



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 07:32 AM EDT

PDB ID : 1LLF  
Title : Cholesterol Esterase (Candida Cylindracea) Crystal Structure at 1.4A resolution  
Authors : Pletnev, V.; Addlagatta, A.; Wawrzak, Z.; Duax, W.  
Deposited on : 2002-04-28  
Resolution : 1.40 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>.

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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 : 2.35  
buster-report : 1.1.7 (2018)  
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) : 2.35

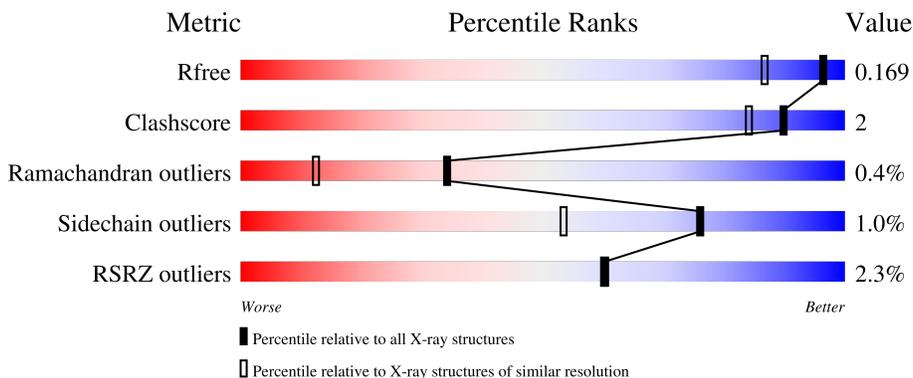
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	534	2% 95% 5%
1	B	534	3% 91% 7%
2	C	2	100%
2	D	2	100%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 17493 atoms, of which 8136 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 Lipase 3.

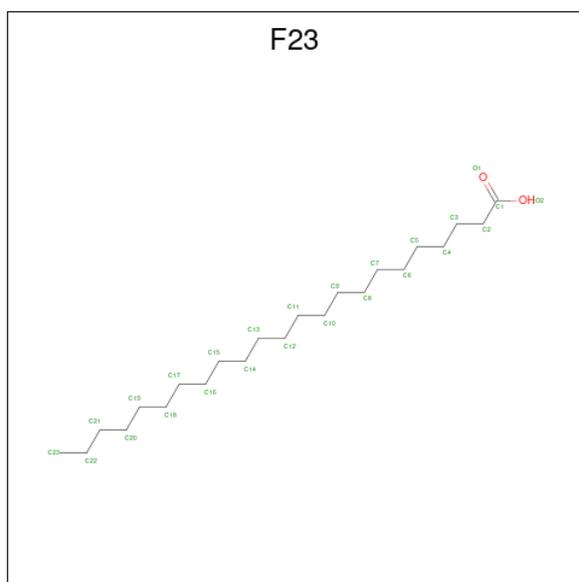
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	534	Total	C	H	N	O	S	0	6	0
			8020	2583	3965	673	778	21			
1	B	534	Total	C	H	N	O	S	0	8	0
			8043	2589	3981	674	778	21			

- 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
			Total	C	H	N	O			
2	C	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	D	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	F	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 3 is TRICOSANOIC ACID (three-letter code: F23) (formula: C<sub>23</sub>H<sub>46</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			66	23	41	2		
3	B	1	Total	C	H	O	0	0
			66	23	41	2		

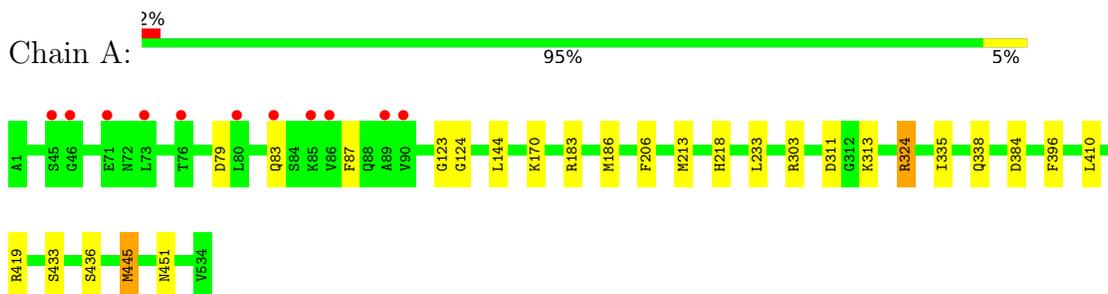
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	540	Total	O	0	0
			540	540		
4	B	538	Total	O	0	0
			538	538		

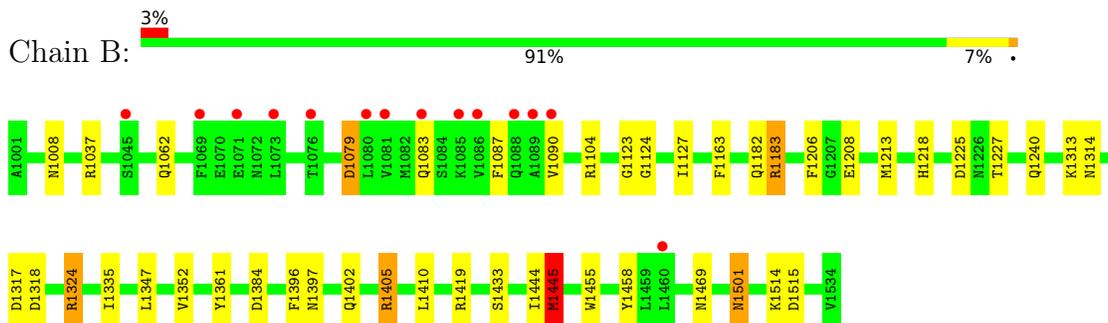
### 3 Residue-property plots [i](#)

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.

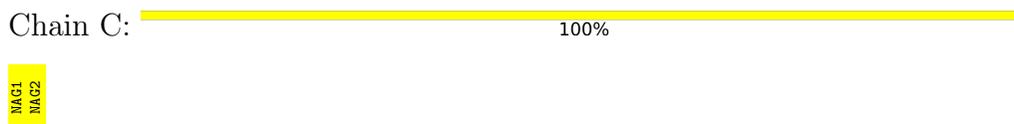
- Molecule 1: Lipase 3



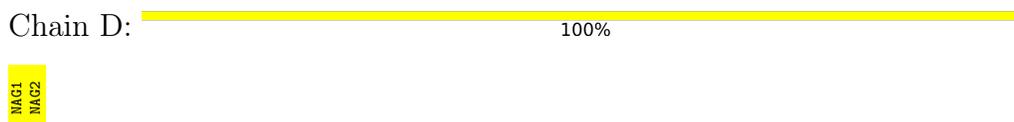
- Molecule 1: Lipase 3



- 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



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

Chain E:  100%

MAG1  
MAG2

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

Chain F:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.46Å 58.48Å 89.52Å 92.71° 97.48° 109.38°	Depositor
Resolution (Å)	30.00 – 1.40 29.76 – 1.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (30.00-1.40) 94.0 (29.76-1.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.37 (at 1.40Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.136 , 0.169 0.140 , 0.169	Depositor DCC
$R_{free}$ test set	10364 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.0	Xtrriage
Anisotropy	0.354	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 59.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.63% 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: NAG, F23

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	0.54	0/4179	1.09	14/5678 (0.2%)
1	B	0.57	0/4195	1.18	29/5699 (0.5%)
All	All	0.55	0/8374	1.14	43/11377 (0.4%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324[A]	ARG	CD-NE-CZ	15.34	145.07	123.60
1	A	324[B]	ARG	CD-NE-CZ	15.34	145.07	123.60
1	B	1183	ARG	NE-CZ-NH1	12.41	126.51	120.30
1	B	1445[A]	MET	CG-SD-CE	10.76	117.41	100.20
1	B	1445[B]	MET	CG-SD-CE	10.76	117.41	100.20
1	A	183	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	B	1183	ARG	NH1-CZ-NH2	-9.24	109.24	119.40
1	A	445[A]	MET	CG-SD-CE	8.96	114.53	100.20
1	A	445[B]	MET	CG-SD-CE	8.96	114.53	100.20
1	B	1405	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	A	303	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	B	1183	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	B	1405	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	B	1405	ARG	NH1-CZ-NH2	-7.54	111.10	119.40
1	B	1324[A]	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	B	1324[B]	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	419	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	1127	ILE	C-N-CA	7.13	137.27	122.30
1	B	1419	ARG	CG-CD-NE	-6.75	97.62	111.80
1	B	1317	ASP	CB-CG-OD1	6.75	124.38	118.30
1	B	1361	TYR	CB-CG-CD1	6.41	124.84	121.00
1	B	1455	TRP	CD1-NE1-CE2	6.37	114.73	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1104	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	183	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
1	B	1079	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	B	1318	ASP	CB-CG-OD1	5.97	123.68	118.30
1	A	324[A]	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	324[B]	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	87	PHE	CB-CG-CD1	5.82	124.87	120.80
1	B	1037	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	B	1396	PHE	CB-CG-CD1	5.71	124.80	120.80
1	A	218	HIS	CG-ND1-CE1	5.70	116.18	108.20
1	A	419	ARG	CG-CD-NE	-5.62	100.01	111.80
1	B	1087	PHE	CB-CG-CD1	5.57	124.70	120.80
1	B	1163	PHE	CB-CG-CD2	5.54	124.68	120.80
1	B	1352	VAL	O-C-N	-5.53	113.85	122.70
1	B	1324[A]	ARG	NH1-CZ-NH2	-5.36	113.51	119.40
1	B	1324[B]	ARG	NH1-CZ-NH2	-5.36	113.51	119.40
1	B	1062	GLN	CG-CD-NE2	-5.34	103.88	116.70
1	A	396	PHE	CB-CG-CD1	5.24	124.47	120.80
1	B	1458	TYR	CB-CG-CD1	5.22	124.13	121.00
1	B	1514	LYS	C-N-CA	5.21	134.72	121.70
1	B	1419	ARG	NE-CZ-NH1	-5.11	117.75	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	4055	3965	3955	12	0
1	B	4062	3981	3965	16	0
2	C	28	27	25	0	0
2	D	28	27	25	0	0
2	E	28	27	25	0	0
2	F	28	27	25	0	0
3	A	25	41	45	4	0
3	B	25	41	45	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	540	0	0	3	0
4	B	538	0	0	3	0
All	All	9357	8136	8110	30	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 (30) 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:1313[B]:LYS:HE2	4:B:2431:HOH:O	1.93	0.68
1:B:1313[B]:LYS:HE3	1:B:1314:ASN:OD1	1.98	0.62
1:A:144:LEU:HD11	4:A:2851:HOH:O	2.06	0.55
1:B:1182:GLN:OE1	1:B:1218:HIS:HE1	1.90	0.54
1:A:170:LYS:HE3	1:A:311:ASP:O	2.06	0.54
1:B:1124:GLY:HA2	3:B:1800:F23:H8B	1.91	0.52
1:B:1397:ASN:ND2	1:B:1444:ILE:H	2.09	0.51
1:A:124:GLY:HA2	3:A:800:F23:H8B	1.93	0.50
1:B:1335:ILE:O	1:B:1433:SER:HA	2.13	0.48
1:A:79:ASP:O	1:A:83:GLN:HG2	2.14	0.47
3:A:800:F23:H5B	4:A:2148:HOH:O	2.14	0.47
1:A:313:LYS:HG3	4:A:3045:HOH:O	2.16	0.45
1:B:1324[B]:ARG:NH1	4:B:2903:HOH:O	2.49	0.45
1:B:1225:ASP:OD1	1:B:1227:THR:HG23	2.16	0.45
1:B:1402:GLN:HE22	1:B:1405:ARG:HH11	1.64	0.45
1:A:335:ILE:O	1:A:433:SER:HA	2.17	0.44
1:B:1347:LEU:HD11	1:B:1445[A]:MET:HE1	1.98	0.44
1:B:1410:LEU:HD21	3:B:1800:F23:H222	1.99	0.44
1:A:186:MET:HE2	1:A:233:LEU:HD13	2.00	0.44
3:B:1800:F23:H5B	4:B:2113:HOH:O	2.17	0.43
1:B:1208:GLU:HA	1:B:1240:GLN:O	2.19	0.43
1:A:213:MET:SD	3:A:800:F23:H101	2.59	0.42
1:B:1183:ARG:HH11	1:B:1218:HIS:HD2	1.66	0.42
1:A:410:LEU:HD21	3:A:800:F23:H222	2.02	0.42
1:B:1213:MET:SD	3:B:1800:F23:H101	2.60	0.42
1:A:338:GLN:HE21	1:A:451:ASN:HD21	1.67	0.41
1:B:1501:ASN:HD21	1:B:1515:ASP:H	1.69	0.41
1:A:338:GLN:NE2	1:A:436:SER:HB3	2.37	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	538/534 (101%)	516 (96%)	20 (4%)	2 (0%)	34	12
1	B	540/534 (101%)	517 (96%)	21 (4%)	2 (0%)	34	12
All	All	1078/1068 (101%)	1033 (96%)	41 (4%)	4 (0%)	34	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ASP
1	B	1384	ASP
1	A	123	GLY
1	B	1123	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	438/432 (101%)	435 (99%)	3 (1%)	84	66
1	B	440/432 (102%)	432 (98%)	8 (2%)	59	28
All	All	878/864 (102%)	867 (99%)	11 (1%)	76	42

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	PHE
1	A	324[A]	ARG

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Mol	Chain	Res	Type
1	A	324[B]	ARG
1	B	1008	ASN
1	B	1079	ASP
1	B	1083	GLN
1	B	1206	PHE
1	B	1445[A]	MET
1	B	1445[B]	MET
1	B	1469	ASN
1	B	1501	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	187	GLN
1	A	338	GLN
1	A	387	GLN
1	A	438	GLN
1	A	468	ASN
1	B	1008	ASN
1	B	1062	GLN
1	B	1063	GLN
1	B	1192	ASN
1	B	1218	HIS
1	B	1339	ASN
1	B	1355	ASN
1	B	1357	GLN
1	B	1383	GLN
1	B	1397	ASN
1	B	1402	GLN
1	B	1438	GLN
1	B	1451	ASN
1	B	1501	ASN

### 5.3.3 RNA

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](#)

8 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	2,1	14,14,15	0.61	0	17,19,21	1.00	1 (5%)
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	1.25	2 (11%)
2	NAG	D	1	2,1	14,14,15	0.50	0	17,19,21	1.46	2 (11%)
2	NAG	D	2	2	14,14,15	0.79	0	17,19,21	1.11	1 (5%)
2	NAG	E	1	2,1	14,14,15	0.54	0	17,19,21	0.98	2 (11%)
2	NAG	E	2	2	14,14,15	0.74	0	17,19,21	1.12	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.60	0	17,19,21	0.86	0
2	NAG	F	2	2	14,14,15	0.81	0	17,19,21	0.91	1 (5%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C2-N2-C7	-3.44	118.01	122.90
2	E	2	NAG	C1-O5-C5	-2.87	108.30	112.19
2	D	1	NAG	C1-C2-N2	-2.82	105.66	110.49
2	E	2	NAG	C3-C4-C5	-2.47	105.83	110.24
2	D	2	NAG	O5-C5-C6	-2.47	103.34	107.20
2	C	2	NAG	C2-N2-C7	-2.45	119.41	122.90
2	E	1	NAG	C2-N2-C7	-2.23	119.73	122.90
2	E	1	NAG	C1-O5-C5	-2.20	109.20	112.19
2	C	1	NAG	O4-C4-C5	-2.14	103.99	109.30
2	C	2	NAG	C1-O5-C5	-2.13	109.31	112.19
2	F	2	NAG	O4-C4-C3	-2.00	105.72	110.35

There are no chirality outliers.

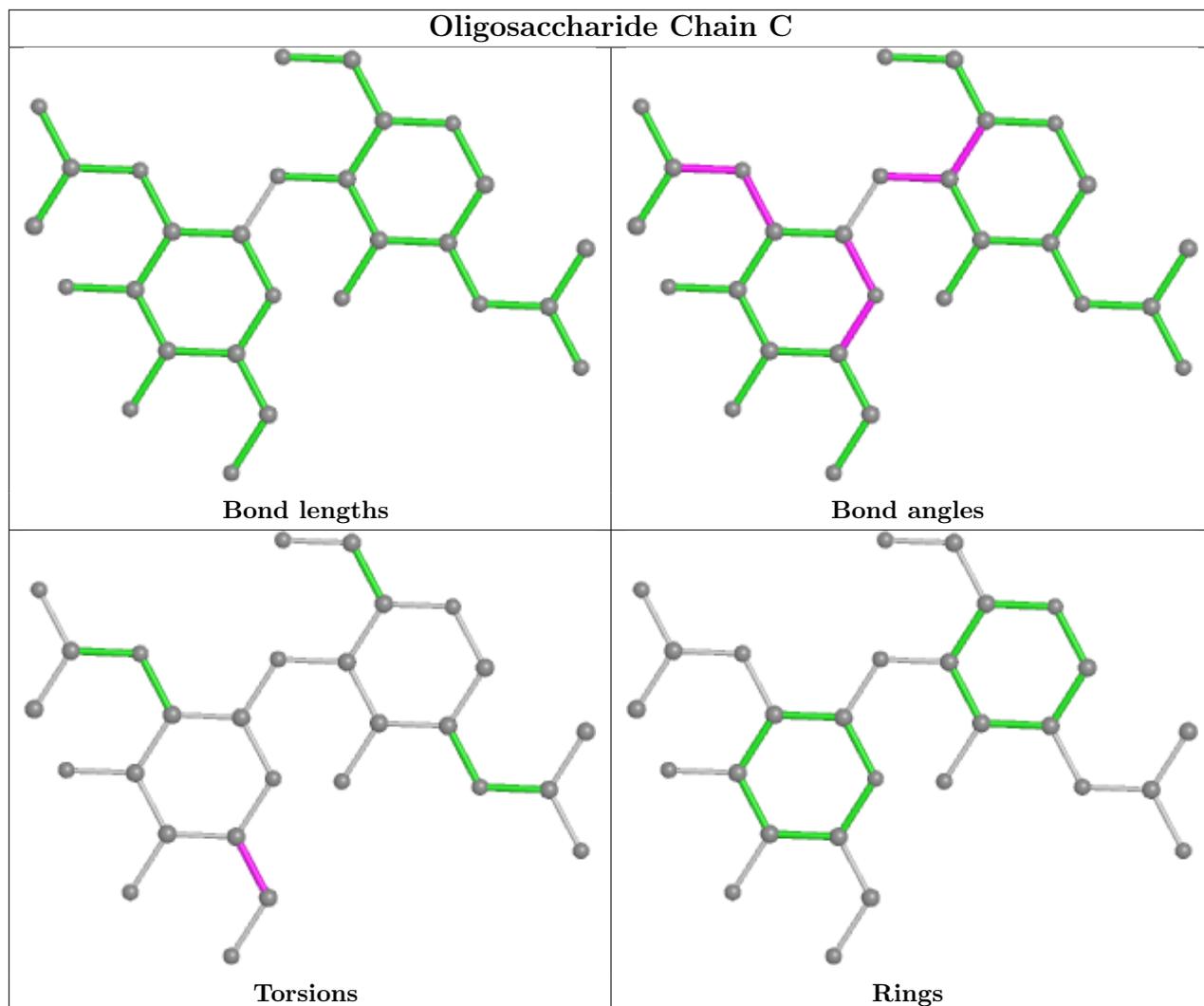
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

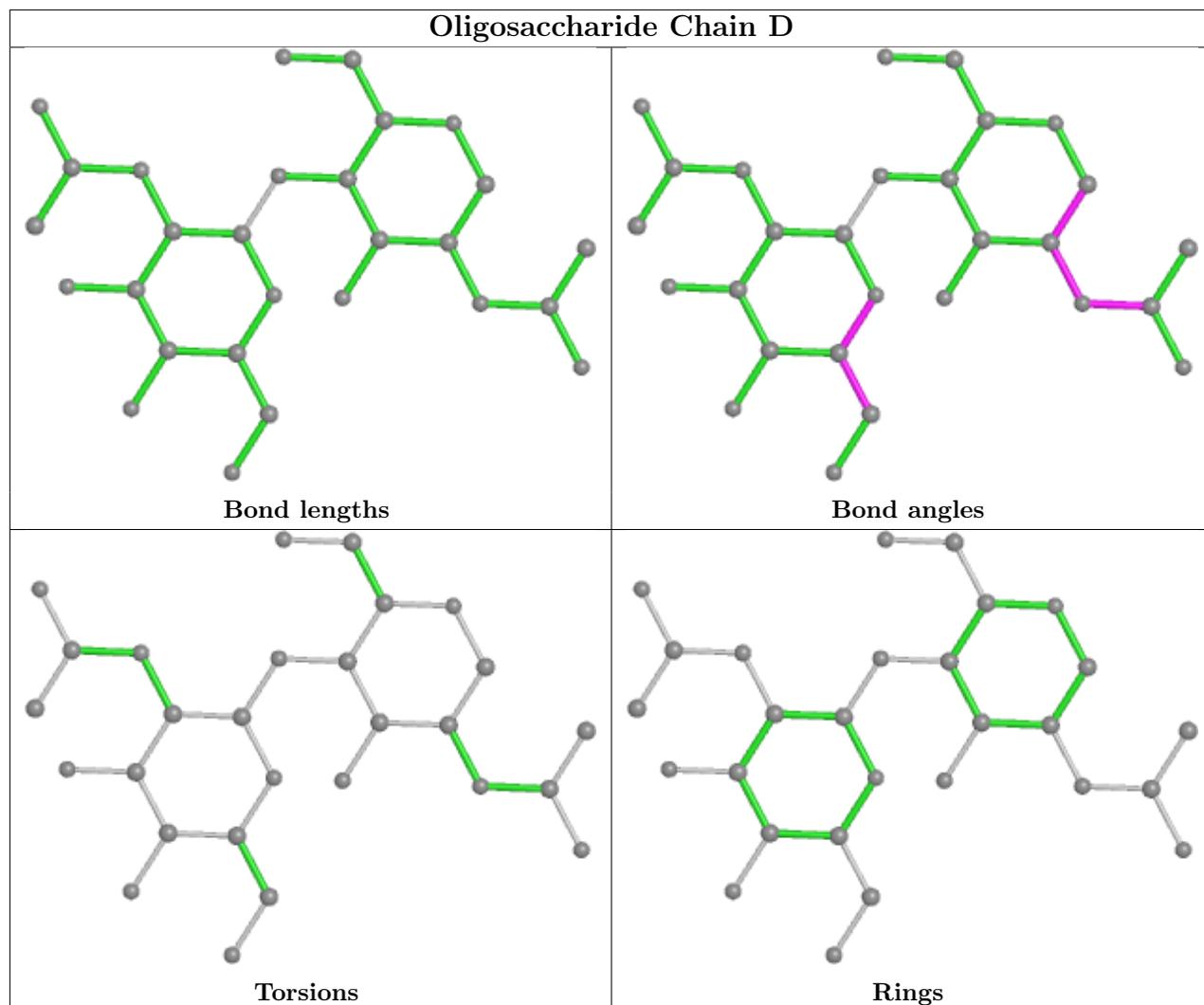
There are no ring outliers.

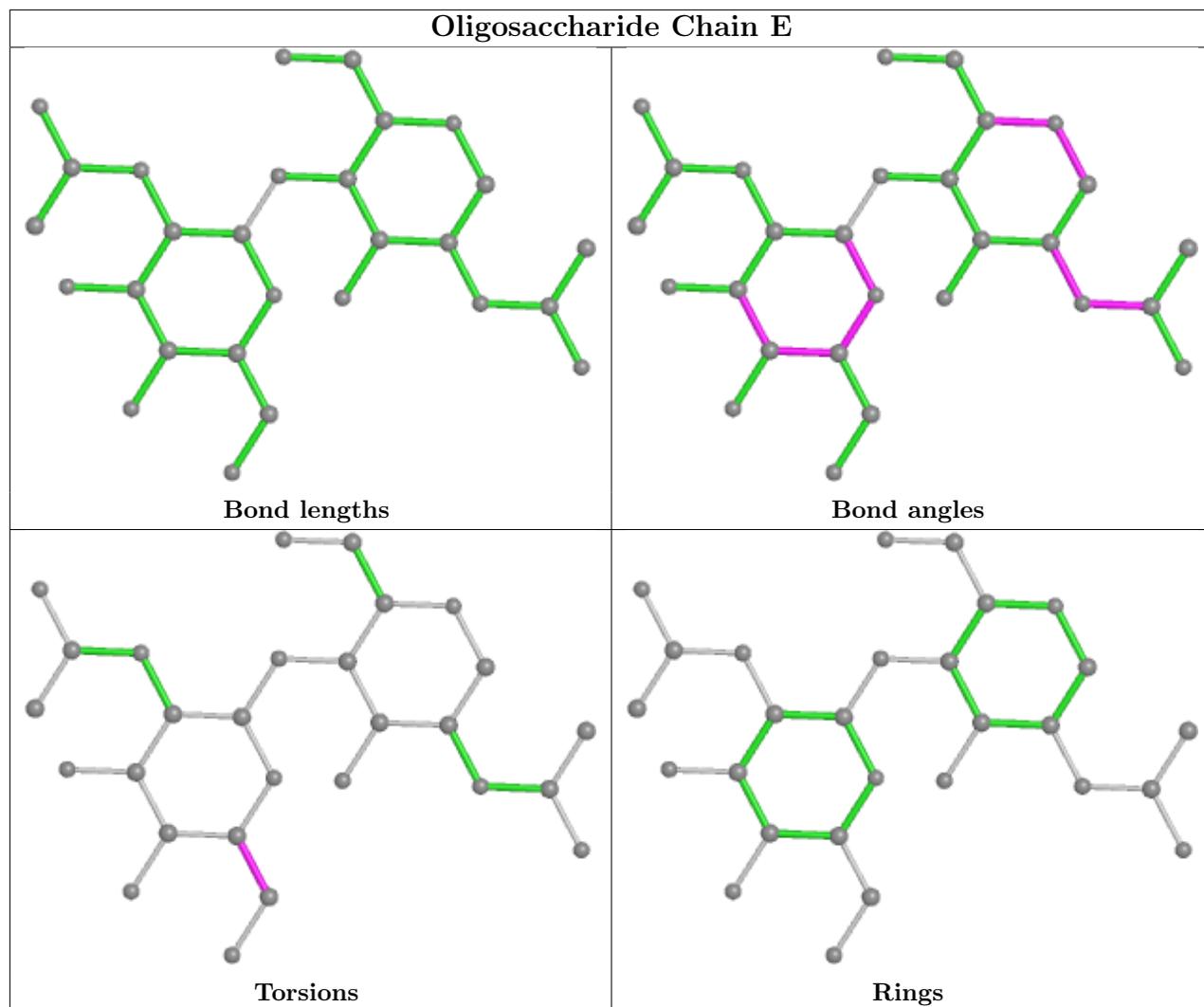
No monomer is involved in short contacts.

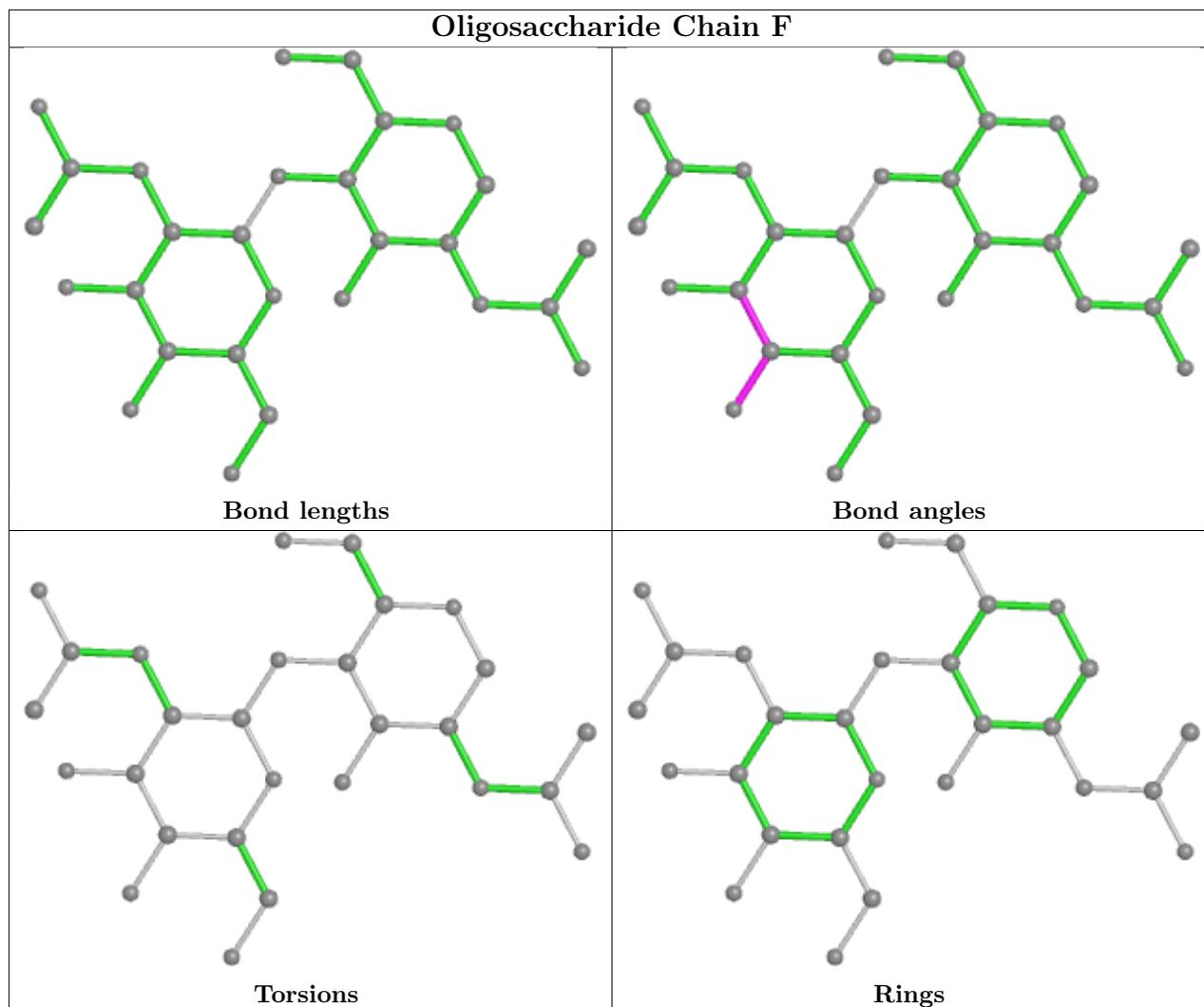
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

2 ligands 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	F23	B	1800	-	24,24,24	1.19	2 (8%)	24,24,24	0.92	2 (8%)
3	F23	A	800	-	24,24,24	1.13	2 (8%)	24,24,24	0.93	1 (4%)

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	F23	B	1800	-	-	9/22/22/22	-
3	F23	A	800	-	-	9/22/22/22	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1800	F23	O2-C1	-4.08	1.17	1.30
3	A	800	F23	O2-C1	-3.94	1.17	1.30
3	B	1800	F23	C2-C1	-3.17	1.43	1.50
3	A	800	F23	C2-C1	-2.80	1.44	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	F23	C9-C8-C7	2.58	127.50	114.42
3	B	1800	F23	C11-C10-C9	-2.05	104.01	114.42
3	B	1800	F23	C9-C8-C7	2.02	124.68	114.42

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	F23	C7-C8-C9-C10
3	B	1800	F23	C7-C8-C9-C10
3	B	1800	F23	C2-C3-C4-C5
3	B	1800	F23	C5-C6-C7-C8
3	A	800	F23	C2-C3-C4-C5
3	A	800	F23	C5-C6-C7-C8
3	A	800	F23	C11-C10-C9-C8
3	A	800	F23	C1-C2-C3-C4
3	B	1800	F23	C11-C10-C9-C8
3	A	800	F23	O1-C1-C2-C3
3	B	1800	F23	O1-C1-C2-C3
3	B	1800	F23	O2-C1-C2-C3
3	A	800	F23	O2-C1-C2-C3
3	B	1800	F23	C16-C17-C18-C19
3	B	1800	F23	C15-C16-C17-C18

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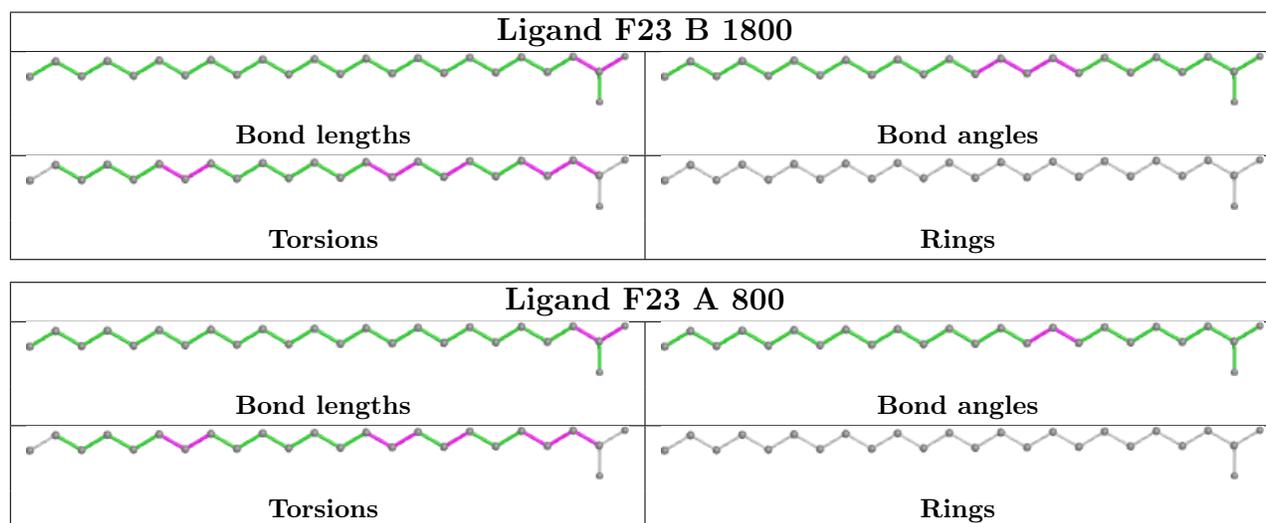
Mol	Chain	Res	Type	Atoms
3	A	800	F23	C15-C16-C17-C18
3	A	800	F23	C16-C17-C18-C19
3	B	1800	F23	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1800	F23	4	0
3	A	800	F23	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	534/534 (100%)	-0.30	11 (2%) 63 63	9, 12, 24, 43	0
1	B	534/534 (100%)	-0.28	14 (2%) 56 55	9, 13, 25, 42	0
All	All	1068/1068 (100%)	-0.29	25 (2%) 60 60	9, 12, 25, 43	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	5.2
1	B	1086[A]	VAL	5.0
1	B	1073	LEU	4.9
1	B	1080	LEU	4.4
1	A	86[A]	VAL	4.4
1	A	80	LEU	4.0
1	B	1090[A]	VAL	3.4
1	A	85	LYS	2.9
1	A	45	SER	2.8
1	B	1045	SER	2.7
1	B	1076	THR	2.7
1	B	1085	LYS	2.7
1	B	1069	PHE	2.7
1	A	76	THR	2.6
1	B	1083	GLN	2.5
1	A	46	GLY	2.4
1	B	1460	LEU	2.3
1	A	71	GLU	2.2
1	A	90	VAL	2.2
1	B	1088	GLN	2.1
1	B	1071	GLU	2.1
1	B	1089	ALA	2.1
1	A	83	GLN	2.0
1	B	1081	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	89	ALA	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

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

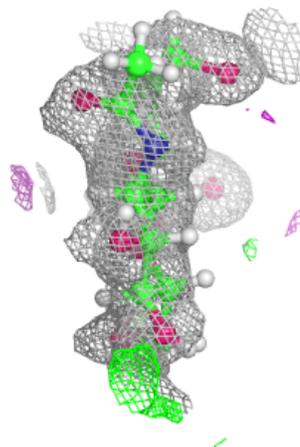
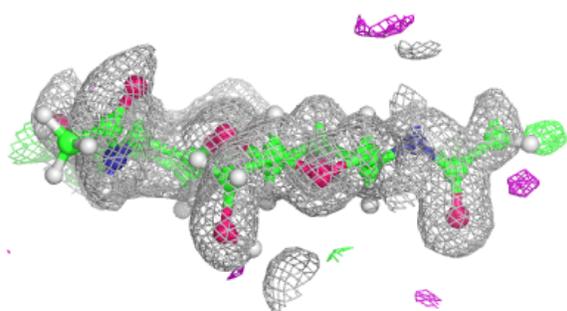
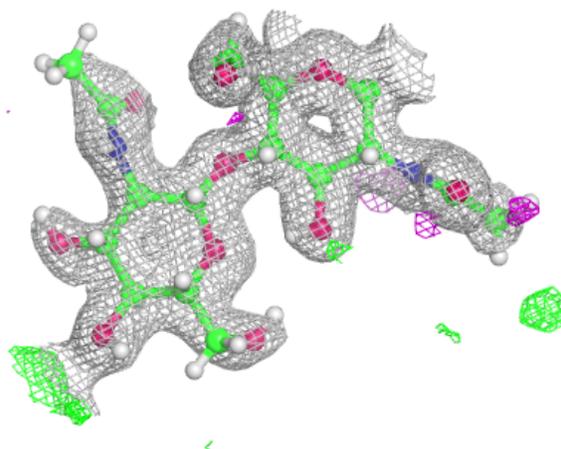
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	C	2	14/15	0.84	0.28	29,44,66,92	0
2	NAG	E	2	14/15	0.90	0.29	38,52,74,97	0
2	NAG	E	1	14/15	0.94	0.11	19,26,43,43	0
2	NAG	D	2	14/15	0.95	0.11	14,24,40,60	0
2	NAG	F	2	14/15	0.95	0.14	16,23,33,50	0
2	NAG	C	1	14/15	0.96	0.13	15,22,38,39	0
2	NAG	F	1	14/15	0.97	0.06	13,18,33,33	0
2	NAG	D	1	14/15	0.98	0.06	12,17,32,32	0

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



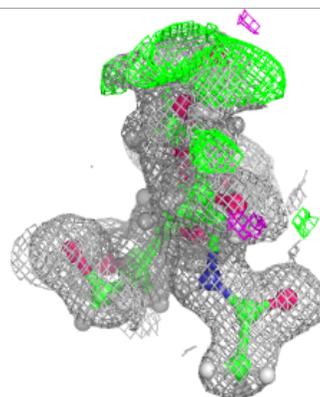
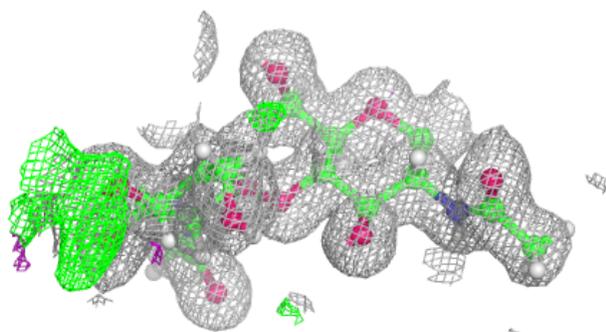
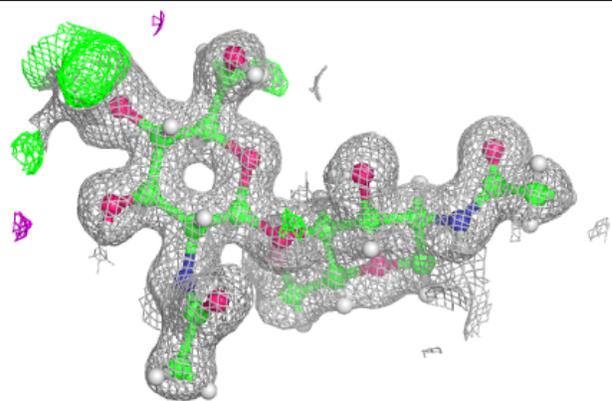
**Electron density around Chain C:**

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

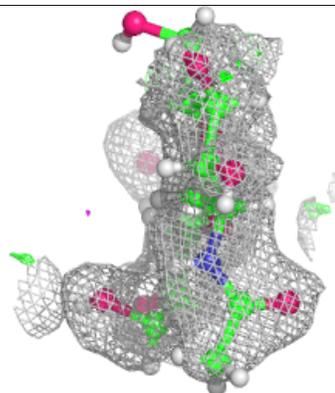
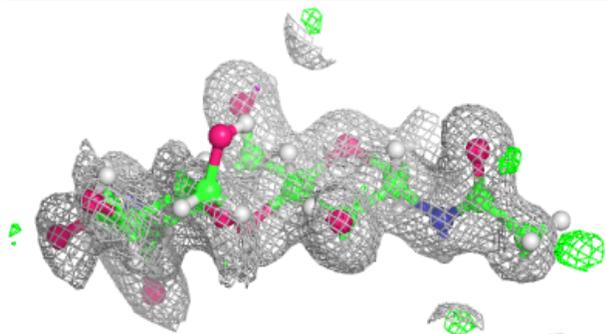
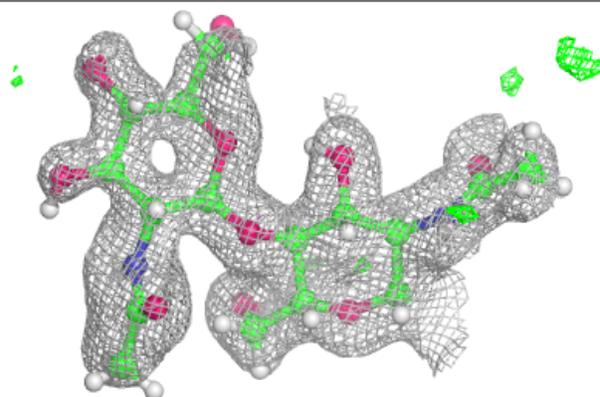


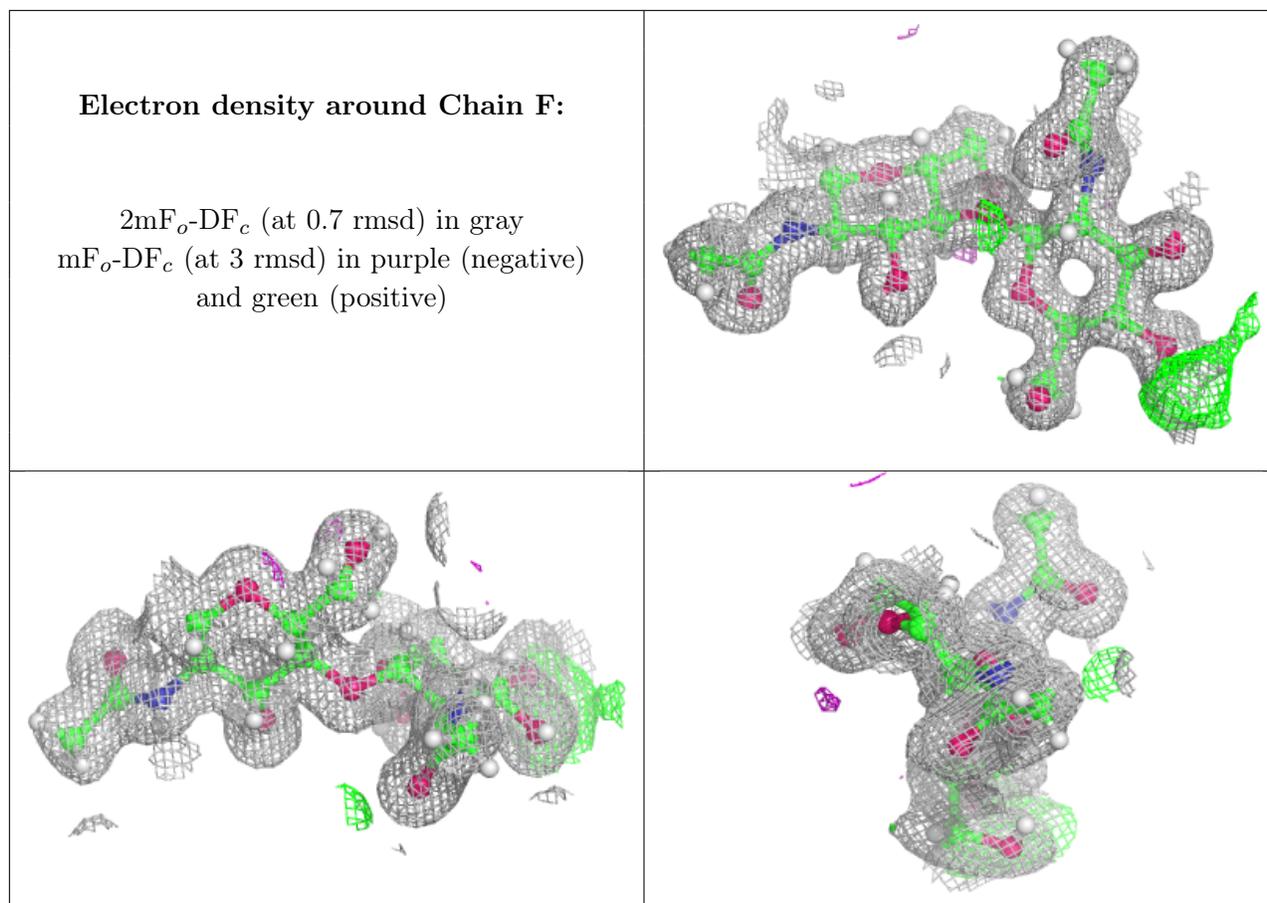
**Electron density around Chain D:**

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

**Electron density around Chain E:**

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



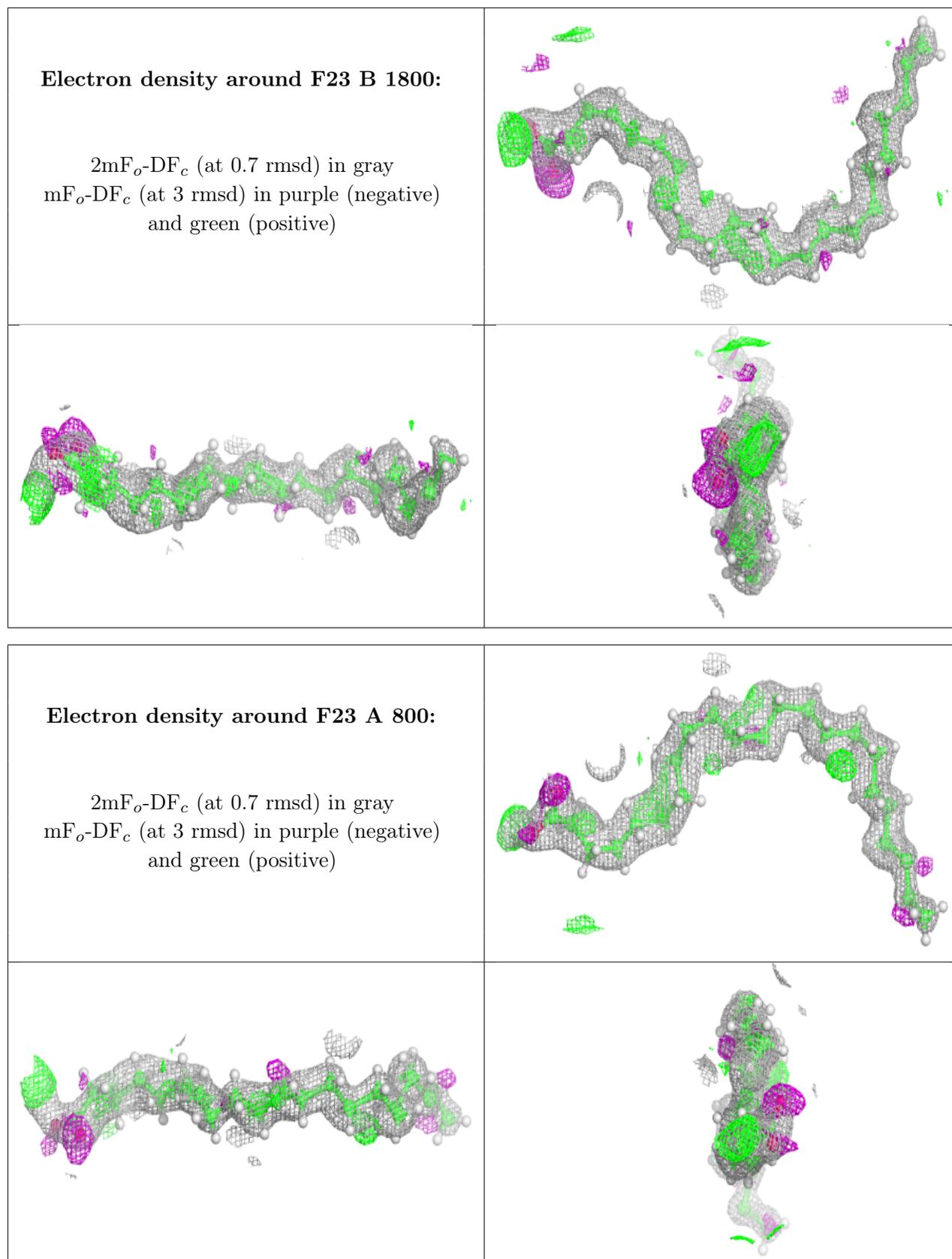


## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q < 0.9
3	F23	B	1800	25/25	0.83	0.17	16,24,33,45	0
3	F23	A	800	25/25	0.86	0.15	16,24,35,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.