



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 07:37 PM UTC

PDB ID : 8Q1K / pdb_00008q1k
Title : Structural analysis of PLD3 reveals insights into the mechanism of lysosomal
5' exonuclease-mediated nucleic acid degradation
Authors : Roske, Y.; Daumke, O.; Damme, M.
Deposited on : 2023-07-31
Resolution : 1.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

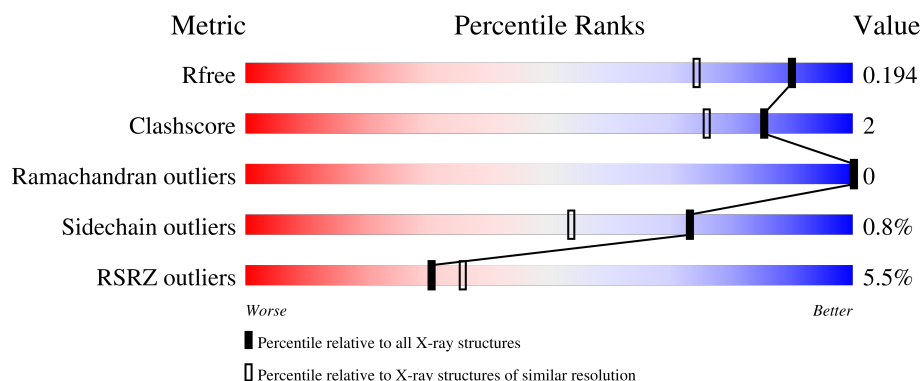
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



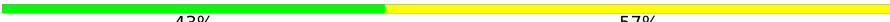
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	5% 94% 5%
1	B	422	6% 94% 6%
2	C	7	43% 57%
3	D	2	100%
3	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	7	 43%57%

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
2	MAN	C	3	X	-	-	-
4	MAN	F	5	X	-	-	-
4	MAN	F	6	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8193 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.

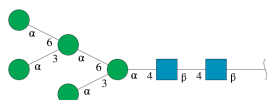
- Molecule 1 is a protein called 5'-3' exonuclease PLD3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	13	0
			3355	2122	585	630	18			
1	B	420	Total	C	N	O	S	0	7	0
			3320	2101	579	623	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	491	ALA	-	expression tag	UNP Q8IV08
A	492	ALA	-	expression tag	UNP Q8IV08
A	493	GLN	-	expression tag	UNP Q8IV08
B	491	ALA	-	expression tag	UNP Q8IV08
B	492	ALA	-	expression tag	UNP Q8IV08
B	493	GLN	-	expression tag	UNP Q8IV08

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



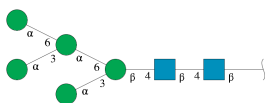
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O		0	0	0
			83	46	2	35				

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



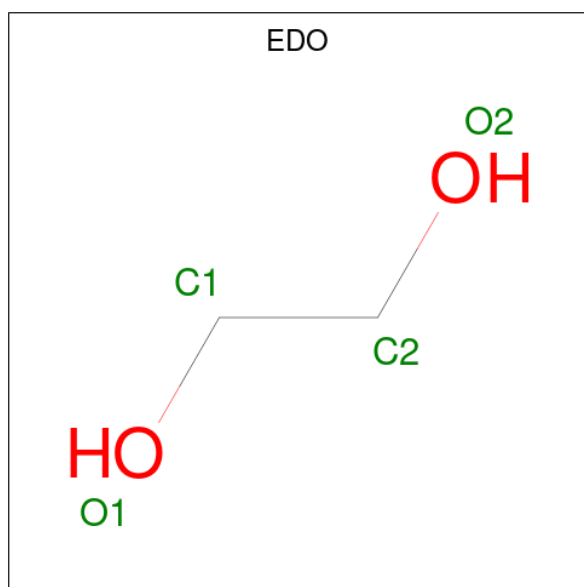
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



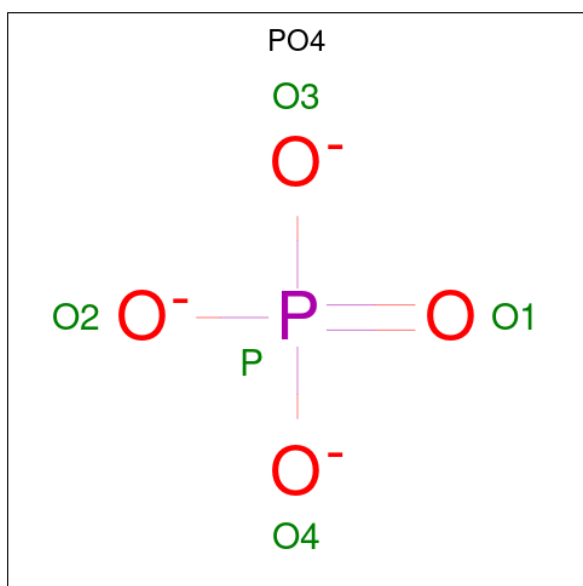
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mn	0	0
			2	2		
7	B	2	Total	Mn	0	0
			2	2		

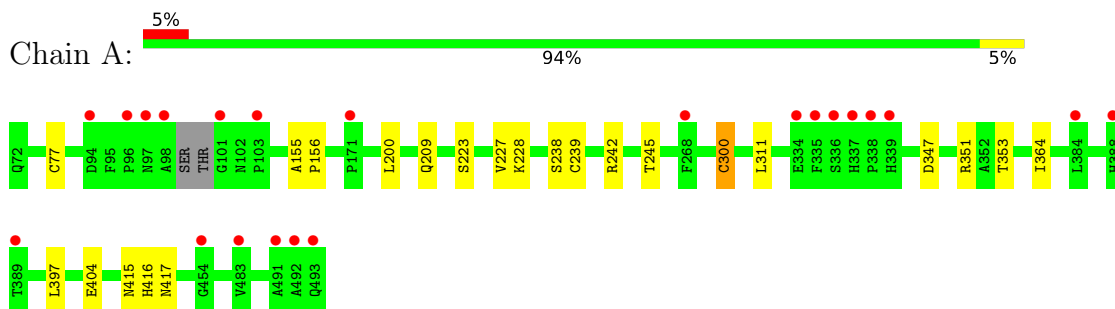
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	635	Total	O	0	0
			635	635		
8	B	589	Total	O	0	0
			589	589		

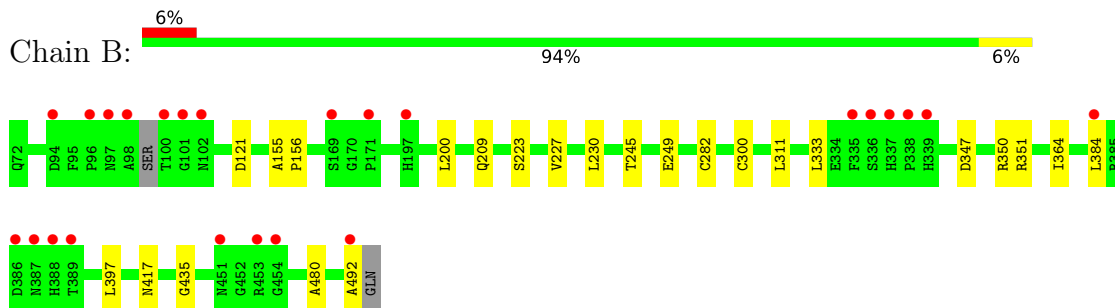
3 Residue-property plots

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.

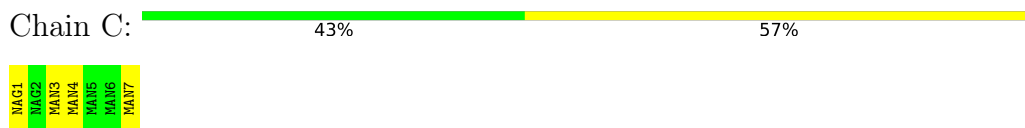
- Molecule 1: 5'-3' exonuclease PLD3



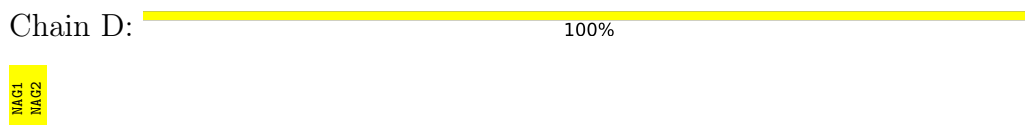
- Molecule 1: 5'-3' exonuclease PLD3



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



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



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

Chain E:  100%

MAG1
MAG2

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

Chain F:  43%  57%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.25Å 115.30Å 101.08Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	44.65 – 1.51 44.65 – 1.51	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.65-1.51) 97.9 (44.65-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.154 , 0.186 0.165 , 0.194	Depositor DCC
R_{free} test set	2105 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8193	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, MAN, NAG, BMA, PO4, OCS, EDO

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	0.95	0/3472	1.17	0/4735
1	B	0.94	0/3419	1.17	0/4663
All	All	0.94	0/6891	1.17	0/9398

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3355	0	3267	15	0
1	B	3320	0	3230	15	0
2	C	83	0	70	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
4	F	83	0	70	0	0
5	A	12	0	18	0	0
5	B	16	0	24	0	0
6	A	20	0	0	1	0
6	B	20	0	0	0	0
7	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	2	0	0	0	0
8	A	635	0	0	4	0
8	B	589	0	0	4	0
All	All	8193	0	6729	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:209:GLN:NE2	8:B:601:HOH:O	2.05	0.87
1:A:300:OCS:OD3	8:A:601:HOH:O	2.01	0.77
1:B:480:ALA:HB3	1:B:492:ALA:HB2	1.78	0.66
1:B:282:CYS:SG	8:B:1013:HOH:O	2.55	0.64
6:A:507:PO4:P	8:A:611:HOH:O	2.58	0.61
1:A:238[B]:SER:OG	1:A:242:ARG:NH1	2.36	0.57
1:A:347:ASP:OD2	1:B:347:ASP:OD2	2.25	0.54
1:A:351:ARG:NH2	8:A:607:HOH:O	2.41	0.52
1:A:223:SER:HA	1:A:227:VAL:HG22	1.95	0.48
1:B:311:LEU:C	1:B:311:LEU:HD23	2.39	0.47
1:A:364:ILE:O	1:A:397:LEU:HA	2.16	0.46
1:A:77:CYS:SG	1:A:239[C]:CYS:HB2	2.56	0.46
1:B:223:SER:HA	1:B:227:VAL:HG22	1.97	0.46
1:B:364:ILE:O	1:B:397:LEU:HA	2.16	0.46
1:A:209:GLN:NE2	1:A:245:THR:OG1	2.50	0.45
1:A:77:CYS:SG	1:A:239[C]:CYS:SG	3.13	0.45
1:A:311:LEU:C	1:A:311:LEU:HD23	2.42	0.44
1:B:223:SER:HA	1:B:227:VAL:CG2	2.48	0.44
1:B:245:THR:O	1:B:249[B]:GLU:HG2	2.17	0.43
1:B:230:LEU:C	1:B:230:LEU:HD13	2.43	0.43
1:A:228:LYS:HB3	1:A:415:ASN:HA	2.01	0.43
1:B:121:ASP:OD2	8:B:601:HOH:O	2.21	0.42
1:A:223:SER:HA	1:A:227:VAL:CG2	2.50	0.42
1:B:155:ALA:HB3	1:B:156:PRO:HD3	2.02	0.41
1:A:209:GLN:HA	1:A:209:GLN:HE21	1.86	0.41
1:B:333:LEU:HD23	1:B:435:GLY:HA3	2.01	0.41
1:A:155:ALA:N	1:A:156:PRO:CD	2.83	0.41
1:A:416:HIS:HD2	8:A:868:HOH:O	2.04	0.40
1:B:350:ARG:NH1	1:B:384:LEU:HD11	2.36	0.40
1:B:351:ARG:NH2	8:B:626:HOH:O	2.54	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	429/422 (102%)	416 (97%)	13 (3%)	0	100	100
1	B	422/422 (100%)	411 (97%)	11 (3%)	0	100	100
All	All	851/844 (101%)	827 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/356 (103%)	363 (99%)	4 (1%)	65	40
1	B	361/356 (101%)	359 (99%)	2 (1%)	78	61
All	All	728/712 (102%)	722 (99%)	6 (1%)	73	53

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	LEU
1	A	353	THR
1	A	404	GLU
1	A	417	ASN
1	B	200	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	417	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	143	GLN
1	A	160	ASN
1	A	178	GLN
1	A	182	GLN
1	A	209	GLN
1	A	256	GLN
1	A	313	ASN
1	A	328	ASN
1	A	416	HIS
1	A	459	GLN
1	B	132	ASN
1	B	142	GLN
1	B	143	GLN
1	B	152	GLN
1	B	209	GLN
1	B	256	GLN
1	B	328	ASN
1	B	390	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	OCS	A	300	1	6,8,9	1.59	1 (16%)	7,11,13	1.41	1 (14%)
1	OCS	B	300	1	6,8,9	1.66	1 (16%)	7,11,13	1.35	1 (14%)

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
1	OCS	A	300	1	-	2/4/7/9	-
1	OCS	B	300	1	-	2/4/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	OCS	OD3-SG	3.69	1.55	1.45
1	A	300	OCS	OD3-SG	3.49	1.55	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	OCS	OD2-SG-OD1	2.59	117.89	111.40
1	A	300	OCS	OD2-SG-OD1	2.52	117.69	111.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	300	OCS	CA-CB-SG-OD1
1	A	300	OCS	CA-CB-SG-OD1
1	B	300	OCS	CA-CB-SG-OD3
1	A	300	OCS	CA-CB-SG-OD3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	300	OCS	1	0

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	0.28	0	17,19,21	1.08	1 (5%)
2	NAG	C	2	2	14,14,15	0.33	0	17,19,21	0.73	0
2	MAN	C	3	2	11,11,12	0.51	0	15,15,17	1.66	3 (20%)
2	MAN	C	4	2	11,11,12	0.68	0	15,15,17	1.20	1 (6%)
2	MAN	C	5	2	11,11,12	0.29	0	15,15,17	0.68	0
2	MAN	C	6	2	11,11,12	0.26	0	15,15,17	0.61	0
2	MAN	C	7	2	11,11,12	0.40	0	15,15,17	1.02	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.37	0	17,19,21	0.98	1 (5%)
3	NAG	D	2	3	14,14,15	0.35	0	17,19,21	1.17	2 (11%)
3	NAG	E	1	3,1	14,14,15	0.26	0	17,19,21	1.46	3 (17%)
3	NAG	E	2	3	14,14,15	0.44	0	17,19,21	1.49	2 (11%)
4	NAG	F	1	4,1	14,14,15	0.34	0	17,19,21	0.80	1 (5%)
4	NAG	F	2	4	14,14,15	0.30	0	17,19,21	0.56	0
4	BMA	F	3	4	11,11,12	0.32	0	15,15,17	0.74	0
4	MAN	F	4	4	11,11,12	0.27	0	15,15,17	0.89	1 (6%)
4	MAN	F	5	4	11,11,12	0.39	0	15,15,17	0.70	0
4	MAN	F	6	4	11,11,12	0.41	0	15,15,17	0.95	1 (6%)
4	MAN	F	7	4	11,11,12	0.32	0	15,15,17	0.88	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	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	MAN	C	3	2	1/1/4/5	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	1/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	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	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	F	6	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C3-C4-C5	4.14	117.74	110.23
3	E	1	NAG	C1-O5-C5	3.80	117.28	112.19
2	C	3	MAN	O5-C5-C6	-3.66	100.53	107.66
2	C	4	MAN	C1-C2-C3	3.65	114.96	109.64
3	E	2	NAG	C4-C3-C2	3.38	115.97	111.02
3	D	1	NAG	C1-O5-C5	3.11	116.35	112.19
2	C	3	MAN	O3-C3-C2	3.03	116.23	110.05
4	F	1	NAG	C4-C3-C2	-2.58	107.24	111.02
3	E	1	NAG	C4-C3-C2	-2.56	107.27	111.02
3	E	1	NAG	O5-C1-C2	-2.52	107.39	111.29
3	D	2	NAG	C1-O5-C5	2.46	115.48	112.19
2	C	3	MAN	O3-C3-C4	-2.44	104.62	110.38
2	C	7	MAN	C1-C2-C3	2.43	113.19	109.64
2	C	1	NAG	C4-C3-C2	-2.39	107.51	111.02
4	F	4	MAN	C1-O5-C5	2.29	115.26	112.19
4	F	6	MAN	C1-O5-C5	2.22	115.16	112.19
4	F	7	MAN	C1-C2-C3	2.05	112.63	109.64
3	D	2	NAG	C3-C4-C5	2.04	113.93	110.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	MAN	C1
4	F	5	MAN	C1
4	F	6	MAN	C1

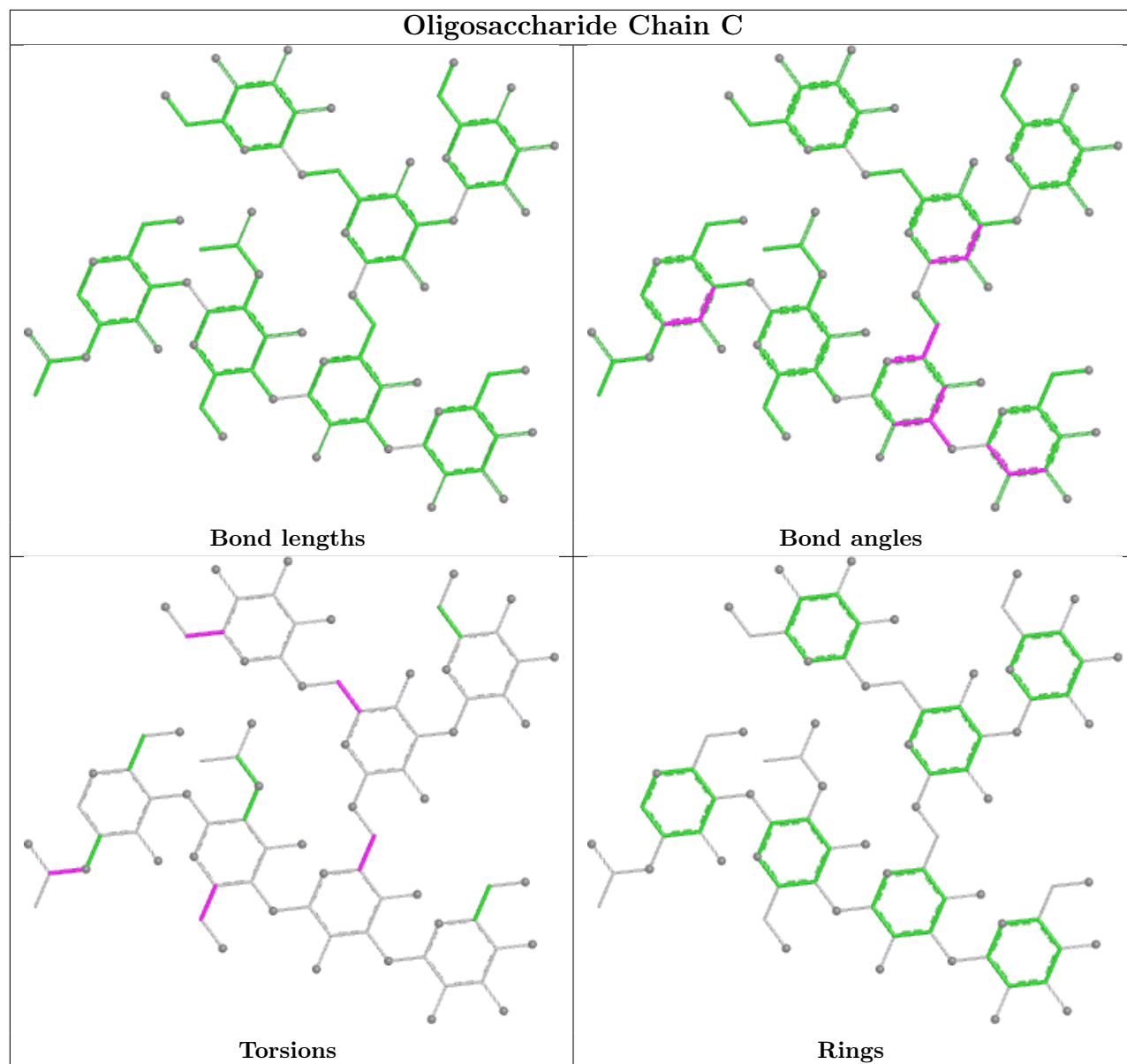
All (15) torsion outliers are listed below:

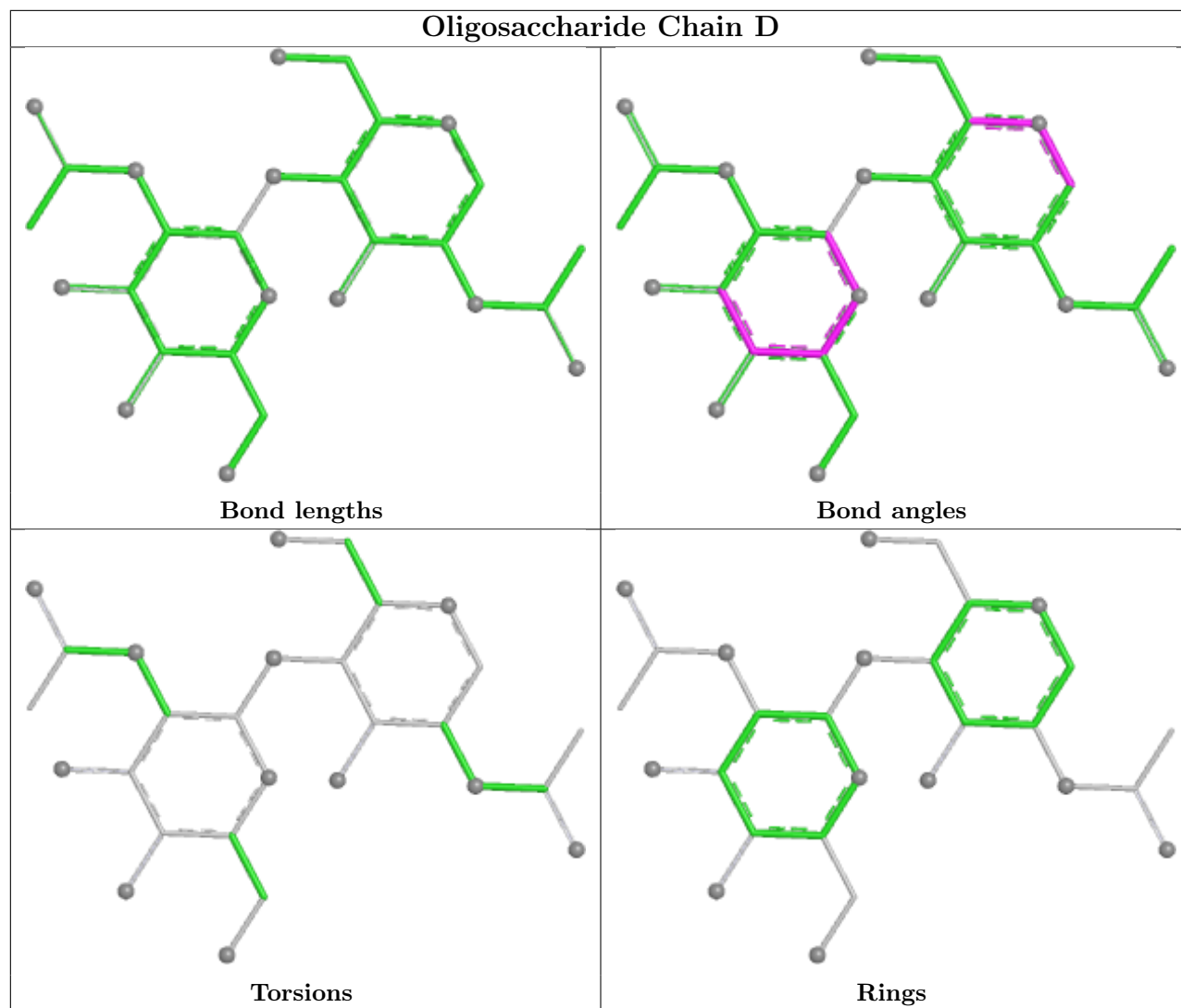
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	3	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
4	F	5	MAN	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6
2	C	3	MAN	C4-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C1-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6

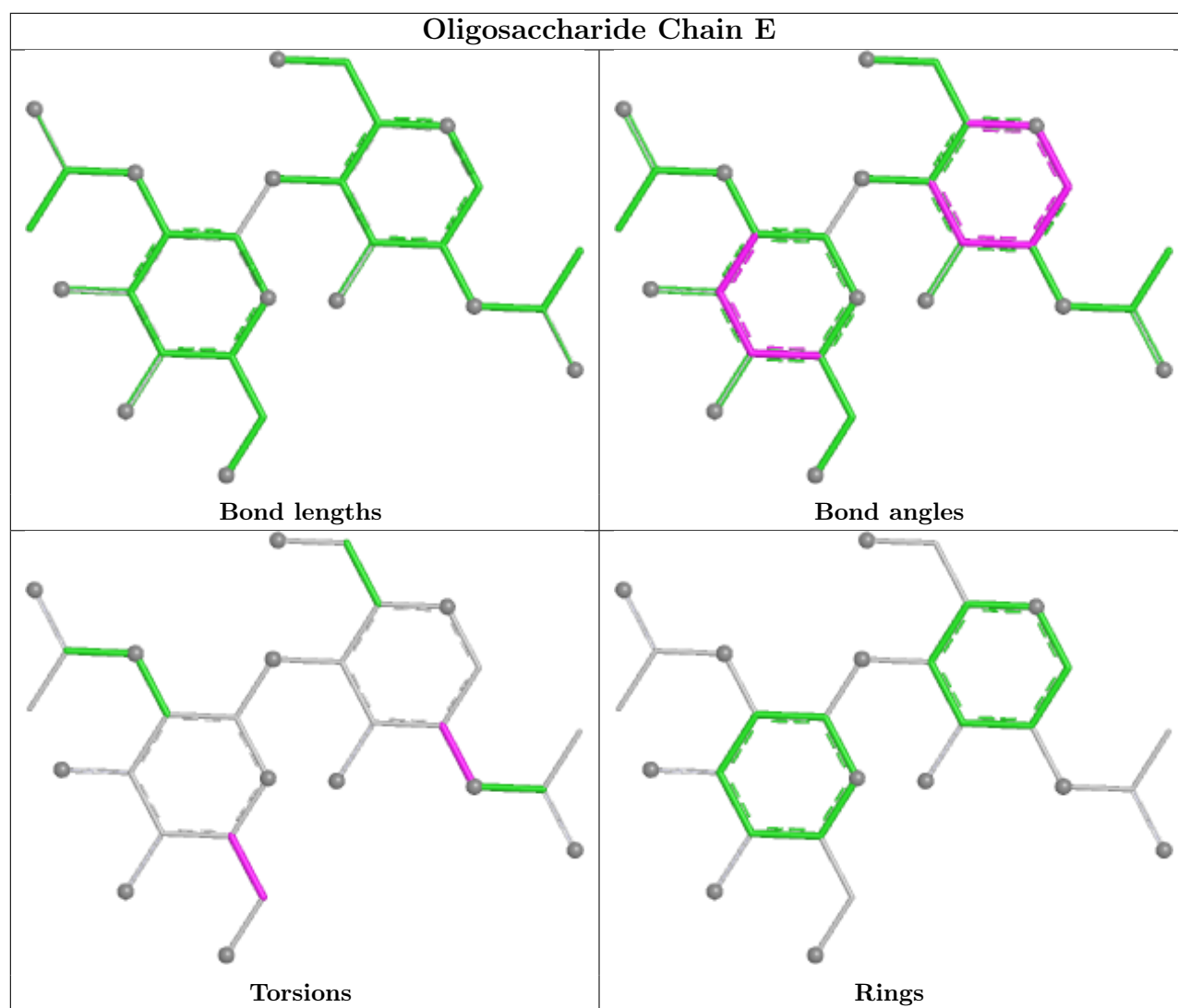
There are no ring outliers.

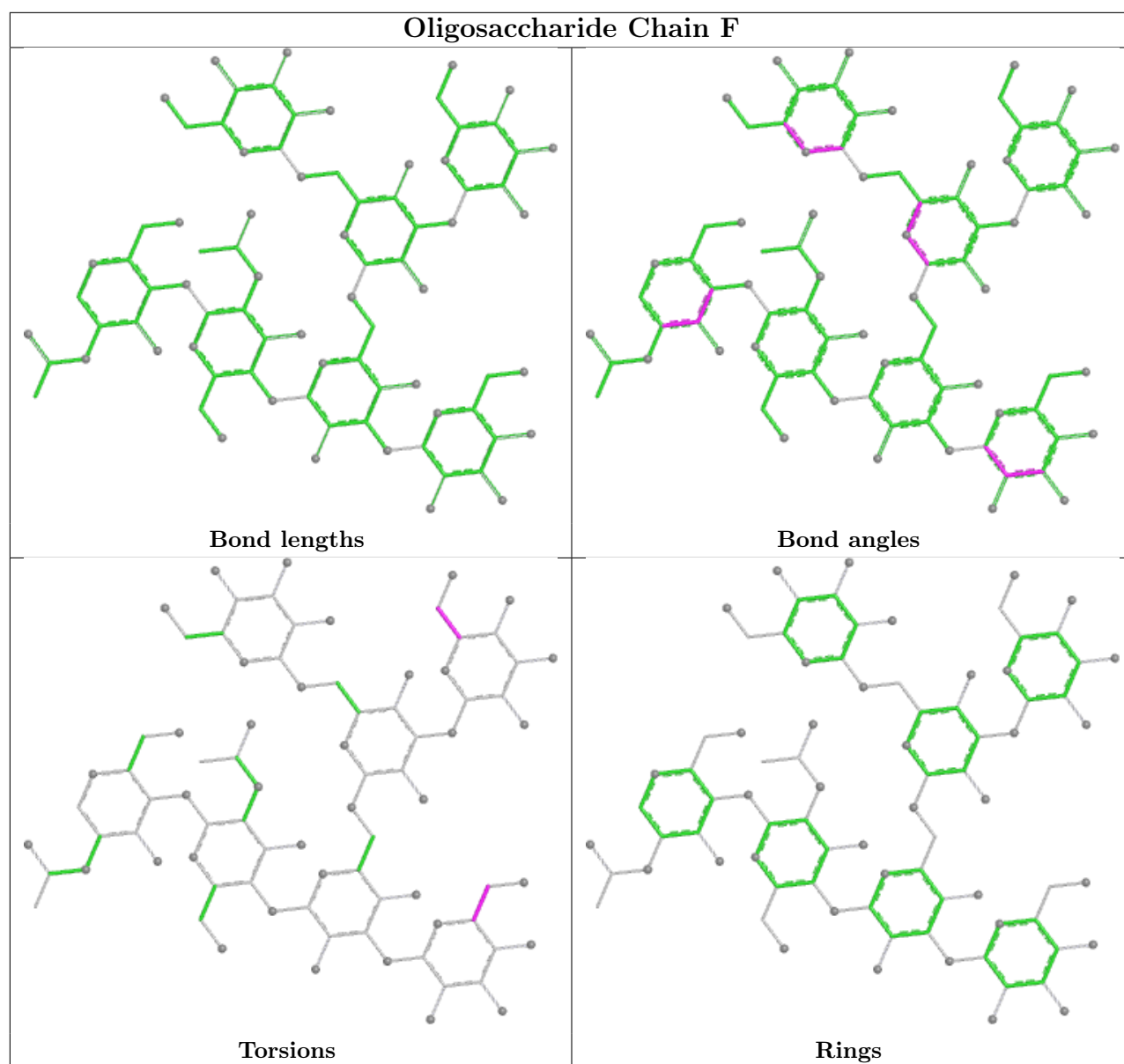
No monomer is involved in short contacts.

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](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PO4	A	504	-	4,4,4	0.58	0	6,6,6	0.47	0
5	EDO	A	503	-	3,3,3	0.06	0	2,2,2	0.15	0
6	PO4	B	506	-	4,4,4	0.73	0	6,6,6	0.49	0
5	EDO	A	502	-	3,3,3	0.07	0	2,2,2	0.13	0
6	PO4	B	507	-	4,4,4	0.66	0	6,6,6	0.47	0
6	PO4	B	505	-	4,4,4	0.71	0	6,6,6	0.54	0
5	EDO	B	502	-	3,3,3	0.07	0	2,2,2	0.11	0
6	PO4	A	507	-	4,4,4	0.64	0	6,6,6	0.54	0
5	EDO	B	501	-	3,3,3	0.07	0	2,2,2	0.12	0
6	PO4	A	505	-	4,4,4	0.71	0	6,6,6	0.46	0
6	PO4	B	508	-	4,4,4	0.67	0	6,6,6	0.47	0
5	EDO	A	501	-	3,3,3	0.07	0	2,2,2	0.14	0
5	EDO	B	503	-	3,3,3	0.06	0	2,2,2	0.13	0
6	PO4	A	506	-	4,4,4	0.73	0	6,6,6	0.48	0
5	EDO	B	504	-	3,3,3	0.06	0	2,2,2	0.11	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
5	EDO	A	503	-	-	1/1/1/1	-
5	EDO	A	502	-	-	1/1/1/1	-
5	EDO	B	502	-	-	0/1/1/1	-
5	EDO	B	501	-	-	1/1/1/1	-
5	EDO	A	501	-	-	0/1/1/1	-
5	EDO	B	503	-	-	1/1/1/1	-
5	EDO	B	504	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	EDO	O1-C1-C2-O2
5	A	503	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	502	EDO	O1-C1-C2-O2
5	B	503	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	507	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	419/422 (99%)	0.20	22 (5%) 32 37	14, 27, 52, 98	13 (3%)
1	B	419/422 (99%)	0.18	24 (5%) 29 34	14, 27, 54, 93	7 (1%)
All	All	838/844 (99%)	0.19	46 (5%) 30 36	14, 27, 53, 98	20 (2%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	PHE	6.6
1	A	98	ALA	6.0
1	B	100	THR	5.8
1	B	335	PHE	5.7
1	B	389	THR	4.7
1	B	492	ALA	4.4
1	B	98	ALA	4.2
1	A	492	ALA	4.0
1	B	96	PRO	3.9
1	B	101	GLY	3.7
1	B	454	GLY	3.7
1	A	388	HIS	3.5
1	A	101	GLY	3.2
1	A	483	VAL	3.2
1	A	339	HIS	3.2
1	B	339	HIS	3.2
1	B	388	HIS	3.1
1	A	336	SER	3.1
1	A	493	GLN	3.0
1	B	97	ASN	3.0
1	A	94	ASP	3.0
1	B	453	ARG	2.8
1	A	491	ALA	2.7
1	A	96	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	102	ASN	2.6
1	B	337	HIS	2.6
1	B	387	ASN	2.6
1	B	384	LEU	2.6
1	B	338	PRO	2.5
1	B	171	PRO	2.5
1	A	338	PRO	2.5
1	A	389	THR	2.4
1	A	337	HIS	2.3
1	A	268	PHE	2.3
1	B	169	SER	2.3
1	A	103	PRO	2.2
1	A	97	ASN	2.2
1	A	384	LEU	2.2
1	A	454	GLY	2.2
1	B	451	ASN	2.2
1	A	334	GLU	2.1
1	B	94	ASP	2.1
1	A	171	PRO	2.1
1	B	386	ASP	2.1
1	B	336	SER	2.1
1	B	197	HIS	2.0

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

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

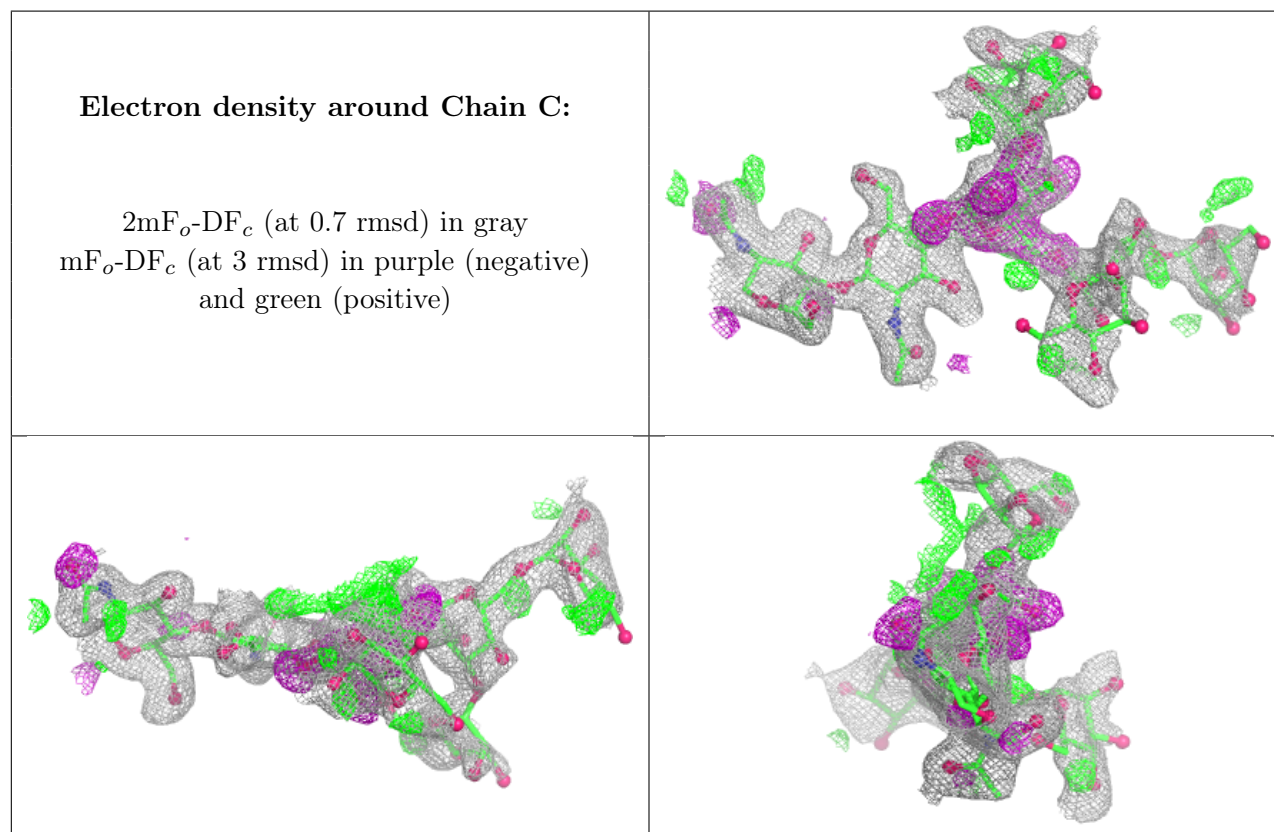
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OCS	B	300	9/10	0.95	0.09	27,30,34,38	4
1	OCS	A	300	9/10	0.96	0.08	25,28,35,38	1

6.3 Carbohydrates [i](#)

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

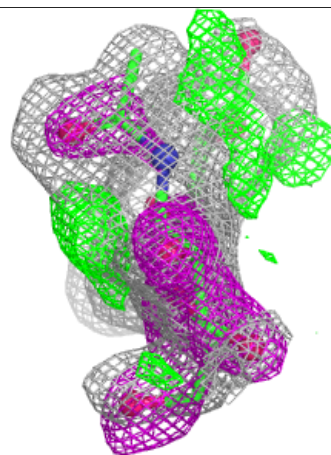
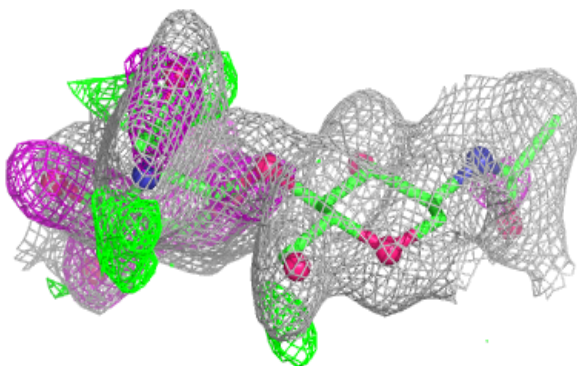
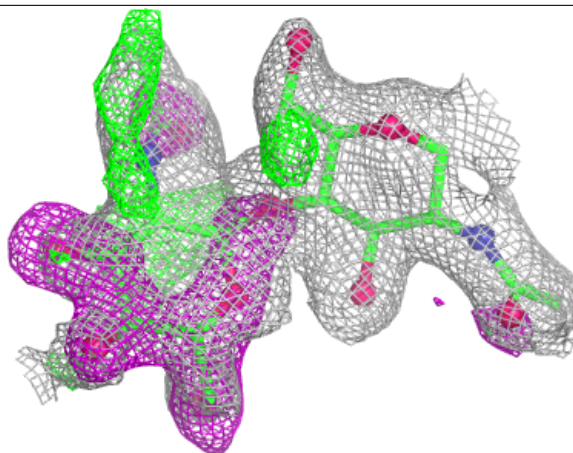
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	F	5	11/12	0.39	0.15	107,113,117,119	0
2	MAN	C	7	11/12	0.60	0.18	49,58,66,68	11
2	MAN	C	5	11/12	0.62	0.17	64,68,71,73	11
4	MAN	F	6	11/12	0.65	0.20	37,39,43,45	0
4	MAN	F	7	11/12	0.65	0.12	94,98,100,103	0
2	MAN	C	6	11/12	0.66	0.21	73,77,81,86	11
3	NAG	E	2	14/15	0.70	0.18	34,37,42,43	0
3	NAG	D	2	14/15	0.72	0.17	34,38,42,43	0
4	BMA	F	3	11/12	0.76	0.12	78,82,90,91	0
2	MAN	C	3	11/12	0.78	0.23	35,37,40,41	0
2	MAN	C	4	11/12	0.81	0.17	45,54,59,63	11
4	MAN	F	4	11/12	0.83	0.12	55,78,90,96	0
3	NAG	D	1	14/15	0.88	0.12	38,45,53,59	0
3	NAG	E	1	14/15	0.88	0.13	40,47,54,59	0
2	NAG	C	2	14/15	0.89	0.13	39,47,53,59	0
4	NAG	F	2	14/15	0.90	0.10	46,58,69,71	0
2	NAG	C	1	14/15	0.92	0.14	35,38,44,51	0
4	NAG	F	1	14/15	0.96	0.07	40,47,49,57	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.



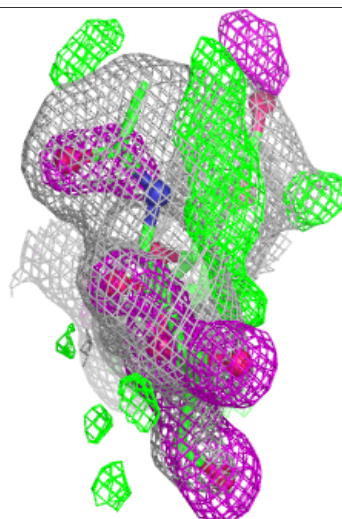
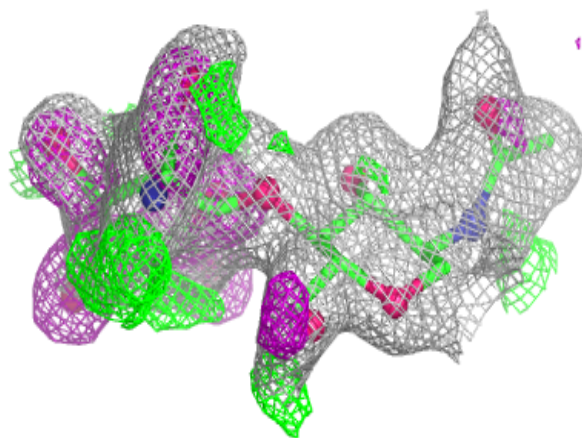
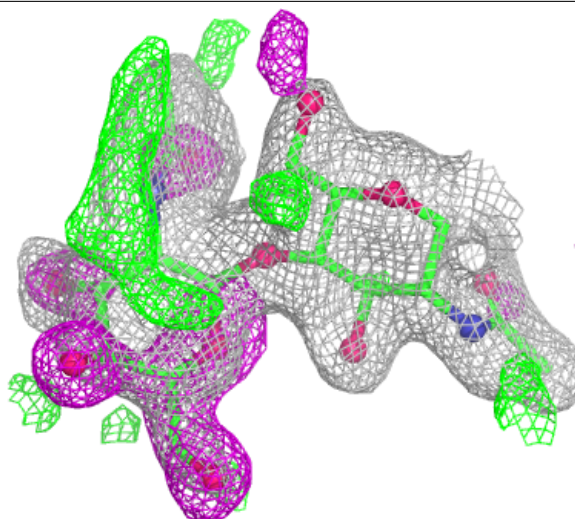
Electron density around Chain D:

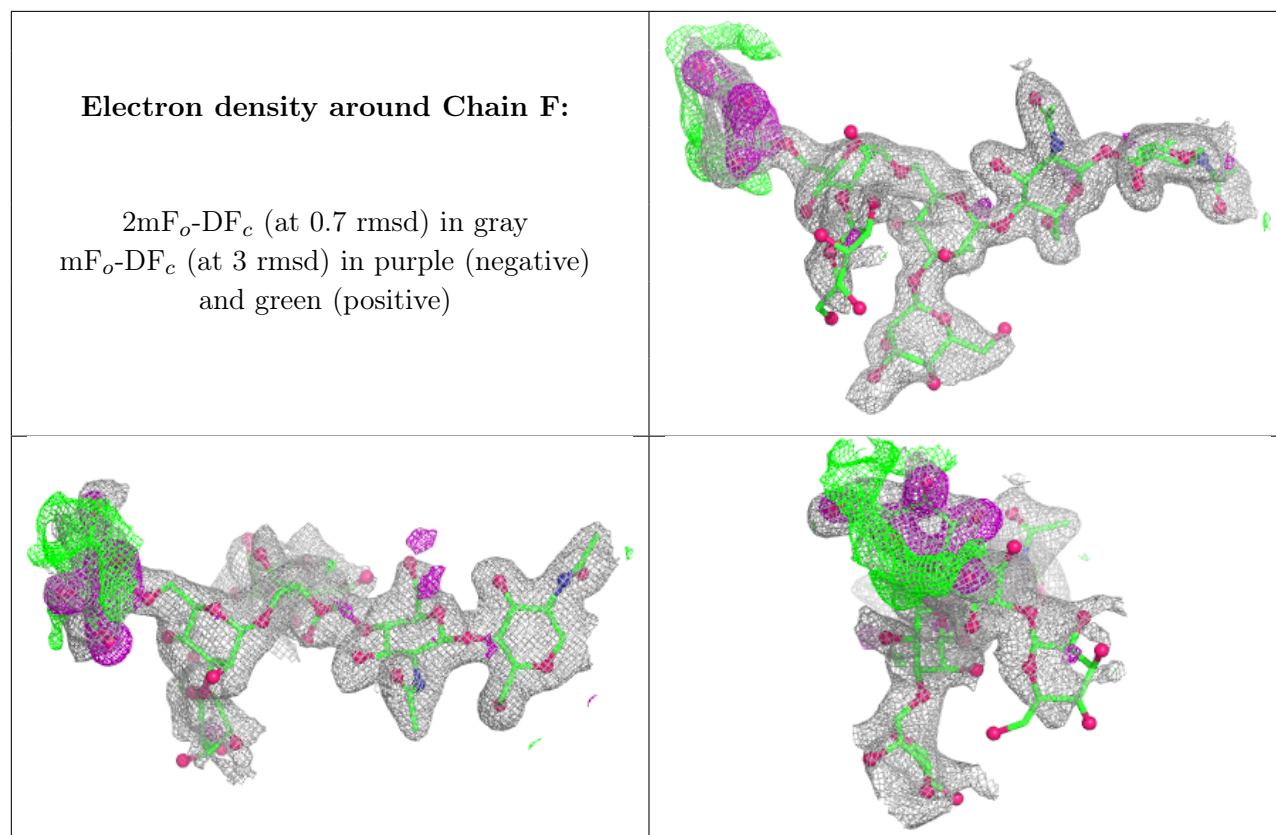
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	503	4/4	0.80	0.17	72,75,76,78	0
5	EDO	A	502	4/4	0.81	0.20	67,71,72,72	0
5	EDO	B	504	4/4	0.81	0.18	73,75,77,78	0
5	EDO	B	502	4/4	0.87	0.19	53,66,69,74	0
6	PO4	A	504	5/5	0.87	0.14	66,68,74,75	0
5	EDO	A	501	4/4	0.90	0.14	52,52,54,54	0
6	PO4	B	507	5/5	0.91	0.10	71,73,81,82	0
6	PO4	B	508	5/5	0.91	0.09	56,76,77,78	0
6	PO4	A	505	5/5	0.94	0.09	54,55,57,64	0
6	PO4	A	506	5/5	0.94	0.08	61,63,66,67	0
6	PO4	A	507	5/5	0.94	0.11	29,34,37,41	5
5	EDO	A	503	4/4	0.94	0.13	70,71,73,74	0
5	EDO	B	501	4/4	0.94	0.08	32,35,38,38	0
6	PO4	B	505	5/5	0.95	0.09	32,37,39,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PO4	B	506	5/5	0.95	0.08	58,64,66,68	0
7	MN	A	509	1/1	0.99	0.02	29,29,29,29	0
7	MN	A	508	1/1	1.00	0.03	27,27,27,27	0
7	MN	B	509	1/1	1.00	0.03	27,27,27,27	0
7	MN	B	510	1/1	1.00	0.02	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.