



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:06 AM UTC

PDB ID : 4KH2 / pdb_00004kh2
Title : Crystal structure of human alpha-L-iduronidase complex with 2-deoxy-2-fluoro-alpha-L-idopyranosyluronic acid fluoride
Authors : Bie, H.; Yin, J.; He, X.; Kermode, A.R.; Goddard-Borger, E.D.; Withers, S.G.; James, M.N.G.
Deposited on : 2013-04-29
Resolution : 2.36 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

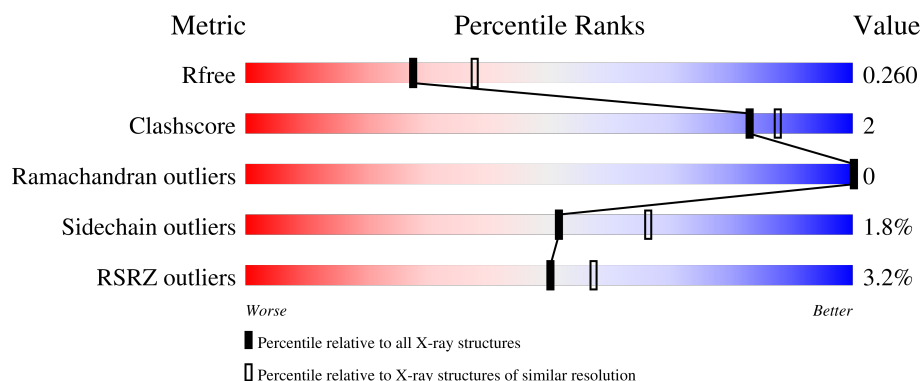
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

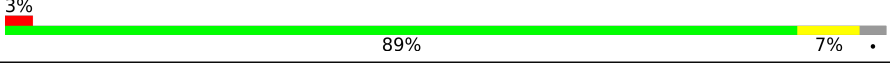
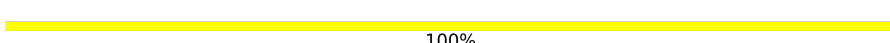
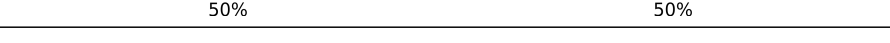
The reported resolution of this entry is 2.36 Å.

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.



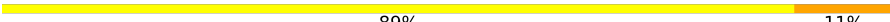
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	627	
1	B	627	
2	C	2	
2	E	2	
3	D	5	

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Mol	Chain	Length	Quality of chain
4	F	9	 89% 11%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10163 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 Alpha-L-iduronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	2	0
			4746	3036	854	842	14			
1	B	607	Total	C	N	O	S	0	5	0
			4862	3105	882	861	14			

There are 6 discrepancies between the modelled and reference sequences:

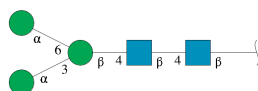
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLN	HIS	SEE REMARK 999	UNP P35475
A	63	PRO	GLN	SEE REMARK 999	UNP P35475
A	105	GLN	ARG	SEE REMARK 999	UNP P35475
B	33	GLN	HIS	SEE REMARK 999	UNP P35475
B	63	PRO	GLN	SEE REMARK 999	UNP P35475
B	105	GLN	ARG	SEE REMARK 999	UNP P35475

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



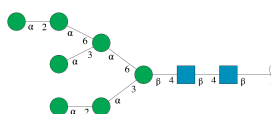
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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.



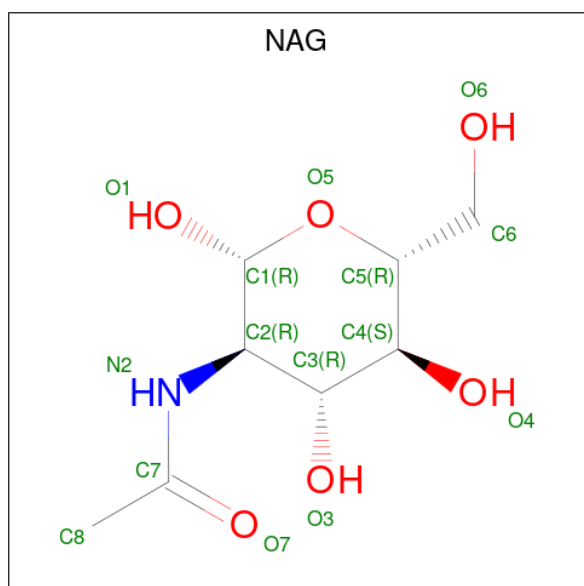
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	9	Total	C	N	O	0	0	0
			105	58	2	45			

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



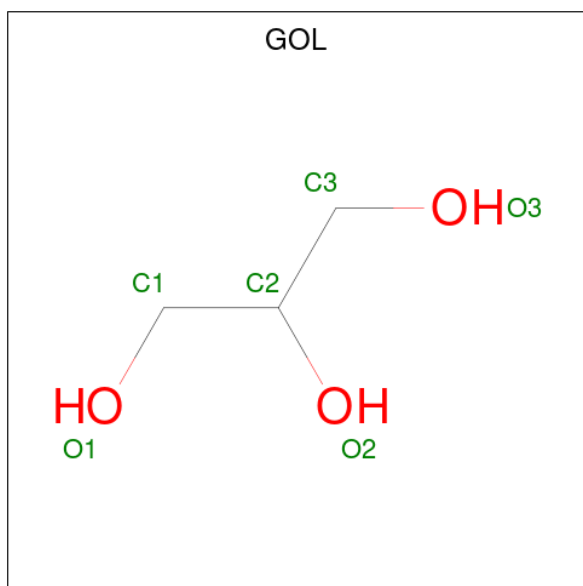
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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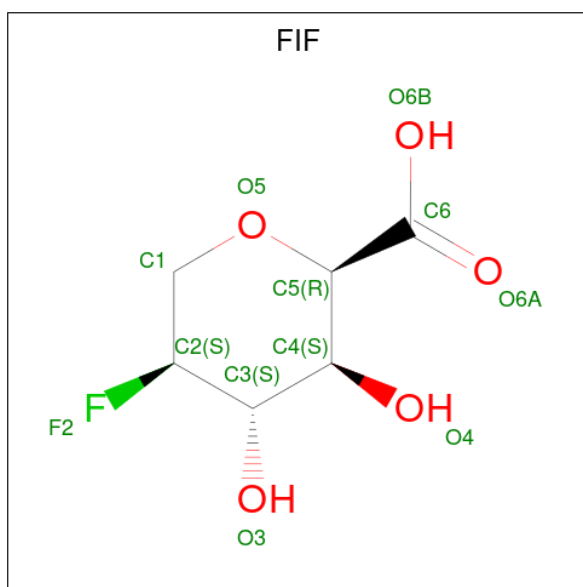
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 2,6-anhydro-5-deoxy-5-fluoro-L-idonic acid (CCD ID: FIF) (formula: $C_6H_9FO_5$).

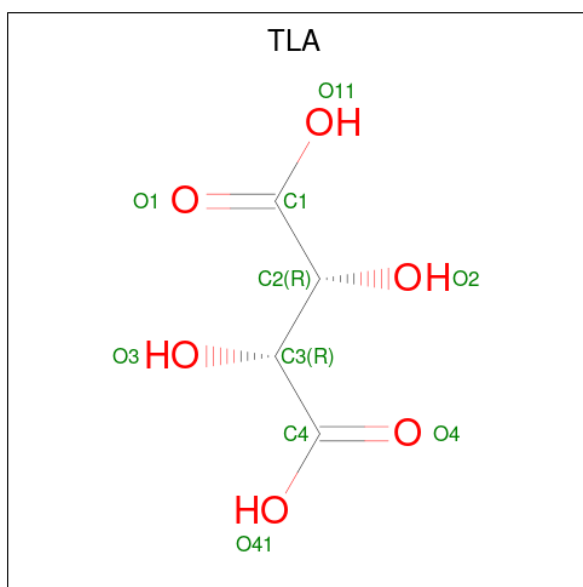


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	F	O	0	0
			12	6	1	5		
7	B	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

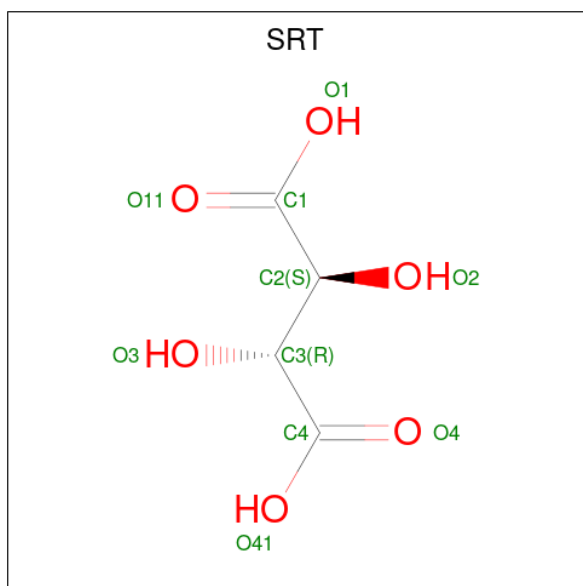
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	B	1	Total	Cl	0	0
			1	1		

- Molecule 9 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



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

- Molecule 10 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: $C_4H_6O_6$).



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

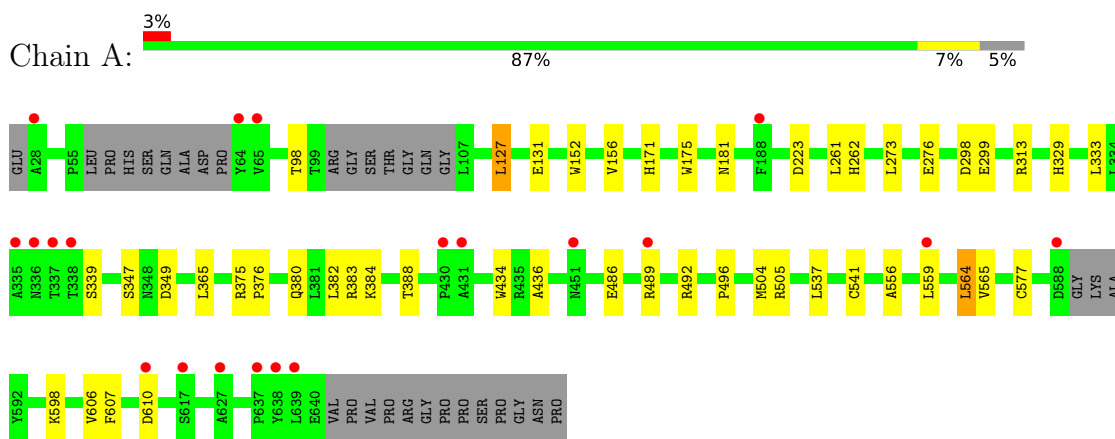
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	95	Total 95	O 95	0	0
11	B	128	Total 128	O 128	0	0

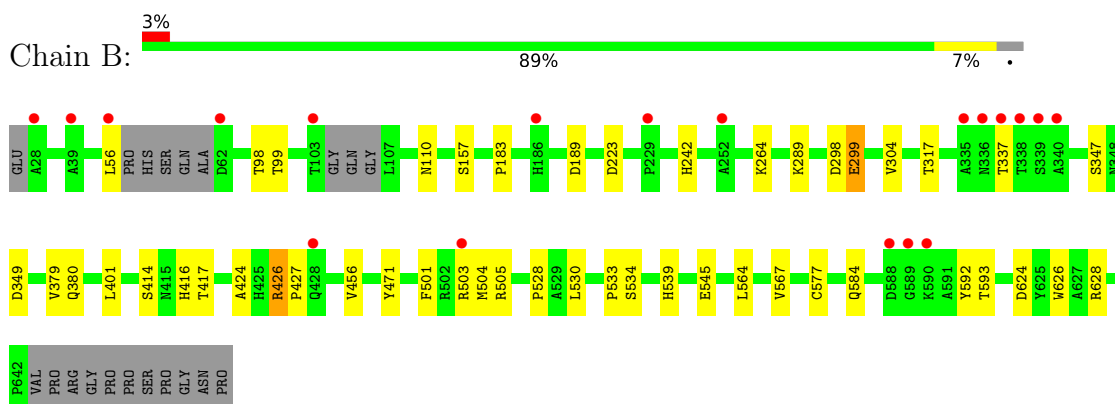
3 Residue-property plots

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: Alpha-L-iduronidase



- Molecule 1: Alpha-L-iduronidase



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



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

Chain E:  50% 50%

MAG1
MAG2

- Molecule 3: 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

Chain D:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 F:  89% 11%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	258.84Å 258.84Å 71.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.72 – 2.36 41.72 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.72-2.36) 98.0 (41.72-2.36)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.220 , 0.261 0.220 , 0.260	Depositor DCC
R_{free} test set	3624 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.827	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10163	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: FIF, BMA, SRT, MAN, NAG, GOL, CL, TLA

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	0.45	2/4891 (0.0%)	0.77	0/6682
1	B	0.46	1/5010 (0.0%)	0.76	1/6843 (0.0%)
All	All	0.46	3/9901 (0.0%)	0.77	1/13525 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	GLU	CD-OE2	11.33	1.46	1.25
1	A	299	GLU	CD-OE2	10.03	1.44	1.25
1	A	299	GLU	C-N	5.20	1.39	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	ASP	CB-CA-C	-5.41	109.88	117.23

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	4746	0	4640	26	0
1	B	4862	0	4765	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	25	0	0
2	E	28	0	25	0	0
3	D	61	0	52	0	0
4	F	105	0	88	1	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	12	0	16	0	0
6	B	24	0	32	0	0
7	A	12	0	7	1	0
7	B	12	0	7	1	0
8	A	1	0	0	1	0
8	B	1	0	0	0	0
9	B	10	0	4	0	0
10	B	10	0	4	0	0
11	A	95	0	0	0	0
11	B	128	0	0	0	0
All	All	10163	0	9691	47	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 2.

All (47) 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:273:LEU:HD11	1:A:333:LEU:HD13	1.85	0.58
1:A:486:GLU:HG2	1:A:489:ARG:HH21	1.72	0.55
1:A:496:PRO:HB3	1:A:504:MET:HE1	1.90	0.54
1:A:565:VAL:HG22	1:A:606:VAL:HG22	1.91	0.53
1:A:380:GLN:NE2	1:A:559:LEU:HB3	2.26	0.51
1:A:262:HIS:HE1	1:A:298:ASP:OD1	1.93	0.50
1:A:223:ASP:O	1:A:261:LEU:HA	2.12	0.50
1:B:242:HIS:CD2	1:B:289:LYS:HB2	2.47	0.50
1:A:564:LEU:HD23	1:A:607:PHE:HB3	1.93	0.50
1:A:541[A]:CYS:SG	1:A:577[A]:CYS:HB3	2.53	0.49
1:B:501:PHE:HA	1:B:504:MET:HE3	1.94	0.49
1:A:127:LEU:HD22	1:A:171:HIS:CE1	2.47	0.49
1:A:262:HIS:CE1	1:A:298:ASP:OD1	2.66	0.49
1:A:383:ARG:HD2	1:A:388:THR:OG1	2.13	0.49
1:A:380:GLN:HE22	1:A:559:LEU:HB3	1.78	0.48
1:A:556:ALA:HB1	1:A:564:LEU:HD11	1.97	0.47
1:A:152:TRP:O	1:A:156:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:LEU:HD21	1:B:424:ALA:HB2	1.97	0.47
1:A:492:ARG:NH2	4:F:3:BMA:O2	2.48	0.47
1:A:349:ASP:OD2	7:A:911:FIF:H5	2.15	0.46
1:B:471:TYR:HA	1:B:539:HIS:O	2.15	0.46
1:A:298:ASP:HA	1:A:347:SER:HB3	1.97	0.45
1:B:530:LEU:HB3	1:B:534:SER:OG	2.16	0.45
1:B:564:LEU:HD12	1:B:564:LEU:C	2.42	0.44
1:B:298:ASP:HA	1:B:347:SER:HB3	1.98	0.44
1:B:584:GLN:HB3	1:B:592:TYR:HB3	1.99	0.44
1:B:577[A]:CYS:SG	1:B:577[A]:CYS:O	2.76	0.43
1:B:577[A]:CYS:SG	1:B:626:TRP:HZ3	2.42	0.43
1:B:317:THR:HA	1:B:533:PRO:HG3	2.01	0.43
1:B:349:ASP:OD2	7:B:919:FIF:H5	2.19	0.43
1:A:171:HIS:CD2	1:A:175:TRP:HE1	2.36	0.42
1:B:456:VAL:O	1:B:528:PRO:HD2	2.19	0.42
1:B:414:SER:C	1:B:416:HIS:H	2.28	0.42
1:B:380:GLN:OE1	1:B:505:ARG:NH2	2.49	0.42
1:B:426:ARG:HA	1:B:427:PRO:HD2	1.90	0.42
1:A:131:GLU:OE2	1:A:181:ASN:HB2	2.20	0.41
1:A:434:TRP:CH2	1:A:436:ALA:HB2	2.55	0.41
1:B:264:LYS:HE3	1:B:304:VAL:HG23	2.01	0.41
1:B:98:THR:OG1	1:B:110:ASN:HB3	2.20	0.41
1:A:365:LEU:O	1:A:384:LYS:HB2	2.21	0.41
1:B:264:LYS:HE2	1:B:299:GLU:OE1	2.21	0.41
1:A:276:GLU:OE1	1:A:329:HIS:NE2	2.48	0.41
1:A:313:ARG:NH2	8:A:912:CL:CL	2.85	0.41
1:B:624:ASP:OD2	1:B:628:ARG:HB2	2.21	0.40
1:A:382:LEU:HD23	1:A:505:ARG:HG2	2.03	0.40
1:A:375:ARG:HA	1:A:376:PRO:HA	1.90	0.40
1:B:183:PRO:HD2	1:B:223:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	589/627 (94%)	564 (96%)	25 (4%)	0	100	100
1	B	606/627 (97%)	582 (96%)	24 (4%)	0	100	100
All	All	1195/1254 (95%)	1146 (96%)	49 (4%)	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	505/527 (96%)	498 (99%)	7 (1%)	59	73
1	B	517/527 (98%)	505 (98%)	12 (2%)	44	58
All	All	1022/1054 (97%)	1003 (98%)	19 (2%)	51	65

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	THR
1	A	127	LEU
1	A	339	SER
1	A	537	LEU
1	A	564	LEU
1	A	598	LYS
1	A	610	ASP
1	B	56	LEU
1	B	99	THR
1	B	157	SER
1	B	337	THR
1	B	379	VAL
1	B	417	THR
1	B	426	ARG
1	B	503[A]	ARG

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Mol	Chain	Res	Type
1	B	503[B]	ARG
1	B	545	GLU
1	B	567	VAL
1	B	593	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	HIS
1	A	185	HIS
1	A	226	HIS
1	A	358	HIS
1	A	416	HIS
1	A	587	GLN
1	B	196	GLN
1	B	226	HIS
1	B	330	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 ⓘ

18 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	C	1	1,2	14,14,15	0.57	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2	2	14,14,15	0.58	0	17,19,21	1.06	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.52	0	17,19,21	0.84	0
3	NAG	D	2	3	14,14,15	0.52	0	17,19,21	1.50	1 (5%)
3	BMA	D	3	3	11,11,12	0.46	0	15,15,17	1.08	2 (13%)
3	MAN	D	4	3	11,11,12	0.54	0	15,15,17	1.00	1 (6%)
3	MAN	D	5	3	11,11,12	0.59	0	15,15,17	1.01	1 (6%)
2	NAG	E	1	1,2	14,14,15	0.55	0	17,19,21	0.81	0
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	0.98	1 (5%)
4	NAG	F	1	4,1	14,14,15	0.49	0	17,19,21	1.19	2 (11%)
4	NAG	F	2	4	14,14,15	0.55	0	17,19,21	0.95	1 (5%)
4	BMA	F	3	4	11,11,12	0.53	0	15,15,17	1.11	2 (13%)
4	MAN	F	4	4	11,11,12	0.67	0	15,15,17	0.97	1 (6%)
4	MAN	F	5	4	11,11,12	0.46	0	15,15,17	1.17	2 (13%)
4	MAN	F	6	4	11,11,12	0.52	0	15,15,17	0.93	1 (6%)
4	MAN	F	7	4	11,11,12	0.56	0	15,15,17	1.10	1 (6%)
4	MAN	F	8	4	11,11,12	0.53	0	15,15,17	1.24	2 (13%)
4	MAN	F	9	4	11,11,12	0.65	0	15,15,17	0.97	1 (6%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	2/2/19/22	0/1/1/1
4	MAN	F	8	4	-	0/2/19/22	0/1/1/1
4	MAN	F	9	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	4.92	118.78	112.19
4	F	5	MAN	C1-O5-C5	3.43	116.78	112.19
4	F	8	MAN	C1-O5-C5	3.38	116.71	112.19
4	F	7	MAN	C1-O5-C5	3.24	116.53	112.19
4	F	6	MAN	C1-O5-C5	3.17	116.44	112.19
3	D	5	MAN	C1-O5-C5	2.85	116.00	112.19
3	D	4	MAN	C1-O5-C5	2.82	115.96	112.19
3	D	3	BMA	C1-O5-C5	2.65	115.74	112.19
4	F	4	MAN	C1-C2-C3	2.45	113.20	109.64
4	F	3	BMA	C1-C2-C3	2.43	113.18	109.64
4	F	1	NAG	O5-C1-C2	-2.40	107.57	111.29
2	C	2	NAG	C1-O5-C5	2.40	115.40	112.19
4	F	9	MAN	C1-C2-C3	2.38	113.10	109.64
4	F	1	NAG	C1-O5-C5	2.30	115.26	112.19
4	F	3	BMA	C1-O5-C5	2.22	115.16	112.19
4	F	2	NAG	C1-O5-C5	2.14	115.06	112.19
3	D	3	BMA	C1-C2-C3	2.11	112.72	109.64
2	E	2	NAG	C2-N2-C7	2.11	125.72	122.90
4	F	5	MAN	O2-C2-C3	-2.09	105.82	110.15
4	F	8	MAN	C3-C4-C5	2.00	113.86	110.23
2	C	1	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	F	7	MAN	C4-C5-C6-O6

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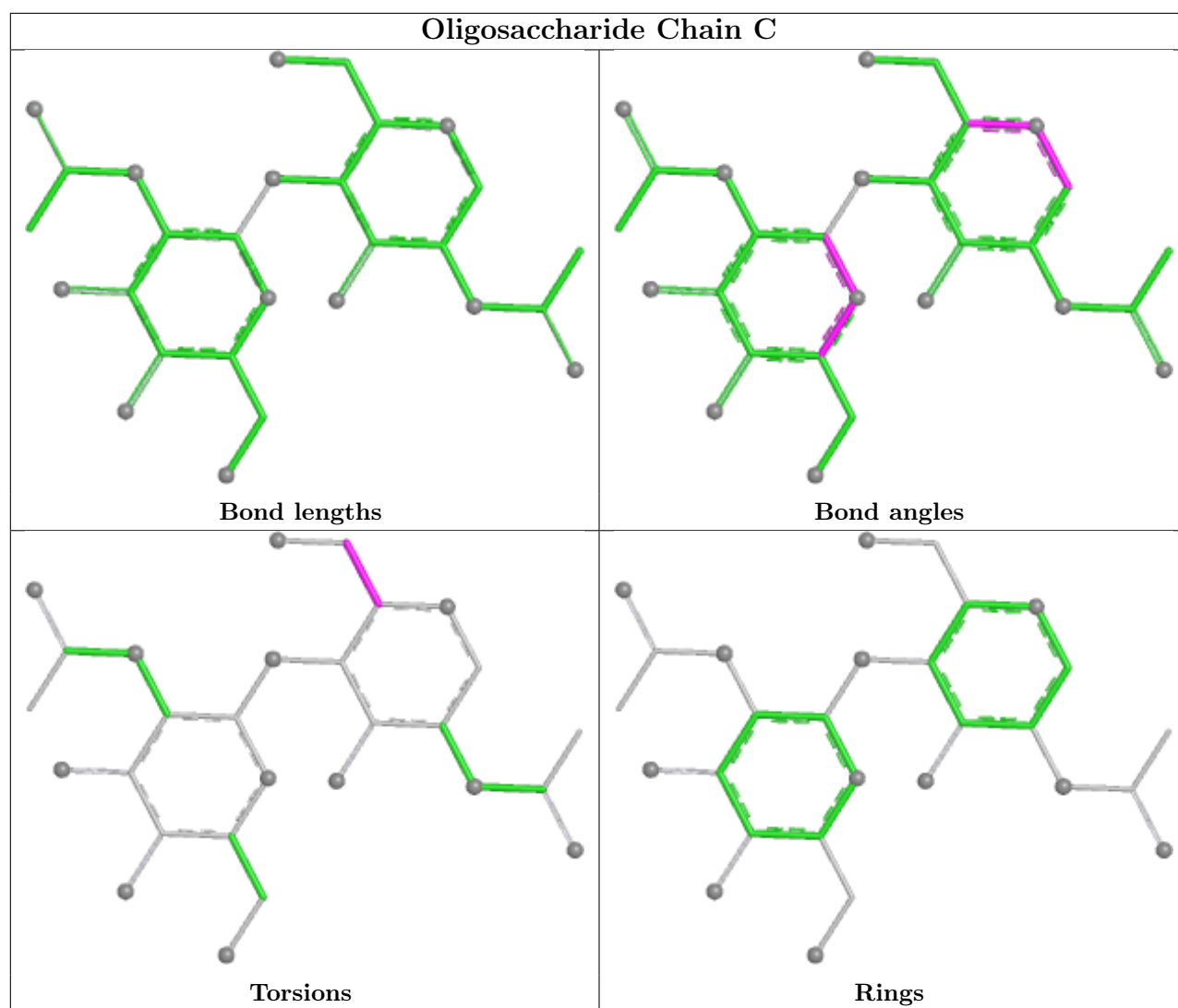
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
4	F	5	MAN	C4-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
4	F	9	MAN	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
4	F	9	MAN	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

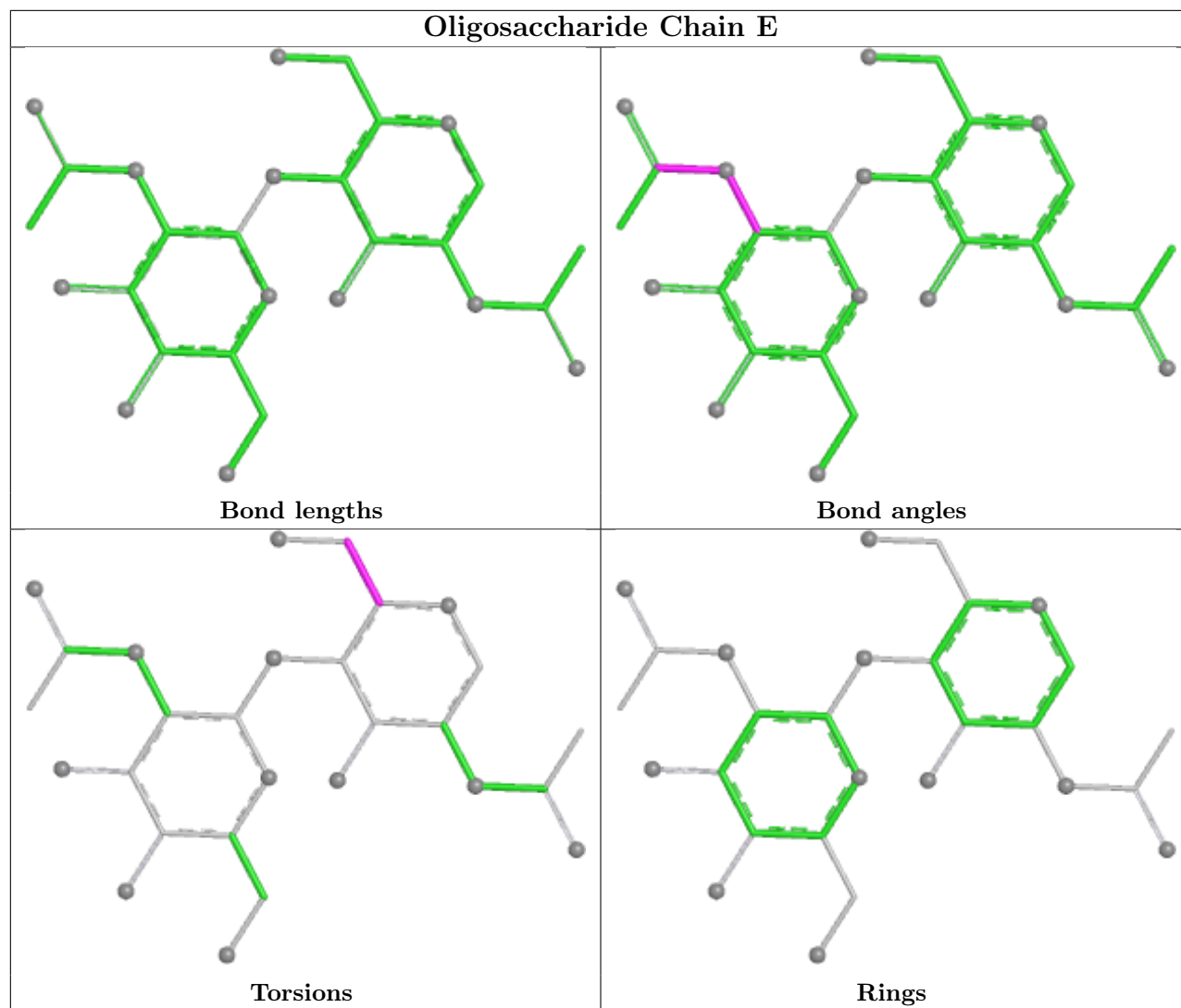
There are no ring outliers.

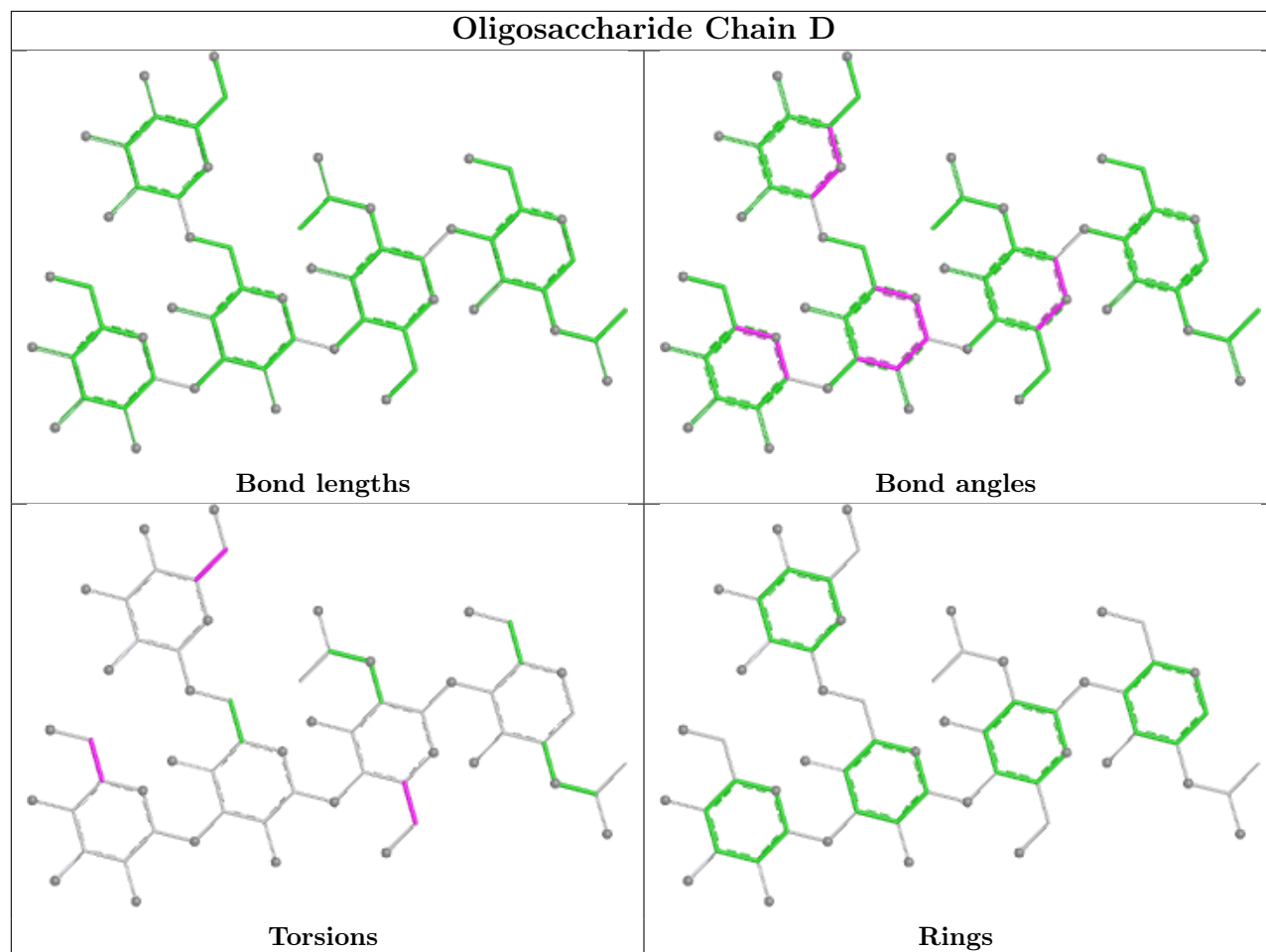
1 monomer is involved in 1 short contact:

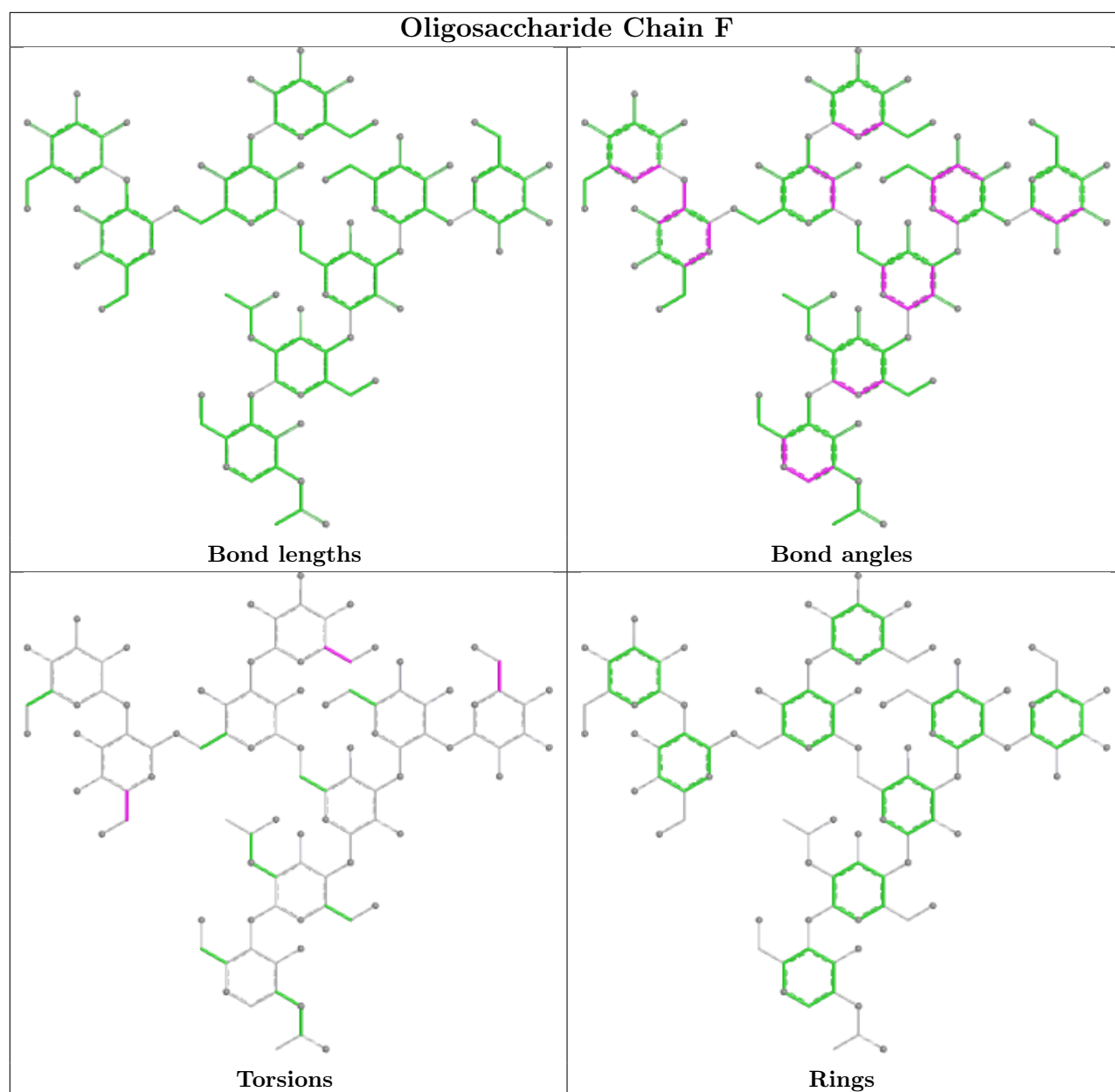
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3	BMA	1	0

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](#)

Of 14 ligands modelled in this entry, 2 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
9	TLA	B	917	-	9,9,9	1.15	0	12,12,12	1.02	1 (8%)
5	NAG	A	901	1	14,14,15	0.66	0	17,19,21	1.13	2 (11%)
6	GOL	A	909	-	5,5,5	0.27	0	5,5,5	0.18	0
7	FIF	B	919	1	12,12,12	1.02	0	11,17,17	1.82	1 (9%)
6	GOL	B	916	-	5,5,5	0.29	0	5,5,5	0.81	0
6	GOL	B	914	-	5,5,5	0.37	0	5,5,5	0.20	0
10	SRT	B	918	-	9,9,9	1.20	0	12,12,12	1.08	0
6	GOL	B	915	-	5,5,5	0.23	0	5,5,5	0.39	0
6	GOL	B	913	-	5,5,5	0.26	0	5,5,5	0.40	0
7	FIF	A	911	1	12,12,12	1.10	0	11,17,17	1.18	2 (18%)
5	NAG	B	901	1	14,14,15	0.43	0	17,19,21	1.38	1 (5%)
6	GOL	A	910	-	5,5,5	0.29	0	5,5,5	0.36	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	TLA	B	917	-	-	0/12/12/12	-
5	NAG	A	901	1	-	2/6/23/26	0/1/1/1
6	GOL	A	909	-	-	1/4/4/4	-
7	FIF	B	919	1	-	0/4/21/21	0/1/1/1
6	GOL	B	916	-	-	4/4/4/4	-
6	GOL	B	914	-	-	4/4/4/4	-
10	SRT	B	918	-	-	7/12/12/12	-
6	GOL	B	915	-	-	1/4/4/4	-
6	GOL	B	913	-	-	0/4/4/4	-
7	FIF	A	911	1	-	0/4/21/21	0/1/1/1
5	NAG	B	901	1	-	0/6/23/26	0/1/1/1
6	GOL	A	910	-	-	2/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	919	FIF	F2-C2-C1	5.18	112.34	108.26
5	B	901	NAG	C1-O5-C5	4.89	118.74	112.19
5	A	901	NAG	C4-C3-C2	2.63	114.87	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	NAG	C1-O5-C5	2.14	115.06	112.19
7	A	911	FIF	C2-C3-C4	2.11	112.14	109.59
9	B	917	TLA	O11-C1-C2	2.06	119.04	113.31
7	A	911	FIF	F2-C2-C1	2.01	109.85	108.26

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	910	GOL	C1-C2-C3-O3
6	B	914	GOL	C1-C2-C3-O3
6	B	914	GOL	O2-C2-C3-O3
10	B	918	SRT	O1-C1-C2-O2
10	B	918	SRT	O11-C1-C2-O2
10	B	918	SRT	O3-C3-C4-O4
10	B	918	SRT	O3-C3-C4-O41
5	A	901	NAG	O5-C5-C6-O6
5	A	901	NAG	C4-C5-C6-O6
6	A	909	GOL	C1-C2-C3-O3
6	B	914	GOL	O1-C1-C2-C3
6	B	915	GOL	C1-C2-C3-O3
6	B	916	GOL	O1-C1-C2-C3
6	B	916	GOL	C1-C2-C3-O3
6	A	910	GOL	O2-C2-C3-O3
10	B	918	SRT	O11-C1-C2-C3
6	B	916	GOL	O1-C1-C2-O2
10	B	918	SRT	O1-C1-C2-C3
10	B	918	SRT	O2-C2-C3-O3
6	B	916	GOL	O2-C2-C3-O3
6	B	914	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	919	FIF	1	0
7	A	911	FIF	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	595/627 (94%)	0.39	20 (3%)	48 55	23, 35, 61, 77	2 (0%)
1	B	607/627 (96%)	0.15	19 (3%)	51 58	13, 32, 53, 84	5 (0%)
All	All	1202/1254 (95%)	0.27	39 (3%)	50 57	13, 34, 59, 84	7 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	LEU	5.1
1	B	337	THR	4.4
1	B	589	GLY	3.8
1	B	340	ALA	3.4
1	A	639	LEU	3.3
1	A	64	TYR	3.2
1	B	338	THR	3.1
1	B	339	SER	3.1
1	B	39	ALA	3.0
1	A	338	THR	2.9
1	A	188	PHE	2.8
1	A	431	ALA	2.8
1	A	610	ASP	2.6
1	A	588	ASP	2.6
1	B	229	PRO	2.6
1	A	638	TYR	2.6
1	A	489	ARG	2.4
1	B	503[A]	ARG	2.4
1	A	337	THR	2.4
1	A	430	PRO	2.4
1	A	28	ALA	2.4
1	B	252	ALA	2.4
1	A	451	ASN	2.3
1	B	62	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	186	HIS	2.3
1	A	559	LEU	2.3
1	A	336	ASN	2.3
1	B	336	ASN	2.2
1	A	637	PRO	2.2
1	B	428	GLN	2.2
1	B	28	ALA	2.2
1	B	103	THR	2.2
1	A	617	SER	2.1
1	B	590	LYS	2.1
1	A	65	VAL	2.1
1	A	335	ALA	2.0
1	A	627	ALA	2.0
1	B	588	ASP	2.0
1	B	335	ALA	2.0

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.

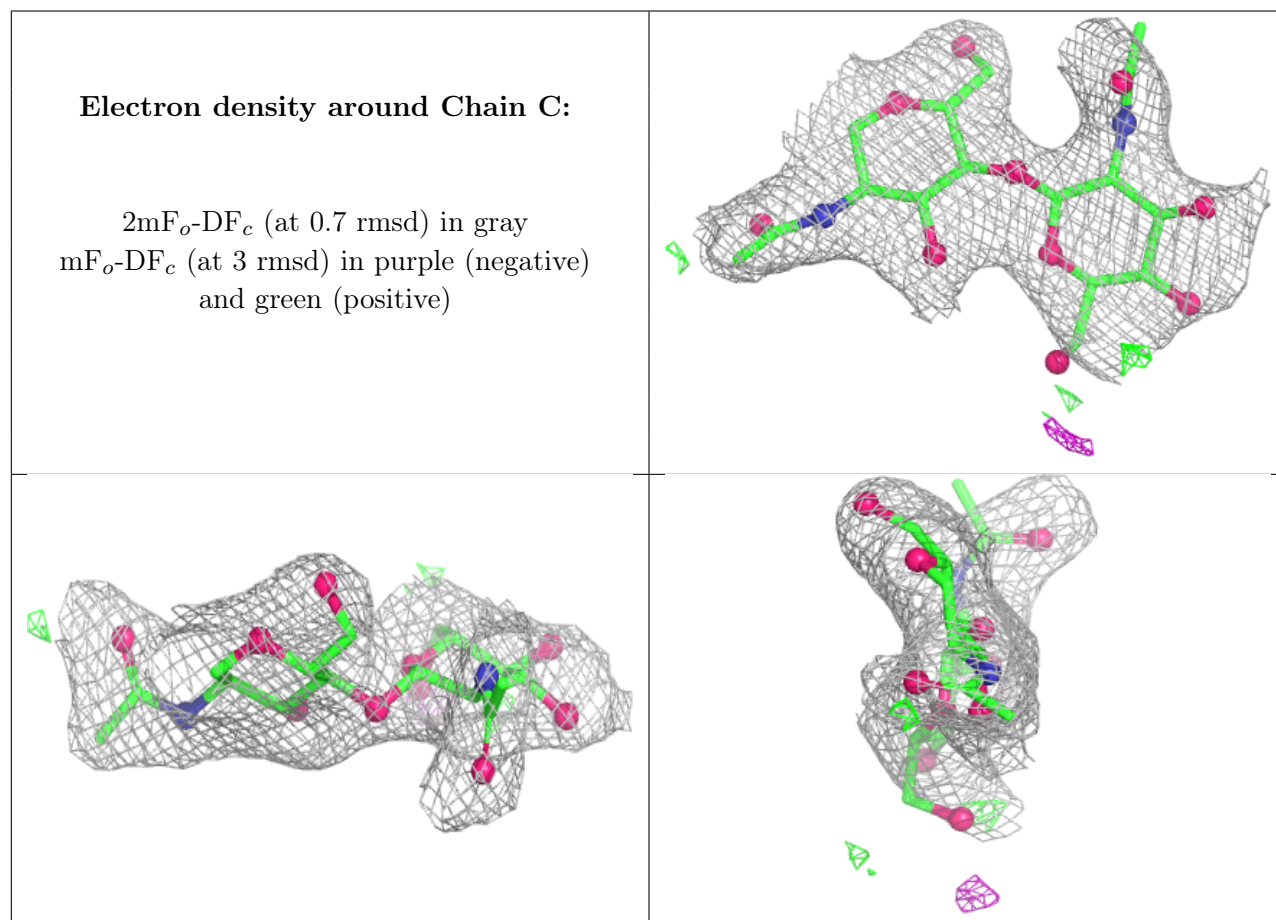
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	D	4	11/12	0.67	0.17	81,83,86,87	0
2	NAG	C	2	14/15	0.68	0.18	66,70,72,72	0
3	MAN	D	5	11/12	0.69	0.19	71,72,74,74	0
4	MAN	F	9	11/12	0.70	0.16	59,61,63,63	0
4	MAN	F	7	11/12	0.75	0.15	61,64,65,66	0
4	MAN	F	5	11/12	0.75	0.18	60,61,62,64	0
2	NAG	E	2	14/15	0.77	0.16	67,70,71,72	0
4	MAN	F	6	11/12	0.83	0.15	56,59,61,62	0
2	NAG	E	1	14/15	0.89	0.11	48,54,58,63	0
4	MAN	F	8	11/12	0.89	0.10	50,54,55,56	0
3	BMA	D	3	11/12	0.89	0.11	62,67,69,74	0
4	MAN	F	4	11/12	0.90	0.11	48,53,57,58	0
3	NAG	D	2	14/15	0.90	0.12	48,52,56,58	0

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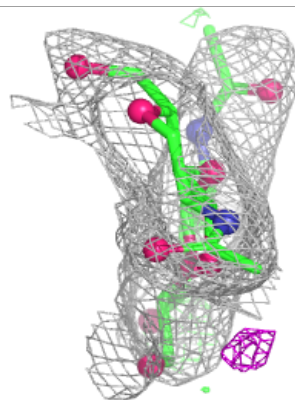
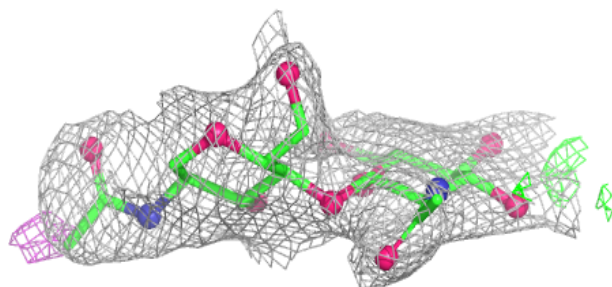
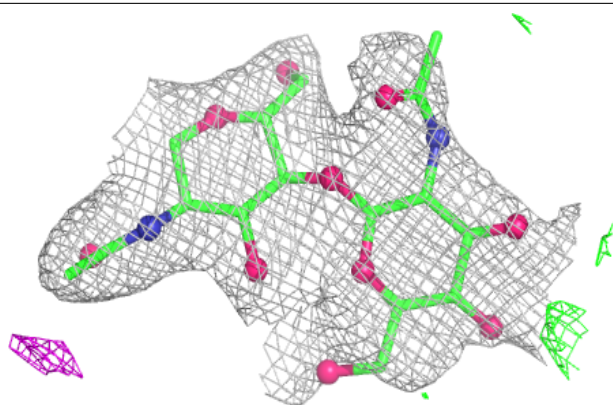
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	1	14/15	0.92	0.10	47,49,54,60	0
3	NAG	D	1	14/15	0.92	0.10	46,47,50,50	0
4	NAG	F	2	14/15	0.92	0.08	30,32,33,34	0
4	BMA	F	3	11/12	0.93	0.09	37,40,44,46	0
4	NAG	F	1	14/15	0.94	0.08	30,30,31,31	0

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.

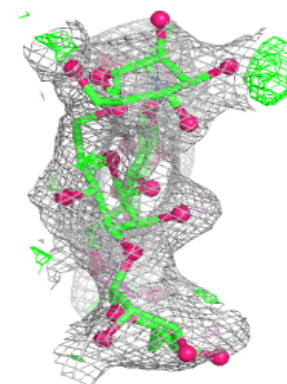
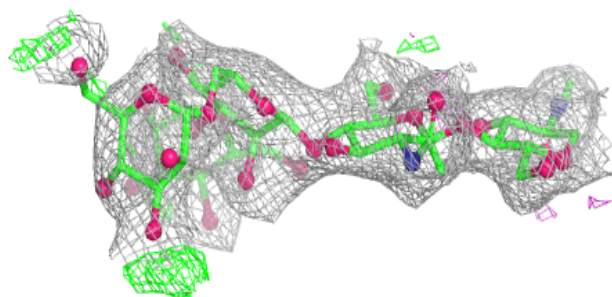
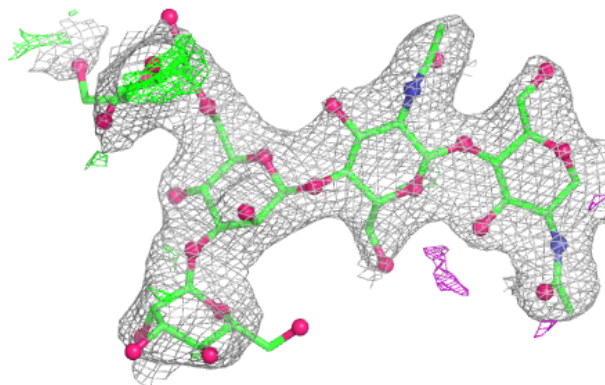


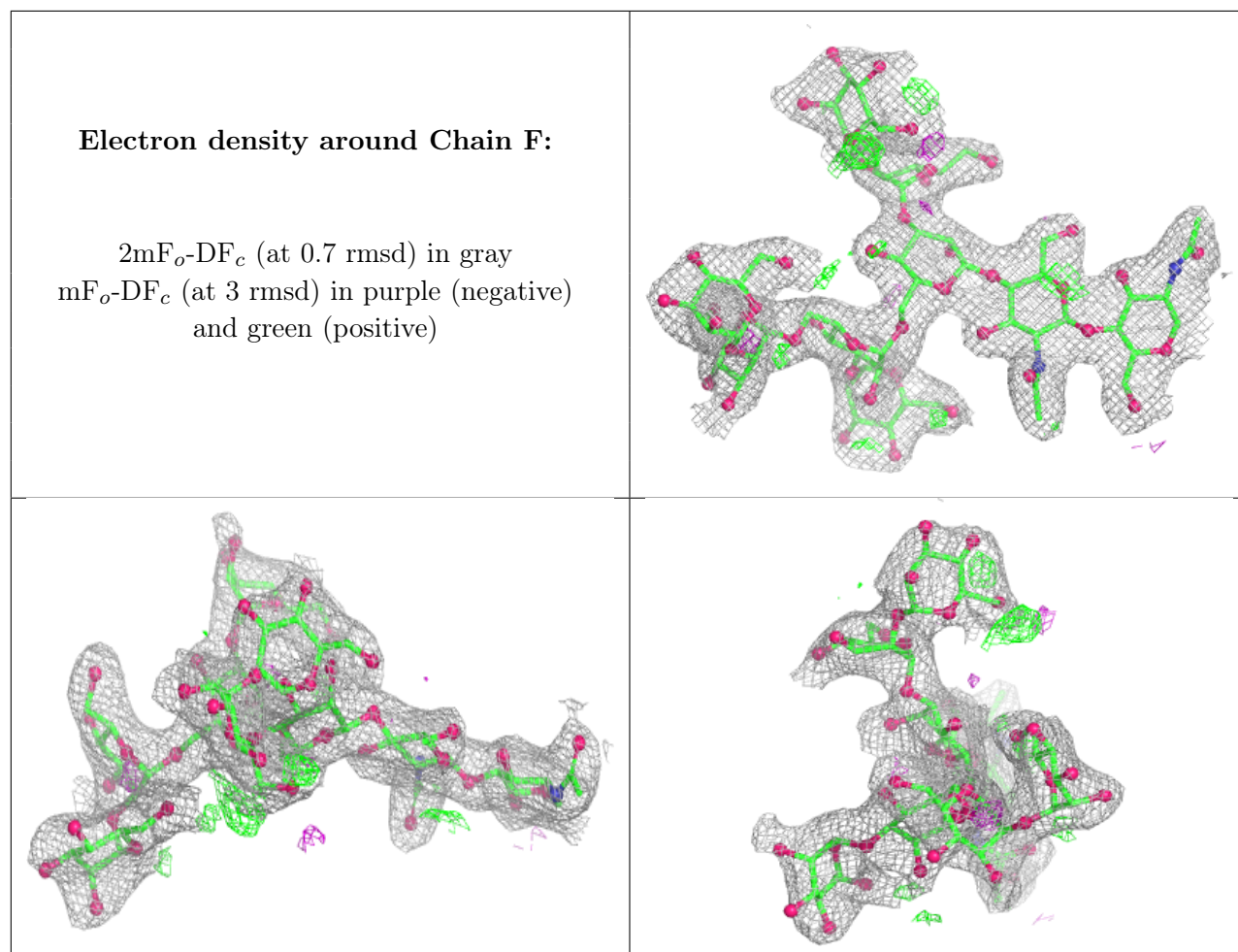
Electron density around Chain E:

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

**Electron density around Chain D:**

$2mF_o-DF_c$ (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
5	NAG	A	901	14/15	0.73	0.17	61,67,70,70	0
6	GOL	A	910	6/6	0.74	0.20	67,67,68,68	0
7	FIF	A	911	12/12	0.83	0.12	42,44,46,47	0
10	SRT	B	918	10/10	0.84	0.12	48,50,51,52	0
6	GOL	B	915	6/6	0.86	0.13	42,43,44,46	0
7	FIF	B	919	12/12	0.87	0.11	44,46,47,47	0
6	GOL	A	909	6/6	0.88	0.12	44,49,49,51	0
6	GOL	B	914	6/6	0.88	0.14	40,42,43,43	0
5	NAG	B	901	14/15	0.89	0.10	42,44,45,46	0
6	GOL	B	913	6/6	0.90	0.12	40,41,42,42	0
6	GOL	B	916	6/6	0.91	0.11	25,27,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	TLA	B	917	10/10	0.93	0.08	39,40,43,43	0
8	CL	A	912	1/1	0.96	0.07	33,33,33,33	0
8	CL	B	920	1/1	0.99	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.