



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:23 PM BST

PDB ID : 6I6X
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

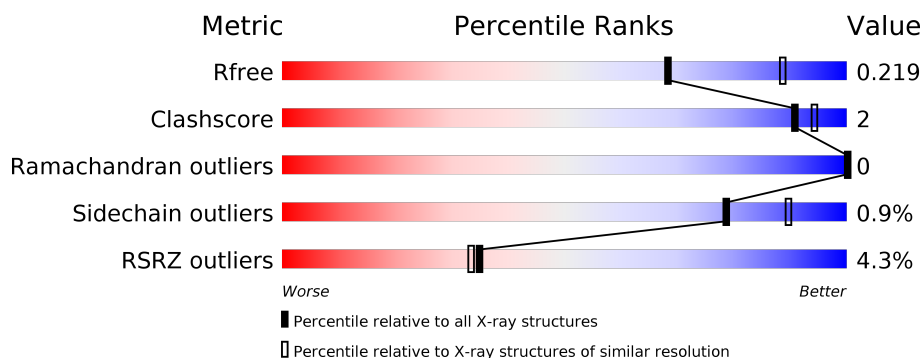
1 Overall quality at a glance

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on 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	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> <div></div> </div>
2	B	627	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> <div></div> </div>
3	C	2	<div> <div></div> <div>100%</div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>
4	D	5	<div> <div></div> <div>100%</div> </div>
5	F	6	<div> <div>17%</div> <div>83%</div> </div>

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	-
3	NAG	C	2	-	-	-	X
3	NAG	E	2	-	-	-	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

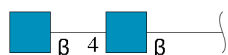
- Molecule 2 is a protein called Alpha-L-iduronidase.

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.



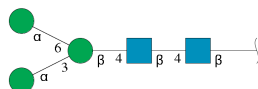
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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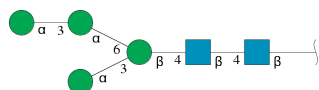
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



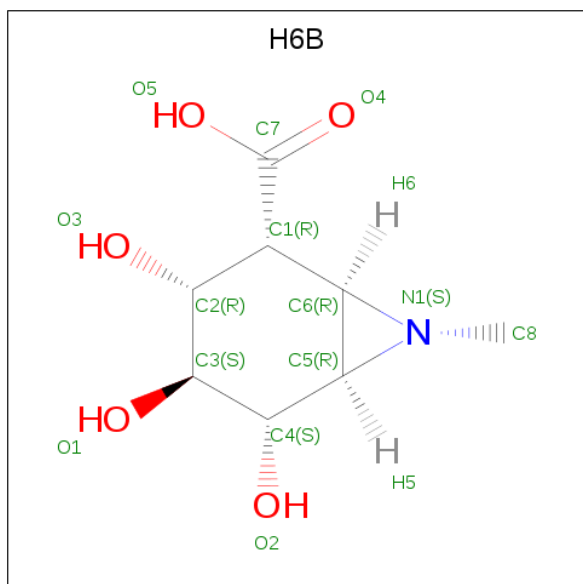
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 (three-letter code: H6B) (formula: C₈H₁₃NO₅).



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

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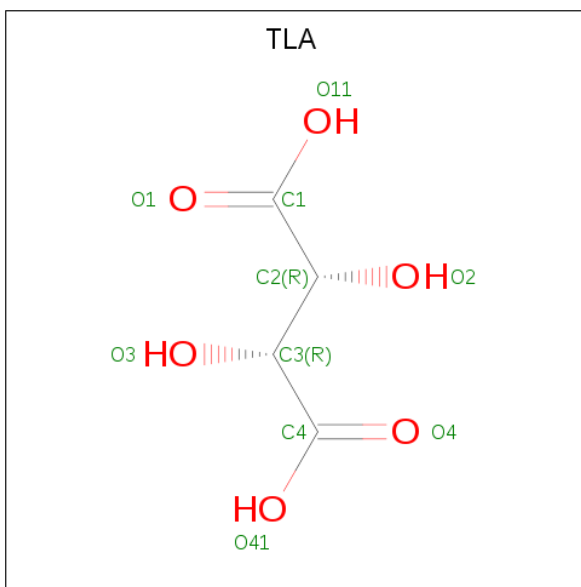
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is GLYCEROL (three-letter code: 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 (three-letter code: TLA) (formula: $C_4H_6O_6$).



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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

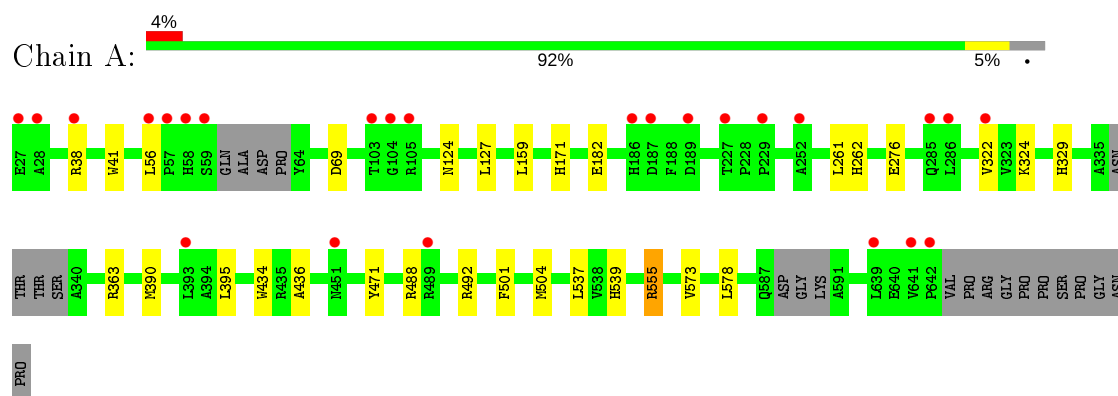
- Molecule 11 is water.

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

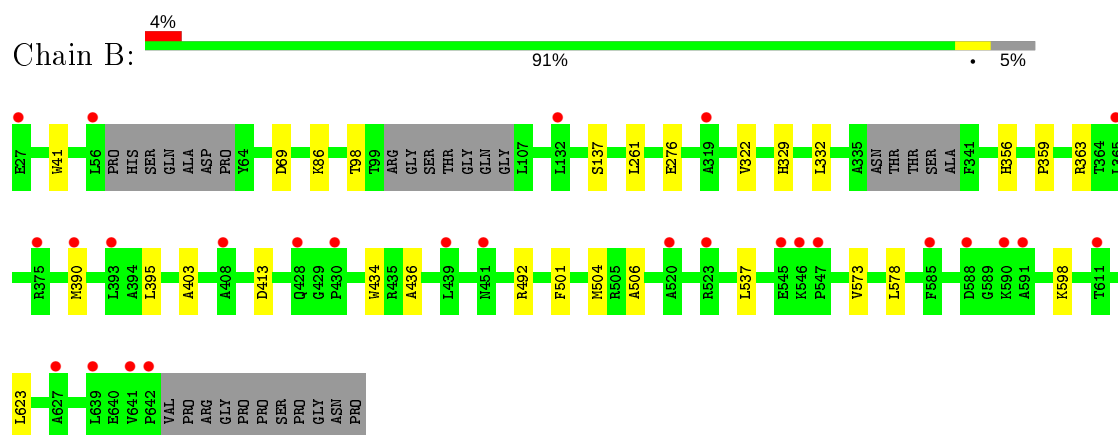
3 Residue-property plots [i](#)

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.

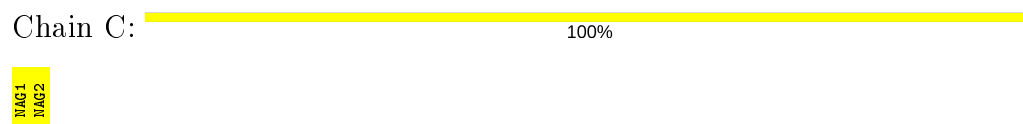
• Molecule 1: Alpha-L-iduronidase



• 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

Chain E:  100%


MAG1
MAG2

- Molecule 4: 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:  100%

MAG1
MAG2
BGL3
MAN4
MAN5

- Molecule 5: 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

Chain F:  17%  83%

MAG1
MAG2
BGL3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	259.18 Å 259.18 Å 71.01 Å 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 2.39 Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.191 , 0.216 0.196 , 0.219	Depositor DCC
R_{free} test set	3444 reflections (4.93%)	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 , 34.9	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: GOL, BMA, NAG, CL, H6B, TLA, 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	0.49	0/4979	0.68	0/6800
2	B	0.48	0/4895	0.67	0/6688
All	All	0.48	0/9874	0.68	0/13488

There are no bond length outliers.

There are no bond angle outliers.

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	16	0
2	B	4746	0	4644	18	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	12	0	16	1	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	34	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 (34) 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
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:86:LYS:NZ	11:B:1001:HOH:O	2.24	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
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:363:ARG:CD	10:B:914:CL:CL	3.00	0.47
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
1:A:363:ARG:CD	10:A:918:CL:CL	3.01	0.45
1:A:501:PHE:HA	1:A:504:MET:HE3	1.99	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:322:VAL:HG11	1:A:390:MET:HE3	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
2:B:322:VAL:HG11	2:B:390:MET:HE3	2.02	0.41
1:A:182:GLU:OE2	1:A:262:HIS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:HD3	1:A:492:ARG:HH21	1.84	0.41
2:B:261:LEU:HD12	2:B:261:LEU:C	2.41	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
2:B:501:PHE:HA	2:B:504:MET:HE3	2.02	0.40
2:B:98:THR:HG22	2:B:137:SER:OG	2.21	0.40
1:A:261:LEU:HD12	1:A:261:LEU:C	2.41	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 [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	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	511/527 (97%)	505 (99%)	6 (1%)	71	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	501/527 (95%)	498 (99%)	3 (1%)	86	94
All	All	1012/1054 (96%)	1003 (99%)	9 (1%)	78	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	41	TRP
1	A	56	LEU
1	A	69	ASP
1	A	159	LEU
1	A	555	ARG
2	B	41	TRP
2	B	69	ASP
2	B	623	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	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	1,3	14,14,15	0.47	0	17,19,21	1.10	2 (11%)
3	NAG	C	2	3	14,14,15	0.56	0	17,19,21	1.55	2 (11%)
4	NAG	D	1	1,4	14,14,15	0.48	0	17,19,21	1.17	1 (5%)
4	NAG	D	2	4	14,14,15	0.48	0	17,19,21	1.03	1 (5%)
4	BMA	D	3	4	11,11,12	0.44	0	15,15,17	0.79	0
4	MAN	D	4	4	11,11,12	0.91	1 (9%)	15,15,17	2.08	7 (46%)
4	MAN	D	5	4	11,11,12	0.56	0	15,15,17	1.41	3 (20%)
3	NAG	E	1	3,2	14,14,15	0.40	0	17,19,21	1.43	3 (17%)
3	NAG	E	2	3	14,14,15	0.69	1 (7%)	17,19,21	1.10	1 (5%)
5	NAG	F	1	2,5	14,14,15	0.51	0	17,19,21	1.13	2 (11%)
5	NAG	F	2	5	14,14,15	0.55	0	17,19,21	1.43	2 (11%)
5	BMA	F	3	5	11,11,12	0.31	0	15,15,17	0.84	0
5	MAN	F	4	5	11,11,12	0.51	0	15,15,17	1.46	3 (20%)
5	MAN	F	5	5	11,11,12	0.33	0	15,15,17	1.42	2 (13%)
5	MAN	F	6	5	11,11,12	0.54	0	15,15,17	1.72	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
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	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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)
4	D	4	MAN	C2-C3	2.26	1.55	1.52
3	E	2	NAG	C1-C2	2.12	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6	MAN	C1-O5-C5	4.75	118.63	112.19
3	C	2	NAG	C4-C3-C2	4.51	117.62	111.02
5	F	2	NAG	C1-O5-C5	3.61	117.08	112.19
5	F	4	MAN	O5-C5-C6	3.45	112.61	107.20
4	D	4	MAN	O2-C2-C1	3.42	116.14	109.15
3	E	1	NAG	C1-O5-C5	3.30	116.67	112.19
4	D	4	MAN	C2-C3-C4	3.26	116.54	110.89
4	D	4	MAN	C3-C4-C5	3.15	115.86	110.24
5	F	4	MAN	C1-C2-C3	3.15	113.53	109.67
5	F	5	MAN	C3-C4-C5	3.13	115.82	110.24
3	C	2	NAG	O5-C5-C6	3.07	112.01	107.20
4	D	4	MAN	O2-C2-C3	2.99	116.12	110.14
4	D	5	MAN	O5-C5-C6	2.92	111.78	107.20
4	D	2	NAG	C1-O5-C5	2.71	115.86	112.19
3	E	2	NAG	C1-O5-C5	2.53	115.62	112.19
4	D	5	MAN	O3-C3-C4	2.45	116.00	110.35
3	E	1	NAG	C2-N2-C7	2.40	126.32	122.90
5	F	5	MAN	O5-C1-C2	-2.39	107.08	110.77
4	D	4	MAN	C1-C2-C3	-2.37	106.75	109.67
4	D	4	MAN	O5-C5-C6	2.36	110.91	107.20
3	C	1	NAG	O5-C1-C2	-2.35	107.57	111.29
5	F	6	MAN	O5-C1-C2	2.35	114.40	110.77
5	F	6	MAN	O5-C5-C6	2.35	110.88	107.20
5	F	2	NAG	O4-C4-C3	-2.30	105.04	110.35
4	D	4	MAN	C6-C5-C4	-2.23	107.78	113.00
4	D	5	MAN	C1-O5-C5	2.23	115.21	112.19
5	F	1	NAG	C6-C5-C4	-2.17	107.91	113.00
3	E	1	NAG	O7-C7-N2	2.14	125.89	121.95
5	F	6	MAN	C3-C4-C5	2.11	114.00	110.24
4	D	1	NAG	O5-C1-C2	-2.07	108.03	111.29
5	F	1	NAG	O5-C1-C2	-2.06	108.04	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

All (15) 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
5	F	5	MAN	C4-C5-C6-O6
3	E	1	NAG	O5-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

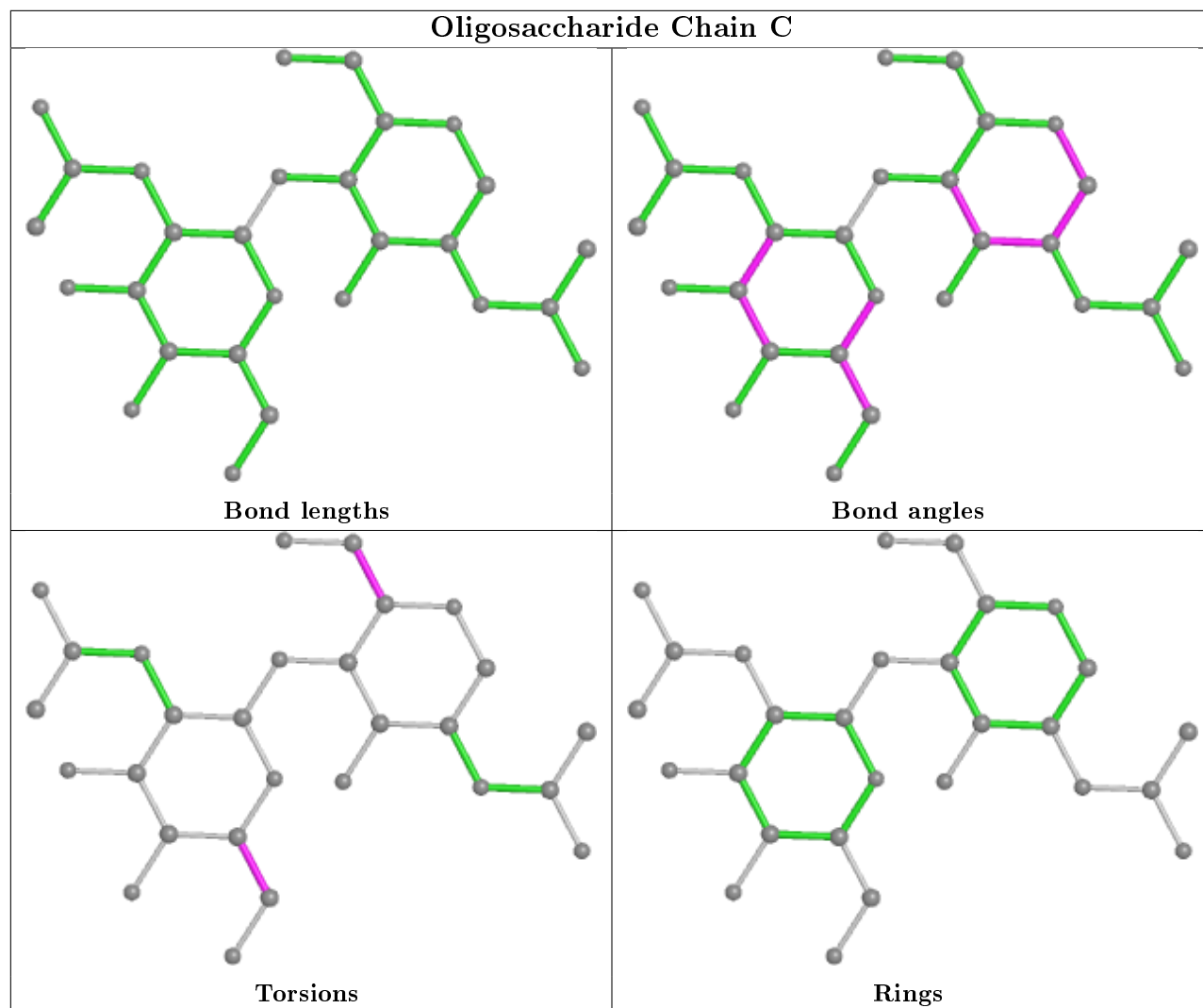
All (1) ring outliers are listed below:

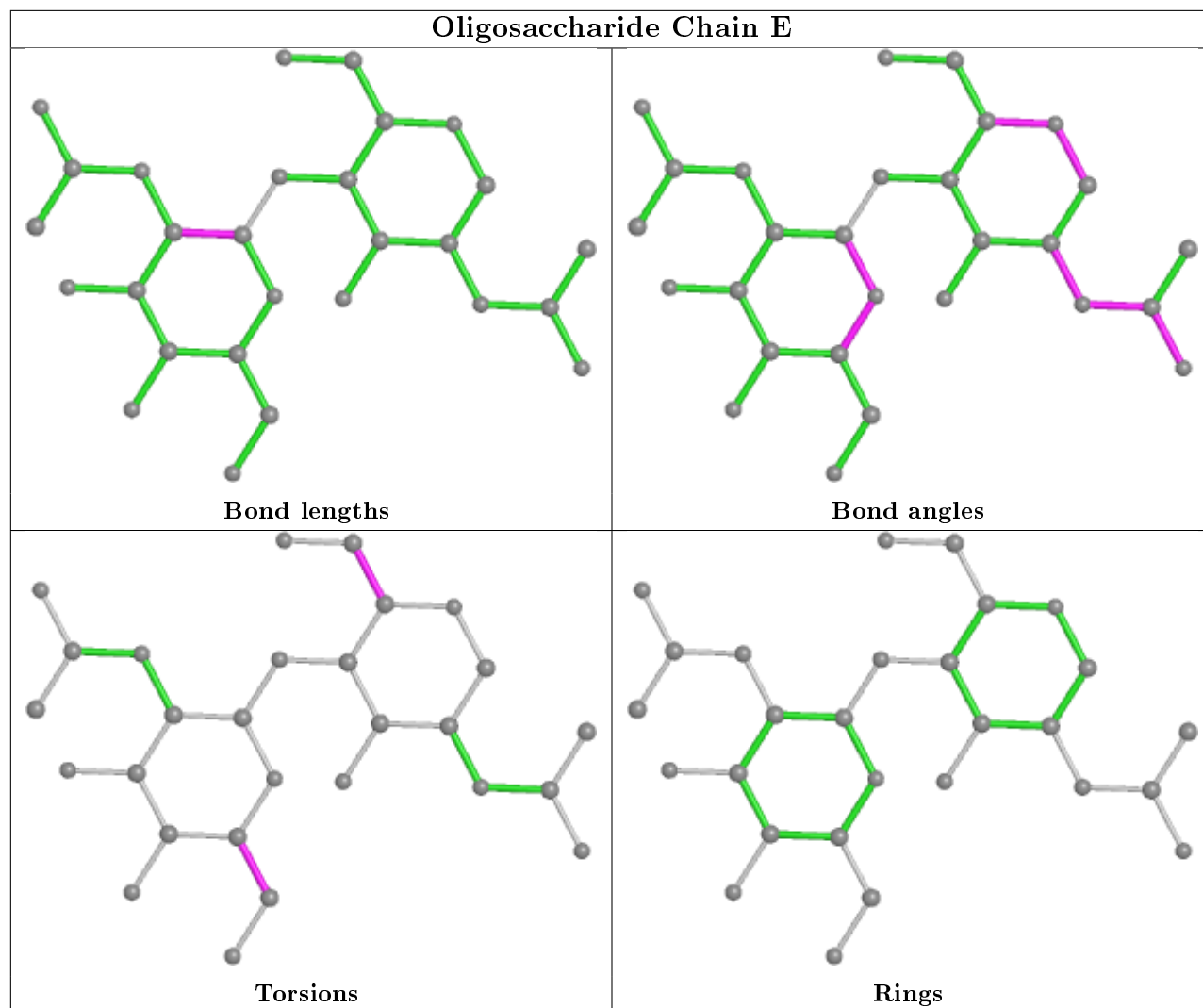
Mol	Chain	Res	Type	Atoms
5	F	6	MAN	C1-C2-C3-C4-C5-O5

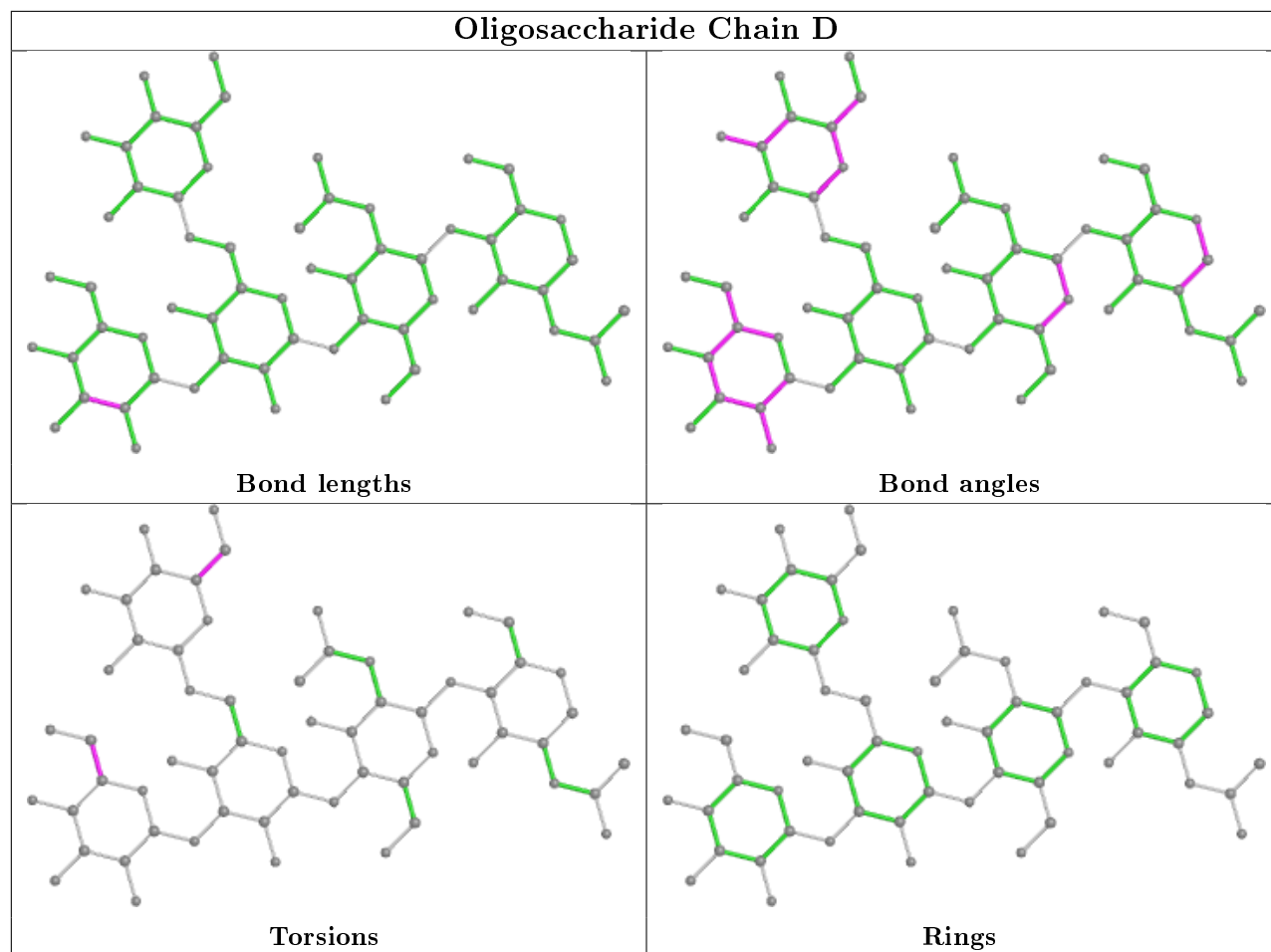
1 monomer is involved in 1 short contact:

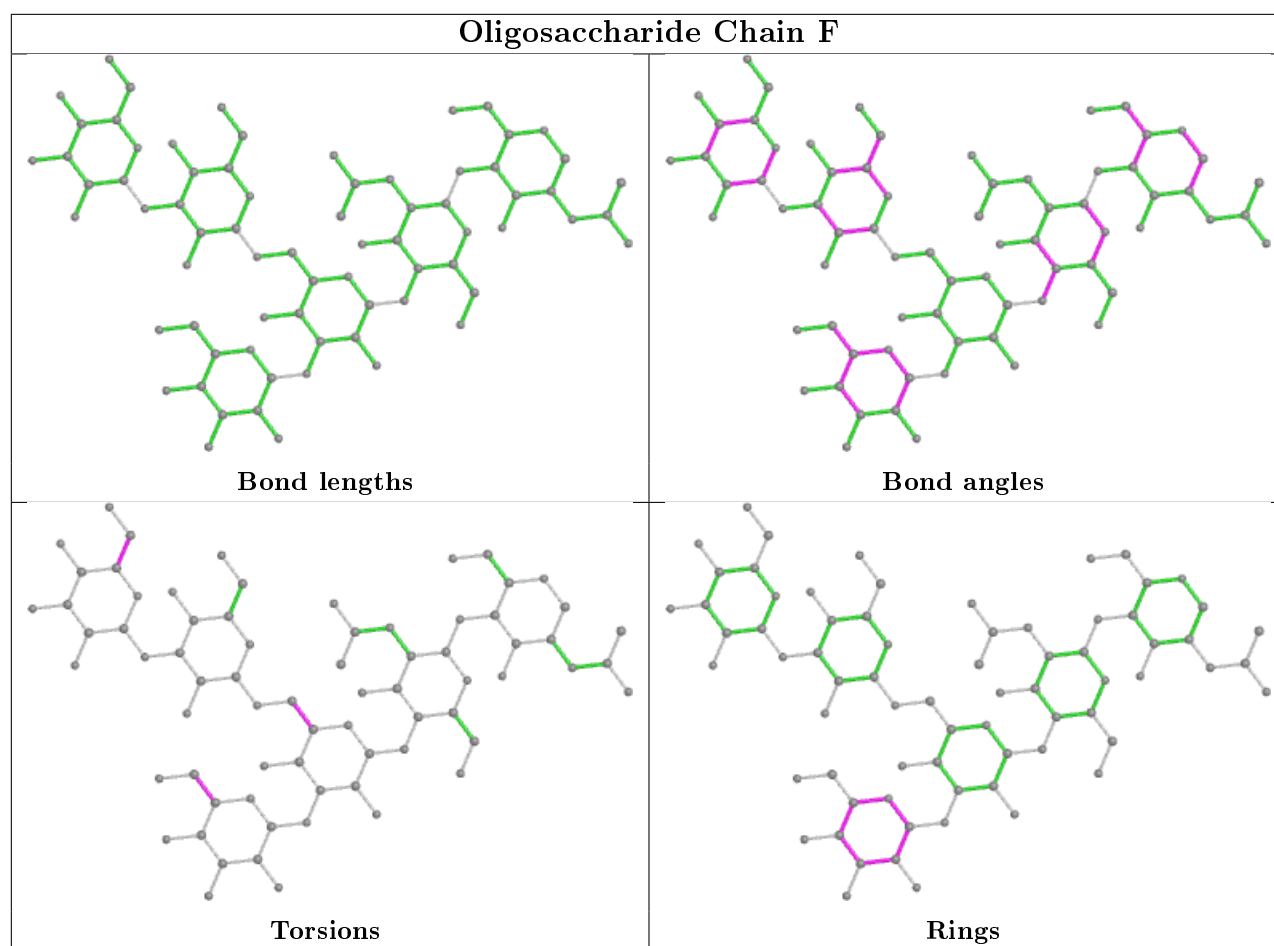
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	BMA	1	0

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	912	-	5,5,5	0.34	0	5,5,5	0.21	0
8	GOL	A	915	-	5,5,5	0.24	0	5,5,5	0.47	0
6	NAG	A	901	1	14,14,15	0.38	0	17,19,21	1.44	3 (17%)
9	TLA	B	913	-	3,9,9	0.43	0	6,12,12	2.39	4 (66%)
8	GOL	A	910	-	5,5,5	0.17	0	5,5,5	0.33	0
8	GOL	A	914	-	5,5,5	0.38	0	5,5,5	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	H6B	B	910	-	12,15,15	0.80	0	12,24,24	2.59	4 (33%)
8	GOL	A	913	-	5,5,5	0.46	0	5,5,5	0.59	0
8	GOL	B	911	-	5,5,5	0.21	0	5,5,5	0.73	0
6	NAG	B	901	2	14,14,15	0.66	0	17,19,21	1.42	1 (5%)
8	GOL	B	912	-	5,5,5	0.27	0	5,5,5	0.32	0
7	H6B	A	909	-	12,15,15	0.74	0	12,24,24	2.46	3 (25%)
9	TLA	A	917	-	3,9,9	0.47	0	6,12,12	0.76	0
8	GOL	A	911	-	5,5,5	0.43	0	5,5,5	0.33	0
8	GOL	A	916	-	5,5,5	0.67	0	5,5,5	0.92	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
8	GOL	A	912	-	-	2/4/4/4	-
8	GOL	A	915	-	-	0/4/4/4	-
6	NAG	A	901	1	-	0/6/23/26	0/1/1/1
9	TLA	B	913	-	-	1/4/12/12	-
8	GOL	A	910	-	-	4/4/4/4	-
8	GOL	A	914	-	-	0/4/4/4	-
7	H6B	B	910	-	-	0/0/33/33	0/2/2/2
8	GOL	A	913	-	-	0/4/4/4	-
8	GOL	B	911	-	-	0/4/4/4	-
6	NAG	B	901	2	-	2/6/23/26	0/1/1/1
8	GOL	B	912	-	-	2/4/4/4	-
7	H6B	A	909	-	-	0/0/33/33	0/2/2/2
9	TLA	A	917	-	-	0/4/12/12	-
8	GOL	A	911	-	-	4/4/4/4	-
8	GOL	A	916	-	-	2/4/4/4	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	909	H6B	C8-N1-C5	7.62	121.43	113.64
7	B	910	H6B	C8-N1-C5	7.48	121.28	113.64
9	B	913	TLA	O3-C3-C4	-4.37	100.57	111.10
6	B	901	NAG	C1-O5-C5	3.73	117.25	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	910	H6B	C8-N1-C6	3.30	117.01	113.64
6	A	901	NAG	C1-O5-C5	3.24	116.58	112.19
6	A	901	NAG	C3-C4-C5	-3.01	104.86	110.24
7	B	910	H6B	C4-C3-C2	2.37	114.97	110.82
6	A	901	NAG	O5-C1-C2	-2.35	107.57	111.29
9	B	913	TLA	O2-C2-C1	-2.26	105.67	111.10
9	B	913	TLA	C1-C2-C3	2.24	117.93	113.11
7	A	909	H6B	C4-C3-C2	2.15	114.58	110.82
7	B	910	H6B	C1-C2-C3	2.11	113.19	110.43
7	A	909	H6B	C8-N1-C6	2.10	115.79	113.64
9	B	913	TLA	O2-C2-C3	-2.00	102.22	108.90

There are no chirality outliers.

All (17) 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	B	912	GOL	O1-C1-C2-C3
8	A	911	GOL	C1-C2-C3-O3
6	B	901	NAG	O5-C5-C6-O6
6	B	901	NAG	C4-C5-C6-O6
8	A	912	GOL	O1-C1-C2-C3
8	A	911	GOL	O1-C1-C2-C3
8	A	916	GOL	C1-C2-C3-O3
8	A	912	GOL	O1-C1-C2-O2
8	A	910	GOL	O1-C1-C2-O2
8	A	911	GOL	O1-C1-C2-O2
8	A	916	GOL	O2-C2-C3-O3
9	B	913	TLA	C1-C2-C3-C4
8	A	910	GOL	O2-C2-C3-O3
8	A	911	GOL	O2-C2-C3-O3
8	B	912	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	915	GOL	1	0
9	B	913	TLA	2	0
7	B	910	H6B	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	911	GOL	1	0
8	A	916	GOL	2	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%)	0.01	25 (4%) 37 36	25, 37, 67, 107	0
2	B	597/627 (95%)	0.18	27 (4%) 33 31	23, 40, 72, 101	0
All	All	1202/1254 (95%)	0.09	52 (4%) 35 33	23, 38, 69, 107	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	591	ALA	6.9
2	B	642	PRO	5.5
1	A	59	SER	5.3
2	B	588	ASP	5.2
1	A	641	VAL	5.1
1	A	642	PRO	5.0
2	B	641	VAL	4.4
1	A	105	ARG	4.3
1	A	27	GLU	3.9
1	A	639	LEU	3.6
1	A	229	PRO	3.6
2	B	451	ASN	3.4
1	A	104	GLY	3.4
2	B	408	ALA	3.2
2	B	430	PRO	3.2
2	B	428	GLN	3.1
1	A	227	THR	3.0
1	A	28	ALA	3.0
1	A	186	HIS	3.0
2	B	523	ARG	3.0
1	A	451	ASN	3.0
2	B	639	LEU	2.9
2	B	56	LEU	2.9
2	B	27	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	611	THR	2.8
1	A	58	HIS	2.7
1	A	57	PRO	2.6
2	B	319	ALA	2.6
1	A	252	ALA	2.6
1	A	56	LEU	2.5
2	B	365	LEU	2.5
2	B	439	LEU	2.5
1	A	38	ARG	2.5
1	A	285	GLN	2.4
2	B	375	ARG	2.4
2	B	545	GLU	2.4
1	A	187	ASP	2.4
2	B	132	LEU	2.3
2	B	627	ALA	2.3
2	B	546	LYS	2.3
2	B	393	LEU	2.3
2	B	520	ALA	2.3
2	B	585	PHE	2.2
2	B	547	PRO	2.2
2	B	390	MET	2.2
1	A	322	VAL	2.1
1	A	189	ASP	2.1
1	A	103	THR	2.1
2	B	590	LYS	2.1
1	A	286	LEU	2.0
1	A	393	LEU	2.0
1	A	489	ARG	2.0

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

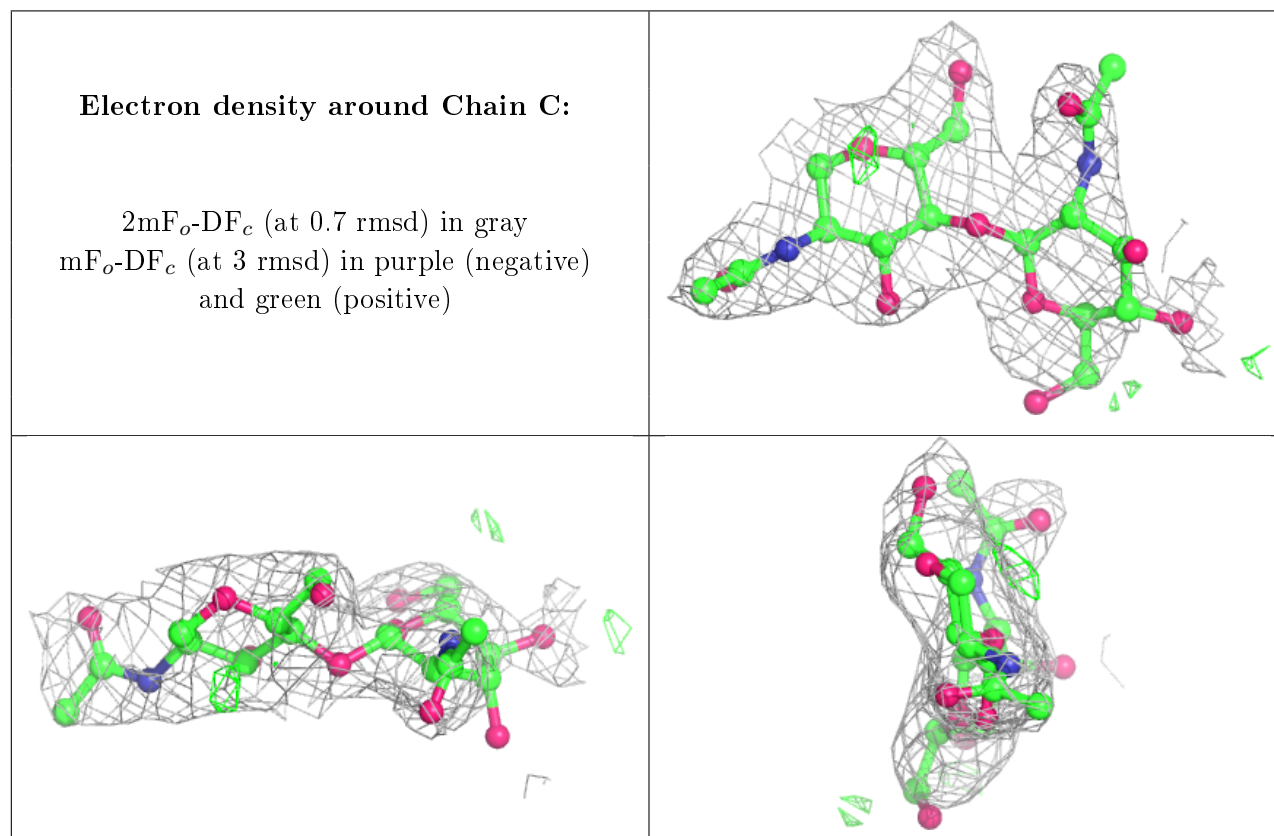
There are no non-standard protein/DNA/RNA residues in this entry.

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.

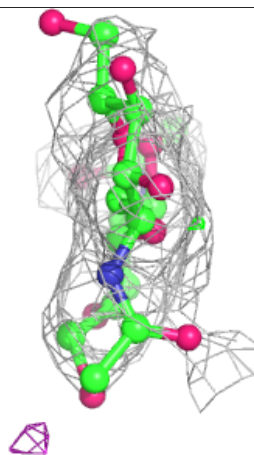
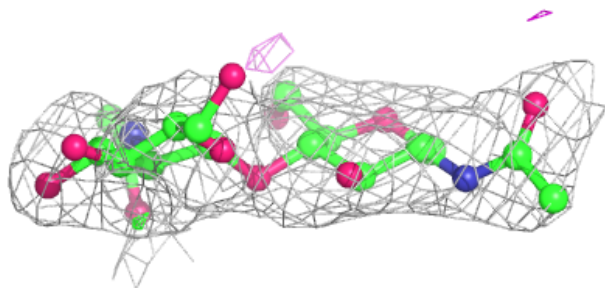
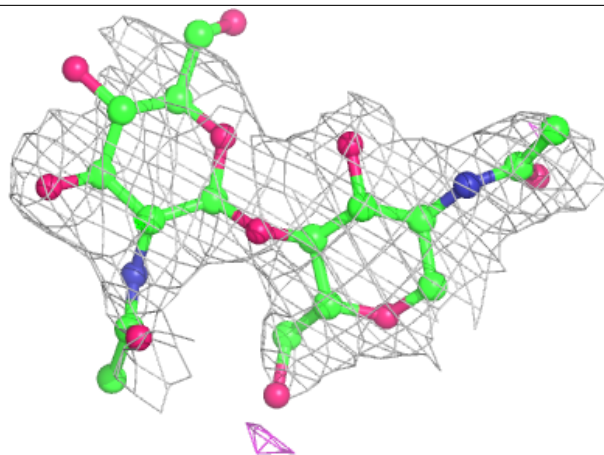
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	F	6	11/12	0.76	0.39	78,83,91,91	0
3	NAG	E	2	14/15	0.77	0.46	87,97,103,106	0
3	NAG	C	2	14/15	0.80	0.41	76,83,89,91	0
4	MAN	D	5	11/12	0.85	0.16	51,54,57,57	0
5	MAN	F	5	11/12	0.85	0.52	72,87,89,91	0
4	MAN	D	4	11/12	0.88	0.14	46,52,56,58	0
3	NAG	E	1	14/15	0.93	0.22	46,52,59,74	0
3	NAG	C	1	14/15	0.93	0.16	53,57,65,72	0
5	MAN	F	4	11/12	0.94	0.36	74,80,84,87	0
5	BMA	F	3	11/12	0.95	0.19	49,57,66,67	0
5	NAG	F	1	14/15	0.96	0.12	40,43,46,52	0
5	NAG	F	2	14/15	0.96	0.14	40,44,49,56	0
4	NAG	D	2	14/15	0.97	0.09	29,34,37,40	0
4	BMA	D	3	11/12	0.98	0.12	36,41,46,49	0
4	NAG	D	1	14/15	0.98	0.09	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.



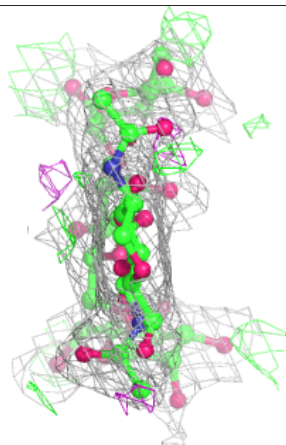
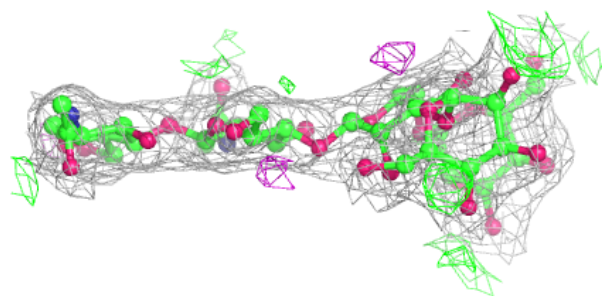
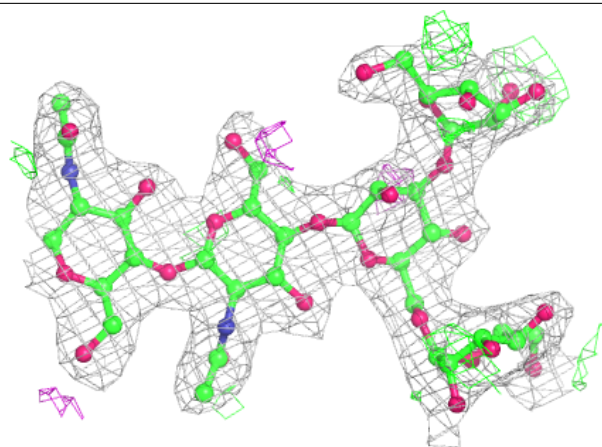
Electron density around Chain E:

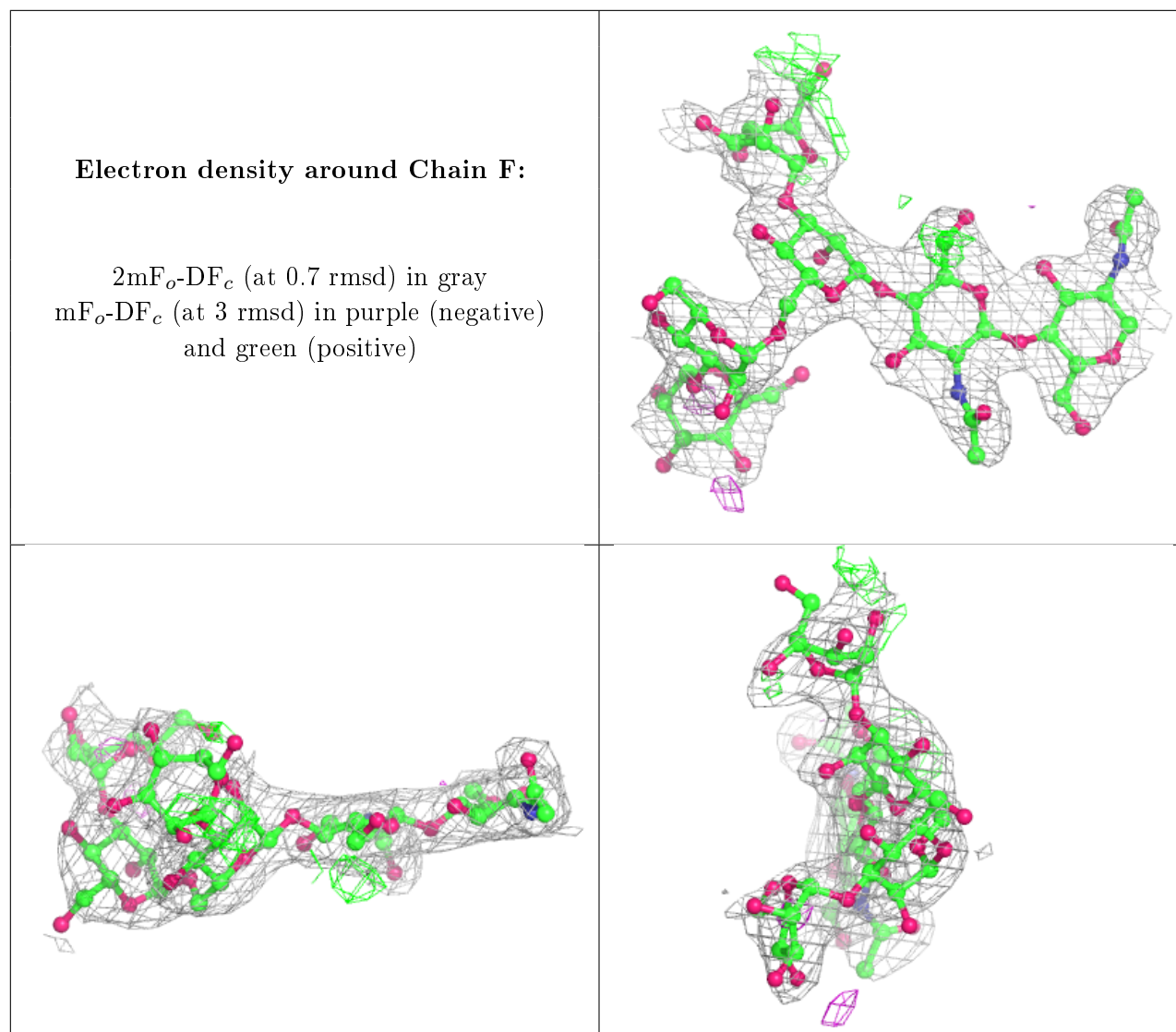
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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	0.83	0.35	67,74,78,79	0
7	H6B	B	910	14/14	0.84	0.21	50,59,65,66	0
7	H6B	A	909	14/14	0.85	0.21	50,60,73,74	0
9	TLA	B	913	10/10	0.90	0.23	60,69,75,76	0
8	GOL	A	911	6/6	0.90	0.31	50,51,52,54	0
8	GOL	A	914	6/6	0.91	0.20	55,57,60,62	0
8	GOL	A	912	6/6	0.91	0.15	50,52,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	A	913	6/6	0.91	0.19	49,54,54,55	0
8	GOL	A	915	6/6	0.93	0.16	48,53,55,60	0
6	NAG	A	901	14/15	0.93	0.21	45,52,58,58	0
8	GOL	B	912	6/6	0.93	0.18	48,49,56,58	0
8	GOL	A	916	6/6	0.93	0.15	33,41,41,44	0
8	GOL	A	910	6/6	0.94	0.12	48,49,52,52	0
8	GOL	B	911	6/6	0.94	0.21	57,60,61,67	0
9	TLA	A	917	10/10	0.95	0.10	43,49,58,61	0
10	CL	B	914	1/1	0.99	0.06	32,32,32,32	0
10	CL	A	918	1/1	0.99	0.10	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.