



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:58 AM UTC

PDB ID : 6I6X / pdb_00006i6x
Title : New Irreversible α -l-Iduronidase Inhibitors and Activity-Based Probes
Authors : Gloster, T.M.; McMahon, S.A.; Oehler, V.
Deposited on : 2018-11-15
Resolution : 2.39 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

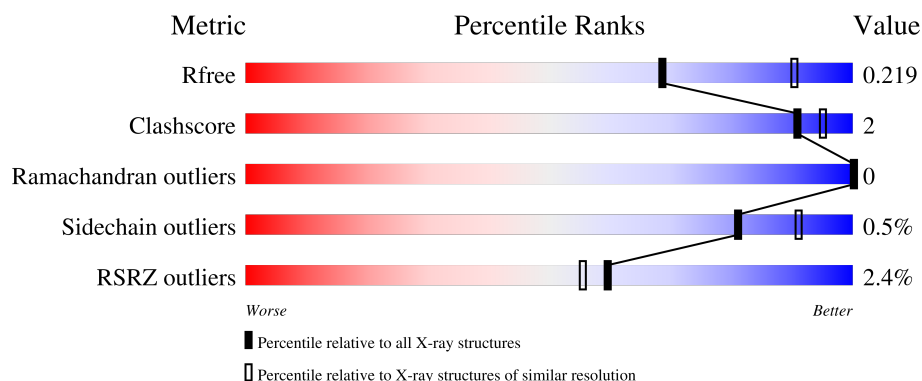
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

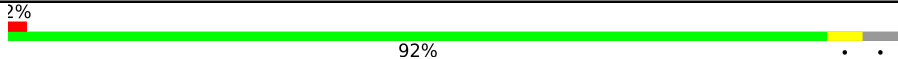
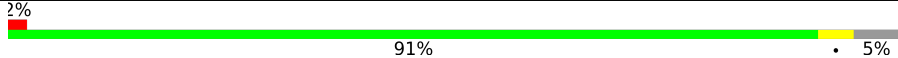
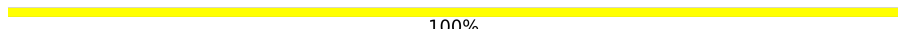
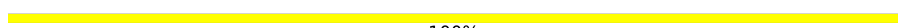
The reported resolution of this entry is 2.39 Å.

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.



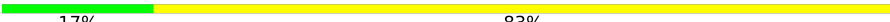
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	 2% 92% 5%
2	B	627	 2% 91% 5%
3	C	2	 100%
3	E	2	 100%
4	D	5	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	6	 17% 83%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CL	A	918	-	-	X	-
10	CL	B	914	-	-	X	-
9	TLA	B	913	-	X	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10186 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	605	Total	C	N	O	S	0	3	0
			4825	3088	875	850	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLN	HIS	conflict	UNP P35475
A	63	PRO	GLN	conflict	UNP P35475

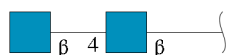
- Molecule 2 is a protein called Alpha-L-iduronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	597	Total	C	N	O	S	0	1	0
			4746	3043	853	838	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	33	GLN	HIS	conflict	UNP P35475
B	63	PRO	GLN	conflict	UNP P35475
B	105	GLN	ARG	conflict	UNP P35475

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



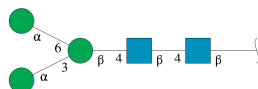
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O		0	0	0
			28	16	2	10				

Continued on next page...

Continued from previous page...

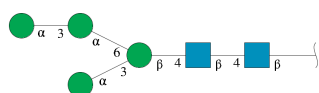
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.



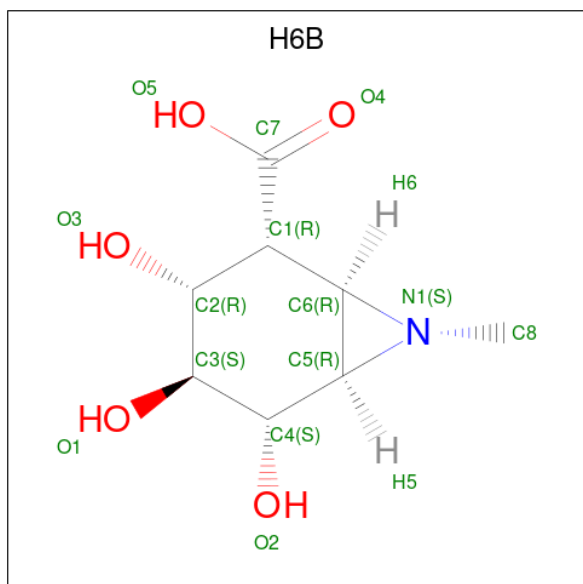
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	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 (1 {R},2 {R},3 {R},4 {S},5 {S},6 {R})-7-methyl-3,4,5-tris(oxidanyl)-7-azabicyclo[4.1.0]heptane-2-carboxylic acid (CCD ID: H6B) (formula: C₈H₁₃NO₅).



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

Continued on next page...

Continued from previous page...

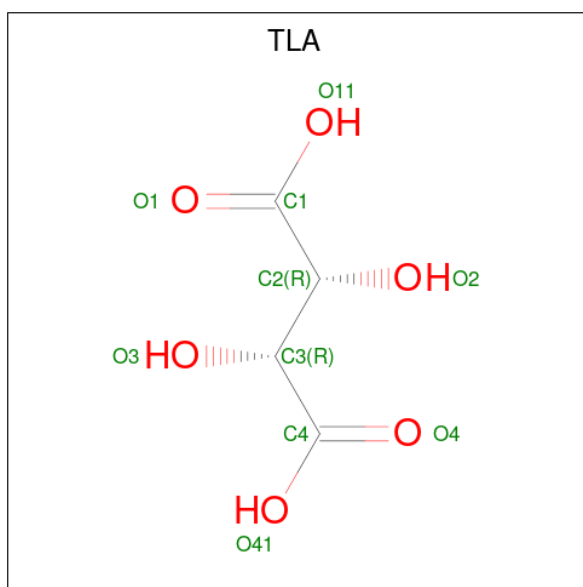
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



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

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

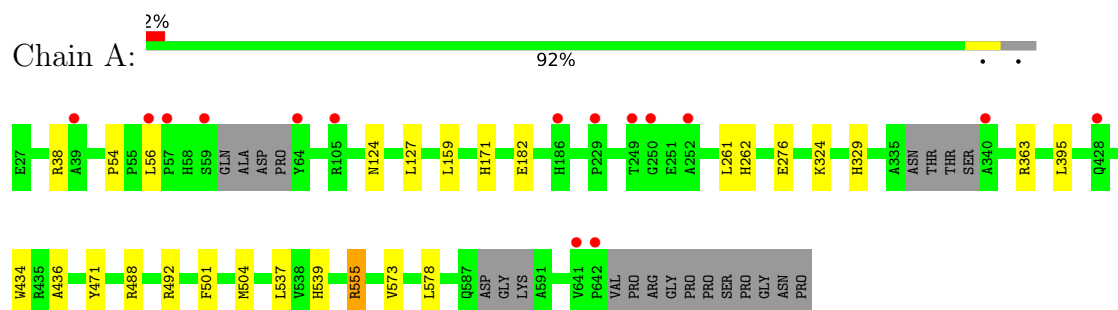
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	154	Total O 154 154	0	0
11	B	140	Total O 140 140	0	0

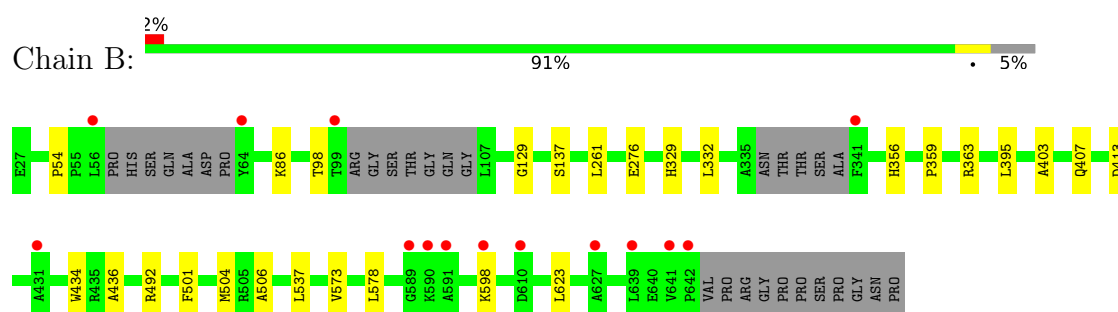
3 Residue-property plots [i](#)

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

- Molecule 1: Alpha-L-iduronidase



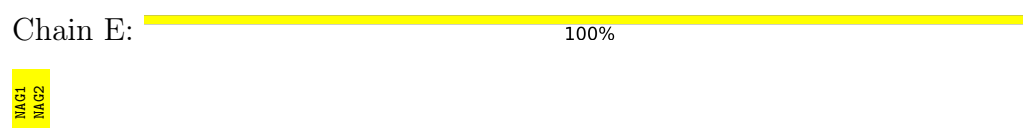
- Molecule 2: Alpha-L-iduronidase



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



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



- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain D:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 5: α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain F:  17%  83%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	259.18Å 259.18Å 71.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.73 – 2.39 29.73 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.73-2.39) 99.6 (29.73-2.39)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.191 , 0.216 0.197 , 0.219	Depositor DCC
R_{free} test set	3444 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10186	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: NAG, GOL, CL, BMA, TLA, MAN, H6B

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	0.66	1/4979 (0.0%)	0.79	0/6800
2	B	0.65	2/4895 (0.0%)	0.78	1/6688 (0.0%)
All	All	0.66	3/9874 (0.0%)	0.78	1/13488 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	407	GLN	CA-C	7.10	1.56	1.52
1	A	54	PRO	CA-C	6.06	1.55	1.51
2	B	54	PRO	CA-C	5.43	1.54	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	129	GLY	N-CA-C	-5.10	101.09	113.18

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	4825	0	4734	15	0
2	B	4746	0	4644	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	25	0	0
3	E	28	0	25	0	0
4	D	61	0	52	1	0
5	F	72	0	61	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
7	A	14	0	0	0	0
7	B	14	0	0	1	0
8	A	42	0	56	3	0
8	B	12	0	16	2	0
9	A	10	0	4	0	0
9	B	10	0	4	2	0
10	A	1	0	0	2	0
10	B	1	0	0	2	0
11	A	154	0	0	0	0
11	B	140	0	0	1	0
All	All	10186	0	9647	33	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 (33) 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:124:ASN:OD1	8:A:916:GOL:O3	2.11	0.68
2:B:86:LYS:NZ	11:B:1001:HOH:O	2.24	0.67
1:A:573:VAL:HG11	1:A:578:LEU:HD11	1.78	0.64
1:A:555:ARG:HE	8:A:916:GOL:H32	1.64	0.62
1:A:324:LYS:NZ	8:A:915:GOL:O1	2.30	0.61
1:A:276:GLU:OE1	1:A:329:HIS:NE2	2.34	0.57
1:A:363:ARG:HD3	10:A:918:CL:CL	2.41	0.56
2:B:276:GLU:OE1	2:B:329:HIS:NE2	2.32	0.53
2:B:359:PRO:HB3	9:B:913:TLA:O2	2.09	0.51
1:A:501:PHE:HA	1:A:504:MET:HE3	1.93	0.50
2:B:363:ARG:NH2	7:B:910:H6B:O3	2.47	0.48
2:B:356:HIS:HB2	9:B:913:TLA:O4	2.13	0.47
2:B:501:PHE:HA	2:B:504:MET:HE3	1.96	0.47
2:B:363:ARG:CD	10:B:914:CL:CL	3.00	0.47
2:B:261:LEU:C	2:B:261:LEU:HD12	2.41	0.46
2:B:492:ARG:NH2	4:D:3:BMA:O2	2.48	0.46
2:B:434:TRP:CH2	2:B:436:ALA:HB2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:C	1:A:261:LEU:HD12	2.41	0.45
1:A:363:ARG:CD	10:A:918:CL:CL	3.01	0.45
2:B:403:ALA:O	8:B:911:GOL:H32	2.17	0.45
1:A:395:LEU:HD12	1:A:537:LEU:HD22	2.00	0.44
1:A:434:TRP:CH2	1:A:436:ALA:HB2	2.53	0.43
2:B:506:ALA:O	2:B:598:LYS:HE3	2.18	0.43
2:B:363:ARG:HD2	10:B:914:CL:CL	2.56	0.42
2:B:573:VAL:HG11	2:B:578:LEU:HD11	2.01	0.42
1:A:127:LEU:CD2	1:A:171:HIS:CE1	3.03	0.42
1:A:182:GLU:OE2	1:A:262:HIS:HD2	2.03	0.41
1:A:488:ARG:HD3	1:A:492:ARG:HH21	1.84	0.41
2:B:395:LEU:HD12	2:B:537:LEU:HD22	2.02	0.41
1:A:471:TYR:HA	1:A:539:HIS:O	2.21	0.41
8:B:911:GOL:O3	8:B:911:GOL:O1	2.38	0.41
2:B:98:THR:HG22	2:B:137:SER:OG	2.21	0.40
2:B:332:LEU:HD21	2:B:413:ASP:HB2	2.03	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	600/627 (96%)	582 (97%)	18 (3%)	0	100	100
2	B	590/627 (94%)	572 (97%)	18 (3%)	0	100	100
All	All	1190/1254 (95%)	1154 (97%)	36 (3%)	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	511/527 (97%)	507 (99%)	4 (1%)	73	86
2	B	501/527 (95%)	500 (100%)	1 (0%)	87	94
All	All	1012/1054 (96%)	1007 (100%)	5 (0%)	81	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	56	LEU
1	A	159	LEU
1	A	555	ARG
2	B	623	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	285	GLN
1	A	356	HIS
1	A	370	GLN
1	A	603	ASN
2	B	70	GLN
2	B	73	ASN
2	B	125	GLN
2	B	196	GLN
2	B	200	ASN
2	B	603	ASN

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 ⓘ

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$
3	NAG	C	1	3,1	14,14,15	0.47	0	17,19,21	1.11	2 (11%)
3	NAG	C	2	3	14,14,15	0.58	0	17,19,21	1.47	2 (11%)
4	NAG	D	1	1,4	14,14,15	0.47	0	17,19,21	1.12	1 (5%)
4	NAG	D	2	4	14,14,15	0.47	0	17,19,21	1.04	1 (5%)
4	BMA	D	3	4	11,11,12	0.42	0	15,15,17	0.70	0
4	MAN	D	4	4	11,11,12	0.89	1 (9%)	15,15,17	1.94	5 (33%)
4	MAN	D	5	4	11,11,12	0.56	0	15,15,17	1.29	3 (20%)
3	NAG	E	1	2,3	14,14,15	0.39	0	17,19,21	1.47	3 (17%)
3	NAG	E	2	3	14,14,15	0.73	1 (7%)	17,19,21	1.11	2 (11%)
5	NAG	F	1	2,5	14,14,15	0.51	0	17,19,21	1.12	2 (11%)
5	NAG	F	2	5	14,14,15	0.56	0	17,19,21	1.45	3 (17%)
5	BMA	F	3	5	11,11,12	0.30	0	15,15,17	0.76	0
5	MAN	F	4	5	11,11,12	0.50	0	15,15,17	1.24	3 (20%)
5	MAN	F	5	5	11,11,12	0.34	0	15,15,17	1.28	1 (6%)
5	MAN	F	6	5	11,11,12	0.54	0	15,15,17	1.59	2 (13%)

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
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	2.32	1.55	1.52
4	D	4	MAN	C2-C3	2.19	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6	MAN	C1-O5-C5	4.81	118.63	112.19
3	C	2	NAG	C4-C3-C2	4.51	117.62	111.02
5	F	2	NAG	C1-O5-C5	3.65	117.08	112.19
3	E	1	NAG	C1-O5-C5	3.34	116.67	112.19
4	D	4	MAN	C2-C3-C4	3.23	116.54	110.86
4	D	4	MAN	C3-C4-C5	3.10	115.86	110.23
5	F	5	MAN	C3-C4-C5	3.08	115.82	110.23
4	D	4	MAN	O2-C2-C1	3.02	116.14	109.22
4	D	4	MAN	O2-C2-C3	2.88	116.12	110.15
4	D	2	NAG	C1-O5-C5	2.75	115.86	112.19
5	F	4	MAN	C1-C2-C3	2.67	113.53	109.64
3	E	2	NAG	C1-O5-C5	2.57	115.62	112.19
3	E	1	NAG	C2-N2-C7	2.55	126.32	122.90
5	F	4	MAN	O5-C5-C6	2.54	112.61	107.66
3	C	1	NAG	O5-C1-C2	-2.40	107.57	111.29
4	D	5	MAN	O3-C3-C4	2.39	116.00	110.38
5	F	2	NAG	O4-C4-C3	-2.26	105.04	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5	MAN	C1-O5-C5	2.26	115.21	112.19
3	C	2	NAG	O5-C5-C6	2.24	112.01	107.66
3	E	1	NAG	O7-C7-N2	2.21	125.89	121.98
5	F	2	NAG	C1-C2-N2	2.19	113.88	110.43
4	D	4	MAN	C6-C5-C4	-2.13	107.78	113.02
4	D	5	MAN	O5-C5-C6	2.11	111.78	107.66
4	D	1	NAG	O5-C1-C2	-2.11	108.03	111.29
5	F	1	NAG	O5-C1-C2	-2.10	108.04	111.29
5	F	6	MAN	C3-C4-C5	2.08	114.00	110.23
5	F	1	NAG	C6-C5-C4	-2.08	107.91	113.02
3	C	1	NAG	C4-C3-C2	2.04	114.01	111.02
5	F	4	MAN	O5-C5-C4	-2.04	105.87	110.83
3	E	2	NAG	O5-C1-C2	2.00	114.39	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
5	F	6	MAN	O5-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
5	F	6	MAN	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	D	5	MAN	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
5	F	5	MAN	C4-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

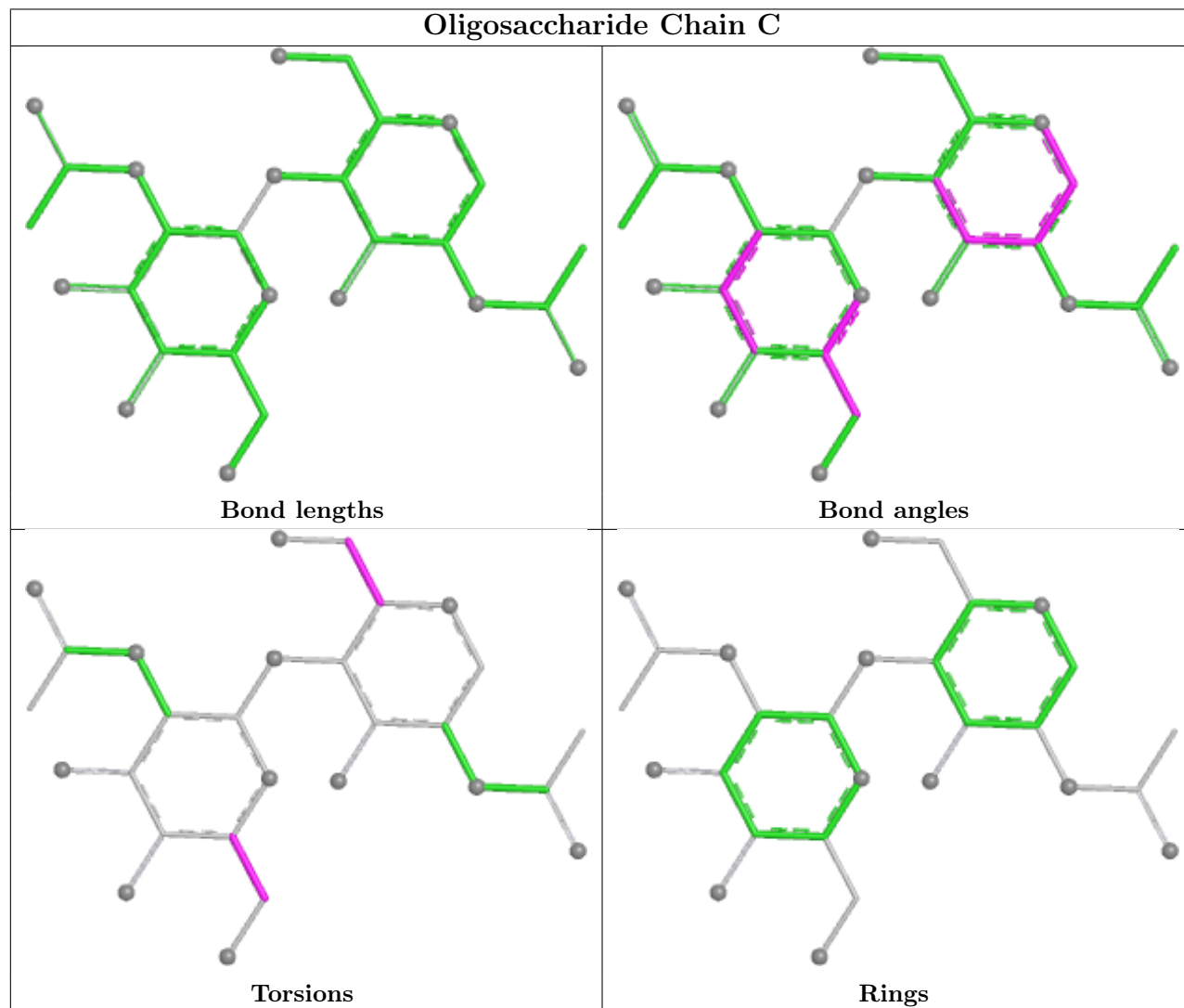
All (1) ring outliers are listed below:

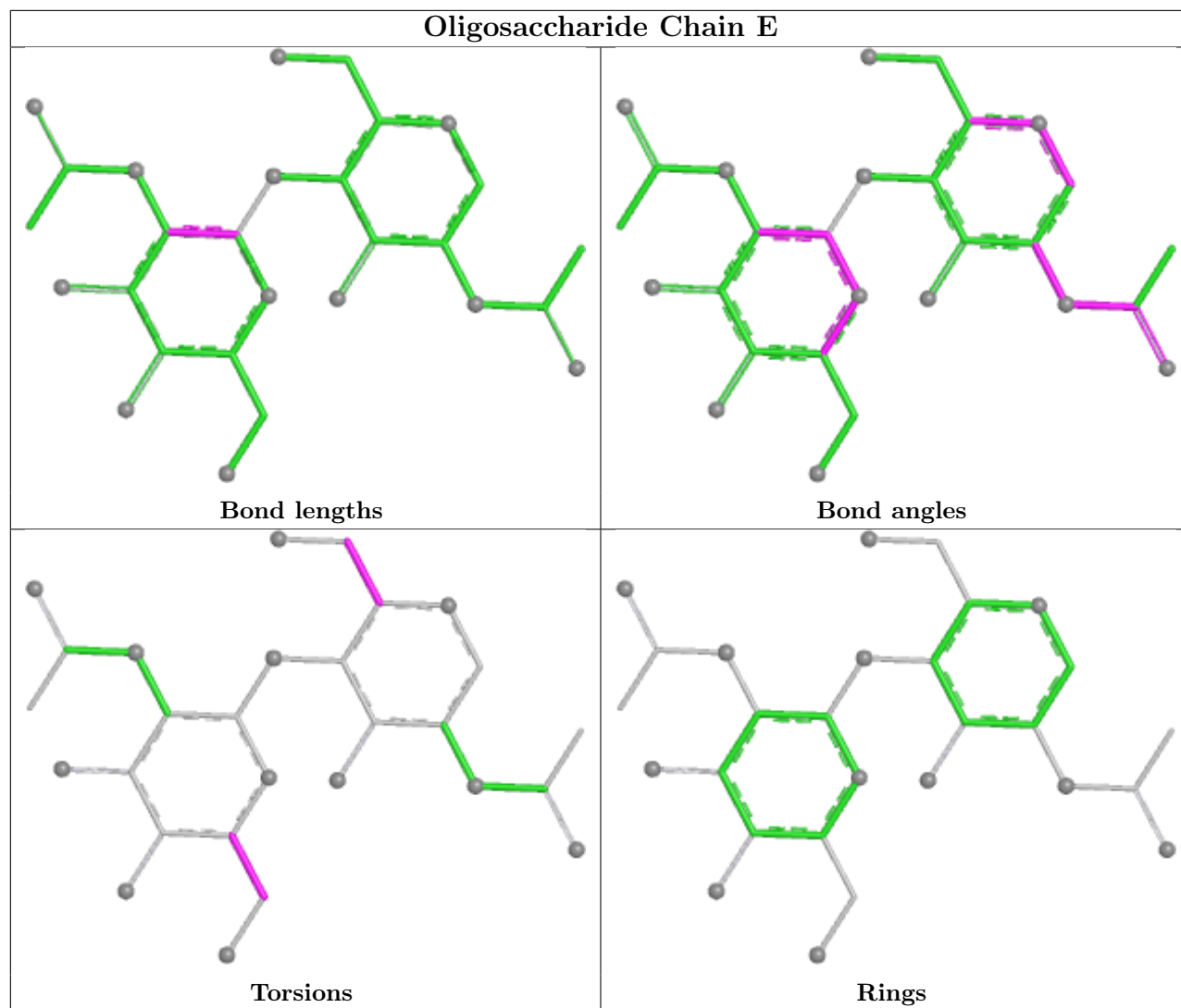
Mol	Chain	Res	Type	Atoms
5	F	6	MAN	C1-C2-C3-C4-C5-O5

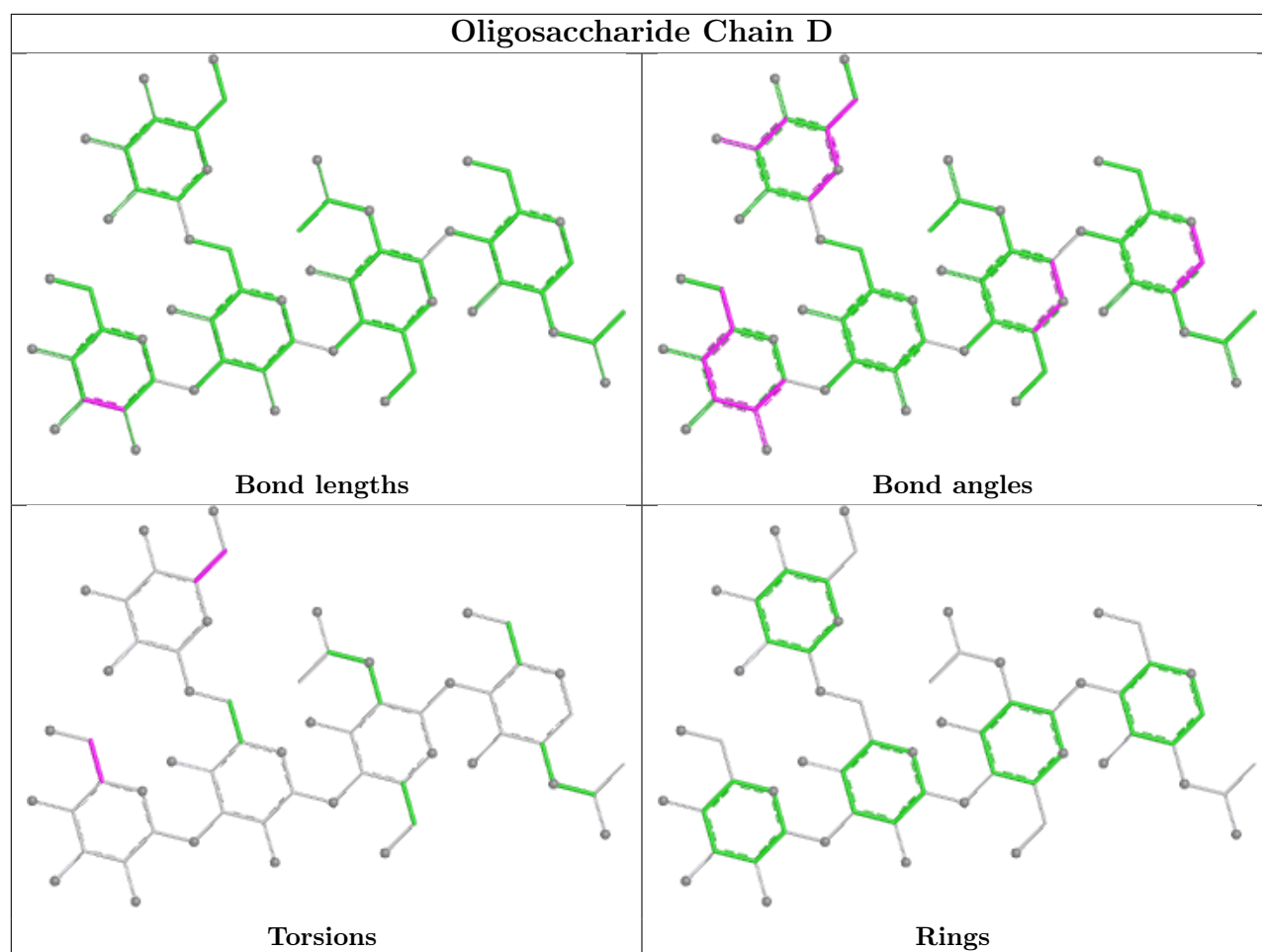
1 monomer is involved in 1 short contact:

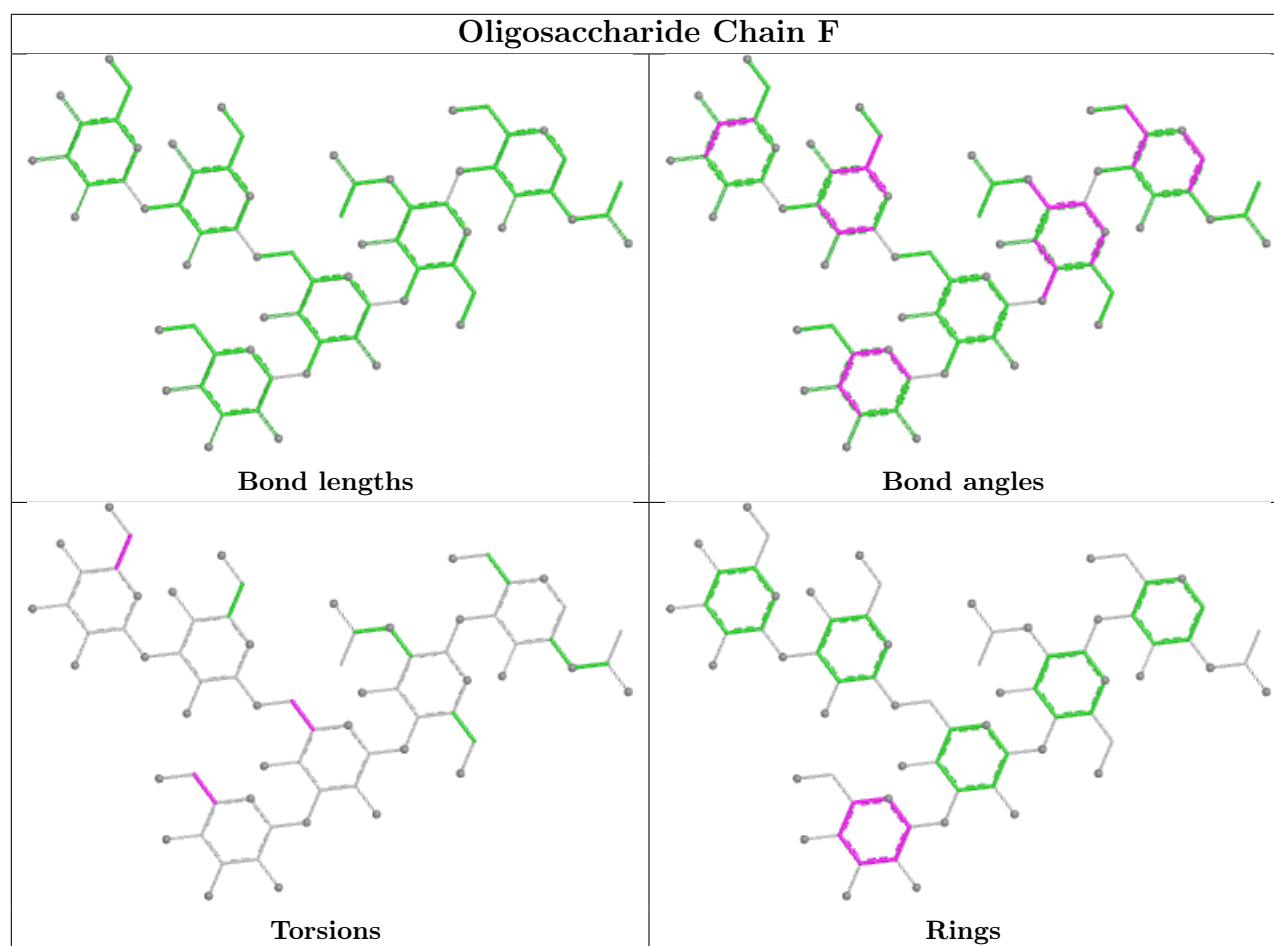
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	BMA	1	0

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 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	GOL	A	911	-	5,5,5	0.44	0	5,5,5	0.34	0
6	NAG	B	901	2	14,14,15	0.68	0	17,19,21	1.39	1 (5%)
9	TLA	B	913	-	9,9,9	1.57	2 (22%)	12,12,12	2.55	7 (58%)
8	GOL	A	916	-	5,5,5	0.70	0	5,5,5	0.97	0
8	GOL	A	915	-	5,5,5	0.24	0	5,5,5	0.51	0
8	GOL	A	910	-	5,5,5	0.17	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	TLA	A	917	-	9,9,9	1.11	0	12,12,12	1.21	1 (8%)
6	NAG	A	901	1	14,14,15	0.38	0	17,19,21	1.42	3 (17%)
8	GOL	B	911	-	5,5,5	0.23	0	5,5,5	0.78	0
8	GOL	A	914	-	5,5,5	0.40	0	5,5,5	0.81	0
8	GOL	A	912	-	5,5,5	0.34	0	5,5,5	0.24	0
7	H6B	A	909	-	15,15,15	1.11	1 (6%)	15,24,24	1.69	4 (26%)
8	GOL	B	912	-	5,5,5	0.28	0	5,5,5	0.36	0
8	GOL	A	913	-	5,5,5	0.47	0	5,5,5	0.62	0
7	H6B	B	910	-	15,15,15	1.10	2 (13%)	15,24,24	1.79	4 (26%)

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
8	GOL	A	911	-	-	4/4/4/4	-
6	NAG	B	901	2	-	2/6/23/26	0/1/1/1
9	TLA	B	913	-	-	7/12/12/12	-
8	GOL	A	916	-	-	2/4/4/4	-
8	GOL	A	915	-	-	0/4/4/4	-
8	GOL	A	910	-	-	4/4/4/4	-
9	TLA	A	917	-	-	0/12/12/12	-
6	NAG	A	901	1	-	0/6/23/26	0/1/1/1
8	GOL	B	911	-	-	0/4/4/4	-
8	GOL	A	914	-	-	0/4/4/4	-
8	GOL	A	912	-	-	2/4/4/4	-
7	H6B	A	909	-	-	4/4/33/33	0/2/2/2
8	GOL	B	912	-	-	2/4/4/4	-
8	GOL	A	913	-	-	0/4/4/4	-
7	H6B	B	910	-	-	2/4/33/33	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	913	TLA	C3-C4	-3.32	1.47	1.52
7	A	909	H6B	O5-C7	-2.93	1.21	1.30
7	B	910	H6B	O5-C7	-2.64	1.22	1.30
7	B	910	H6B	C1-C6	-2.45	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	913	TLA	O1-C1	2.01	1.28	1.22

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	913	TLA	O3-C3-C4	-4.73	100.57	110.69
7	A	909	H6B	C8-N1-C5	4.42	121.43	114.03
7	B	910	H6B	C8-N1-C5	4.33	121.28	114.03
9	B	913	TLA	O2-C2-C3	-3.90	102.22	110.17
6	B	901	NAG	C1-O5-C5	3.77	117.25	112.19
9	B	913	TLA	C3-C2-C1	3.66	117.93	109.82
6	A	901	NAG	C1-O5-C5	3.28	116.58	112.19
6	A	901	NAG	C3-C4-C5	-2.96	104.86	110.23
9	B	913	TLA	O4-C4-C3	-2.83	114.07	121.62
7	B	910	H6B	O4-C7-C1	-2.76	115.80	122.84
7	A	909	H6B	O4-C7-C1	-2.62	116.15	122.84
7	B	910	H6B	O5-C7-C1	2.45	120.97	113.91
7	A	909	H6B	O5-C7-C1	2.45	120.95	113.91
9	A	917	TLA	O3-C3-C2	-2.41	105.25	110.17
6	A	901	NAG	O5-C1-C2	-2.40	107.57	111.29
9	B	913	TLA	C2-C3-C4	2.36	115.06	109.82
7	B	910	H6B	C4-C3-C2	2.36	114.97	110.83
9	B	913	TLA	O2-C2-C1	-2.35	105.67	110.69
9	B	913	TLA	O41-C4-C3	2.28	119.63	113.31
7	A	909	H6B	C4-C3-C2	2.14	114.58	110.83

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	910	GOL	O1-C1-C2-C3
8	A	910	GOL	C1-C2-C3-O3
8	A	911	GOL	C1-C2-C3-O3
8	B	912	GOL	O1-C1-C2-C3
9	B	913	TLA	O3-C3-C4-O4
9	B	913	TLA	O3-C3-C4-O41
9	B	913	TLA	O1-C1-C2-O2
9	B	913	TLA	O11-C1-C2-O2
6	B	901	NAG	O5-C5-C6-O6
6	B	901	NAG	C4-C5-C6-O6
8	A	911	GOL	O1-C1-C2-C3
8	A	912	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	916	GOL	C1-C2-C3-O3
8	A	910	GOL	O1-C1-C2-O2
8	A	911	GOL	O1-C1-C2-O2
8	A	912	GOL	O1-C1-C2-O2
8	A	916	GOL	O2-C2-C3-O3
9	B	913	TLA	C1-C2-C3-O3
9	B	913	TLA	O2-C2-C3-C4
8	A	910	GOL	O2-C2-C3-O3
8	A	911	GOL	O2-C2-C3-O3
9	B	913	TLA	C1-C2-C3-C4
8	B	912	GOL	O1-C1-C2-O2
7	A	909	H6B	C6-C1-C7-O5
7	A	909	H6B	C6-C1-C7-O4
7	B	910	H6B	C2-C1-C7-O5
7	A	909	H6B	C2-C1-C7-O5
7	B	910	H6B	C2-C1-C7-O4
7	A	909	H6B	C2-C1-C7-O4

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	913	TLA	2	0
8	A	916	GOL	2	0
8	A	915	GOL	1	0
8	B	911	GOL	2	0
7	B	910	H6B	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	605/627 (96%)	-0.16	15 (2%) 58 54	17, 37, 67, 107	3 (0%)
2	B	597/627 (95%)	0.05	14 (2%) 61 57	23, 40, 72, 101	1 (0%)
All	All	1202/1254 (95%)	-0.06	29 (2%) 59 55	17, 38, 69, 107	4 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	SER	5.3
2	B	642	PRO	4.2
2	B	56	LEU	4.1
2	B	591	ALA	3.8
2	B	641	VAL	3.8
1	A	250	GLY	3.7
1	A	642	PRO	3.6
1	A	340	ALA	3.6
1	A	252	ALA	3.4
2	B	589	GLY	3.4
1	A	428	GLN	3.3
1	A	56	LEU	3.3
1	A	249	THR	2.8
1	A	57	PRO	2.7
1	A	186	HIS	2.6
1	A	105	ARG	2.5
2	B	590	LYS	2.5
1	A	641	VAL	2.4
2	B	431	ALA	2.4
2	B	610	ASP	2.3
2	B	64	TYR	2.3
1	A	39	ALA	2.3
1	A	229	PRO	2.2
2	B	341	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	598	LYS	2.2
2	B	99	THR	2.1
1	A	64	TYR	2.1
2	B	639	LEU	2.1
2	B	627	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](#)

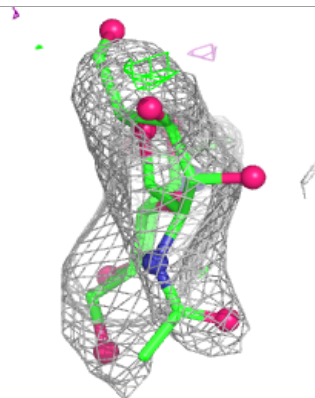
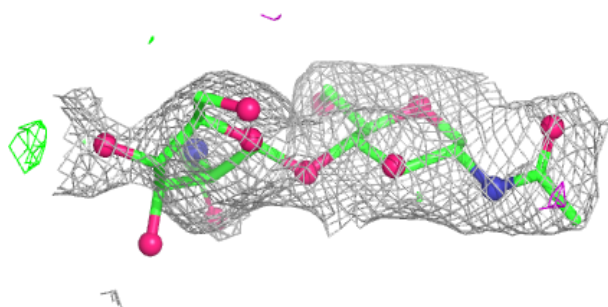
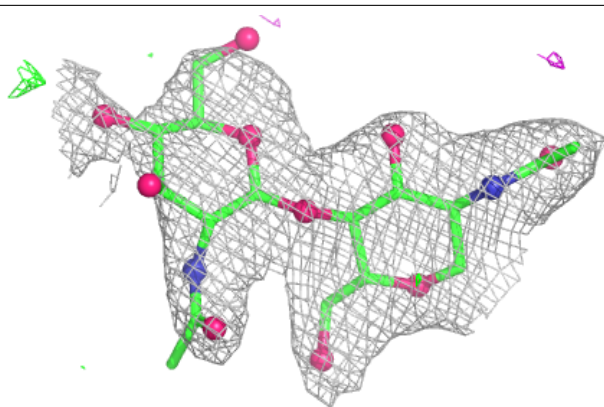
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	F	6	11/12	0.59	0.15	78,83,91,91	0
3	NAG	E	2	14/15	0.67	0.17	87,97,103,106	0
5	MAN	F	5	11/12	0.71	0.15	72,87,89,91	0
3	NAG	C	2	14/15	0.78	0.16	76,83,89,91	0
5	MAN	F	4	11/12	0.83	0.13	74,80,84,87	0
4	MAN	D	5	11/12	0.84	0.11	51,54,57,57	0
4	MAN	D	4	11/12	0.87	0.11	46,52,56,58	0
3	NAG	C	1	14/15	0.91	0.09	53,57,65,72	0
3	NAG	E	1	14/15	0.92	0.10	46,52,59,74	0
5	NAG	F	2	14/15	0.93	0.08	40,44,49,56	0
4	NAG	D	2	14/15	0.94	0.07	29,34,37,40	0
5	NAG	F	1	14/15	0.94	0.07	40,43,46,52	0
5	BMA	F	3	11/12	0.95	0.07	49,57,66,67	0
4	BMA	D	3	11/12	0.97	0.06	36,41,46,49	0
4	NAG	D	1	14/15	0.98	0.05	29,31,36,37	0

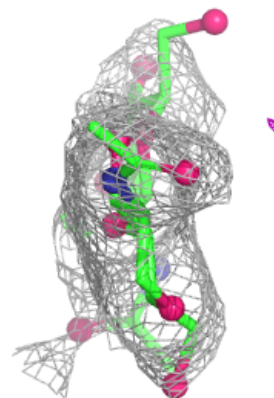
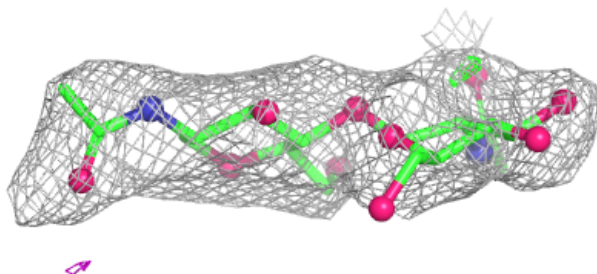
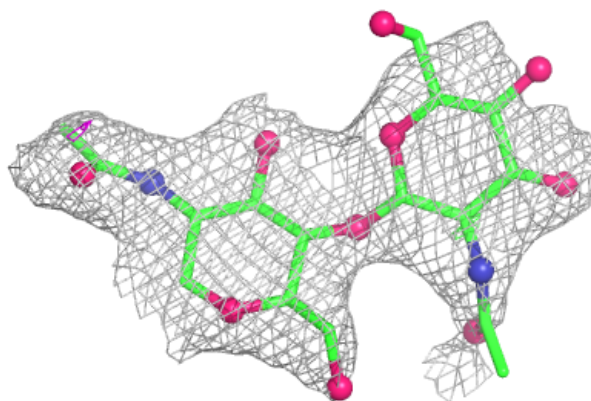
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

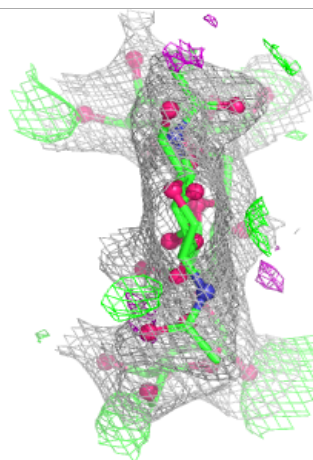
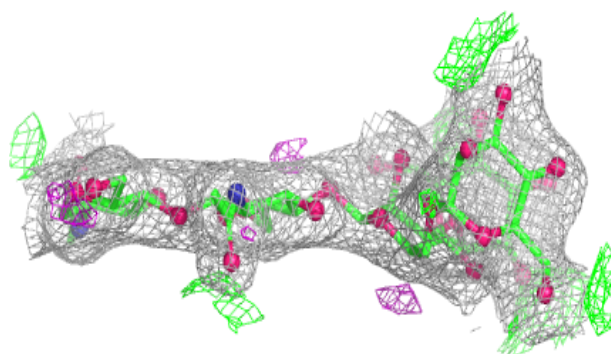
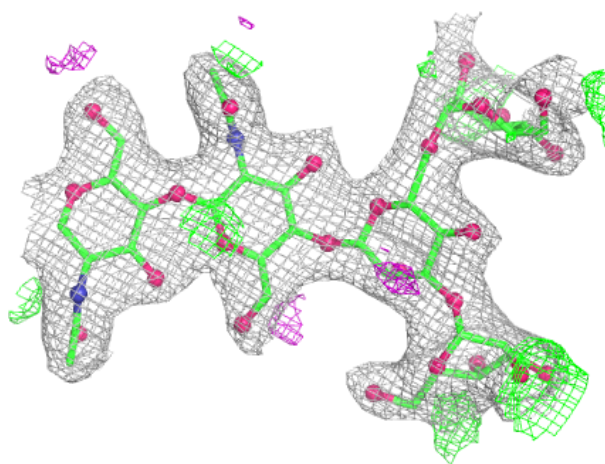
**Electron density around Chain E:**

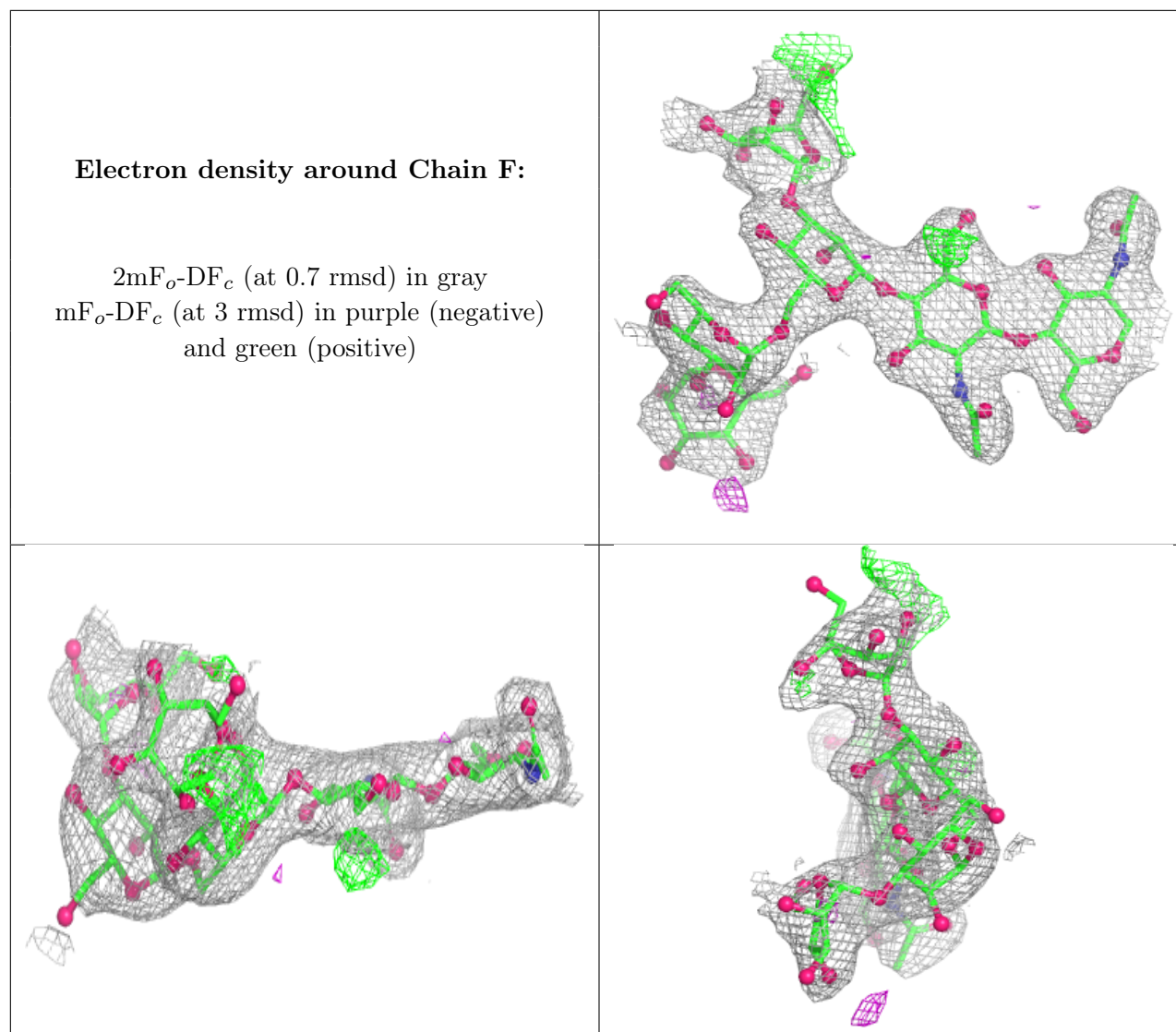
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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(Å ²)	Q<0.9
6	NAG	B	901	14/15	0.79	0.14	67,74,78,79	0
7	H6B	B	910	14/14	0.82	0.14	50,59,65,66	0
9	TLA	B	913	10/10	0.86	0.14	60,69,75,76	0
7	H6B	A	909	14/14	0.87	0.14	50,60,73,74	0
8	GOL	A	911	6/6	0.89	0.14	50,51,52,54	0
8	GOL	B	911	6/6	0.90	0.13	57,60,61,67	0
8	GOL	A	912	6/6	0.91	0.12	50,52,54,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	901	14/15	0.92	0.08	45,52,58,58	0
8	GOL	B	912	6/6	0.92	0.11	48,49,56,58	0
8	GOL	A	916	6/6	0.92	0.10	33,41,41,44	0
8	GOL	A	914	6/6	0.93	0.11	55,57,60,62	0
8	GOL	A	915	6/6	0.93	0.08	48,53,55,60	0
8	GOL	A	913	6/6	0.93	0.12	49,54,54,55	0
9	TLA	A	917	10/10	0.94	0.07	43,49,58,61	0
8	GOL	A	910	6/6	0.94	0.09	48,49,52,52	0
10	CL	B	914	1/1	0.98	0.10	32,32,32,32	0
10	CL	A	918	1/1	0.99	0.04	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.