



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:46 AM UTC

PDB ID : 7Q3P / pdb_00007q3p
Title : Crystal structure of IgG1-Fc-MST-HN (efgartigimod)
Authors : Pannecoucke, E.; Savvides, S.N.
Deposited on : 2021-10-28
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

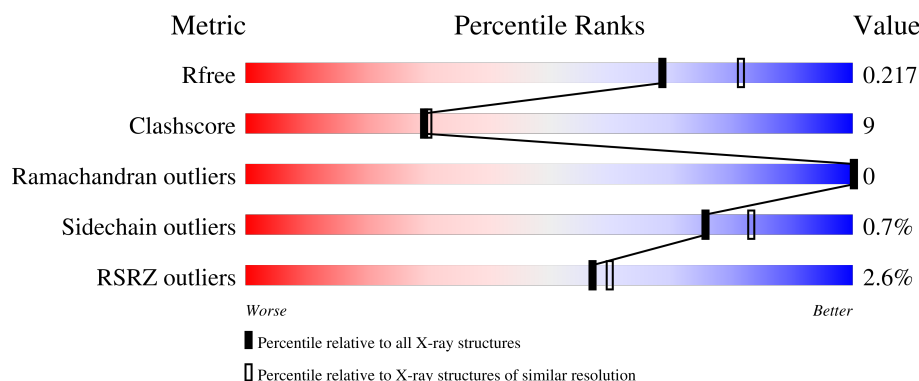
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

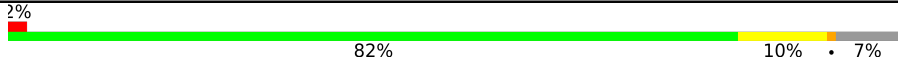
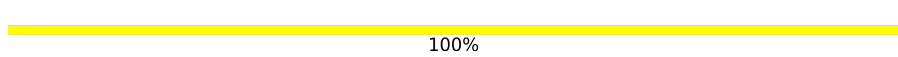
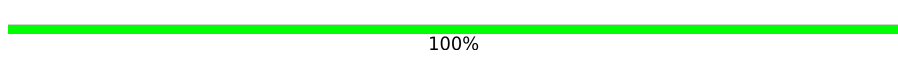
The reported resolution of this entry is 2.10 Å.

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.



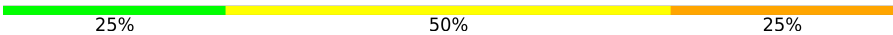
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	225	
1	B	225	
1	C	225	
2	D	2	
2	G	2	

Continued on next page...

Continued from previous page...

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

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5730 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 IgG1-Fc-MST-HN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	2	0
			1679	1076	279	319	5			
1	B	208	Total	C	N	O	S	0	1	0
			1623	1040	269	309	5			
1	C	208	Total	C	N	O	S	0	1	0
			1673	1069	279	320	5			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



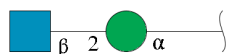
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	G	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



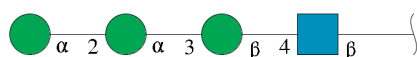
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



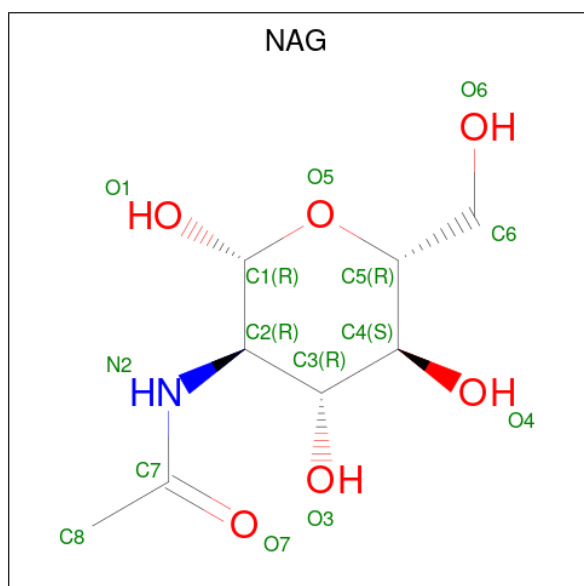
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			25	14	1	10			
4	I	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



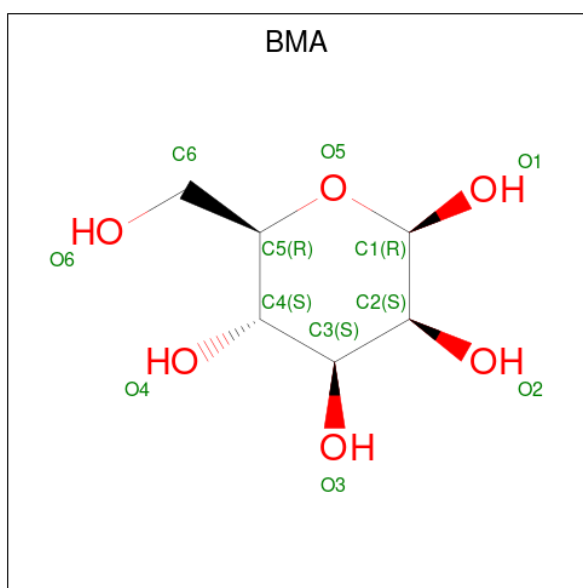
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	4	Total	C	N	O	0	0	0
			47	26	1	20			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



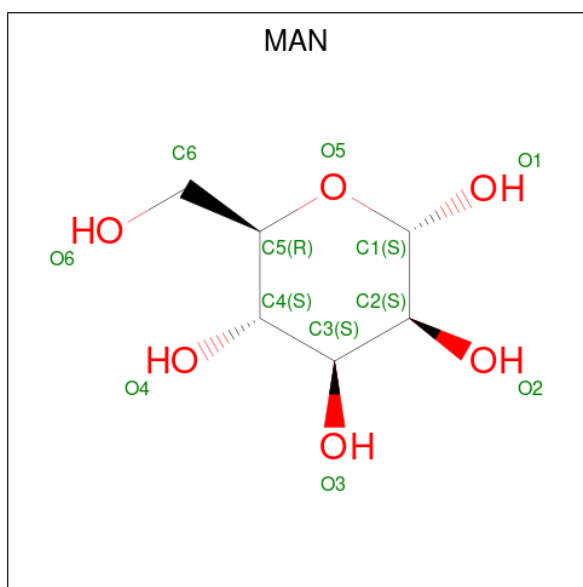
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



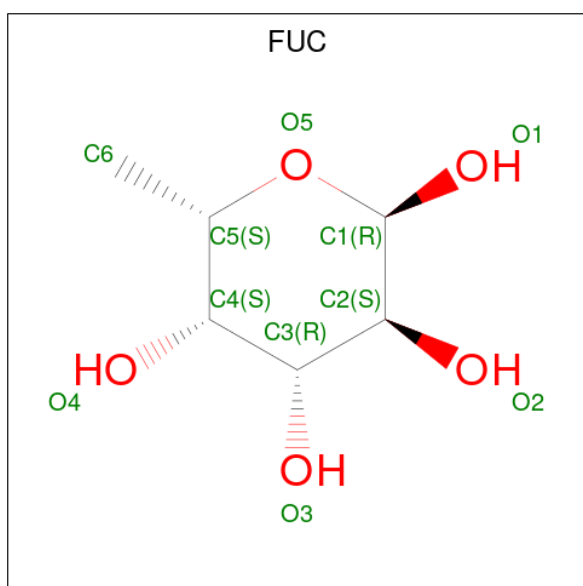
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 9 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	6	4		

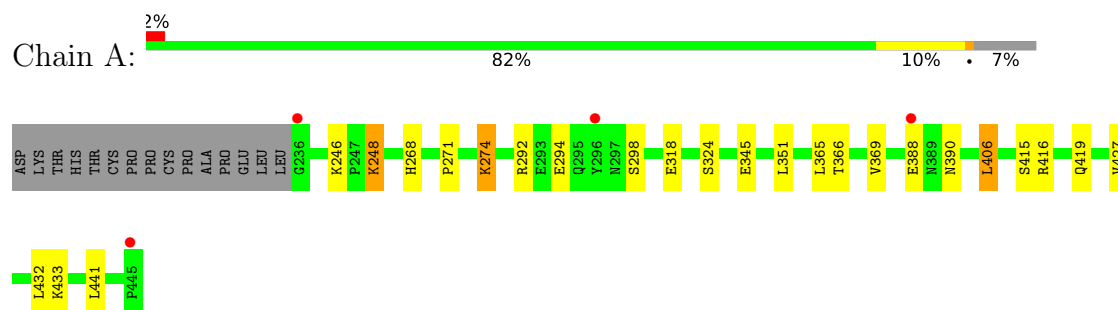
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	173	Total 173	O 173	0	0
10	B	101	Total 101	O 101	0	0
10	C	187	Total 187	O 187	0	0

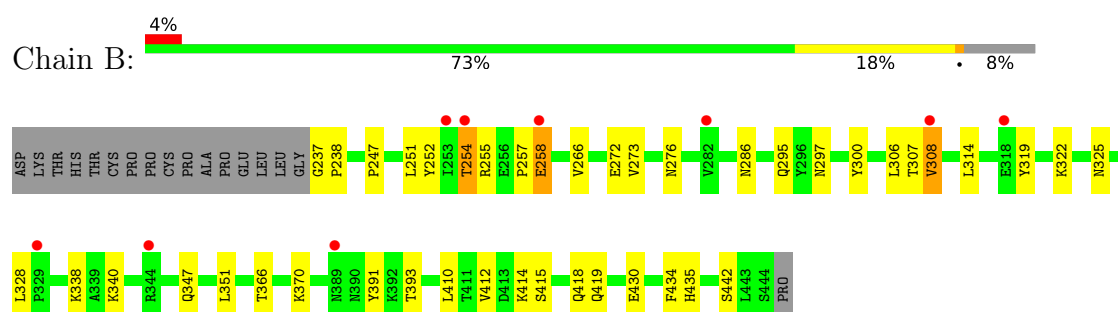
3 Residue-property plots

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.

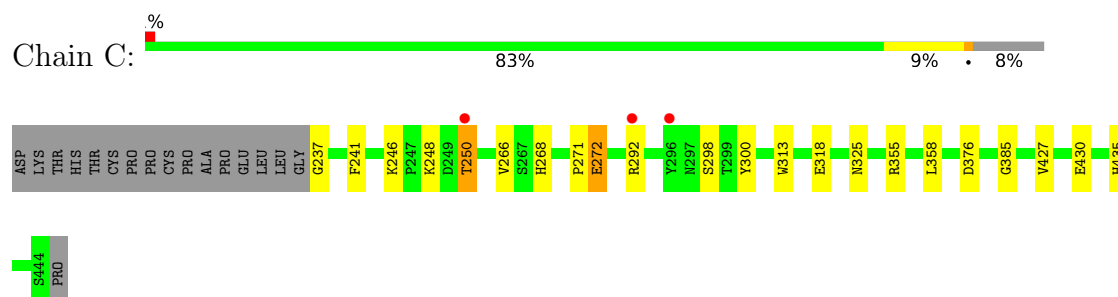
• Molecule 1: IgG1-Fc-MST-HN



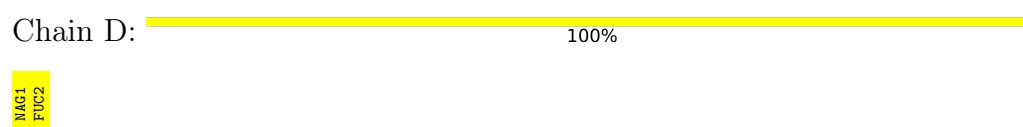
• Molecule 1: IgG1-Fc-MST-HN



• Molecule 1: IgG1-Fc-MST-HN



• Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
FUC2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  75% 25%

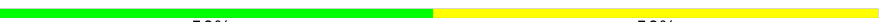
MAG1
BNA2
MAN3
MAG4

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

Chain F:  50% 50%

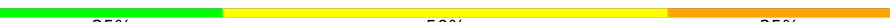
MAG1
MAG2

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

Chain I:  50% 50%

MAN1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  25% 50% 25%

MAG1
BNA2
MAN3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.41Å 87.94Å 106.09Å 90.00° 114.04° 90.00°	Depositor
Resolution (Å)	48.14 – 2.10 48.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.14-2.10) 88.9 (48.14-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.189 , 0.214 0.191 , 0.217	Depositor DCC
R_{free} test set	2344 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5730	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUC, NAG, 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	0.39	2/1730 (0.1%)	0.64	5/2360 (0.2%)
1	B	0.38	1/1670 (0.1%)	0.77	9/2287 (0.4%)
1	C	0.31	0/1720	0.61	6/2345 (0.3%)
All	All	0.36	3/5120 (0.1%)	0.67	20/6992 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	258	GLU	CD-OE2	8.12	1.40	1.25
1	A	248	LYS	CE-NZ	7.82	1.72	1.49
1	A	388	GLU	CD-OE2	7.01	1.38	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	LYS	CA-CB-CG	-12.54	89.02	114.10
1	B	340	LYS	CD-CE-NZ	-9.35	81.98	111.90
1	A	248	LYS	CD-CE-NZ	-8.94	83.29	111.90
1	C	246	LYS	CB-CG-CD	-8.85	90.95	111.30
1	B	340	LYS	CG-CD-CE	8.82	131.58	111.30
1	B	254	THR	OG1-CB-CG2	-7.12	95.05	109.30
1	A	248	LYS	CA-CB-CG	6.69	127.48	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	THR	OG1-CB-CG2	6.67	122.64	109.30
1	B	273	VAL	CG1-CB-CG2	-6.46	96.60	110.80
1	A	274	LYS	CB-CG-CD	-6.16	97.12	111.30
1	C	250	THR	CA-CB-OG1	5.98	118.57	109.60
1	C	246	LYS	CA-CB-CG	5.74	125.57	114.10
1	C	246	LYS	CG-CD-CE	5.66	124.31	111.30
1	B	340	LYS	CB-CG-CD	5.53	124.03	111.30
1	A	248	LYS	N-CA-CB	5.47	119.62	110.32
1	B	254	THR	CB-CA-C	-5.28	99.62	110.38
1	A	388	GLU	N-CA-CB	-5.23	101.76	110.80
1	B	308	VAL	CG1-CB-CG2	5.08	121.98	110.80
1	C	246	LYS	N-CA-CB	-5.04	99.02	109.45
1	B	308	VAL	CA-CB-CG2	5.01	118.92	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	250	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	272	GLU	Sidechain

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	1679	0	1631	22	0
1	B	1623	0	1537	43	0
1	C	1673	0	1630	19	0
2	D	24	0	22	0	0
2	G	24	0	22	0	0
3	E	50	0	43	2	0
4	F	25	0	22	2	0
4	I	25	0	22	0	0
5	H	47	0	40	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	56	0	50	2	0
7	B	11	0	9	1	0
8	B	22	0	18	1	0
9	B	10	0	10	2	0
10	A	173	0	0	8	0
10	B	101	0	0	10	1
10	C	187	0	0	7	0
All	All	5730	0	5056	89	1

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 9.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:CE	1:A:248:LYS:NZ	1.72	1.51
1:A:248:LYS:NZ	1:A:248:LYS:CD	2.17	1.07
1:A:271:PRO:HB2	1:A:292[B]:ARG:HH12	1.10	1.06
1:C:248:LYS:NZ	10:C:501:HOH:O	1.93	1.00
1:B:297:ASN:ND2	10:B:601:HOH:O	1.94	0.97
1:A:271:PRO:HB2	1:A:292[B]:ARG:NH1	1.82	0.94
1:B:258:GLU:HA	1:B:308:VAL:HG22	1.50	0.94
1:B:258:GLU:HA	1:B:308:VAL:CG2	1.99	0.92
1:C:237:GLY:N	10:C:502:HOH:O	2.05	0.88
1:A:298:SER:O	10:A:501:HOH:O	1.89	0.88
10:B:618:HOH:O	4:F:1:MAN:O4	1.92	0.86
1:A:248:LYS:NZ	1:A:248:LYS:HD3	1.91	0.84
1:B:319:TYR:OH	10:B:602:HOH:O	1.97	0.83
1:B:442:SER:O	10:B:603:HOH:O	1.97	0.82
1:B:391:TYR:HB3	1:B:410:LEU:HD23	1.62	0.81
1:A:246:LYS:NZ	3:E:4:NAG:O4	2.15	0.79
1:B:308:VAL:HG13	1:B:319:TYR:CZ	2.17	0.79
1:B:295:GLN:NE2	10:B:606:HOH:O	2.16	0.77
1:A:416[B]:ARG:NH1	10:A:504:HOH:O	2.19	0.74
1:A:248:LYS:CD	1:A:248:LYS:HZ3	2.00	0.74
1:B:308:VAL:CG1	1:B:319:TYR:CZ	2.72	0.72
1:B:258:GLU:HB3	1:B:307:THR:HA	1.71	0.72
1:A:248:LYS:HD3	1:A:248:LYS:HZ3	1.53	0.71
1:C:318:GLU:OE2	10:C:503:HOH:O	2.08	0.70
1:B:276:ASN:HB2	1:B:322:LYS:HE2	1.75	0.69
1:A:271:PRO:CB	1:A:292[B]:ARG:HH12	1.97	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLN:NE2	10:B:608:HOH:O	2.25	0.69
1:C:430:GLU:OE2	10:C:504:HOH:O	2.09	0.68
10:A:514:HOH:O	1:B:370:LYS:HE3	1.96	0.66
1:A:433:LYS:NZ	10:A:503:HOH:O	2.10	0.64
1:B:322:LYS:HE3	10:B:625:HOH:O	1.97	0.64
1:C:268:HIS:NE2	1:C:298:SER:O	2.31	0.62
1:C:271:PRO:HB2	1:C:292:ARG:NH1	2.14	0.61
1:A:318:GLU:CD	10:A:505:HOH:O	2.44	0.60
1:C:355:ARG:HA	1:C:358:LEU:CD2	2.32	0.59
1:B:308:VAL:CG1	1:B:319:TYR:OH	2.49	0.59
6:B:501:NAG:H61	9:B:508:FUC:O5	2.02	0.59
1:C:355:ARG:HA	1:C:358:LEU:HD23	1.83	0.59
1:B:258:GLU:OE2	1:B:307:THR:OG1	2.17	0.58
3:E:2:BMA:O3	4:F:1:MAN:H3	2.04	0.58
1:B:258:GLU:HA	1:B:308:VAL:HG23	1.85	0.57
1:C:250:THR:HG21	1:C:313:TRP:CD1	2.41	0.56
1:C:266:VAL:HB	1:C:300:TYR:HB2	1.89	0.54
1:A:390:ASN:ND2	10:A:502:HOH:O	1.93	0.54
1:B:414:LYS:HG2	1:B:418:GLN:NE2	2.23	0.54
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.89	0.53
1:B:308:VAL:HG12	1:B:319:TYR:OH	2.08	0.53
1:A:274:LYS:HD3	1:A:324:SER:HB2	1.89	0.53
1:B:308:VAL:HG13	1:B:319:TYR:CE1	2.45	0.52
1:C:250:THR:HG21	1:C:313:TRP:HD1	1.73	0.51
1:B:252:TYR:C	1:B:254:THR:H	2.19	0.51
1:B:442:SER:N	10:B:603:HOH:O	2.26	0.50
1:B:258:GLU:CA	1:B:308:VAL:CG2	2.83	0.49
1:B:257:PRO:C	1:B:308:VAL:HG23	2.37	0.49
1:B:415:SER:O	1:B:419:GLN:HG2	2.13	0.49
1:B:276:ASN:CB	1:B:322:LYS:HE2	2.43	0.49
1:B:347:GLN:NE2	10:B:605:HOH:O	2.16	0.48
1:C:272:GLU:O	1:C:325:ASN:ND2	2.44	0.48
1:B:414:LYS:O	1:B:418:GLN:HG2	2.14	0.48
1:B:430:GLU:HA	1:B:435:HIS:CD2	2.49	0.48
1:B:237:GLY:HA2	1:B:238:PRO:C	2.38	0.48
6:B:501:NAG:H61	9:B:508:FUC:C5	2.44	0.48
1:B:258:GLU:CB	1:B:307:THR:HA	2.44	0.46
7:B:503:BMA:H61	8:B:505:MAN:C1	2.46	0.46
1:B:434:PHE:N	10:B:607:HOH:O	2.18	0.45
1:A:268:HIS:NE2	1:A:294:GLU:OE2	2.48	0.45
1:B:254:THR:OG1	1:B:255:ARG:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:HIS:CE1	1:C:298:SER:HB3	2.53	0.44
1:A:369:VAL:HB	1:A:406:LEU:HD22	2.00	0.44
1:A:345:GLU:HG3	1:A:432:LEU:HD23	2.00	0.44
1:A:318:GLU:CG	10:A:505:HOH:O	2.64	0.44
1:A:365:LEU:HD13	1:A:441:LEU:HD23	1.99	0.43
1:B:314:LEU:HA	1:B:338:LYS:HD3	2.00	0.43
1:C:271:PRO:HB2	1:C:292:ARG:HH12	1.83	0.43
1:B:238:PRO:HG2	1:B:328:LEU:HD21	2.02	0.42
1:C:376:ASP:OD1	10:C:507:HOH:O	2.22	0.42
1:C:385:GLY:N	10:C:505:HOH:O	2.11	0.42
1:B:276:ASN:HB2	1:B:322:LYS:CE	2.48	0.42
1:A:351:LEU:HB2	1:A:366:THR:HB	2.02	0.41
1:C:248:LYS:CE	10:C:501:HOH:O	2.59	0.41
1:B:410:LEU:CD1	1:B:412:VAL:HG13	2.50	0.41
1:B:272:GLU:O	1:B:325:ASN:ND2	2.50	0.41
1:B:247:PRO:O	1:B:251:LEU:HG	2.20	0.41
1:A:415:SER:O	1:A:419:GLN:HG3	2.21	0.41
1:B:351:LEU:HB2	1:B:366:THR:HB	2.02	0.41
1:C:241:PHE:CZ	5:H:1:NAG:H61	2.57	0.40
1:B:252:TYR:C	1:B:254:THR:N	2.79	0.40
1:B:286:ASN:OD1	1:B:306:LEU:HD11	2.21	0.40
10:A:581:HOH:O	1:C:435:HIS:HD2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:616:HOH:O	10:B:685:HOH:O[4_445]	2.12	0.08

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	210/225 (93%)	209 (100%)	1 (0%)	0	100	100
1	B	207/225 (92%)	204 (99%)	3 (1%)	0	100	100
1	C	207/225 (92%)	206 (100%)	1 (0%)	0	100	100
All	All	624/675 (92%)	619 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/209 (91%)	189 (99%)	2 (1%)	68	76
1	B	180/209 (86%)	179 (99%)	1 (1%)	78	86
1	C	193/209 (92%)	192 (100%)	1 (0%)	81	88
All	All	564/627 (90%)	560 (99%)	4 (1%)	76	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	LEU
1	A	427	VAL
1	B	393	THR
1	C	427	VAL

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

Mol	Chain	Res	Type
1	A	276	ASN
1	B	362	GLN
1	C	276	ASN
1	C	342	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

16 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	D	1	1,2	14,14,15	0.21	0	17,19,21	0.77	1 (5%)
2	FUC	D	2	2	10,10,11	0.88	0	14,14,16	1.05	1 (7%)
3	NAG	E	1	3	14,14,15	1.20	1 (7%)	17,19,21	0.78	0
3	BMA	E	2	3	11,11,12	0.68	0	15,15,17	0.82	1 (6%)
3	MAN	E	3	3	11,11,12	1.21	2 (18%)	15,15,17	1.32	1 (6%)
3	NAG	E	4	3	14,14,15	0.14	0	17,19,21	0.58	0
4	MAN	F	1	4	11,11,12	1.47	1 (9%)	15,15,17	1.58	2 (13%)
4	NAG	F	2	4	14,14,15	0.42	0	17,19,21	1.53	3 (17%)
2	NAG	G	1	1,2	14,14,15	0.21	0	17,19,21	0.84	0
2	FUC	G	2	2	10,10,11	0.84	0	14,14,16	0.92	0
5	NAG	H	1	5	14,14,15	0.97	1 (7%)	17,19,21	0.75	0
5	BMA	H	2	5	11,11,12	0.63	0	15,15,17	0.92	0
5	MAN	H	3	5	11,11,12	1.00	1 (9%)	15,15,17	1.02	1 (6%)
5	MAN	H	4	5	11,11,12	1.09	1 (9%)	15,15,17	1.62	2 (13%)
4	MAN	I	1	4	11,11,12	1.07	0	15,15,17	1.07	1 (6%)
4	NAG	I	2	4	14,14,15	0.37	0	17,19,21	0.52	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	D	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	D	2	2	-	-	0/1/1/1
3	NAG	E	1	3	-	0/6/23/26	0/1/1/1
3	BMA	E	2	3	-	0/2/19/22	0/1/1/1
3	MAN	E	3	3	-	2/2/19/22	0/1/1/1
3	NAG	E	4	3	-	2/6/23/26	0/1/1/1
4	MAN	F	1	4	-	0/2/19/22	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
5	NAG	H	1	5	-	1/6/23/26	0/1/1/1
5	BMA	H	2	5	-	2/2/19/22	0/1/1/1
5	MAN	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	1/2/19/22	1/1/1/1
4	MAN	I	1	4	-	1/2/19/22	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-4.07	1.36	1.43
4	F	1	MAN	C2-C3	3.01	1.57	1.52
5	H	1	NAG	O5-C1	-2.98	1.38	1.43
5	H	3	MAN	O5-C1	-2.63	1.39	1.43
3	E	3	MAN	O5-C1	-2.53	1.39	1.43
5	H	4	MAN	O5-C5	2.53	1.48	1.43
3	E	3	MAN	C1-C2	2.01	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	4	MAN	C1-O5-C5	5.12	119.05	112.19
4	F	2	NAG	C2-N2-C7	4.47	128.88	122.90
4	F	1	MAN	O2-C2-C1	4.19	118.83	109.22
3	E	3	MAN	O2-C2-C3	-3.95	101.97	110.15
4	F	2	NAG	C1-C2-N2	3.36	115.73	110.43
4	F	1	MAN	O2-C2-C3	3.01	116.39	110.15
4	I	1	MAN	C1-O5-C5	2.62	115.70	112.19
5	H	4	MAN	O2-C2-C3	-2.34	105.30	110.15
2	D	2	FUC	C1-O5-C5	2.24	118.24	112.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	O4-C4-C5	-2.19	103.93	109.32
3	E	2	BMA	O2-C2-C3	-2.16	105.69	110.15
5	H	3	MAN	C1-C2-C3	-2.06	106.65	109.64
4	F	2	NAG	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C1-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
5	H	2	BMA	O5-C5-C6-O6
3	E	3	MAN	C4-C5-C6-O6
3	E	3	MAN	O5-C5-C6-O6
5	H	3	MAN	C4-C5-C6-O6
5	H	2	BMA	C4-C5-C6-O6
3	E	4	NAG	O5-C5-C6-O6
5	H	3	MAN	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
4	I	1	MAN	O5-C5-C6-O6
3	E	4	NAG	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6

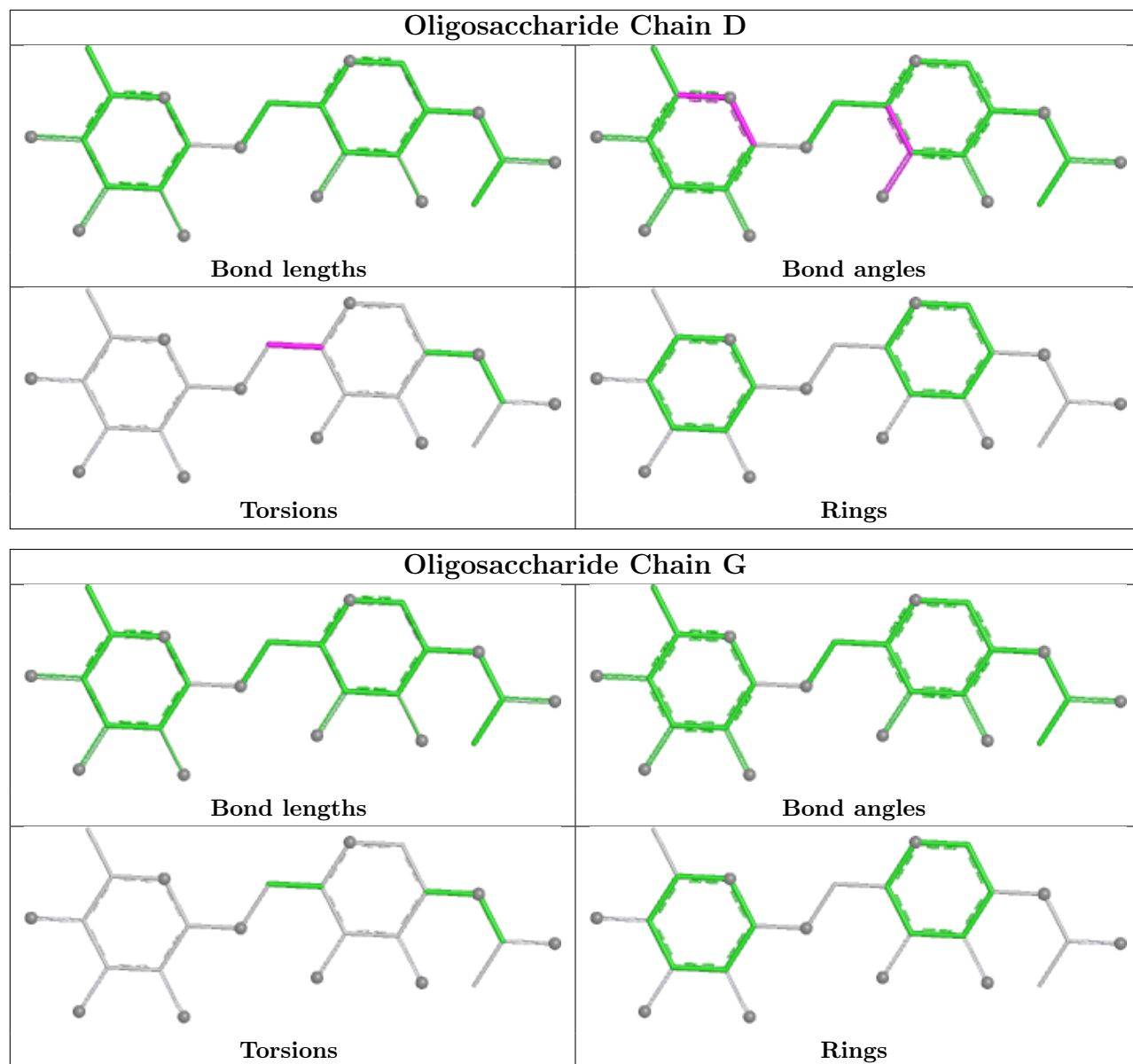
All (1) ring outliers are listed below:

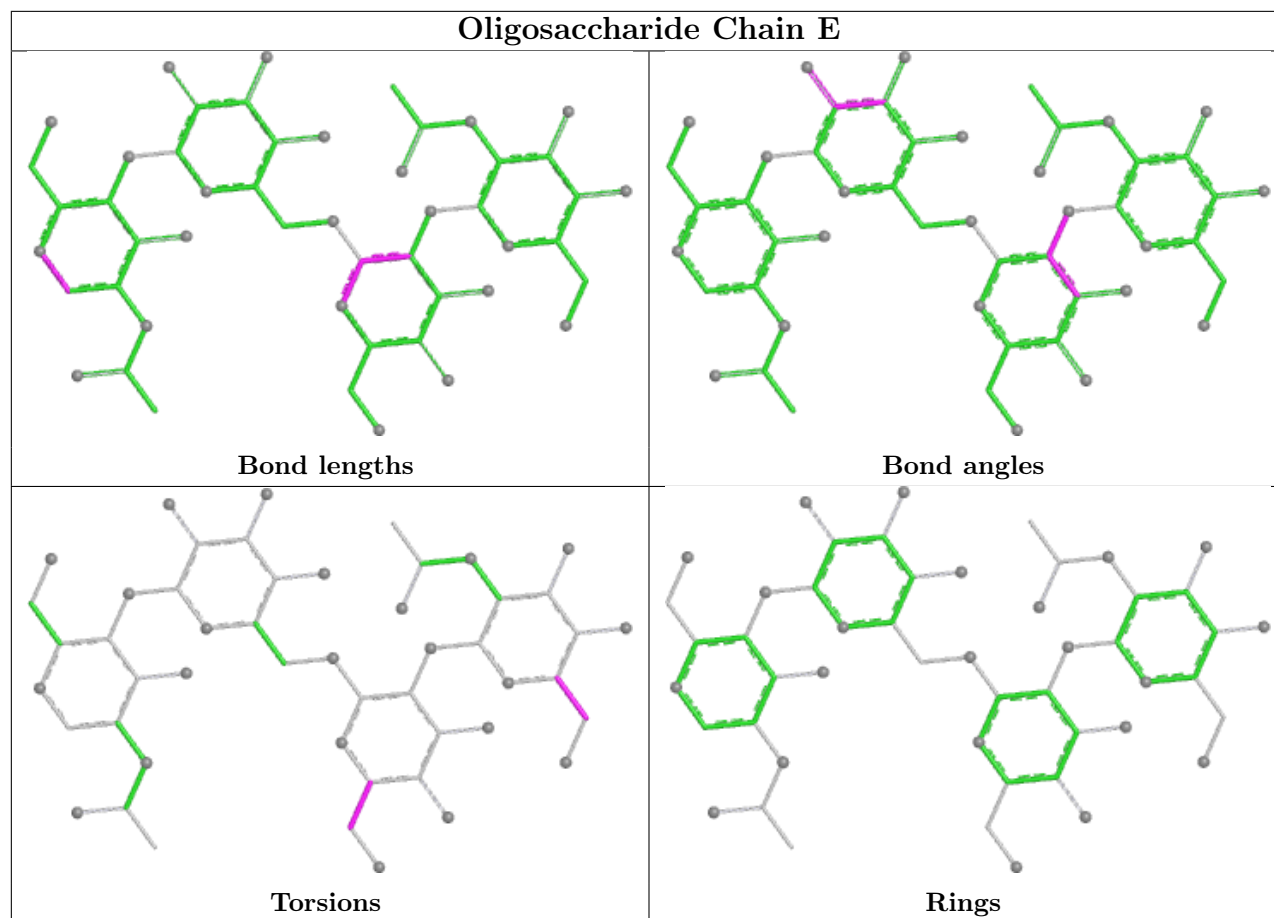
Mol	Chain	Res	Type	Atoms
5	H	4	MAN	C1-C2-C3-C4-C5-O5

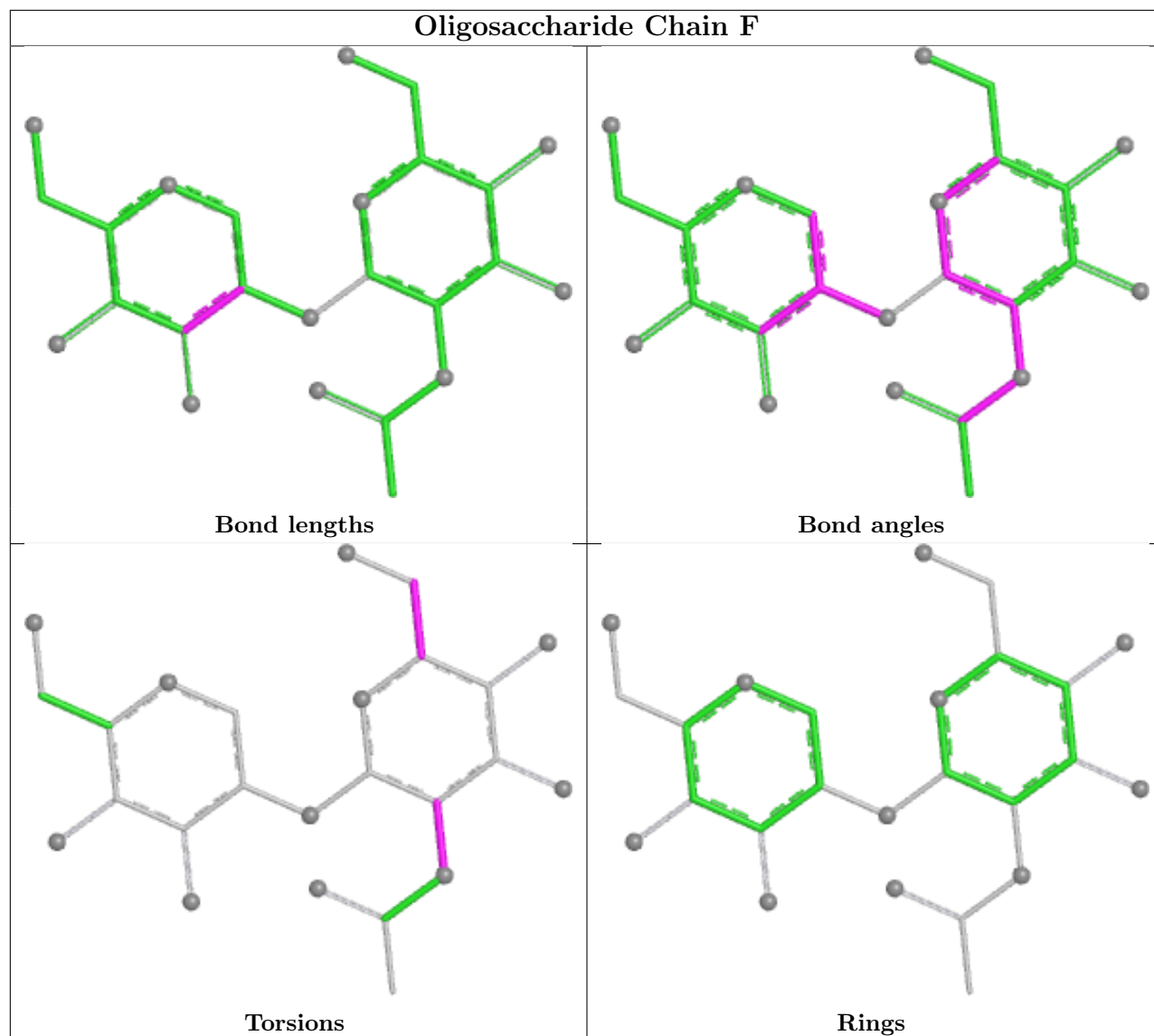
4 monomers are involved in 4 short contacts:

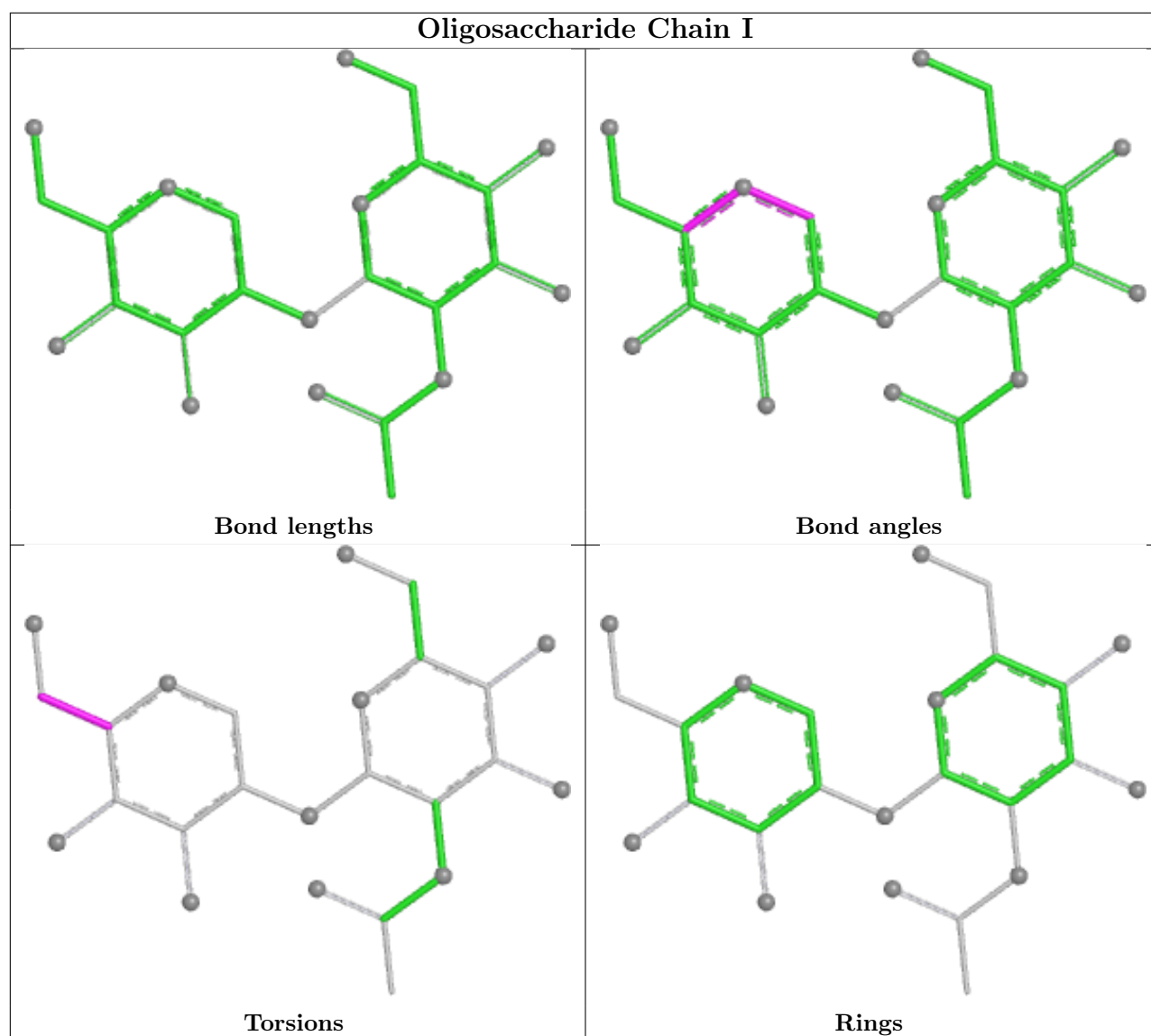
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	1	0
3	E	4	NAG	1	0
4	F	1	MAN	2	0
3	E	2	BMA	1	0

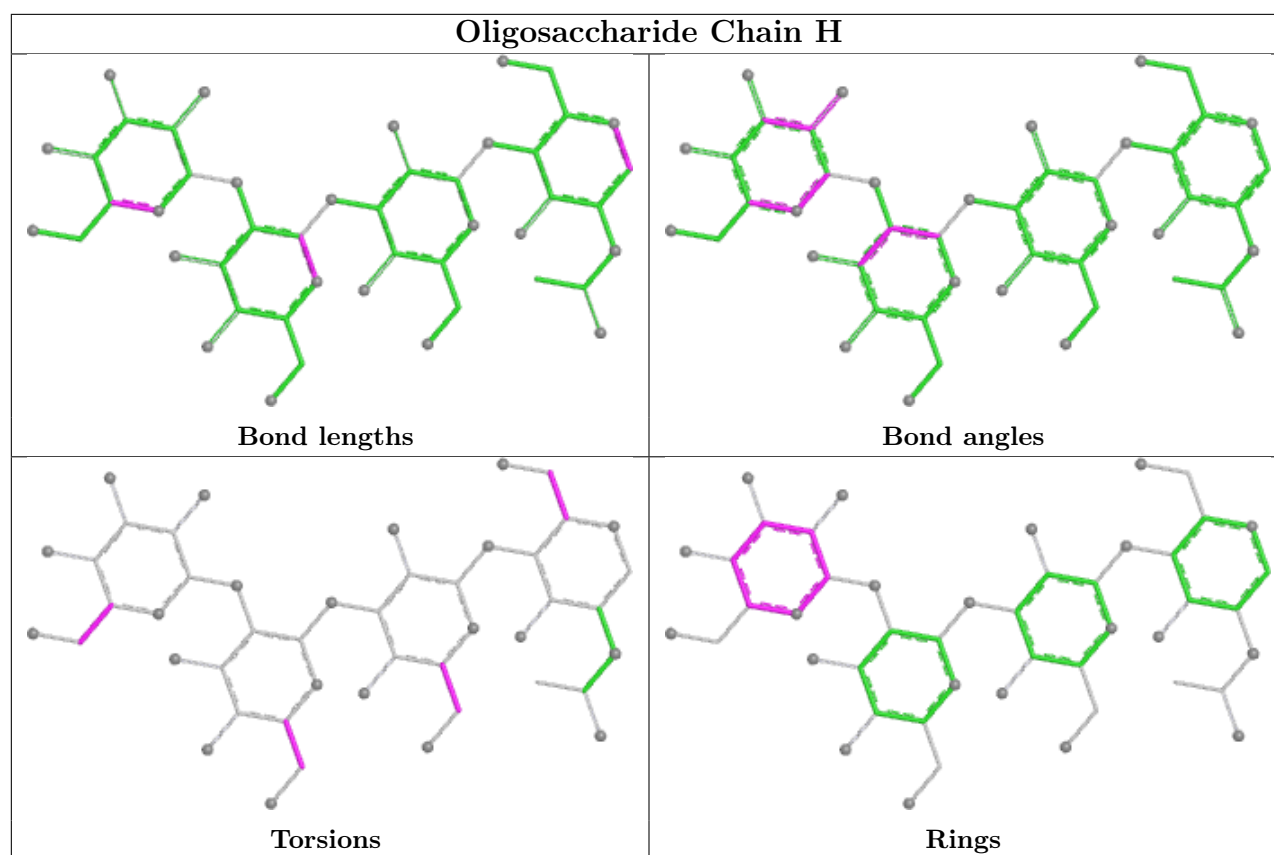
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	FUC	B	508	-	10,10,11	1.35	2 (20%)	14,14,16	1.71	3 (21%)
6	NAG	B	502	7,6	14,14,15	0.87	1 (7%)	17,19,21	0.62	0
7	BMA	B	503	8,6	11,11,12	1.75	3 (27%)	15,15,17	1.94	3 (20%)
6	NAG	B	501	1,6	14,14,15	0.39	0	17,19,21	0.77	0
6	NAG	B	506	8	14,14,15	0.71	1 (7%)	17,19,21	0.63	1 (5%)
8	MAN	B	505	6	11,11,12	1.27	3 (27%)	15,15,17	1.17	1 (6%)
8	MAN	B	504	7,6	11,11,12	0.90	0	15,15,17	0.98	2 (13%)
6	NAG	B	507	8	14,14,15	0.23	0	17,19,21	0.57	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	FUC	B	508	-	-	-	0/1/1/1
6	NAG	B	502	7,6	-	0/6/23/26	0/1/1/1
7	BMA	B	503	8,6	-	2/2/19/22	0/1/1/1
6	NAG	B	501	1,6	-	2/6/23/26	0/1/1/1
6	NAG	B	506	8	-	2/6/23/26	0/1/1/1
8	MAN	B	505	6	-	2/2/19/22	0/1/1/1
8	MAN	B	504	7,6	-	0/2/19/22	0/1/1/1
6	NAG	B	507	8	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	503	BMA	O5-C1	-4.48	1.36	1.43
6	B	502	NAG	O5-C1	-3.06	1.38	1.43
7	B	503	BMA	C6-C5	-2.71	1.42	1.51
9	B	508	FUC	C1-C2	2.54	1.58	1.52
6	B	506	NAG	O5-C1	-2.51	1.39	1.43
8	B	505	MAN	O5-C1	-2.45	1.39	1.43
8	B	505	MAN	C1-C2	-2.28	1.46	1.52
9	B	508	FUC	O5-C5	2.15	1.47	1.43
7	B	503	BMA	O5-C5	-2.06	1.39	1.43
8	B	505	MAN	O2-C2	-2.02	1.39	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	503	BMA	C1-O5-C5	4.88	118.72	112.19
7	B	503	BMA	O5-C5-C6	-3.40	101.05	107.66
9	B	508	FUC	C1-O5-C5	3.39	120.97	112.97
9	B	508	FUC	C1-C2-C3	3.33	114.49	109.64
7	B	503	BMA	C6-C5-C4	-3.26	105.00	113.02
9	B	508	FUC	O5-C1-C2	2.65	117.10	110.79
8	B	504	MAN	C1-O5-C5	2.16	115.09	112.19
8	B	505	MAN	O2-C2-C3	-2.16	105.68	110.15
8	B	504	MAN	O2-C2-C3	-2.14	105.72	110.15
6	B	506	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	505	MAN	O5-C5-C6-O6
6	B	506	NAG	C4-C5-C6-O6
6	B	501	NAG	O5-C5-C6-O6
6	B	506	NAG	O5-C5-C6-O6
8	B	505	MAN	C4-C5-C6-O6
6	B	501	NAG	C4-C5-C6-O6
6	B	507	NAG	C8-C7-N2-C2
6	B	507	NAG	O7-C7-N2-C2
7	B	503	BMA	O5-C5-C6-O6
7	B	503	BMA	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	508	FUC	2	0
7	B	503	BMA	1	0
6	B	501	NAG	2	0
8	B	505	MAN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	210/225 (93%)	-0.00	4 (1%)	66 69	23, 44, 66, 91	2 (0%)
1	B	208/225 (92%)	0.41	9 (4%)	40 41	27, 59, 80, 91	1 (0%)
1	C	208/225 (92%)	-0.03	3 (1%)	73 75	17, 40, 67, 84	1 (0%)
All	All	626/675 (92%)	0.12	16 (2%)	57 60	17, 47, 75, 91	4 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	250	THR	3.9
1	A	388	GLU	3.0
1	B	254	THR	2.9
1	A	445	PRO	2.7
1	B	282	VAL	2.5
1	B	344[A]	ARG	2.3
1	B	253	ILE	2.3
1	B	329	PRO	2.2
1	C	296	TYR	2.2
1	C	292	ARG	2.2
1	B	258	GLU	2.2
1	B	308	VAL	2.1
1	B	318	GLU	2.1
1	B	389	ASN	2.1
1	A	236	GLY	2.0
1	A	296	TYR	2.0

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

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

6.3 Carbohydrates

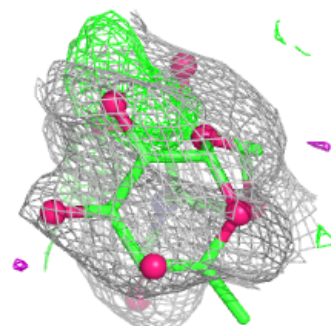
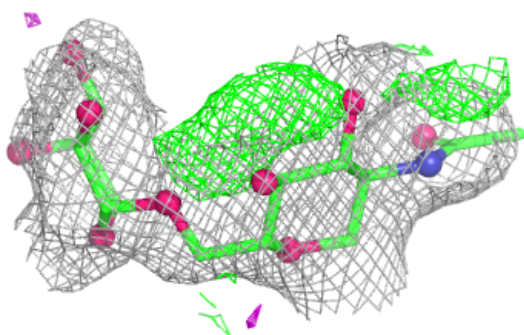
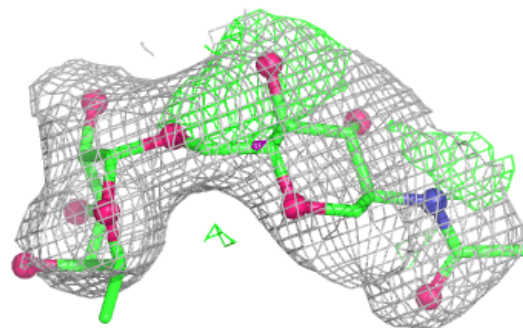
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	2	14/15	0.45	0.18	98,103,106,109	0
5	MAN	H	4	11/12	0.66	0.18	88,91,98,99	0
2	FUC	D	2	10/11	0.74	0.16	75,79,83,85	0
5	MAN	H	3	11/12	0.77	0.13	71,79,88,88	0
4	MAN	F	1	11/12	0.78	0.13	89,96,99,101	0
4	MAN	I	1	11/12	0.81	0.14	52,57,66,70	0
3	MAN	E	3	11/12	0.83	0.12	63,65,70,72	0
2	NAG	D	1	14/15	0.83	0.14	49,61,68,69	0
2	FUC	G	2	10/11	0.84	0.12	62,68,73,77	0
3	NAG	E	1	14/15	0.86	0.11	50,53,57,58	0
5	BMA	H	2	11/12	0.87	0.12	51,58,67,71	0
3	NAG	E	4	14/15	0.88	0.11	64,65,68,69	0
2	NAG	G	1	14/15	0.89	0.10	46,53,61,64	0
3	BMA	E	2	11/12	0.89	0.09	50,57,63,69	0
5	NAG	H	1	14/15	0.90	0.12	43,49,63,68	0
4	NAG	I	2	14/15	0.92	0.09	48,52,57,57	0

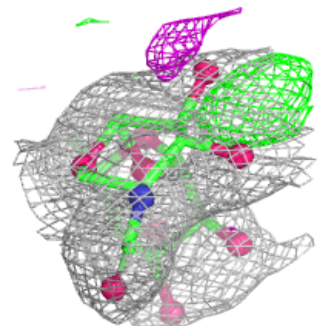
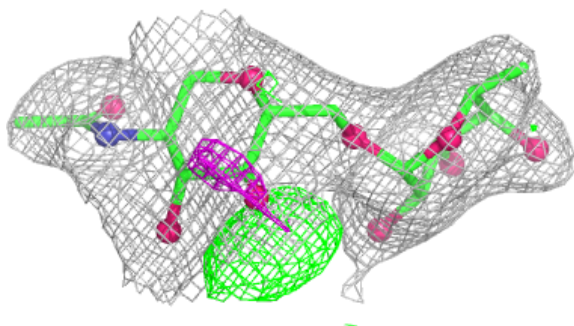
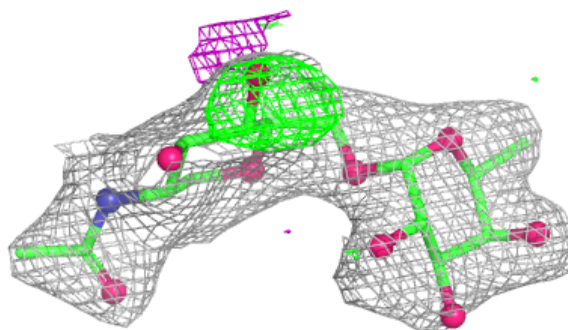
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

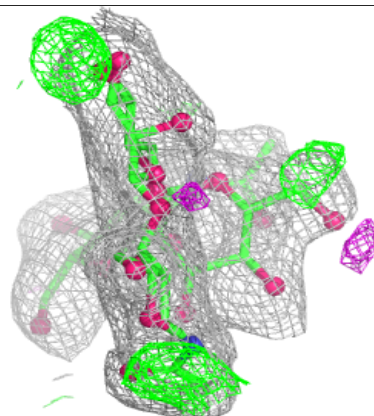
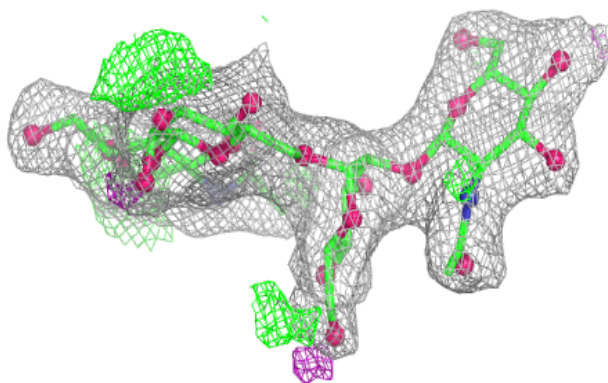
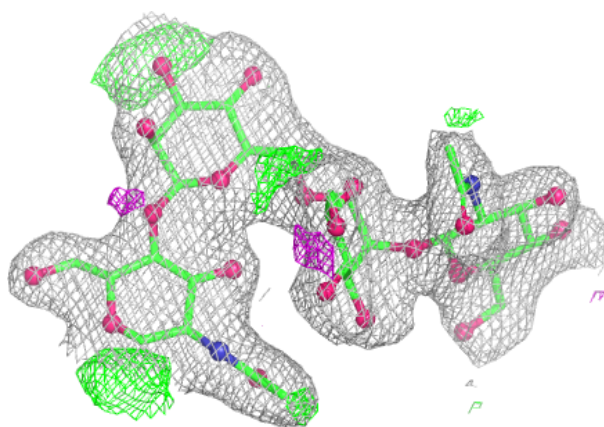
**Electron density around Chain G:**

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



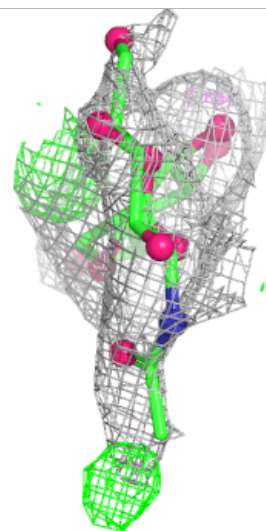
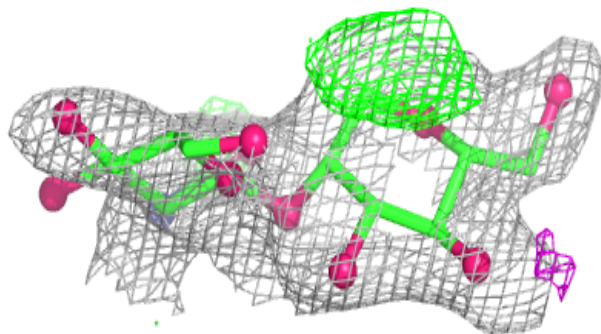
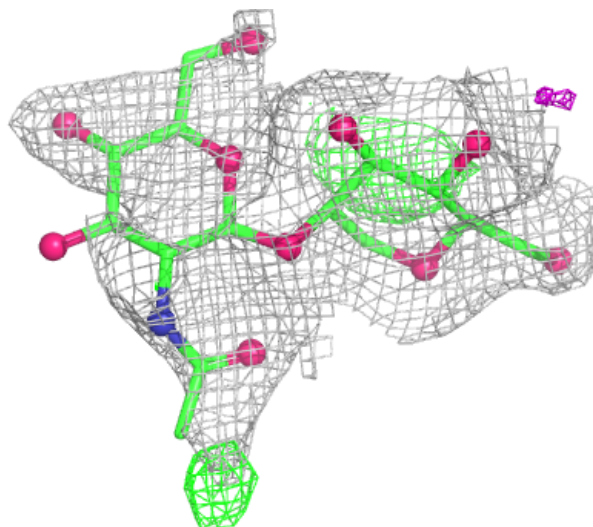
Electron density around Chain E:

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



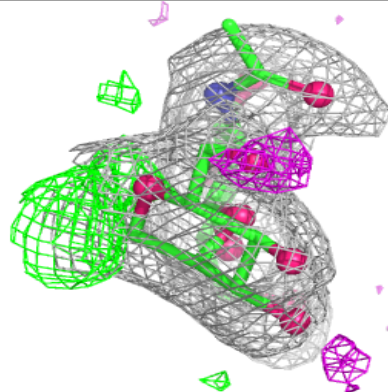
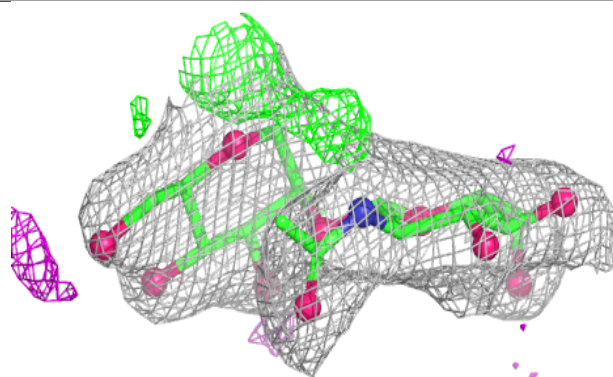
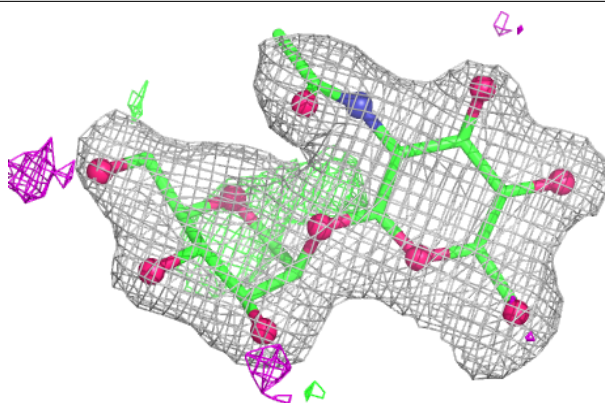
Electron density around Chain F:

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

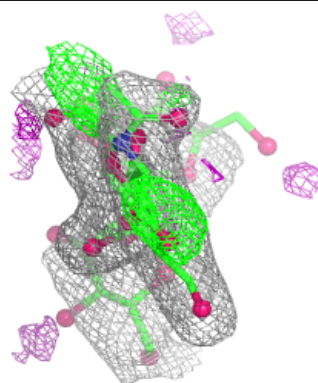
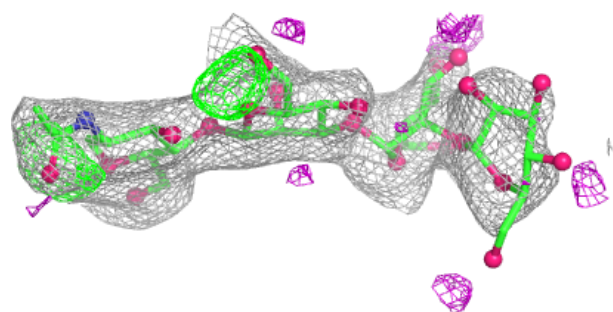
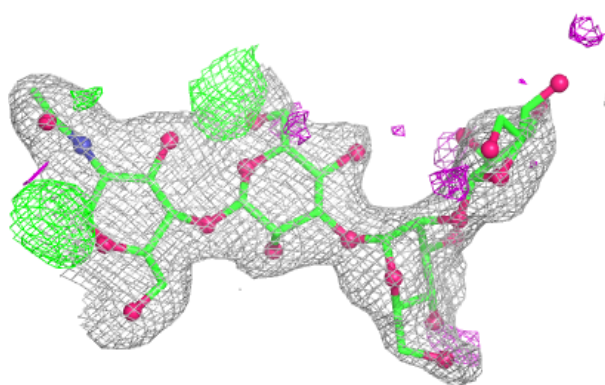


Electron density around Chain I:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
6	NAG	B	507	14/15	0.67	0.13	82,87,92,92	0
7	BMA	B	503	11/12	0.79	0.13	49,59,67,76	0
8	MAN	B	505	11/12	0.81	0.12	60,64,67,70	0
9	FUC	B	508	10/11	0.81	0.14	84,87,90,92	0
6	NAG	B	506	14/15	0.84	0.12	60,67,70,77	0
8	MAN	B	504	11/12	0.84	0.11	70,72,76,76	0
6	NAG	B	501	14/15	0.87	0.12	55,64,71,72	0
6	NAG	B	502	14/15	0.91	0.09	49,59,64,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.