



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:54 PM BST

PDB ID : 4KH2  
Title : Crystal structure of human alpha-L-iduronidase complex with 2-deoxy-2-fluoro-alpha-L-idopyranosyluronic acid fluoride  
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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](mailto: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.

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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

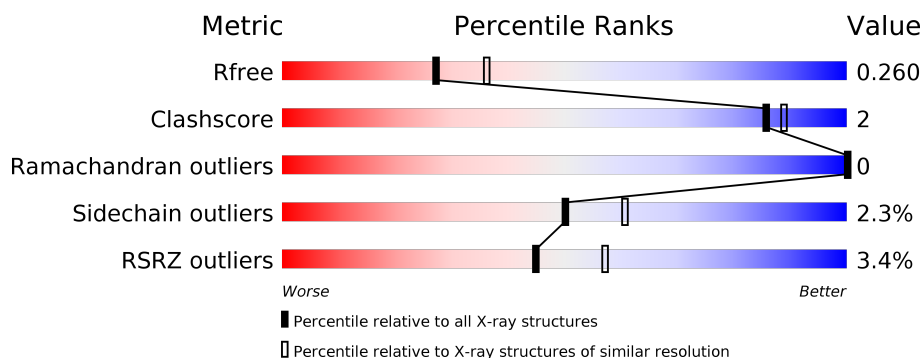
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	627	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>•</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>100%</div> </div>
3	D	5	<div> <div>20%</div> <div>80%</div> </div>
4	F	9	<div> <div>89%</div> <div>11%</div> </div>

## 2 Entry composition

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:

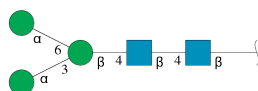
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLN	HIS	SEE REMARK 999	UNP P35475
A	63	PRO	GLN	SEE REMARK 999	UNP P35475
A	105	GLN	ARG	SEE REMARK 999	UNP P35475
B	33	GLN	HIS	SEE REMARK 999	UNP P35475
B	63	PRO	GLN	SEE REMARK 999	UNP P35475
B	105	GLN	ARG	SEE REMARK 999	UNP P35475

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



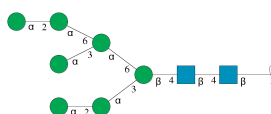
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



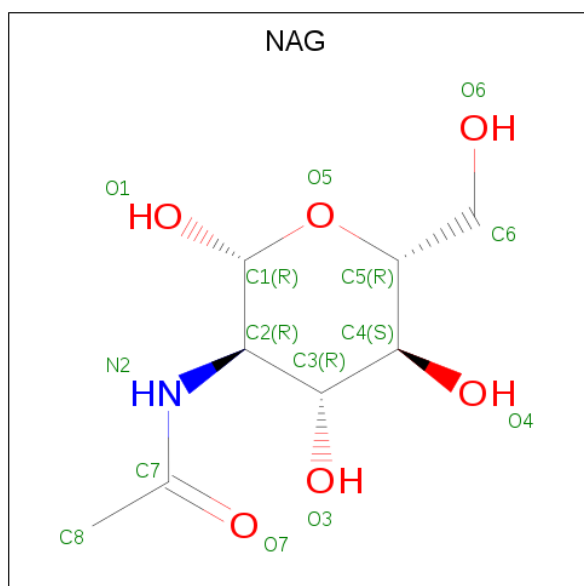
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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 (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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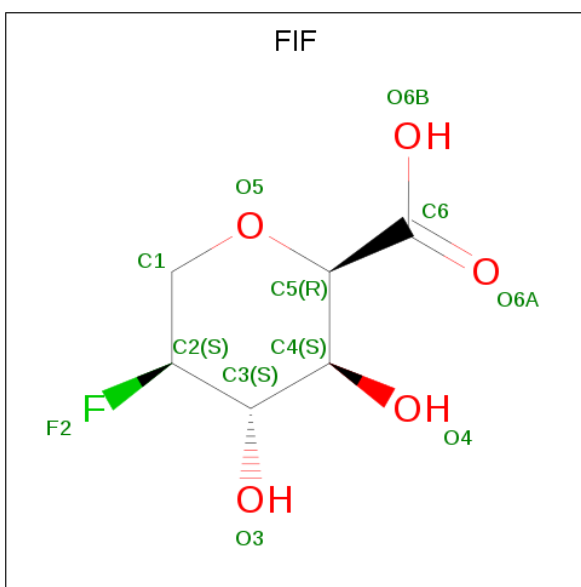
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (three-letter code: 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 (three-letter code: FIF) (formula:  $C_6H_9FO_5$ ).

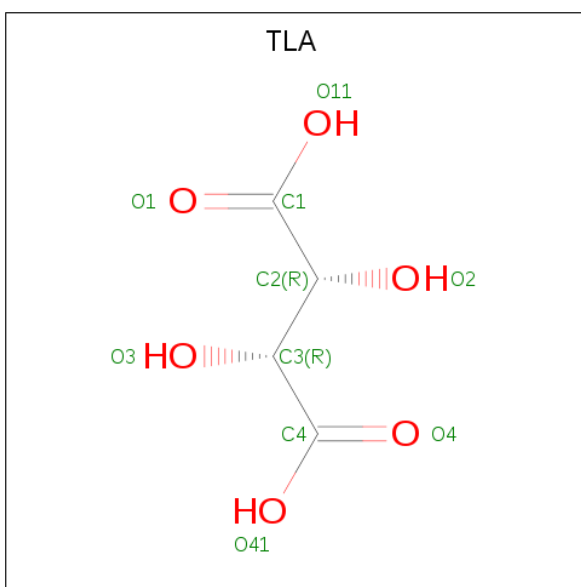


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	F	O	0	0
			12	6	1	5		
7	B	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

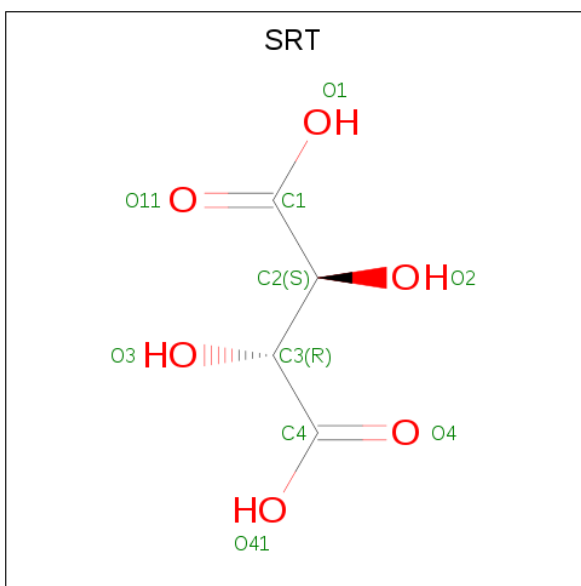
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



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 (three-letter code: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



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

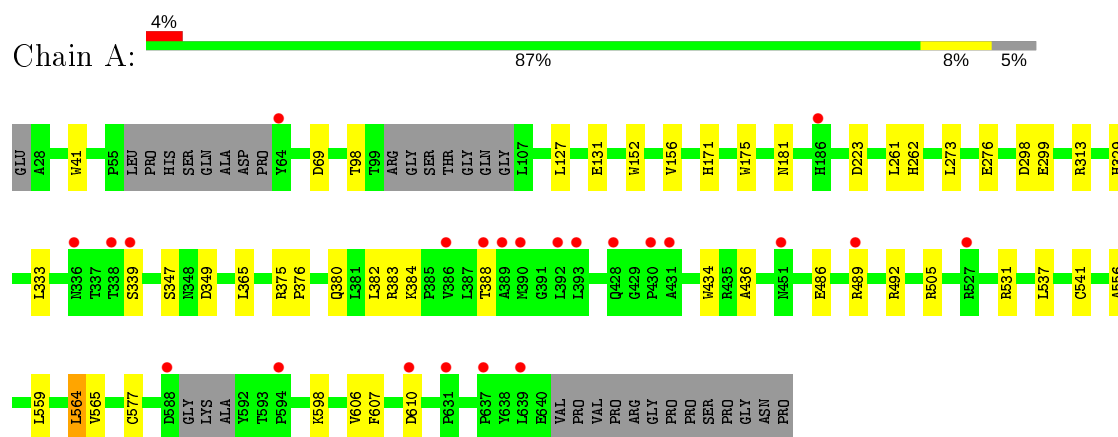
- Molecule 11 is water.

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

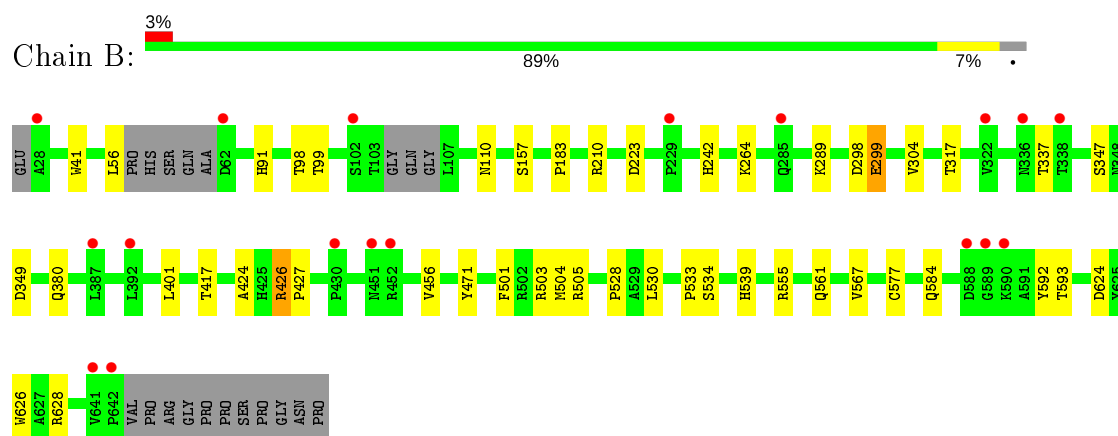
### 3 Residue-property plots [i](#)

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 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:  100%



MAN1  
MAN2

- 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%

MAN1  
MAN2  
BGL3  
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%

MAN1  
MAN2  
BGL3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.220 , 0.261 0.219 , 0.260	Depositor DCC
$R_{free}$ test set	3624 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.827	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, TLA, FIF, SRT, 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	0.41	1/4891 (0.0%)	0.52	0/6682
1	B	0.43	1/5010 (0.0%)	0.54	0/6843
All	All	0.42	2/9901 (0.0%)	0.53	0/13525

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	GLU	CD-OE2	19.30	1.46	1.25
1	A	299	GLU	CD-OE2	17.05	1.44	1.25

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	4746	0	4640	25	0
1	B	4862	0	4765	19	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	44	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 (44) 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: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: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
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:298:ASP:HA	1:B:347:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:GLN:HB3	1:B:592:TYR:HB3	1.99	0.44
1:B:577[A]:CYS:O	1:B:577[A]:CYS:SG	2.76	0.43
1:B:577[A]:CYS:SG	1:B:626:TRP:HZ3	2.42	0.43
1:B:349:ASP:OD2	7:B:919:FIF:H5	2.19	0.43
1:B:317:THR:HA	1:B:533:PRO:HG3	2.01	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: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:501:PHE:HA	1:B:504:MET:HE3	2.02	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 [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	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%)	496 (98%)	9 (2%)	59	70
1	B	517/527 (98%)	502 (97%)	15 (3%)	42	52
All	All	1022/1054 (97%)	998 (98%)	24 (2%)	50	61

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TRP
1	A	69	ASP
1	A	98	THR
1	A	339	SER
1	A	531	ARG
1	A	537	LEU
1	A	564	LEU
1	A	598	LYS
1	A	610	ASP
1	B	41	TRP
1	B	56	LEU
1	B	91	HIS
1	B	99	THR
1	B	157	SER
1	B	210	ARG
1	B	337	THR
1	B	417	THR
1	B	426	ARG
1	B	503[A]	ARG
1	B	503[B]	ARG
1	B	555	ARG
1	B	561	GLN
1	B	567	VAL
1	B	593	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	171	HIS

### 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	0
2	NAG	C	2	2	14,14,15	0.57	0	17,19,21	1.06	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.53	0	17,19,21	0.83	0
3	NAG	D	2	3	14,14,15	0.53	0	17,19,21	1.48	1 (5%)
3	BMA	D	3	3	11,11,12	0.47	0	15,15,17	1.13	2 (13%)
3	MAN	D	4	3	11,11,12	0.56	0	15,15,17	1.05	1 (6%)
3	MAN	D	5	3	11,11,12	0.60	0	15,15,17	1.08	1 (6%)
2	NAG	E	1	1,2	14,14,15	0.55	0	17,19,21	0.84	0
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	0.97	0
4	NAG	F	1	1,4	14,14,15	0.50	0	17,19,21	1.23	2 (11%)
4	NAG	F	2	4	14,14,15	0.56	0	17,19,21	0.93	1 (5%)
4	BMA	F	3	4	11,11,12	0.55	0	15,15,17	1.19	2 (13%)
4	MAN	F	4	4	11,11,12	0.69	0	15,15,17	1.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	F	5	4	11,11,12	0.48	0	15,15,17	1.20	2 (13%)
4	MAN	F	6	4	11,11,12	0.53	0	15,15,17	1.00	1 (6%)
4	MAN	F	7	4	11,11,12	0.57	0	15,15,17	1.15	1 (6%)
4	MAN	F	8	4	11,11,12	0.55	0	15,15,17	1.28	2 (13%)
4	MAN	F	9	4	11,11,12	0.67	0	15,15,17	1.12	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
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	1,4	-	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
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 (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	4.86	118.78	112.19
4	F	5	MAN	C1-O5-C5	3.39	116.78	112.19
4	F	8	MAN	C1-O5-C5	3.34	116.71	112.19
4	F	7	MAN	C1-O5-C5	3.20	116.53	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	6	MAN	C1-O5-C5	3.14	116.44	112.19
4	F	4	MAN	C1-C2-C3	2.88	113.20	109.67
4	F	3	BMA	C1-C2-C3	2.86	113.18	109.67
3	D	5	MAN	C1-O5-C5	2.81	116.00	112.19
4	F	9	MAN	C1-C2-C3	2.80	113.10	109.67
3	D	4	MAN	C1-O5-C5	2.78	115.96	112.19
3	D	3	BMA	C1-O5-C5	2.62	115.74	112.19
3	D	3	BMA	C1-C2-C3	2.48	112.72	109.67
2	C	2	NAG	C1-O5-C5	2.37	115.40	112.19
4	F	1	NAG	O5-C1-C2	-2.35	107.57	111.29
4	F	1	NAG	C1-O5-C5	2.27	115.26	112.19
4	F	9	MAN	O5-C5-C6	2.20	110.65	107.20
4	F	3	BMA	C1-O5-C5	2.19	115.16	112.19
4	F	5	MAN	O2-C2-C3	-2.15	105.82	110.14
4	F	2	NAG	C1-O5-C5	2.12	115.06	112.19
4	F	8	MAN	C3-C4-C5	2.03	113.86	110.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

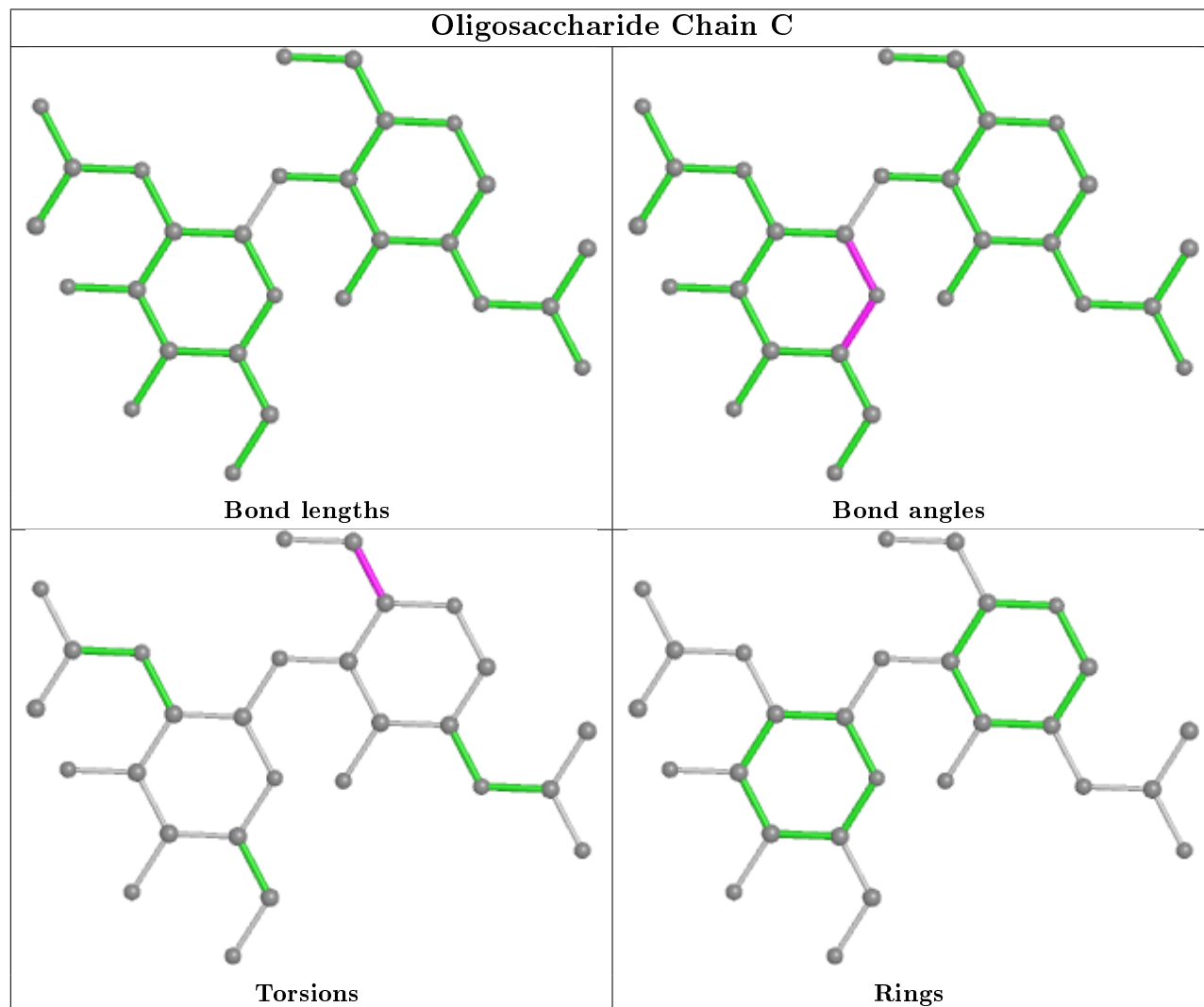
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
4	F	5	MAN	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	F	7	MAN	C4-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
4	F	9	MAN	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
4	F	9	MAN	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

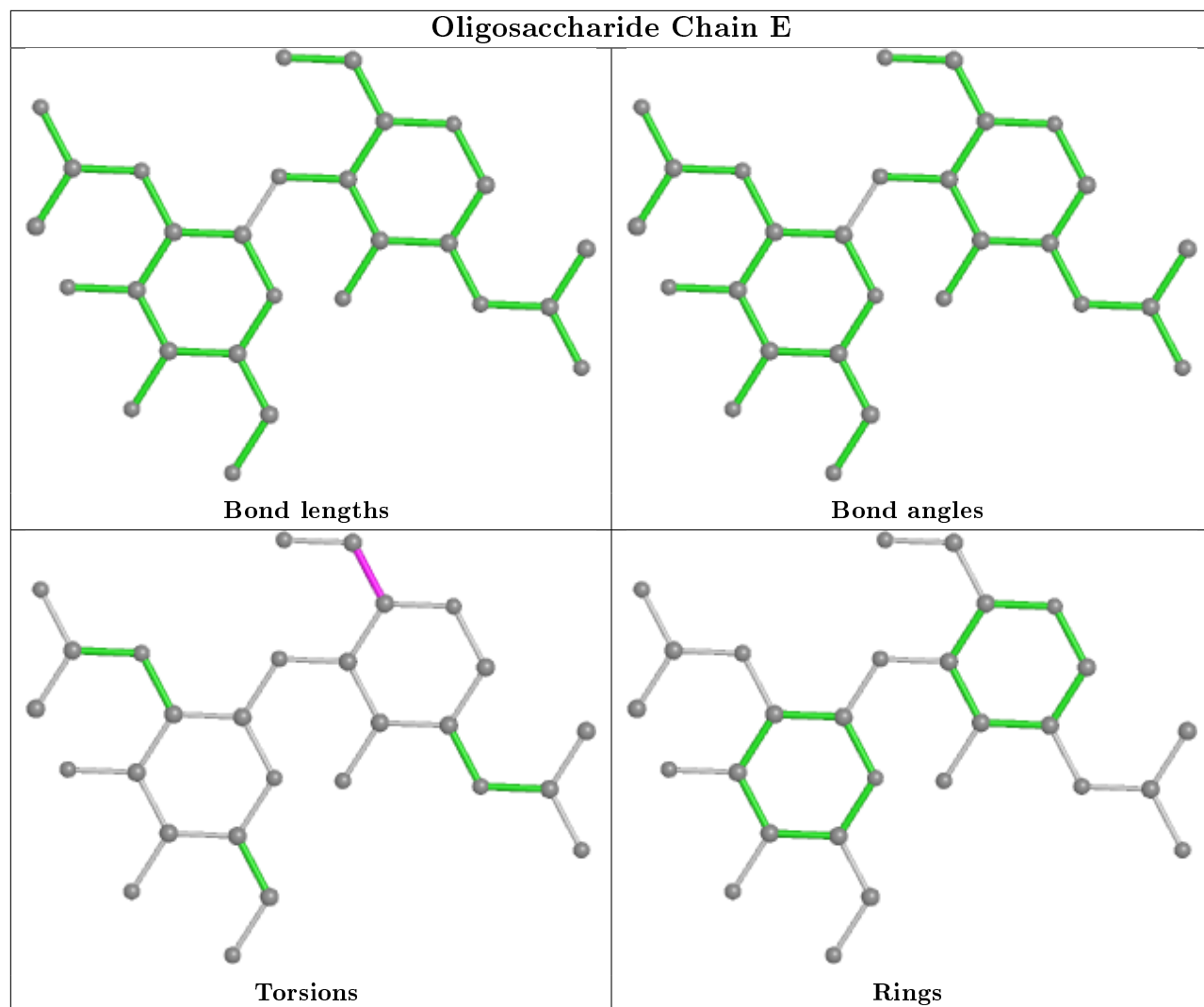
There are no ring outliers.

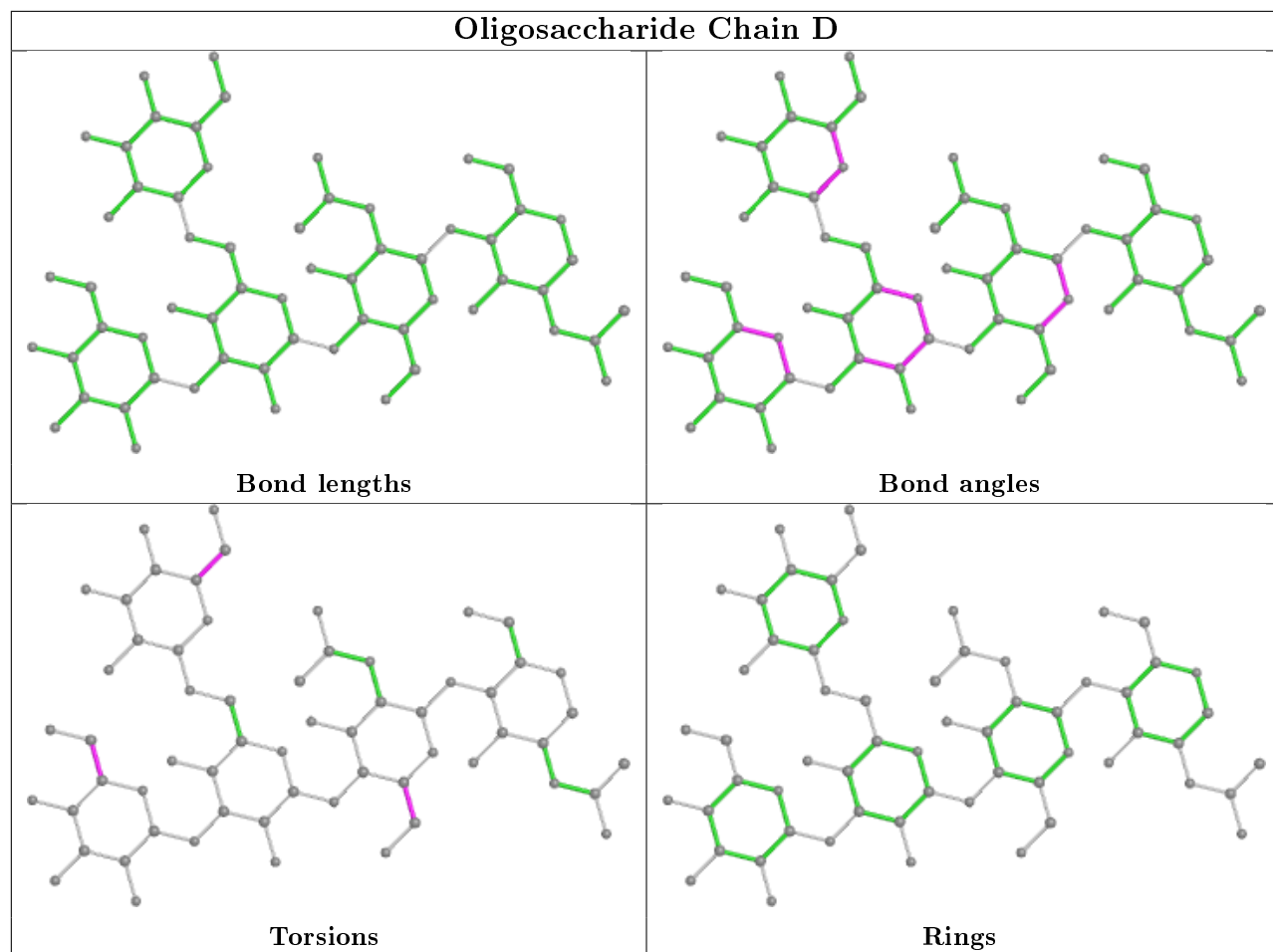
1 monomer is involved in 1 short contact:

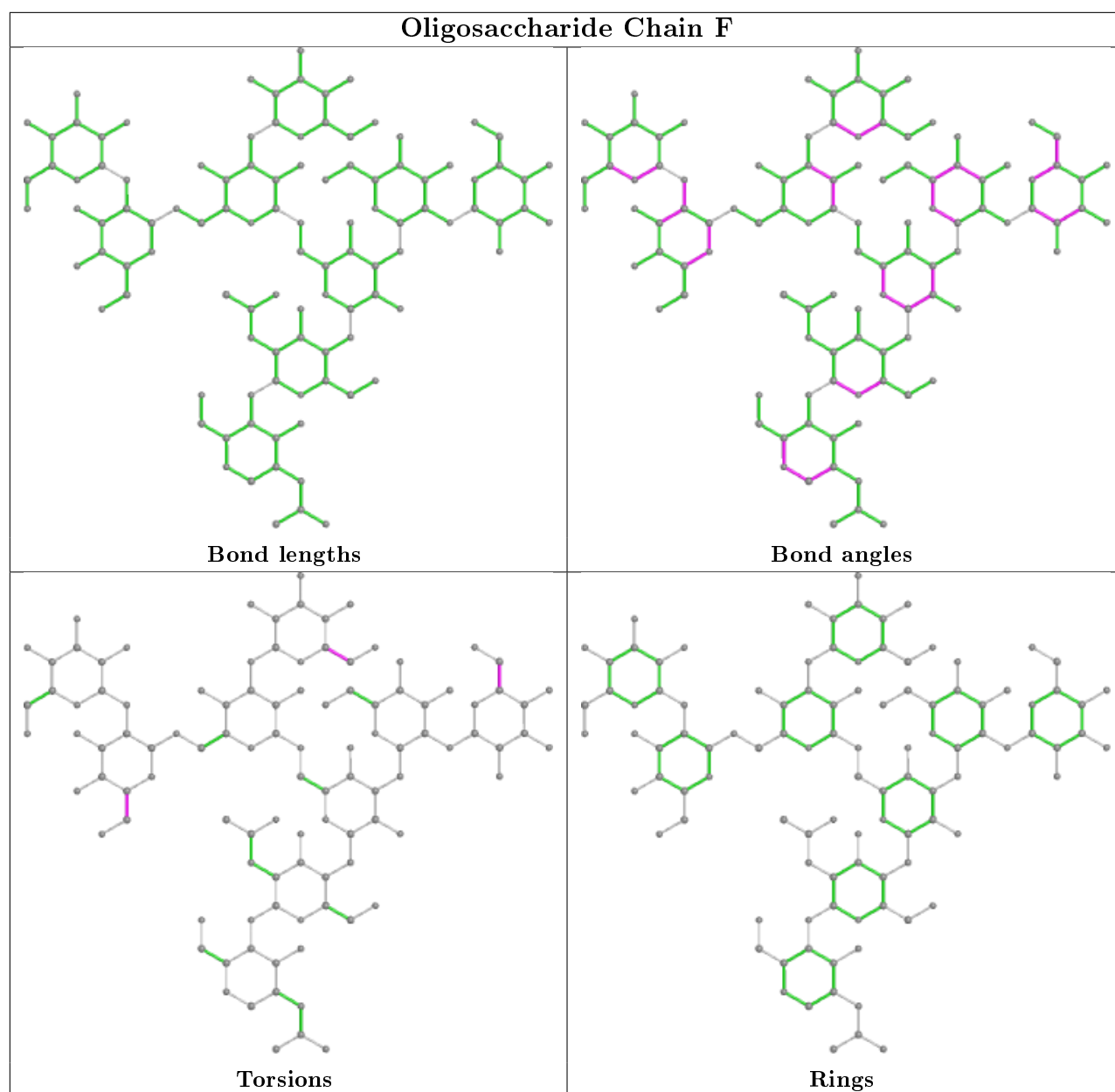
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3	BMA	1	0

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
6	GOL	A	910	-	5,5,5	0.28	0	5,5,5	0.32	0
5	NAG	A	901	1	14,14,15	0.65	0	17,19,21	1.17	2 (11%)
6	GOL	B	914	-	5,5,5	0.36	0	5,5,5	0.19	0
5	NAG	B	901	1	14,14,15	0.44	0	17,19,21	1.36	1 (5%)
6	GOL	A	909	-	5,5,5	0.27	0	5,5,5	0.16	0
9	TLA	B	917	-	3,9,9	0.38	0	6,12,12	0.87	0
6	GOL	B	915	-	5,5,5	0.23	0	5,5,5	0.35	0
6	GOL	B	916	-	5,5,5	0.28	0	5,5,5	0.75	0
7	FIF	A	911	1	9,12,12	1.02	0	7,17,17	1.51	2 (28%)
7	FIF	B	919	1	9,12,12	0.93	0	7,17,17	1.42	1 (14%)
6	GOL	B	913	-	5,5,5	0.25	0	5,5,5	0.36	0
10	SRT	B	918	-	3,9,9	0.32	0	6,12,12	1.02	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
6	GOL	A	910	-	-	2/4/4/4	-
5	NAG	A	901	1	-	2/6/23/26	0/1/1/1
6	GOL	B	914	-	-	4/4/4/4	-
5	NAG	B	901	1	-	0/6/23/26	0/1/1/1
6	GOL	A	909	-	-	1/4/4/4	-
9	TLA	B	917	-	-	0/4/12/12	-
6	GOL	B	915	-	-	1/4/4/4	-
6	GOL	B	916	-	-	4/4/4/4	-
7	FIF	A	911	1	-	0/0/21/21	0/1/1/1
7	FIF	B	919	1	-	0/0/21/21	0/1/1/1
6	GOL	B	913	-	-	0/4/4/4	-
10	SRT	B	918	-	-	0/4/12/12	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	901	NAG	C1-O5-C5	4.83	118.74	112.19
7	B	919	FIF	C1-O5-C5	3.07	117.58	112.17
7	A	911	FIF	C1-O5-C5	2.96	117.39	112.17
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(°)
7	A	911	FIF	C6-C5-C4	-2.15	107.68	113.04
5	A	901	NAG	C1-O5-C5	2.12	115.06	112.19

There are no chirality outliers.

All (14) 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
6	B	916	GOL	O1-C1-C2-C3
6	B	916	GOL	C1-C2-C3-O3
5	A	901	NAG	O5-C5-C6-O6
5	A	901	NAG	C4-C5-C6-O6
6	B	914	GOL	O1-C1-C2-C3
6	A	909	GOL	C1-C2-C3-O3
6	B	915	GOL	C1-C2-C3-O3
6	A	910	GOL	O2-C2-C3-O3
6	B	916	GOL	O1-C1-C2-O2
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	A	911	FIF	1	0
7	B	919	FIF	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	595/627 (94%)	0.13	23 (3%)	39 52	23, 35, 61, 77	0
1	B	607/627 (96%)	0.08	18 (2%)	50 61	21, 32, 53, 84	0
All	All	1202/1254 (95%)	0.11	41 (3%)	45 57	21, 34, 59, 84	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	589	GLY	4.8
1	A	336	ASN	4.7
1	A	338	THR	4.5
1	B	642	PRO	4.3
1	A	639	LEU	4.0
1	A	637	PRO	3.7
1	B	588	ASP	3.6
1	B	338	THR	3.2
1	B	590	LYS	3.1
1	A	428	GLN	3.1
1	A	389	ALA	2.9
1	B	229	PRO	2.8
1	B	28	ALA	2.7
1	B	322	VAL	2.7
1	B	641	VAL	2.7
1	A	390	MET	2.6
1	A	610	ASP	2.6
1	A	393	LEU	2.5
1	B	336	ASN	2.5
1	A	588	ASP	2.4
1	A	386	VAL	2.4
1	B	452	ARG	2.4
1	A	431	ALA	2.3
1	A	392	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	285	GLN	2.3
1	B	102	SER	2.2
1	A	186	HIS	2.2
1	A	339	SER	2.2
1	B	451	ASN	2.2
1	B	387	LEU	2.2
1	A	451	ASN	2.1
1	A	64	TYR	2.1
1	A	527	ARG	2.1
1	B	392	LEU	2.1
1	A	594	PRO	2.1
1	B	430	PRO	2.1
1	A	631	PRO	2.1
1	B	62	ASP	2.0
1	A	388	THR	2.0
1	A	430	PRO	2.0
1	A	489	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

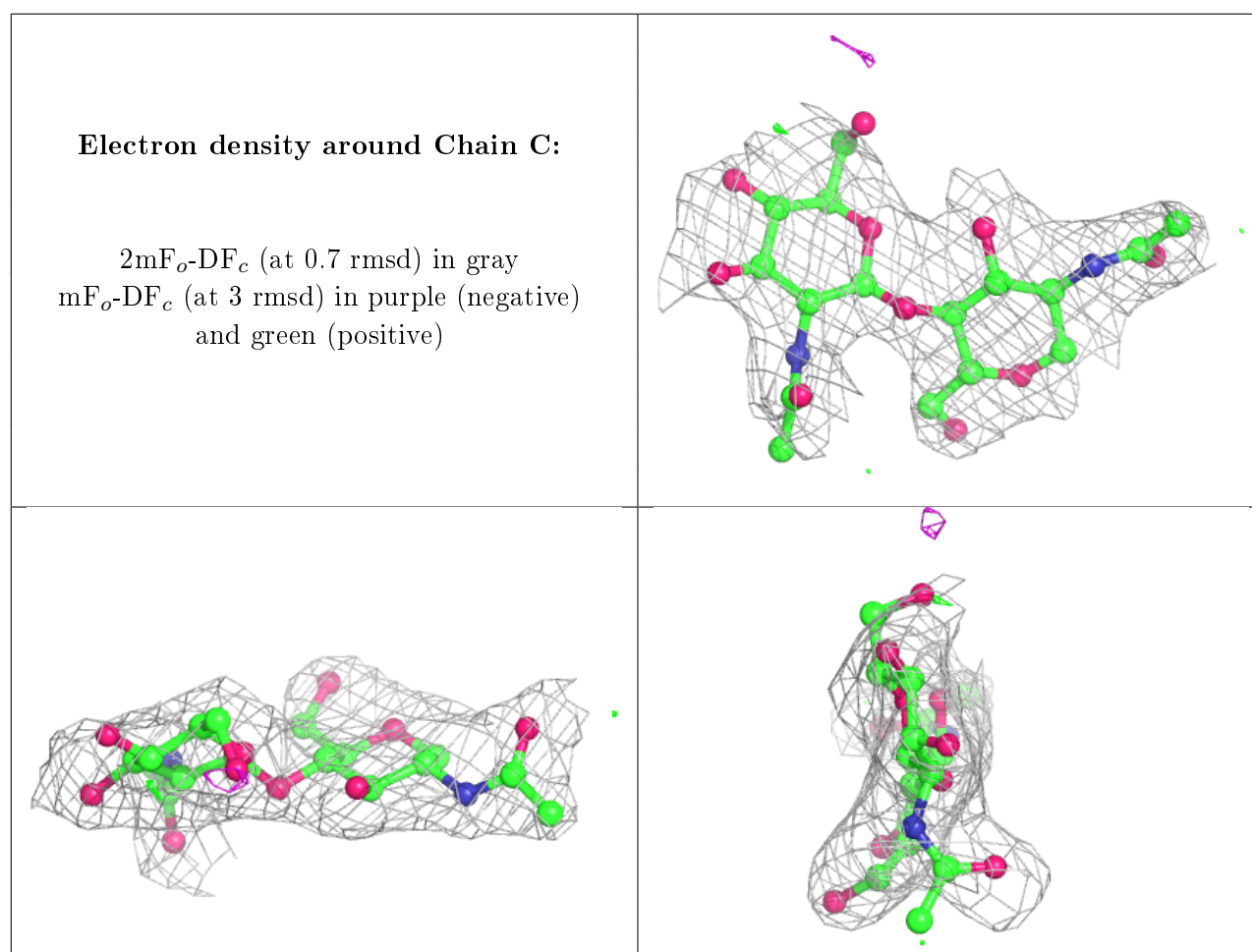
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	D	5	11/12	0.71	0.30	71,72,74,74	0
4	MAN	F	9	11/12	0.75	0.23	59,61,63,63	0
4	MAN	F	5	11/12	0.82	0.18	60,61,62,64	0
4	MAN	F	6	11/12	0.83	0.18	56,59,61,62	0
3	MAN	D	4	11/12	0.84	0.41	81,83,86,87	0
2	NAG	C	2	14/15	0.85	0.35	66,70,72,72	0
2	NAG	E	2	14/15	0.86	0.32	67,70,71,72	0
4	MAN	F	7	11/12	0.86	0.21	61,64,65,66	0
2	NAG	E	1	14/15	0.88	0.18	48,54,58,63	0
3	BMA	D	3	11/12	0.90	0.14	62,67,69,74	0
4	MAN	F	4	11/12	0.91	0.15	48,53,57,58	0

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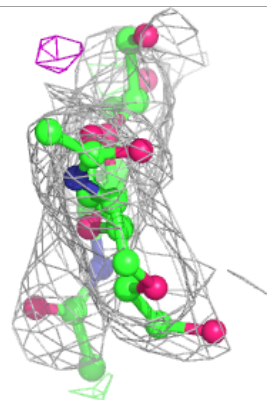
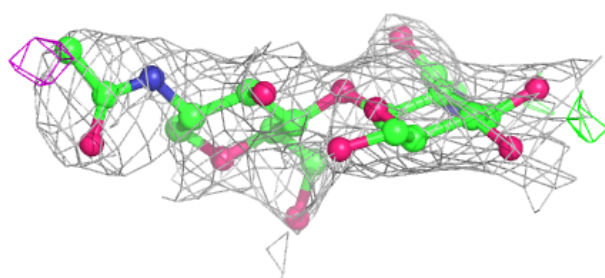
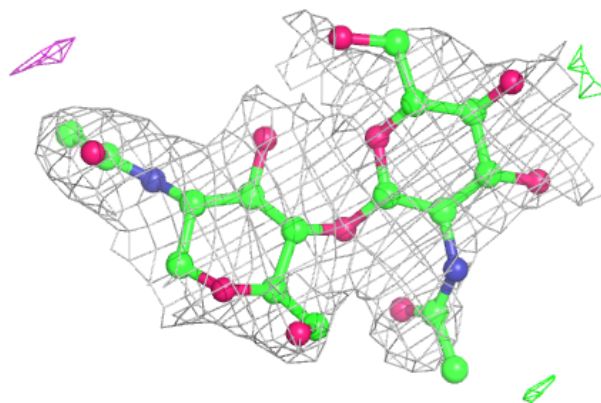
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	2	14/15	0.92	0.14	48,52,56,58	0
2	NAG	C	1	14/15	0.93	0.12	47,49,54,60	0
4	BMA	F	3	11/12	0.94	0.11	37,40,44,46	0
4	MAN	F	8	11/12	0.94	0.18	50,54,55,56	0
3	NAG	D	1	14/15	0.94	0.15	46,47,50,50	0
4	NAG	F	1	14/15	0.94	0.13	30,30,31,31	0
4	NAG	F	2	14/15	0.95	0.11	30,32,33,34	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.

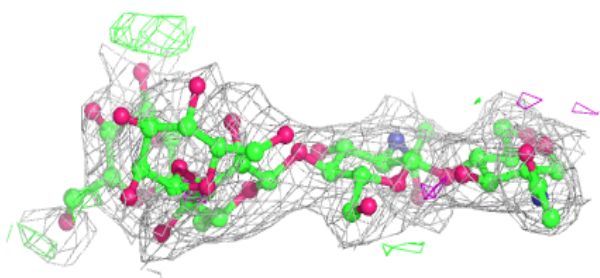
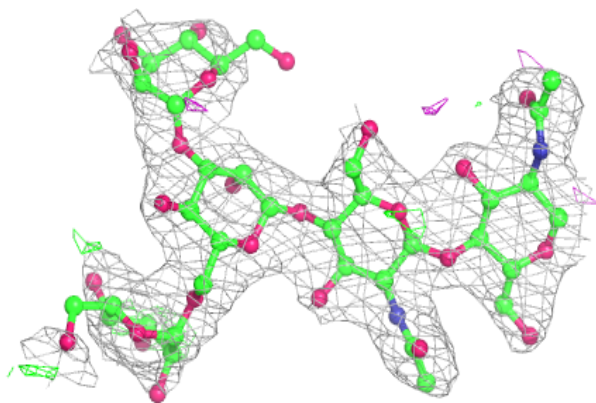


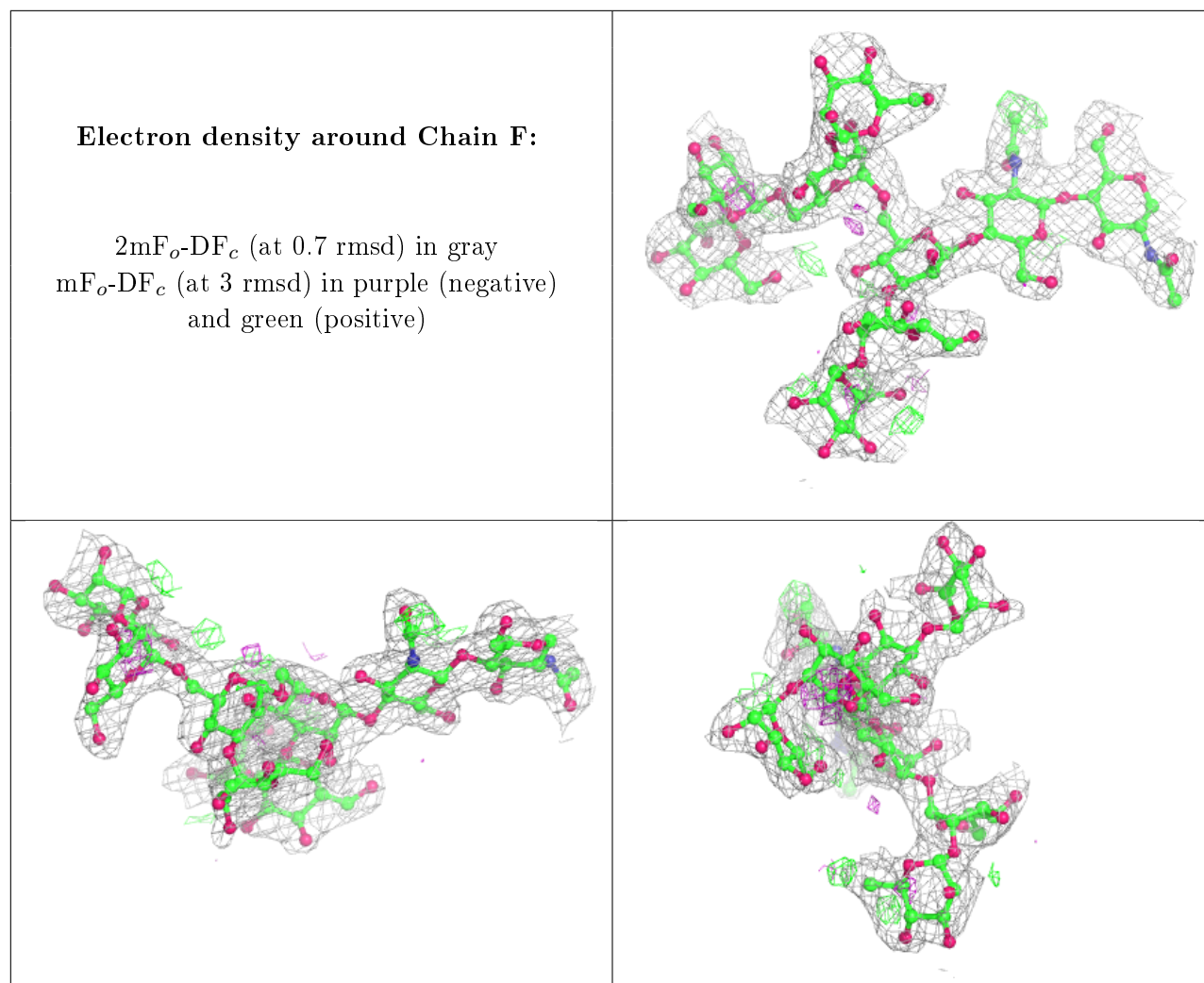
**Electron density around Chain E:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	GOL	A	910	6/6	0.72	0.18	67,67,68,68	0
6	GOL	A	909	6/6	0.85	0.20	44,49,49,51	0
5	NAG	A	901	14/15	0.86	0.28	61,67,70,70	0
6	GOL	B	914	6/6	0.88	0.17	40,42,43,43	0
7	FIF	A	911	12/12	0.88	0.14	42,44,46,47	0
6	GOL	B	915	6/6	0.89	0.15	42,43,44,46	0
5	NAG	B	901	14/15	0.90	0.21	42,44,45,46	0
7	FIF	B	919	12/12	0.90	0.12	44,46,47,47	0
6	GOL	B	913	6/6	0.90	0.23	40,41,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	SRT	B	918	10/10	0.91	0.23	48,50,51,52	0
6	GOL	B	916	6/6	0.93	0.16	25,27,27,28	0
9	TLA	B	917	10/10	0.93	0.14	39,40,43,43	0
8	CL	A	912	1/1	0.97	0.08	33,33,33,33	0
8	CL	B	920	1/1	0.99	0.16	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.