



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 10:52 am GMT

PDB ID : 5NXU  
Title : Complex structure with maltose of Providencia stuartii Omp-Pst1 porin  
Authors : Colletier, J.P.; Nasrallah, C.  
Deposited on : 2017-05-10  
Resolution : 3.00 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.

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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

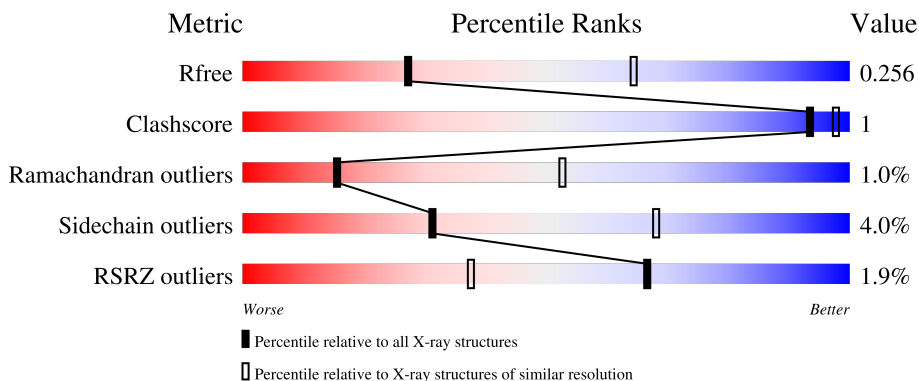
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



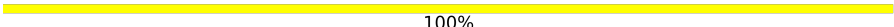
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	352	 2% 92% 8%
1	B	352	 3% 92% 7%
1	C	352	 93% 7%
2	D	2	 100%
2	E	2	 50% 50%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	2	 100%

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
3	LDA	A	401	-	-	-	X
3	LDA	B	406	-	-	-	X
3	LDA	B	407	-	-	-	X
3	LDA	B	409	-	-	-	X
3	LDA	C	405	-	-	-	X
3	LDA	C	406	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9181 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 Porin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	Total 2758	C 1728	N 469	O 556	S 5	0	0	0
1	B	352	Total 2775	C 1738	N 472	O 559	S 6	0	2	0
1	C	352	Total 2767	C 1734	N 471	O 557	S 5	0	1	0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	D	2	Total 23	C 12	O 11	0	0	0
2	E	2	Total 23	C 12	O 11	0	0	0
2	F	2	Total 23	C 12	O 11	0	0	0

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			11	9	1	1		
3	B	1	Total	C			0	0
			10	10				
3	B	1	Total	C	N	O	0	0
			15	13	1	1		
3	B	1	Total	C	N	O	0	0
			11	9	1	1		
3	B	1	Total	C	N	O	0	0
			11	9	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			13	11	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			11	9	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

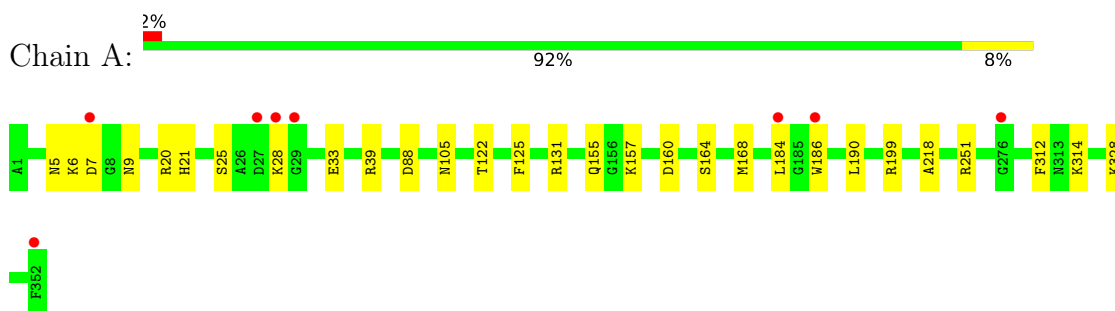
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	226	Total	O	0	0
			226	226		
5	B	166	Total	O	0	0
			166	166		
5	C	145	Total	O	0	0
			145	145		

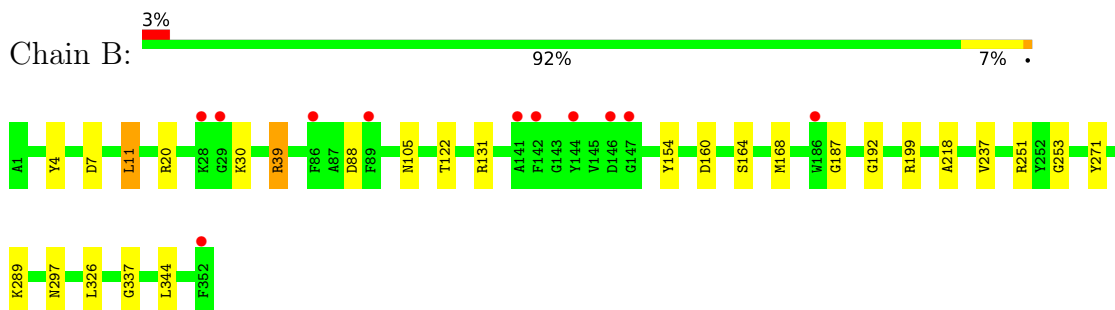
### 3 Residue-property plots [i](#)

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.

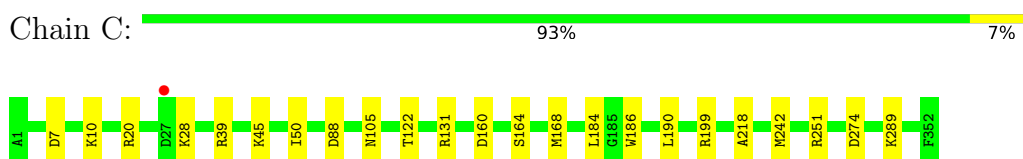
- Molecule 1: Porin 1



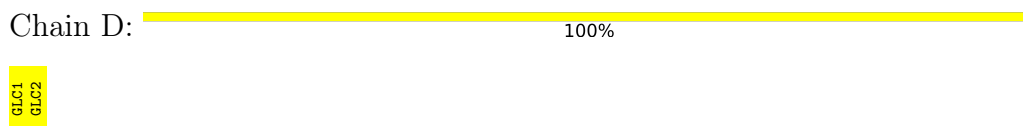
- Molecule 1: Porin 1



- Molecule 1: Porin 1



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



GLC1  
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:

100%

GLC1  
GLC2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.20Å 127.12Å 150.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.17 – 3.00 39.41 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (97.17-3.00) 99.6 (39.41-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.211 , 0.255 0.210 , 0.256	Depositor DCC
$R_{free}$ test set	2030 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.3	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, GLC, CA

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	0/2815	0.79	4/3800 (0.1%)
1	B	0.40	0/2832	0.73	4/3822 (0.1%)
1	C	0.39	0/2824	0.68	4/3811 (0.1%)
All	All	0.40	0/8471	0.74	12/11433 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ARG	NE-CZ-NH1	18.43	129.51	120.30
1	A	20	ARG	NE-CZ-NH2	-17.84	111.38	120.30
1	B	39	ARG	NE-CZ-NH2	13.21	126.90	120.30
1	B	20	ARG	NE-CZ-NH1	-10.20	115.20	120.30
1	B	39	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	B	20	ARG	NE-CZ-NH2	9.47	125.03	120.30
1	C	20	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	C	20	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	C	39	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	39	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	C	39	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	39	ARG	NE-CZ-NH1	5.83	123.21	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2758	0	2591	7	0
1	B	2775	0	2606	11	0
1	C	2767	0	2603	4	0
2	D	23	0	21	0	0
2	E	23	0	21	2	0
2	F	23	0	21	0	0
3	A	32	0	62	0	0
3	B	122	0	223	4	0
3	C	120	0	226	3	0
4	B	1	0	0	0	0
5	A	226	0	0	1	0
5	B	166	0	0	1	0
5	C	145	0	0	1	0
All	All	9181	0	8374	23	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 1.

All (23) 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:B:344:LEU:HD22	3:B:402:LDA:H51	1.65	0.79
1:B:192:GLY:HA3	3:B:405:LDA:H101	1.66	0.77
1:B:199:ARG:NH1	5:B:501:HOH:O	2.31	0.63
1:B:4:TYR:HB3	1:B:11:LEU:HB2	1.87	0.56
1:B:154:TYR:CE2	3:B:401:LDA:H32	2.40	0.56
1:B:122:THR:O	1:B:251:ARG:NH2	2.41	0.54
1:C:122:THR:O	1:C:251:ARG:NH2	2.41	0.53
1:A:122:THR:O	1:A:251:ARG:NH2	2.41	0.53
1:A:199:ARG:NH2	1:A:218:ALA:O	2.44	0.51
1:C:199:ARG:NH2	1:C:218:ALA:O	2.44	0.50
1:B:199:ARG:NH2	1:B:218:ALA:O	2.45	0.49
1:A:125:PHE:HA	1:A:155:GLN:HE22	1.78	0.49
1:A:21:HIS:NE2	3:C:401:LDA:HM21	2.29	0.47
1:A:199:ARG:NH1	5:A:502:HOH:O	2.48	0.47
1:C:184:LEU:HD11	1:C:190:LEU:HD12	2.00	0.44
1:B:253:GLY:N	2:E:2:GLC:O2	2.48	0.43
1:A:312:PHE:HB3	1:C:50:ILE:HD12	2.01	0.43
1:B:326:LEU:HD22	3:B:407:LDA:HM21	2.02	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:401:LDA:H82	3:C:401:LDA:H52	1.71	0.41
1:A:184:LEU:HD11	1:A:190:LEU:HD12	2.02	0.41
1:B:337:GLY:O	2:E:1:GLC:H2	2.21	0.41
3:C:404:LDA:HM22	5:C:514:HOH:O	2.20	0.41
1:B:237:VAL:HG22	1:B:271:TYR:HD1	1.86	0.41

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	350/352 (99%)	321 (92%)	26 (7%)	3 (1%)	17	55
1	B	352/352 (100%)	321 (91%)	28 (8%)	3 (1%)	17	55
1	C	351/352 (100%)	323 (92%)	24 (7%)	4 (1%)	14	50
All	All	1053/1056 (100%)	965 (92%)	78 (7%)	10 (1%)	15	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	B	7	ASP
1	C	7	ASP
1	A	186	TRP
1	C	88	ASP
1	C	186	TRP
1	A	160	ASP
1	B	160	ASP
1	C	160	ASP
1	B	187	GLY

### 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	284/284 (100%)	270 (95%)	14 (5%)	25	61
1	B	286/284 (101%)	276 (96%)	10 (4%)	36	71
1	C	285/284 (100%)	275 (96%)	10 (4%)	36	71
All	All	855/852 (100%)	821 (96%)	34 (4%)	31	68

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	6	LYS
1	A	9	ASN
1	A	25	SER
1	A	28	LYS
1	A	33	GLU
1	A	88	ASP
1	A	105	ASN
1	A	131	ARG
1	A	157	LYS
1	A	164	SER
1	A	168	MET
1	A	314	LYS
1	A	328	LYS
1	B	11	LEU
1	B	30	LYS
1	B	39	ARG
1	B	88	ASP
1	B	105	ASN
1	B	131	ARG
1	B	164	SER
1	B	168	MET
1	B	289	LYS
1	B	297	ASN
1	C	10	LYS
1	C	28	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	45	LYS
1	C	105	ASN
1	C	131	ARG
1	C	164	SER
1	C	168	MET
1	C	242	MET
1	C	274	ASP
1	C	289	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	155	GLN
1	A	235	ASN
1	A	270	GLN
1	B	297	ASN
1	C	202	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

6 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	GLC	D	1	2	12,12,12	0.73	0	17,17,17	1.44	3 (17%)
2	GLC	D	2	2	11,11,12	0.71	0	15,15,17	1.78	3 (20%)
2	GLC	E	1	2	12,12,12	0.58	0	17,17,17	0.81	0
2	GLC	E	2	2	11,11,12	0.56	0	15,15,17	1.72	3 (20%)
2	GLC	F	1	2	12,12,12	0.68	0	17,17,17	1.26	2 (11%)
2	GLC	F	2	2	11,11,12	0.52	0	15,15,17	0.89	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C1-O5-C5	4.57	118.39	112.19
2	E	2	GLC	C1-C2-C3	3.72	114.24	109.67
2	E	2	GLC	C1-O5-C5	3.47	116.90	112.19
2	D	2	GLC	C1-C2-C3	3.43	113.89	109.67
2	F	1	GLC	O4-C4-C5	3.23	117.33	109.30
2	D	1	GLC	O5-C5-C4	2.92	115.00	109.69
2	D	1	GLC	C1-O5-C5	2.84	119.03	113.66
2	F	1	GLC	O4-C4-C3	-2.49	104.60	110.35
2	E	2	GLC	C3-C4-C5	2.33	114.39	110.24
2	D	1	GLC	O4-C4-C5	2.31	115.03	109.30
2	D	2	GLC	C3-C4-C5	-2.14	106.42	110.24
2	F	2	GLC	O2-C2-C1	2.01	113.26	109.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	GLC	O5-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6

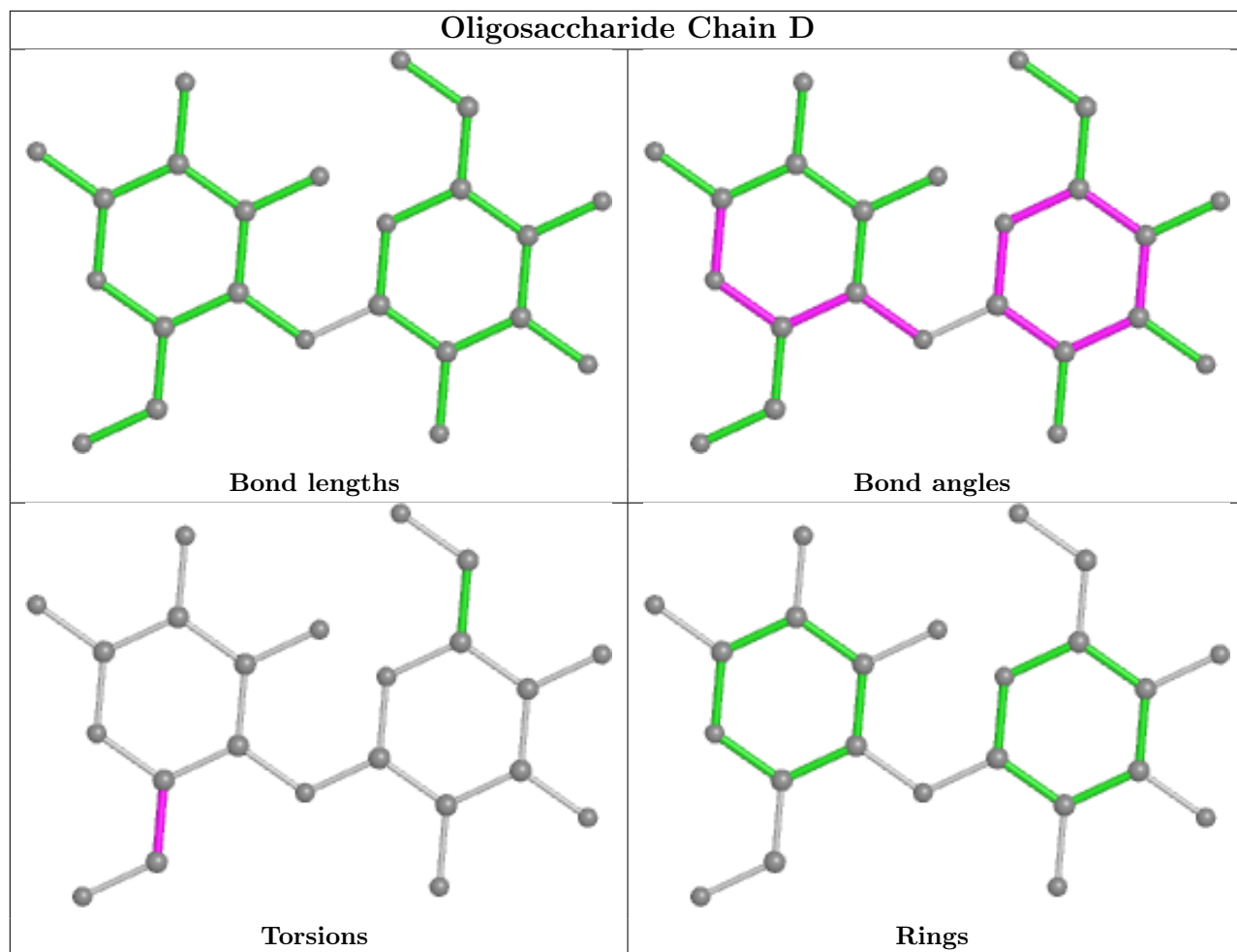
There are no ring outliers.

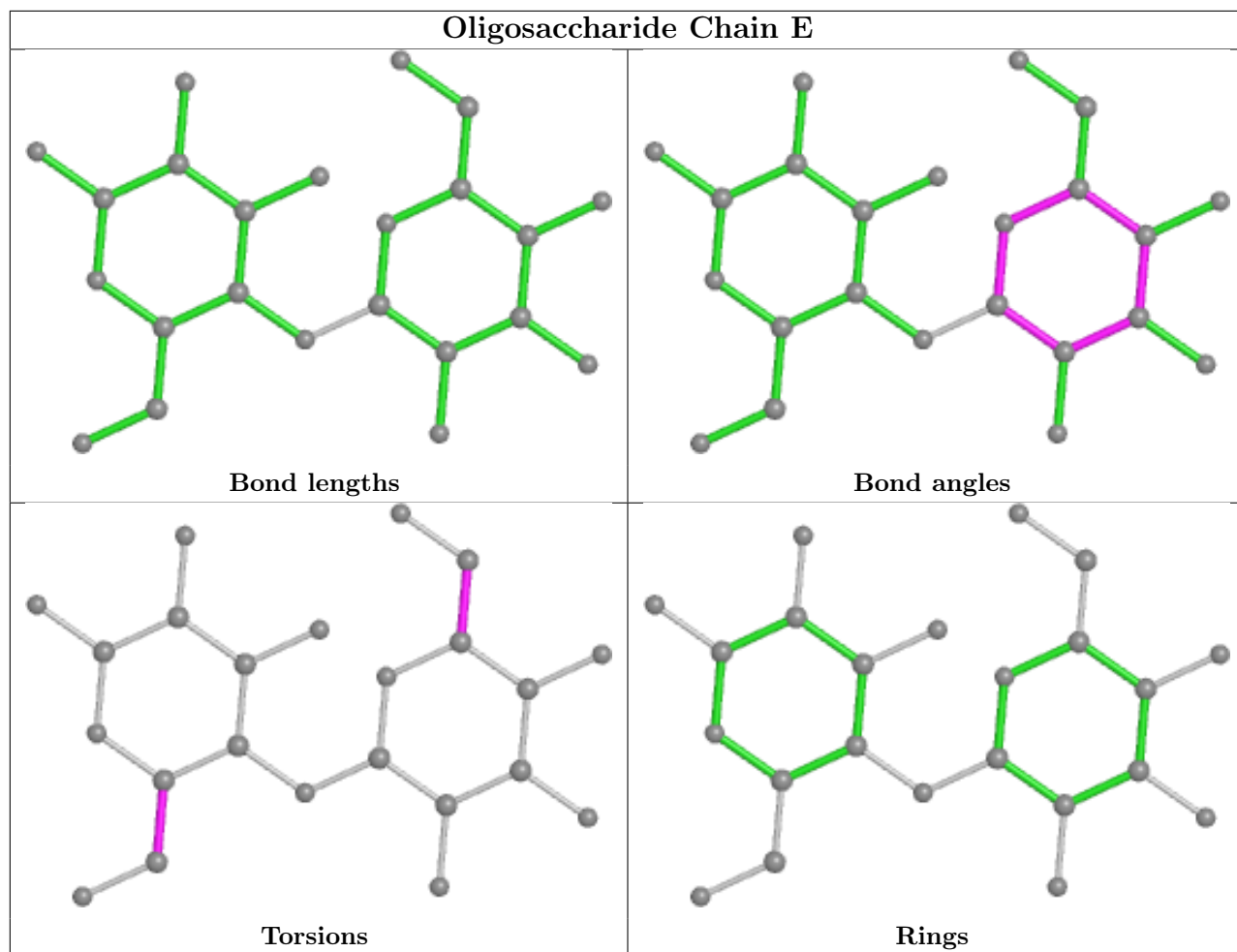
2 monomers are involved in 2 short contacts:

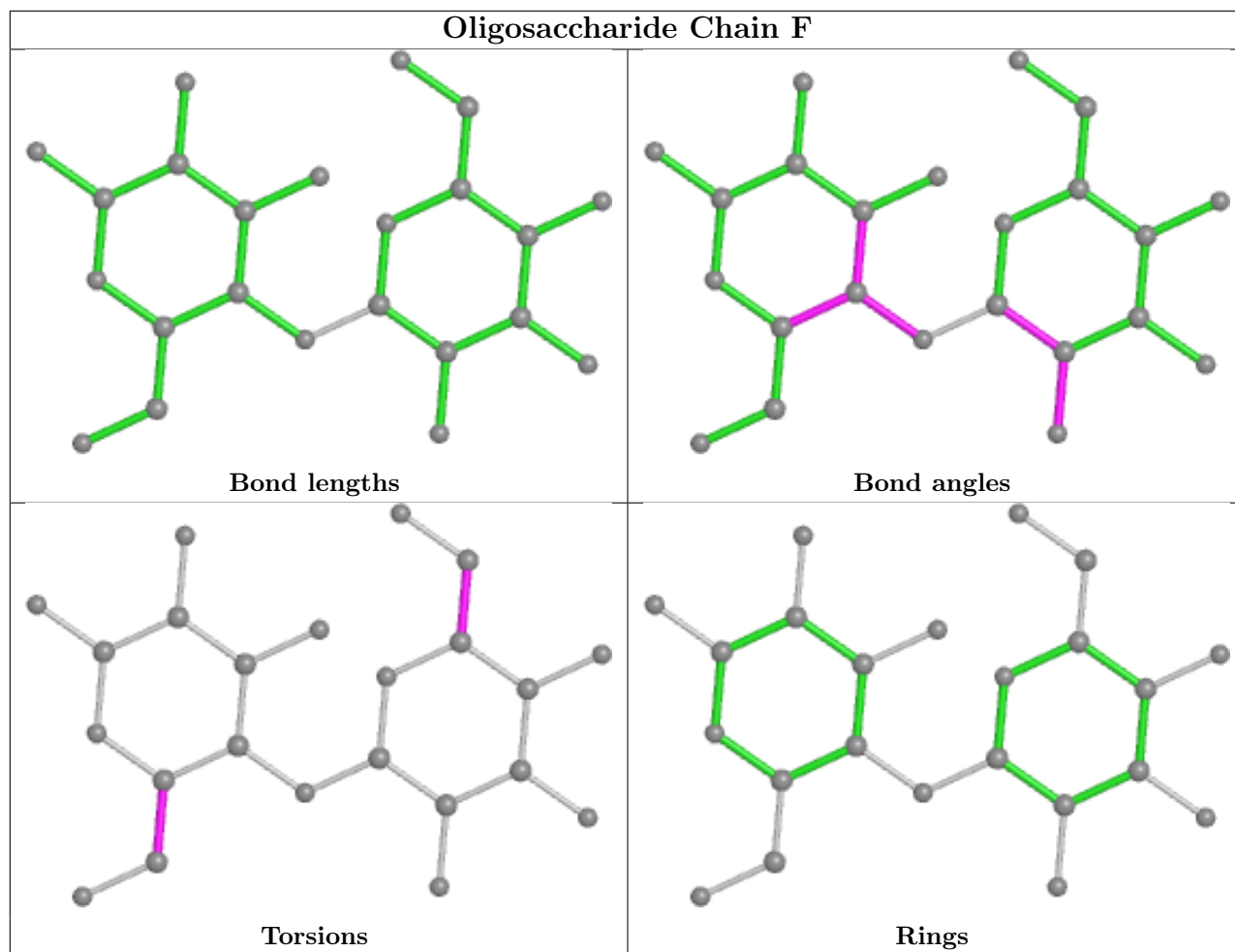
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	GLC	1	0
2	E	1	GLC	1	0

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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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
3	LDA	B	407	-	7,10,15	1.37	1 (14%)	9,12,17	3.44	3 (33%)
3	LDA	C	404	-	12,15,15	1.10	1 (8%)	14,17,17	3.03	3 (21%)
3	LDA	B	401	-	12,15,15	1.06	1 (8%)	14,17,17	2.99	3 (21%)
3	LDA	B	406	-	7,10,15	1.35	1 (14%)	9,12,17	3.68	3 (33%)
3	LDA	B	409	-	12,15,15	0.74	1 (8%)	14,17,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LDA	C	402	-	12,15,15	0.76	1 (8%)	14,17,17	0.46	0
3	LDA	C	405	-	7,10,15	1.53	1 (14%)	9,12,17	3.49	3 (33%)
3	LDA	B	408	-	12,15,15	1.05	1 (8%)	14,17,17	3.05	3 (21%)
3	LDA	A	402	-	12,15,15	0.74	1 (8%)	14,17,17	0.50	0
3	LDA	C	401	-	9,12,15	1.25	1 (11%)	11,14,17	3.42	3 (27%)
3	LDA	B	405	-	11,14,15	1.11	1 (9%)	13,16,17	2.96	3 (23%)
3	LDA	B	403	-	7,10,15	0.94	1 (14%)	9,12,17	0.41	0
3	LDA	C	406	-	12,15,15	0.86	1 (8%)	14,17,17	0.55	0
3	LDA	B	404	-	9,9,15	0.42	0	8,8,17	0.46	0
3	LDA	C	407	-	12,15,15	0.72	1 (8%)	14,17,17	0.47	0
3	LDA	B	402	-	12,15,15	0.78	1 (8%)	14,17,17	0.50	0
3	LDA	C	408	-	12,15,15	0.73	1 (8%)	14,17,17	0.46	0
3	LDA	A	401	-	12,15,15	0.78	1 (8%)	14,17,17	0.47	0
3	LDA	C	403	-	12,15,15	0.78	1 (8%)	14,17,17	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	B	407	-	-	2/8/8/13	-
3	LDA	C	404	-	-	7/13/13/13	-
3	LDA	B	401	-	-	7/13/13/13	-
3	LDA	B	406	-	-	6/8/8/13	-
3	LDA	B	409	-	-	2/13/13/13	-
3	LDA	C	402	-	-	2/13/13/13	-
3	LDA	C	405	-	-	5/8/8/13	-
3	LDA	B	408	-	-	5/13/13/13	-
3	LDA	A	402	-	-	6/13/13/13	-
3	LDA	C	401	-	-	7/10/10/13	-
3	LDA	B	405	-	-	6/12/12/13	-
3	LDA	B	403	-	-	0/8/8/13	-
3	LDA	C	406	-	-	9/13/13/13	-
3	LDA	B	404	-	-	3/7/7/13	-
3	LDA	C	407	-	-	5/13/13/13	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	B	402	-	-	5/13/13/13	-
3	LDA	C	408	-	-	3/13/13/13	-
3	LDA	A	401	-	-	3/13/13/13	-
3	LDA	C	403	-	-	3/13/13/13	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	405	LDA	O1-N1	3.86	1.51	1.42
3	C	401	LDA	O1-N1	3.55	1.50	1.42
3	C	404	LDA	O1-N1	3.51	1.50	1.42
3	B	405	LDA	O1-N1	3.44	1.50	1.42
3	B	407	LDA	O1-N1	3.41	1.50	1.42
3	B	401	LDA	O1-N1	3.39	1.50	1.42
3	B	408	LDA	O1-N1	3.39	1.50	1.42
3	B	406	LDA	O1-N1	3.35	1.50	1.42
3	C	406	LDA	O1-N1	2.48	1.47	1.42
3	B	402	LDA	O1-N1	2.28	1.47	1.42
3	A	402	LDA	O1-N1	2.26	1.47	1.42
3	A	401	LDA	O1-N1	2.26	1.47	1.42
3	C	403	LDA	O1-N1	2.19	1.47	1.42
3	B	403	LDA	O1-N1	2.16	1.47	1.42
3	C	408	LDA	O1-N1	2.13	1.47	1.42
3	B	409	LDA	O1-N1	2.09	1.47	1.42
3	C	402	LDA	O1-N1	2.08	1.47	1.42
3	C	407	LDA	O1-N1	2.00	1.46	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	408	LDA	O1-N1-C1	-9.18	86.75	109.27
3	B	401	LDA	O1-N1-C1	-9.11	86.93	109.27
3	B	406	LDA	O1-N1-C1	-8.72	87.88	109.27
3	C	401	LDA	O1-N1-C1	-8.71	87.90	109.27
3	B	405	LDA	O1-N1-C1	-8.38	88.71	109.27
3	C	405	LDA	O1-N1-C1	-8.26	89.02	109.27
3	B	407	LDA	O1-N1-C1	-8.03	89.57	109.27
3	C	404	LDA	CM1-N1-C1	7.79	126.59	110.23
3	C	404	LDA	O1-N1-C1	-7.58	90.67	109.27
3	C	401	LDA	CM2-N1-C1	5.43	121.64	110.23
3	B	406	LDA	CM2-N1-C1	4.92	120.56	110.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	408	LDA	CM1-N1-C1	4.90	120.52	110.23
3	B	401	LDA	CM2-N1-C1	4.61	119.92	110.23
3	B	405	LDA	CM2-N1-C1	4.60	119.91	110.23
3	C	401	LDA	CM1-N1-C1	4.59	119.87	110.23
3	C	405	LDA	CM1-N1-C1	4.51	119.70	110.23
3	B	407	LDA	CM2-N1-C1	4.49	119.67	110.23
3	B	406	LDA	CM1-N1-C1	4.44	119.56	110.23
3	B	407	LDA	CM1-N1-C1	4.39	119.46	110.23
3	C	405	LDA	CM2-N1-C1	4.37	119.42	110.23
3	B	405	LDA	CM1-N1-C1	4.30	119.26	110.23
3	B	408	LDA	CM2-N1-C1	4.17	119.00	110.23
3	B	401	LDA	CM1-N1-C1	4.11	118.87	110.23
3	C	404	LDA	CM2-N1-C1	2.68	115.86	110.23

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	LDA	C2-C1-N1-O1
3	B	401	LDA	N1-C1-C2-C3
3	B	405	LDA	C2-C1-N1-CM1
3	B	405	LDA	C2-C1-N1-CM2
3	B	406	LDA	C2-C1-N1-O1
3	B	407	LDA	C2-C1-N1-O1
3	B	408	LDA	C2-C1-N1-O1
3	B	408	LDA	N1-C1-C2-C3
3	C	401	LDA	C2-C1-N1-O1
3	C	401	LDA	C2-C1-N1-CM2
3	C	401	LDA	N1-C1-C2-C3
3	C	404	LDA	C2-C1-N1-CM1
3	C	405	LDA	C2-C1-N1-O1
3	C	406	LDA	C2-C1-N1-CM1
3	C	406	LDA	C2-C1-N1-CM2
3	C	406	LDA	N1-C1-C2-C3
3	C	407	LDA	N1-C1-C2-C3
3	A	401	LDA	C1-C2-C3-C4
3	C	402	LDA	C11-C10-C9-C8
3	C	406	LDA	C5-C6-C7-C8
3	A	401	LDA	C4-C5-C6-C7
3	C	406	LDA	C4-C5-C6-C7
3	B	402	LDA	C11-C10-C9-C8
3	C	407	LDA	C3-C4-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	401	LDA	C6-C7-C8-C9
3	C	408	LDA	C6-C7-C8-C9
3	C	407	LDA	C1-C2-C3-C4
3	B	405	LDA	C2-C3-C4-C5
3	C	401	LDA	C1-C2-C3-C4
3	B	408	LDA	C1-C2-C3-C4
3	C	406	LDA	C7-C8-C9-C10
3	B	409	LDA	C4-C5-C6-C7
3	A	401	LDA	C2-C3-C4-C5
3	B	402	LDA	C2-C3-C4-C5
3	C	404	LDA	C3-C4-C5-C6
3	B	402	LDA	C1-C2-C3-C4
3	C	401	LDA	C2-C3-C4-C5
3	A	402	LDA	C3-C4-C5-C6
3	C	408	LDA	C1-C2-C3-C4
3	B	405	LDA	C1-C2-C3-C4
3	B	408	LDA	C2-C3-C4-C5
3	C	406	LDA	C6-C7-C8-C9
3	B	409	LDA	C1-C2-C3-C4
3	C	401	LDA	C4-C5-C6-C7
3	B	401	LDA	C4-C5-C6-C7
3	B	404	LDA	C6-C7-C8-C9
3	C	403	LDA	C1-C2-C3-C4
3	C	407	LDA	C2-C3-C4-C5
3	C	404	LDA	C1-C2-C3-C4
3	A	402	LDA	C2-C3-C4-C5
3	B	402	LDA	C7-C8-C9-C10
3	B	406	LDA	C3-C4-C5-C6
3	B	404	LDA	C5-C6-C7-C8
3	A	402	LDA	C5-C6-C7-C8
3	C	405	LDA	C2-C3-C4-C5
3	B	401	LDA	C2-C1-N1-CM2
3	B	406	LDA	C2-C1-N1-CM2
3	B	407	LDA	C2-C1-N1-CM2
3	B	408	LDA	C2-C1-N1-CM2
3	C	404	LDA	C2-C1-N1-CM2
3	C	405	LDA	C2-C1-N1-CM2
3	C	404	LDA	C11-C10-C9-C8
3	B	406	LDA	C1-C2-C3-C4
3	C	406	LDA	C2-C1-N1-O1
3	B	406	LDA	C4-C5-C6-C7
3	B	404	LDA	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	401	LDA	C2-C3-C4-C5
3	B	405	LDA	C11-C10-C9-C8
3	C	401	LDA	C5-C6-C7-C8
3	A	402	LDA	C7-C8-C9-C10
3	B	401	LDA	C5-C6-C7-C8
3	B	406	LDA	C2-C3-C4-C5
3	B	405	LDA	N1-C1-C2-C3
3	C	404	LDA	N1-C1-C2-C3
3	C	405	LDA	N1-C1-C2-C3
3	B	402	LDA	C9-C10-C11-C12
3	A	402	LDA	C11-C10-C9-C8
3	A	402	LDA	C1-C2-C3-C4
3	C	402	LDA	C5-C6-C7-C8
3	C	403	LDA	C2-C1-N1-CM2
3	C	407	LDA	C5-C6-C7-C8
3	C	406	LDA	C2-C3-C4-C5
3	C	405	LDA	C3-C4-C5-C6
3	C	408	LDA	C7-C8-C9-C10
3	C	403	LDA	C9-C10-C11-C12
3	C	404	LDA	C6-C7-C8-C9

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	407	LDA	1	0
3	C	404	LDA	1	0
3	B	401	LDA	1	0
3	C	401	LDA	2	0
3	B	405	LDA	1	0
3	B	402	LDA	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	352/352 (100%)	-0.14	8 (2%) 60 31	65, 92, 146, 193	0
1	B	352/352 (100%)	-0.16	11 (3%) 49 21	66, 91, 142, 175	0
1	C	352/352 (100%)	-0.34	1 (0%) 94 84	69, 97, 139, 184	0
All	All	1056/1056 (100%)	-0.21	20 (1%) 66 37	65, 93, 145, 193	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	LYS	5.2
1	A	7	ASP	4.8
1	B	142	PHE	3.2
1	A	352	PHE	3.2
1	B	186	TRP	3.1
1	A	27	ASP	3.0
1	A	29	GLY	3.0
1	A	186	TRP	2.9
1	B	144	TYR	2.9
1	B	147	GLY	2.7
1	B	86	PHE	2.7
1	B	141	ALA	2.4
1	C	27	ASP	2.3
1	B	146	ASP	2.2
1	B	352	PHE	2.2
1	B	89	PHE	2.2
1	B	28	LYS	2.1
1	B	29	GLY	2.1
1	A	276	GLY	2.1
1	A	184	LEU	2.1

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

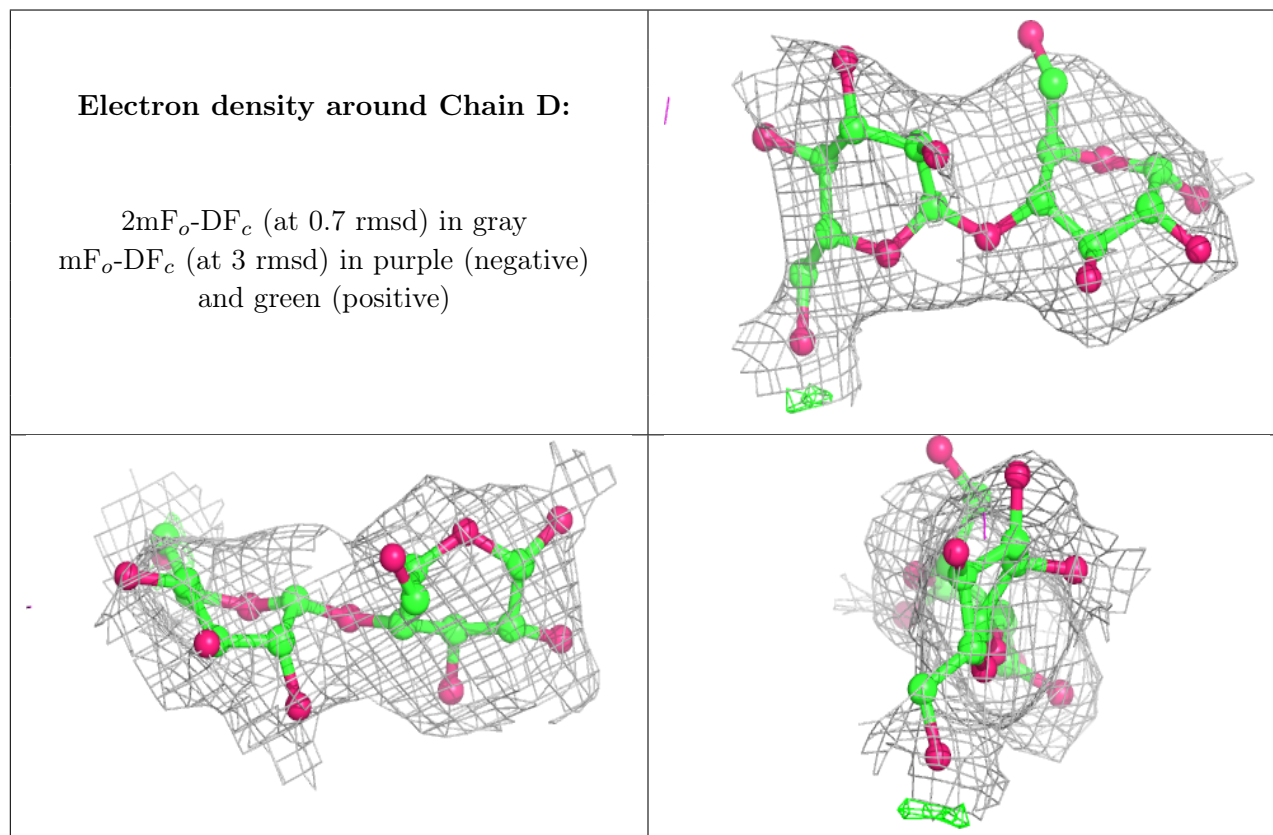
There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 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.

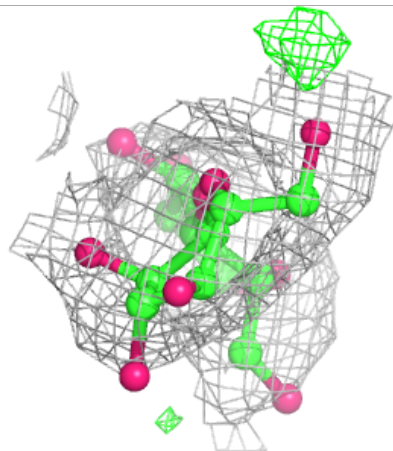
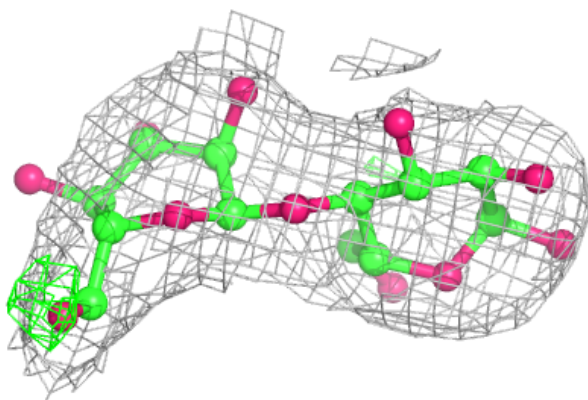
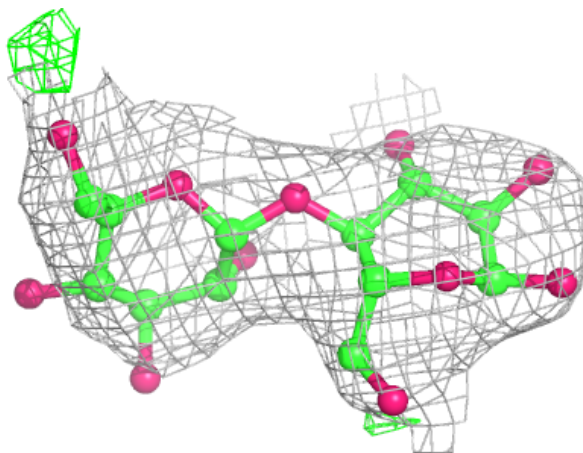
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	F	2	11/12	0.85	0.28	139,147,149,151	0
2	GLC	D	2	11/12	0.86	0.20	115,122,125,125	0
2	GLC	E	2	11/12	0.88	0.21	103,116,118,119	0
2	GLC	F	1	12/12	0.89	0.19	148,153,155,156	0
2	GLC	D	1	12/12	0.91	0.16	120,126,129,129	0
2	GLC	E	1	12/12	0.93	0.15	110,116,116,119	0

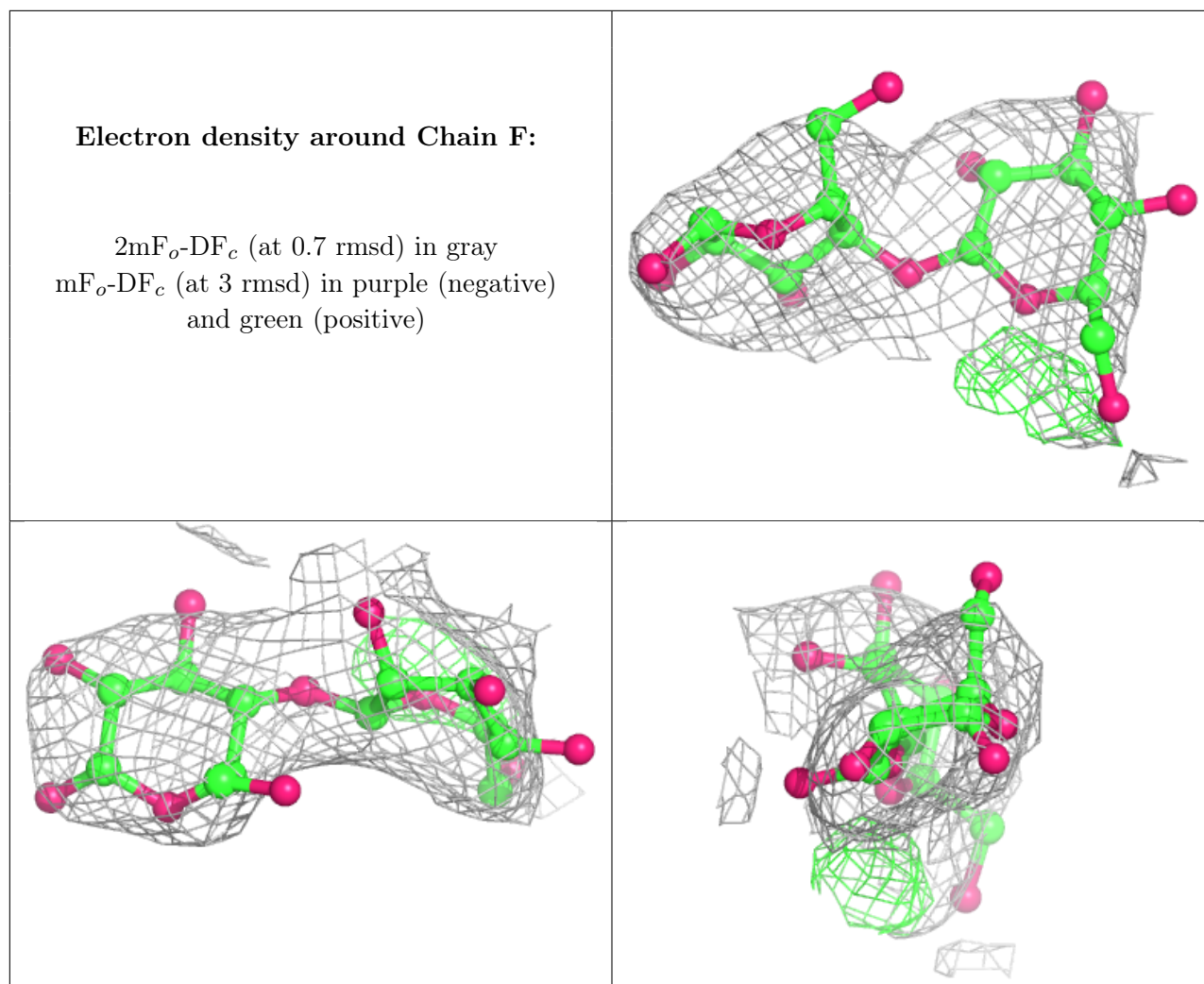
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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)





## 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
3	LDA	B	407	11/16	0.71	0.59	101,109,137,137	0
3	LDA	C	406	16/16	0.71	0.45	104,112,141,142	0
3	LDA	A	401	16/16	0.73	0.70	97,119,151,151	0
3	LDA	B	403	11/16	0.77	0.33	101,122,136,136	0
3	LDA	B	406	11/16	0.77	0.48	94,110,127,127	0
3	LDA	B	409	16/16	0.78	0.44	85,104,156,157	0
3	LDA	C	405	11/16	0.79	0.40	94,118,146,148	0
3	LDA	C	402	16/16	0.81	0.47	98,109,121,121	0
3	LDA	C	408	16/16	0.83	0.49	105,117,161,161	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LDA	C	407	16/16	0.84	0.36	100,121,149,150	0
4	CA	B	411	1/1	0.84	0.48	101,101,101,101	0
3	LDA	A	402	16/16	0.87	0.42	88,111,145,145	0
3	LDA	B	405	15/16	0.89	0.26	87,93,127,131	0
3	LDA	C	401	13/16	0.89	0.40	93,102,120,124	0
3	LDA	B	402	16/16	0.91	0.34	93,101,119,122	0
3	LDA	B	408	16/16	0.91	0.51	90,101,152,154	0
3	LDA	C	404	16/16	0.92	0.24	78,102,130,131	0
3	LDA	B	404	10/16	0.93	0.32	87,88,93,94	0
3	LDA	B	401	16/16	0.93	0.28	65,94,129,132	0
3	LDA	C	403	16/16	0.93	0.29	82,90,101,101	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.