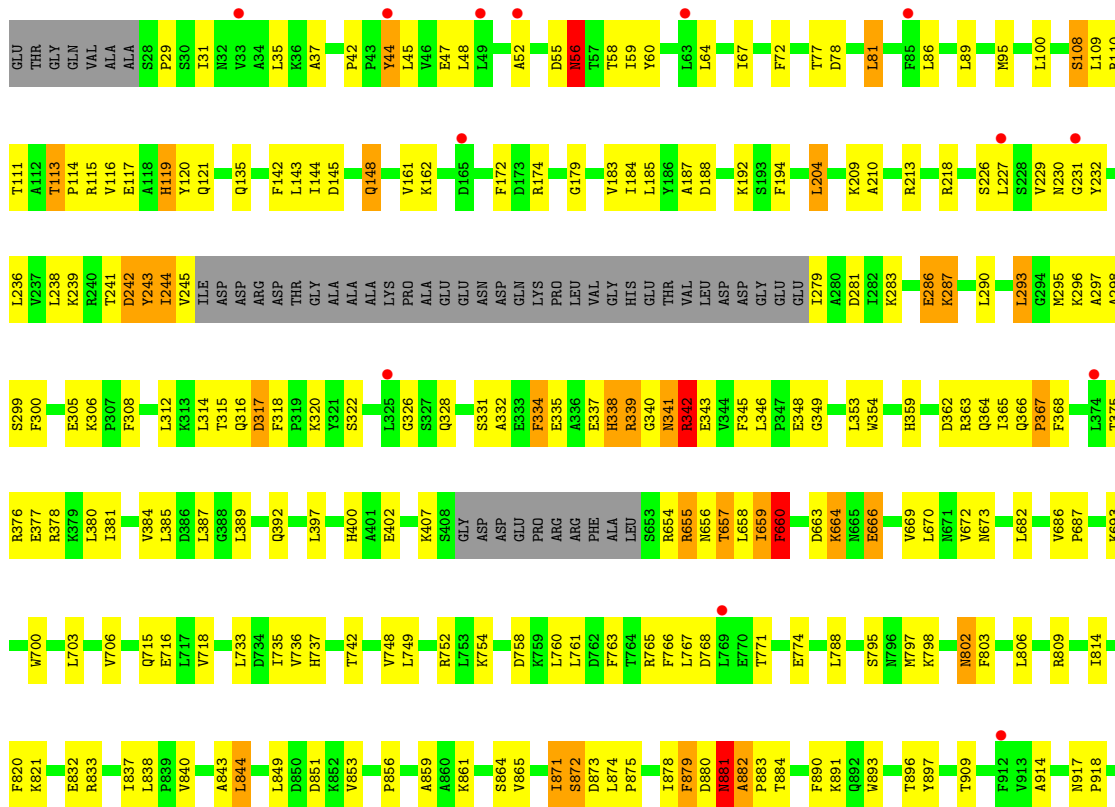
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein





• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein



Chain G:  100%

MAG1
MAG2
BGA3
MAN4

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.15Å 191.01Å 158.81Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	140.60 – 5.74 140.60 – 5.74	Depositor EDS
% Data completeness (in resolution range)	74.9 (140.60-5.74) 75.4 (140.60-5.74)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 5.77Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.249 0.184 , 0.253	Depositor DCC
R_{free} test set	829 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	290.4	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 466.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	36079	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, CA, MAN, NAG

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	0.79	8/9087 (0.1%)	1.22	48/12325 (0.4%)
1	B	0.83	5/9162 (0.1%)	1.27	79/12428 (0.6%)
1	C	0.79	7/9104 (0.1%)	1.20	43/12349 (0.3%)
1	D	0.78	3/9191 (0.0%)	1.23	53/12467 (0.4%)
All	All	0.80	23/36544 (0.1%)	1.23	223/49569 (0.4%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	663	ASP	CA-C	7.28	1.62	1.52
1	C	666	GLU	CA-C	7.25	1.61	1.52
1	A	664	LYS	C-N	6.73	1.43	1.33
1	A	882	ALA	CA-C	6.57	1.61	1.52
1	A	665	ASN	CA-C	6.25	1.61	1.52

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASN	CA-CB-CG	12.12	124.72	112.60
1	A	308	PHE	CA-CB-CG	9.60	123.39	113.80
1	D	881	ASN	CA-CB-CG	9.54	122.14	112.60
1	B	871	ILE	CA-C-N	8.32	136.68	121.70
1	B	871	ILE	C-N-CA	8.32	136.68	121.70

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	8882	0	8770	234	0
1	B	8955	0	8846	337	0
1	C	8898	0	8788	282	0
1	D	8983	0	8881	293	0
2	E	61	0	52	4	0
3	F	39	0	34	0	0
3	H	39	0	34	0	0
4	G	50	0	43	0	0
5	A	42	0	39	0	0
5	B	42	0	39	0	0
5	C	42	0	39	0	0
5	D	42	0	39	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	36079	0	35604	1116	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 16.

The worst 5 of 1116 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:D:78:ASP:HB2	1:D:975:LYS:HA	1.23	1.16
1:B:1376:ASP:HA	1:B:1379:ARG:HD3	1.26	1.15
1:B:1333:ARG:HG3	1:B:1424:SER:HA	1.17	1.13
1:D:1241:PRO:HA	1:D:1244:LYS:HB2	1.32	1.12
1:B:869:SER:HB2	1:B:886:ARG:HE	1.07	1.10

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	1101/1260 (87%)	1009 (92%)	78 (7%)	14 (1%)	9	41
1	B	1110/1260 (88%)	947 (85%)	134 (12%)	29 (3%)	4	25
1	C	1105/1260 (88%)	991 (90%)	98 (9%)	16 (1%)	9	39
1	D	1115/1260 (88%)	987 (88%)	100 (9%)	28 (2%)	4	25
All	All	4431/5040 (88%)	3934 (89%)	410 (9%)	87 (2%)	6	30

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	ALA
1	A	873	ASP
1	A	874	LEU
1	A	876	GLN
1	A	883	PRO

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	965/1088 (89%)	884 (92%)	81 (8%)	10	29
1	B	974/1088 (90%)	838 (86%)	136 (14%)	3	13
1	C	967/1088 (89%)	873 (90%)	94 (10%)	8	24
1	D	977/1088 (90%)	884 (90%)	93 (10%)	8	25
All	All	3883/4352 (89%)	3479 (90%)	404 (10%)	7	22

5 of 404 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	295	MET
1	C	1048	ILE
1	D	1370	ARG
1	C	341	ASN
1	C	844	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	316	GLN
1	D	1082	GLN
1	D	392	GLN
1	D	881	ASN
1	D	1367	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](#)

15 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	0.31	0	17,19,21	1.14	2 (11%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	2.56	3 (17%)

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	0.41	0	15,15,17	0.97	1 (6%)
2	MAN	E	4	2	11,11,12	0.93	0	15,15,17	1.89	2 (13%)
2	MAN	E	5	2	11,11,12	0.79	0	15,15,17	1.85	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	1.21	2 (11%)
3	NAG	F	2	3	14,14,15	0.36	0	17,19,21	1.13	1 (5%)
3	BMA	F	3	3	11,11,12	0.32	0	15,15,17	0.49	0
4	NAG	G	1	4,1	14,14,15	0.29	0	17,19,21	1.08	2 (11%)
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	1.58	4 (23%)
4	BMA	G	3	4	11,11,12	0.35	0	15,15,17	0.91	1 (6%)
4	MAN	G	4	4	11,11,12	0.74	0	15,15,17	1.31	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.29	0	17,19,21	1.07	2 (11%)
3	NAG	H	2	3	14,14,15	0.31	0	17,19,21	1.07	2 (11%)
3	BMA	H	3	3	11,11,12	0.30	0	15,15,17	0.40	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	NAG	E	1	2,1	-	0/6/23/26	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	1/1/1/1
2	MAN	E	5	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-C2-N2	6.24	120.27	110.43
2	E	4	MAN	C1-O5-C5	6.16	120.44	112.19
2	E	2	NAG	O5-C1-C2	-5.94	102.10	111.29
2	E	5	MAN	C1-O5-C5	5.93	120.13	112.19
2	E	2	NAG	C1-O5-C5	5.03	118.93	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6

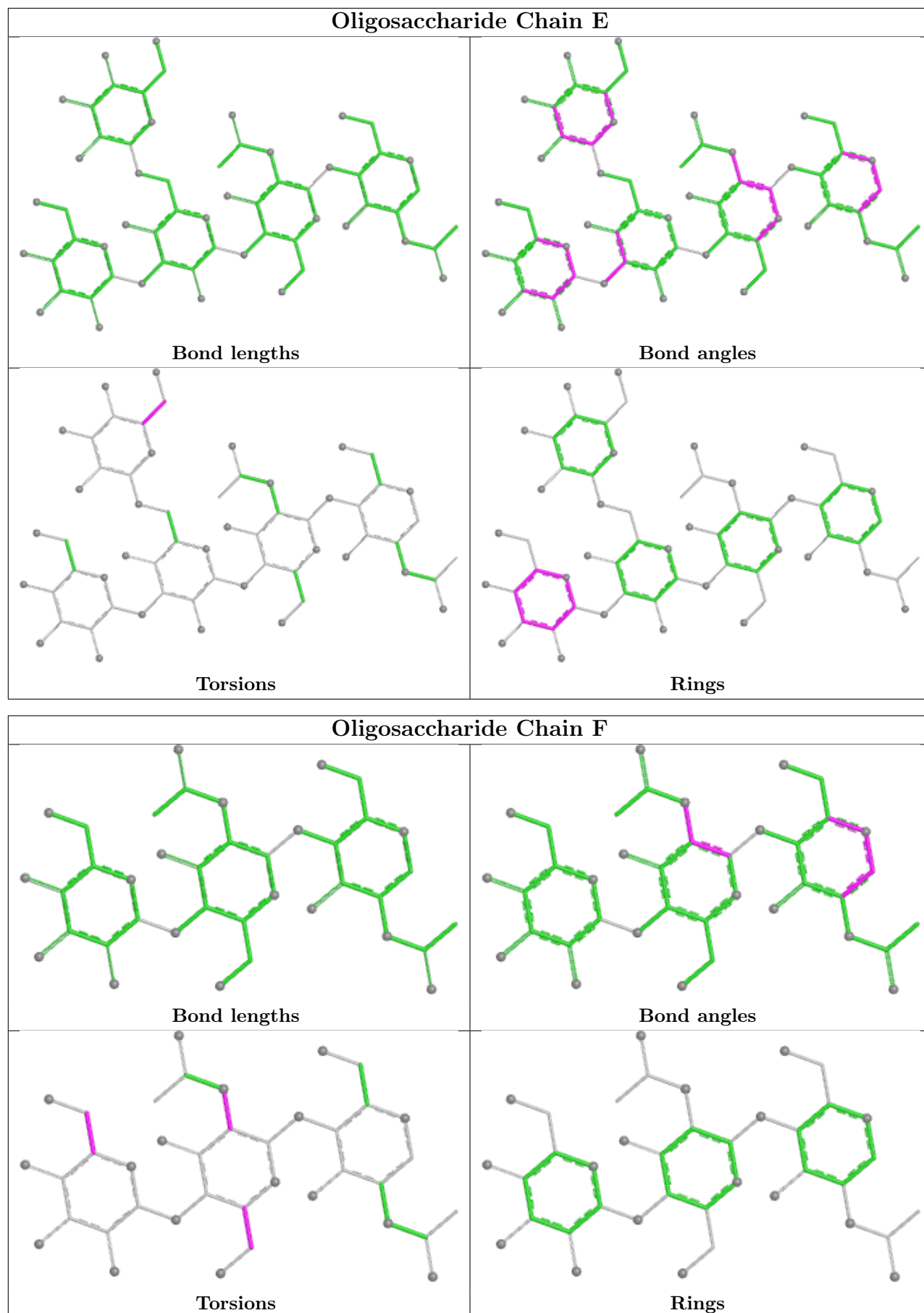
All (1) ring outliers are listed below:

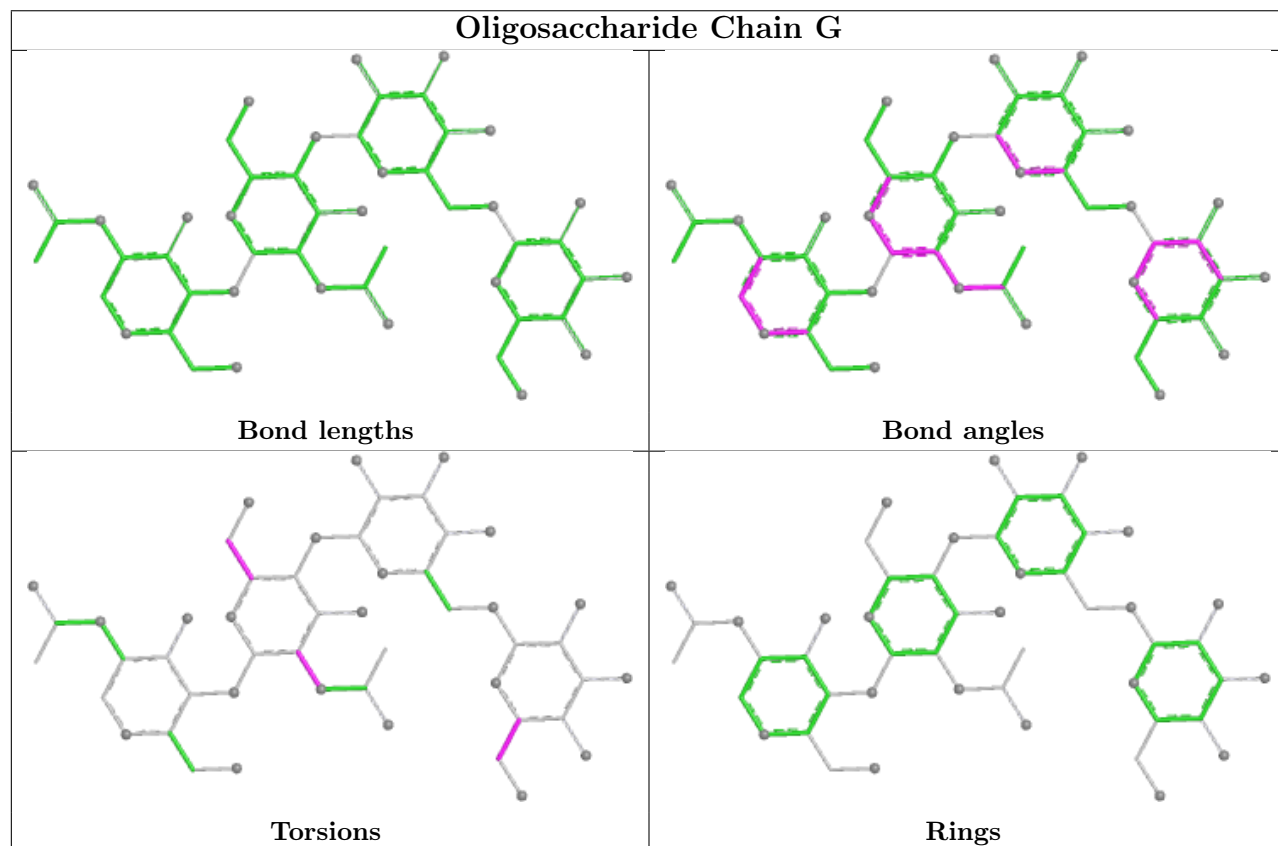
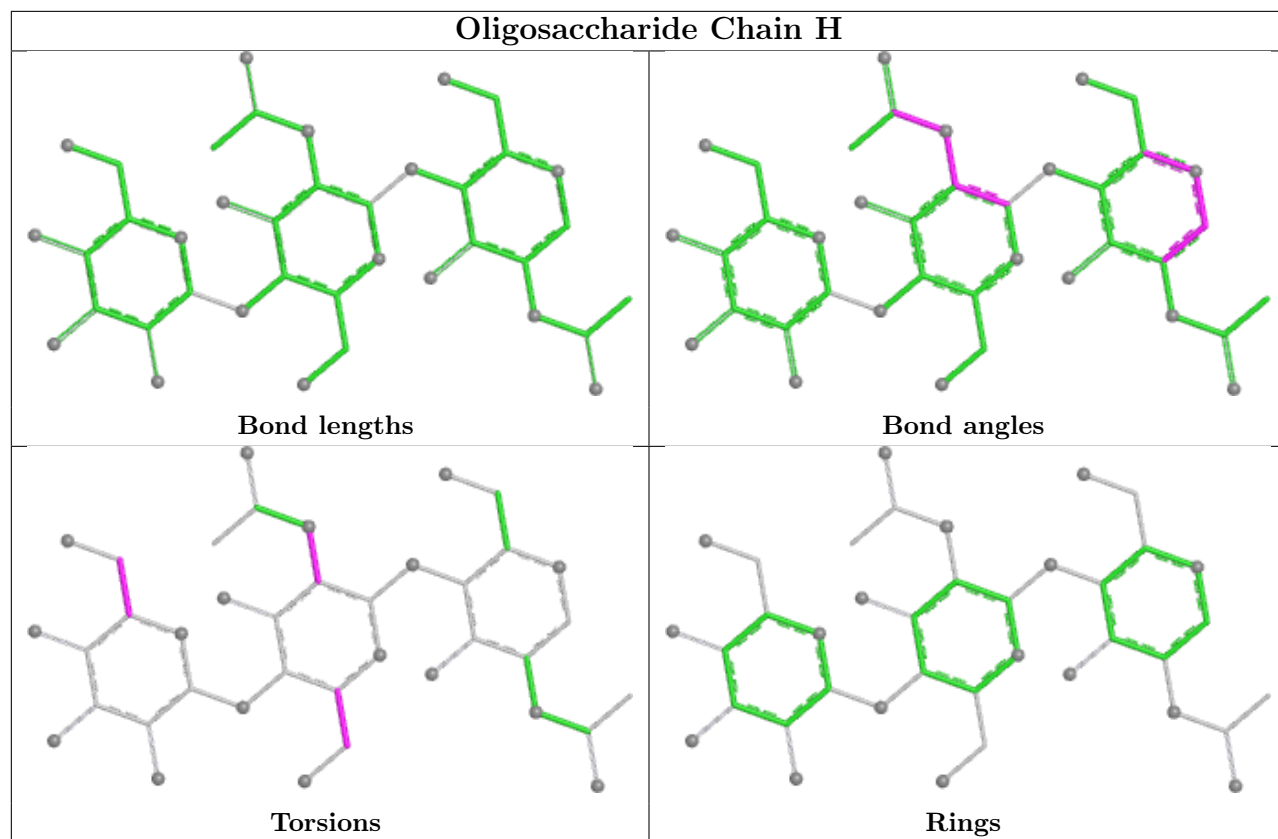
Mol	Chain	Res	Type	Atoms
2	E	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	4	0
2	E	1	NAG	4	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, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1602	1	14,14,15	0.30	0	17,19,21	0.80	1 (5%)
5	NAG	B	1602	1	14,14,15	0.37	0	17,19,21	1.20	1 (5%)
5	NAG	B	1603	1	14,14,15	0.39	0	17,19,21	1.02	2 (11%)
5	NAG	D	1601	-	14,14,15	0.32	0	17,19,21	0.68	0
5	NAG	A	1601	-	14,14,15	0.36	0	17,19,21	0.70	0
5	NAG	C	1607	1	14,14,15	0.30	0	17,19,21	0.58	0
5	NAG	C	1606	1	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
5	NAG	C	1601	-	14,14,15	0.53	0	17,19,21	0.82	0
5	NAG	D	1606	1	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
5	NAG	A	1603	1	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
5	NAG	D	1605	1	14,14,15	0.37	0	17,19,21	0.72	1 (5%)
5	NAG	B	1601	-	14,14,15	0.31	0	17,19,21	0.53	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
5	NAG	A	1602	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1602	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1603	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1607	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1606	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	D	1606	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1603	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1605	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1601	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	1602	NAG	C1-O5-C5	4.07	117.64	112.19
5	C	1606	NAG	C1-O5-C5	3.07	116.29	112.19
5	A	1602	NAG	C1-O5-C5	2.98	116.17	112.19
5	B	1603	NAG	C1-O5-C5	2.97	116.17	112.19
5	A	1603	NAG	C1-O5-C5	2.81	115.96	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1111/1260 (88%)	-0.34	8 (0%) 84 73	22, 100, 190, 292	0
1	B	1120/1260 (88%)	-0.38	11 (0%) 79 67	23, 105, 185, 292	0
1	C	1113/1260 (88%)	-0.34	6 (0%) 87 77	56, 165, 300, 300	0
1	D	1123/1260 (89%)	-0.24	24 (2%) 63 54	29, 114, 279, 300	0
All	All	4467/5040 (88%)	-0.32	49 (1%) 78 66	22, 120, 282, 300	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	85	PHE	4.0
1	B	241	THR	3.9
1	C	28	SER	3.9
1	C	1399	LEU	3.7
1	C	1207	SER	3.6

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.

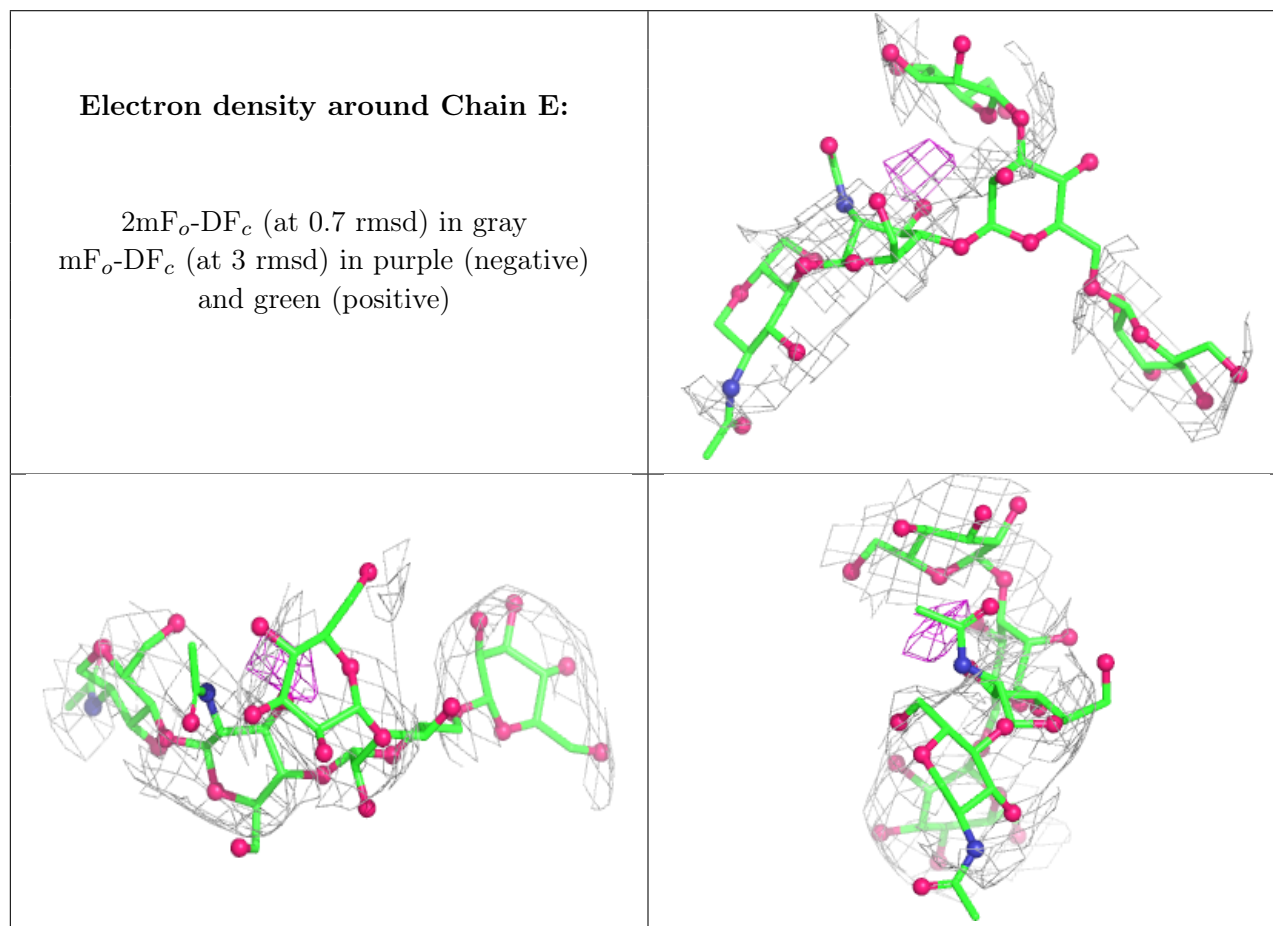
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	H	3	11/12	0.36	0.14	270,279,283,286	0
3	NAG	H	2	14/15	0.55	0.11	178,199,259,268	0

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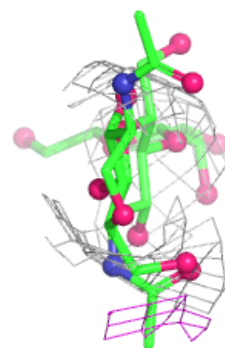
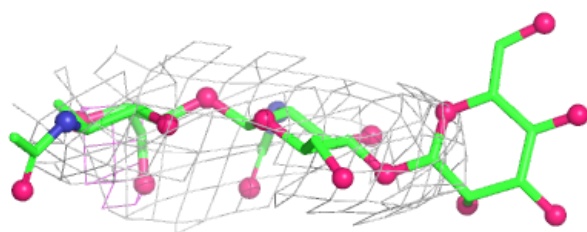
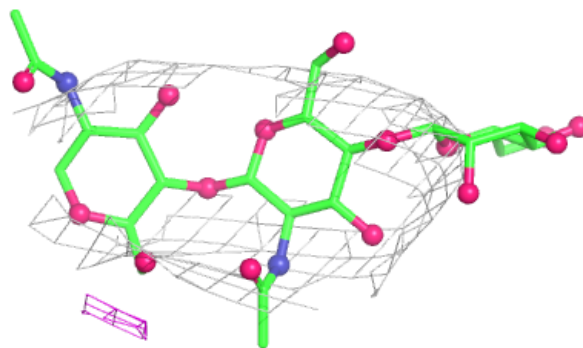
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BMA	E	3	11/12	0.55	0.08	234,265,279,280	0
4	BMA	G	3	11/12	0.65	0.07	283,284,285,285	0
3	BMA	F	3	11/12	0.68	0.06	273,297,300,300	0
2	MAN	E	4	11/12	0.68	0.10	68,78,97,105	0
2	MAN	E	5	11/12	0.69	0.10	99,119,146,149	0
4	MAN	G	4	11/12	0.73	0.19	139,177,250,260	0
4	NAG	G	2	14/15	0.74	0.10	212,277,285,286	0
3	NAG	F	2	14/15	0.79	0.07	167,184,223,252	0
2	NAG	E	1	14/15	0.90	0.09	119,132,157,157	0
2	NAG	E	2	14/15	0.90	0.10	148,183,239,243	0
4	NAG	G	1	14/15	0.94	0.12	169,178,200,205	0
3	NAG	H	1	14/15	0.94	0.09	141,151,174,177	0
3	NAG	F	1	14/15	0.95	0.06	126,135,157,162	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.

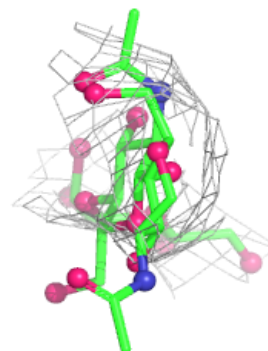
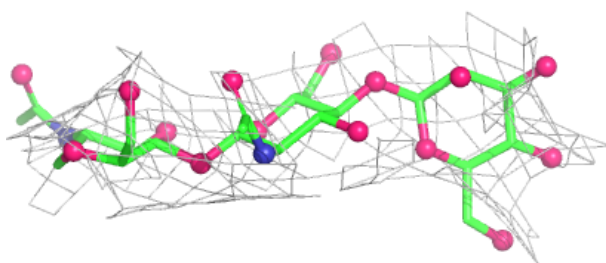
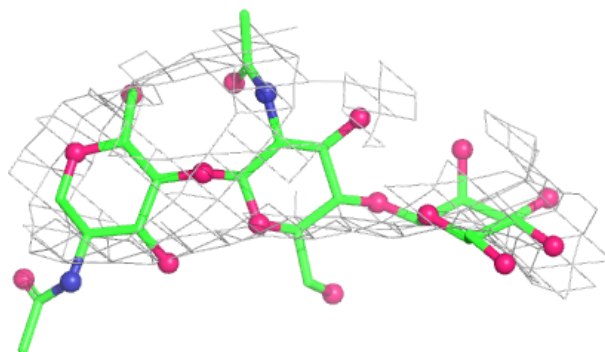


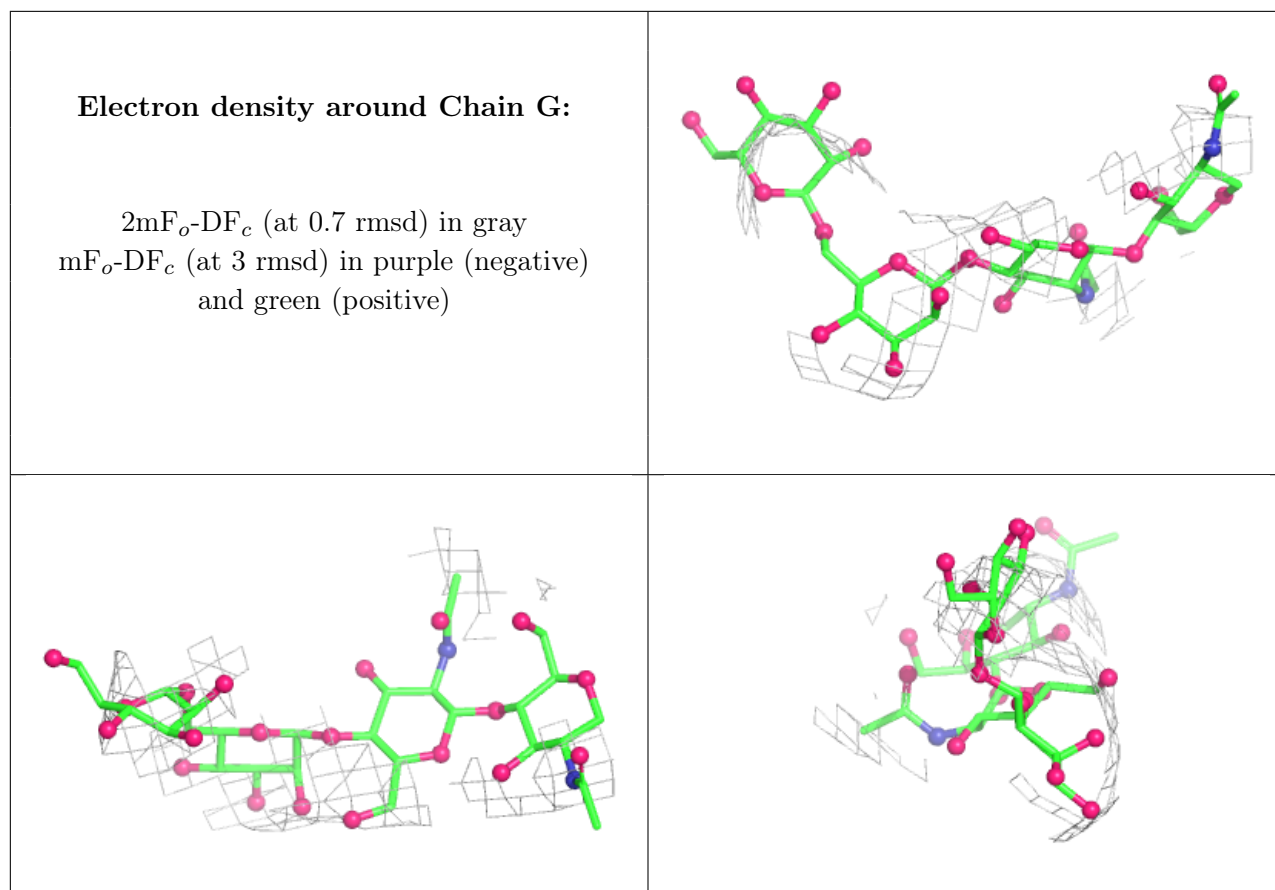
Electron density around Chain F:

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

**Electron density around Chain H:**

$2mF_o-DF_c$ (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
5	NAG	A	1601	14/15	0.45	0.22	148,153,161,162	0
5	NAG	C	1601	14/15	0.55	0.11	148,153,161,162	0
5	NAG	C	1606	14/15	0.57	0.06	292,292,293,293	0
5	NAG	D	1601	14/15	0.67	0.11	148,153,161,162	0
5	NAG	B	1603	14/15	0.68	0.09	189,255,283,283	0
5	NAG	A	1602	14/15	0.69	0.10	250,256,259,262	0
5	NAG	B	1601	14/15	0.69	0.11	148,153,161,162	0
5	NAG	C	1607	14/15	0.71	0.09	295,295,295,296	0
5	NAG	A	1603	14/15	0.71	0.10	199,247,278,280	0
5	NAG	D	1605	14/15	0.79	0.07	282,282,282,283	0
5	NAG	B	1602	14/15	0.82	0.09	250,257,261,262	0
6	CA	C	1608	1/1	0.85	0.14	234,234,234,234	1
5	NAG	D	1606	14/15	0.87	0.10	218,227,252,254	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CA	D	1607	1/1	0.97	0.11	191,191,191,191	1
6	CA	A	1604	1/1	0.98	0.04	152,152,152,152	1
6	CA	B	1604	1/1	1.00	0.03	142,142,142,142	1

6.5 Other polymers [i](#)

There are no such residues in this entry.