



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2026 – 09:38 am BST

PDB ID : 9T7G / pdb_00009t7g
Title : XN-IL lectin from Xenorhabdus nematophila in complex with heparosan trisaccharide
Authors : Korsak, M.; Wimmerova, M.
Deposited on : 2025-11-10
Resolution : 1.80 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 : 1.8.4, CSD as541be (2020)
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

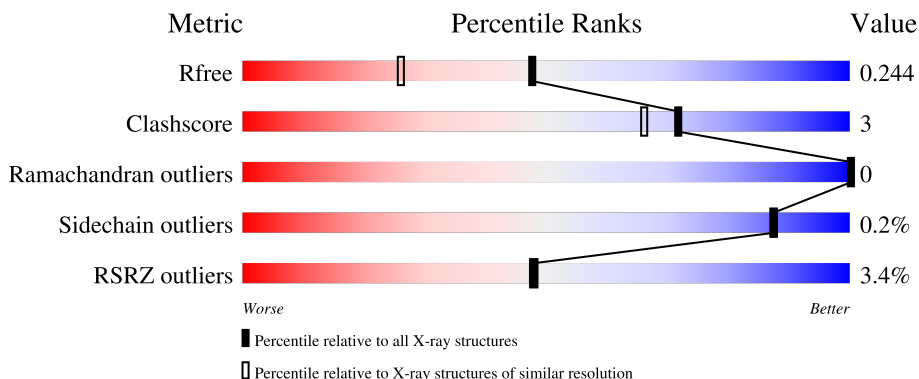
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	AAA	125	 3% 91% 8% .
1	BBB	125	 2% 98% .
1	CCC	125	 2% 90% 8% ..
1	DDD	125	 7% 93% 7%
2	HHH	3	 100%

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Mol	Chain	Length	Quality of chain
2	KKK	3	 100%
3	JaJ	3	 33% 67%

2 Entry composition [i](#)

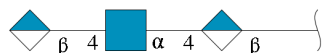
There are 9 unique types of molecules in this entry. The entry contains 4340 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	124	964	627	154	182	1	0	1	0
1	BBB	125	967	629	153	184	1	0	1	0
1	CCC	124	955	620	152	182	1	0	0	0
1	DDD	125	957	621	153	183		0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	HHH	3	39	20	1	18	0	0	0
2	KKK	3	39	20	1	18	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-1-O-pentylamine-beta-D-glucopyranuronic acid.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	JaJ	3	45	25	2	18	0	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	DDD	1	Total C O 4 2 2	0	0

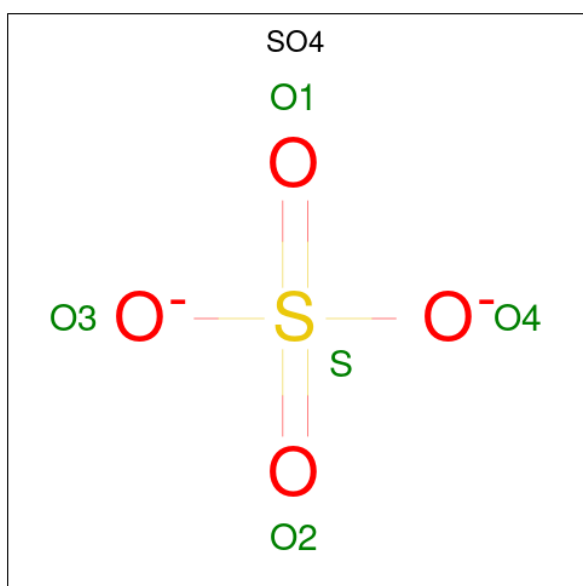
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total Ca 1 1	0	0
5	BBB	1	Total Ca 1 1	0	0
5	CCC	1	Total Ca 1 1	0	0
5	DDD	1	Total Ca 1 1	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total Mg 1 1	0	0
6	BBB	1	Total Mg 1 1	0	0
6	CCC	1	Total Mg 1 1	0	0
6	DDD	1	Total Mg 1 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total O S 5 4 1	0	0
7	DDD	1	Total O S 5 4 1	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	1	Total Na 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	94	Total 94	O 94	0	0
9	BBB	87	Total 87	O 87	0	0
9	CCC	83	Total 83	O 83	0	0
9	DDD	63	Total 63	O 63	0	0

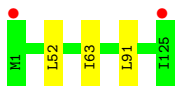
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)



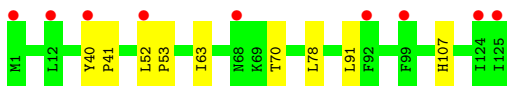
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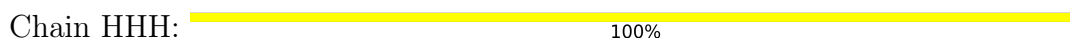
- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)



- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)



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




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

Chain KKK:  100%

BDF1
MDG2
BDF3

- Molecule 3: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-1-O-pentylamine-beta-D-glucopyranuronic acid

Chain JaJ:  33% 67%

ALJUC1
MDG2
BDF3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.98Å 77.05Å 146.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 1.80 49.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.05-1.80) 99.9 (49.05-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.237 0.202 , 0.244	Depositor DCC
R_{free} test set	2742 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4340	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: CA, NDG, EDO, A1JUC, MG, BDP, NA, SO4

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	AAA	1.03	0/994	1.15	0/1355
1	BBB	1.02	0/996	1.15	0/1359
1	CCC	1.00	0/981	1.18	0/1338
1	DDD	1.08	0/983	1.22	0/1342
All	All	1.03	0/3954	1.17	0/5394

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	AAA	964	0	950	8	0
1	BBB	967	0	957	3	0
1	CCC	955	0	939	11	0
1	DDD	957	0	934	8	0
2	HHH	39	0	24	0	0
2	KKK	39	0	24	0	0
3	JaJ	45	0	18	0	0
4	AAA	12	0	18	0	0
4	BBB	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CCC	4	0	6	0	0
4	DDD	4	0	6	2	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
6	DDD	1	0	0	0	0
7	AAA	5	0	0	0	0
7	DDD	5	0	0	0	0
8	AAA	1	0	0	0	0
9	AAA	94	0	0	3	0
9	BBB	87	0	0	0	0
9	CCC	83	0	0	0	0
9	DDD	63	0	0	0	0
All	All	4340	0	3888	26	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 3.

All (26) 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:CCC:15:GLY:HA3	1:CCC:91:LEU:HD12	1.54	0.89
1:CCC:15:GLY:HA3	1:CCC:91:LEU:CD1	2.16	0.74
1:AAA:45:TRP:HB2	1:AAA:52:LEU:HD22	1.72	0.71
1:BBB:63:ILE:HD11	1:BBB:91:LEU:HD23	1.74	0.70
1:DDD:107:HIS:ND1	4:DDD:201:EDO:O1	2.27	0.64
1:CCC:63:ILE:HG13	1:CCC:91:LEU:HD23	1.82	0.61
1:AAA:107[B]:HIS:CD2	9:AAA:379:HOH:O	2.55	0.58
1:AAA:63:ILE:HD11	1:AAA:91:LEU:HD23	1.86	0.57
1:DDD:63:ILE:HD12	1:DDD:70:THR:HG23	1.86	0.57
1:AAA:31:VAL:HG23	1:DDD:78:LEU:HD13	1.88	0.55
1:BBB:52:LEU:HD21	1:CCC:52:LEU:HD21	1.91	0.52
1:AAA:65:LYS:HE2	1:AAA:91:LEU:HD22	1.93	0.51
1:DDD:52:LEU:HB3	1:DDD:53:PRO:HD3	1.93	0.50
1:CCC:124:ILE:HD12	1:DDD:70:THR:HG22	1.93	0.49
1:DDD:40:TYR:N	1:DDD:41:PRO:CD	2.76	0.48
1:AAA:14:GLN:HG2	9:AAA:376:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:40:TYR:N	1:CCC:41:PRO:CD	2.79	0.46
1:CCC:91:LEU:N	1:CCC:91:LEU:HD22	2.31	0.45
1:DDD:107:HIS:CE1	4:DDD:201:EDO:HO1	2.30	0.44
1:CCC:7:THR:HA	1:CCC:106:PHE:O	2.18	0.43
1:CCC:89:ILE:HG22	1:CCC:91:LEU:CD1	2.49	0.43
1:CCC:90:LEU:C	1:CCC:91:LEU:HD13	2.45	0.42
1:AAA:40:TYR:CG	1:AAA:41:PRO:HD3	2.55	0.41
1:BBB:52:LEU:CD2	1:CCC:52:LEU:HD21	2.50	0.41
1:AAA:107[A]:HIS:HE1	9:AAA:385:HOH:O	2.03	0.40
1:DDD:63:ILE:HD11	1:DDD:91:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	123/125 (98%)	123 (100%)	0	0	100	100
1	BBB	124/125 (99%)	123 (99%)	1 (1%)	0	100	100
1	CCC	122/125 (98%)	122 (100%)	0	0	100	100
1	DDD	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
All	All	492/500 (98%)	488 (99%)	4 (1%)	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	AAA	102/104 (98%)	102 (100%)	0	100	100
1	BBB	103/104 (99%)	103 (100%)	0	100	100
1	CCC	101/104 (97%)	100 (99%)	1 (1%)	68	64
1	DDD	100/104 (96%)	100 (100%)	0	100	100
All	All	406/416 (98%)	405 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	91	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

9 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	BDP	HHH	1	2,5	13,13,13	1.12	1 (7%)	18,19,19	1.61	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDG	HHH	2	2	14,14,15	0.46	0	17,19,21	1.48	3 (17%)
2	BDP	HHH	3	2	12,12,13	0.74	0	14,17,19	0.99	1 (7%)
3	A1JUC	JaJ	1	3,5	19,19,19	1.26	2 (10%)	24,25,25	1.24	2 (8%)
3	NDG	JaJ	2	3	14,14,15	0.44	0	17,19,21	0.57	0
3	BDP	JaJ	3	3	12,12,13	0.83	0	14,17,19	1.54	3 (21%)
2	BDP	KKK	1	2,5	13,13,13	1.10	0	18,19,19	1.39	3 (16%)
2	NDG	KKK	2	2	14,14,15	0.45	0	17,19,21	1.41	2 (11%)
2	BDP	KKK	3	2	12,12,13	0.88	0	14,17,19	1.96	3 (21%)

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	BDP	HHH	1	2,5	-	0/4/24/24	0/1/1/1
2	NDG	HHH	2	2	-	1/6/23/26	0/1/1/1
2	BDP	HHH	3	2	-	0/4/21/24	0/1/1/1
3	A1JUC	JaJ	1	3,5	-	2/11/31/31	0/1/1/1
3	NDG	JaJ	2	3	-	2/6/23/26	0/1/1/1
3	BDP	JaJ	3	3	-	0/4/21/24	0/1/1/1
2	BDP	KKK	1	2,5	-	0/4/24/24	0/1/1/1
2	NDG	KKK	2	2	-	0/6/23/26	0/1/1/1
2	BDP	KKK	3	2	-	0/4/21/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	JaJ	1	A1JUC	C4-C5	2.93	1.58	1.53
3	JaJ	1	A1JUC	O1-C1	2.93	1.45	1.40
2	HHH	1	BDP	O3-C3	2.10	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	KKK	3	BDP	O5-C1-C2	-3.99	104.61	110.77
2	KKK	3	BDP	C1-C2-C3	-3.96	104.80	109.67
2	HHH	2	NDG	C1-C2-N2	3.88	117.11	110.49
2	KKK	2	NDG	O5-C1-C2	-3.75	105.37	111.29
3	JaJ	3	BDP	C1-C2-C3	3.72	114.23	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	KKK	3	BDP	C3-C4-C5	3.51	115.26	109.25
2	KKK	2	NDG	C1-C2-N2	3.44	116.37	110.49
2	HHH	1	BDP	O3-C3-C4	2.84	116.92	110.35
2	HHH	2	NDG	C1-O5-C5	2.77	115.95	112.19
2	HHH	1	BDP	O2-C2-C3	-2.72	104.05	110.35
3	JaJ	3	BDP	O2-C2-C3	-2.65	104.83	110.14
2	HHH	1	BDP	O4-C4-C3	-2.53	104.51	110.35
2	HHH	1	BDP	O2-C2-C1	2.37	114.66	109.16
2	HHH	2	NDG	O5-C1-C2	-2.37	107.55	111.29
2	KKK	1	BDP	O3-C3-C4	2.28	115.61	110.35
2	HHH	3	BDP	O5-C5-C6	2.26	113.73	106.31
2	KKK	1	BDP	C1-O5-C5	2.25	115.53	112.22
3	JaJ	1	A1JUC	O1-C1-C2	2.24	111.80	108.30
2	HHH	1	BDP	O1-C1-C2	2.16	115.12	109.03
3	JaJ	1	A1JUC	O3-C3-C4	2.13	115.28	110.35
2	KKK	1	BDP	O6B-C6-C5	2.11	121.36	113.65
3	JaJ	3	BDP	O4-C4-C3	-2.02	105.68	110.35

There are no chirality outliers.

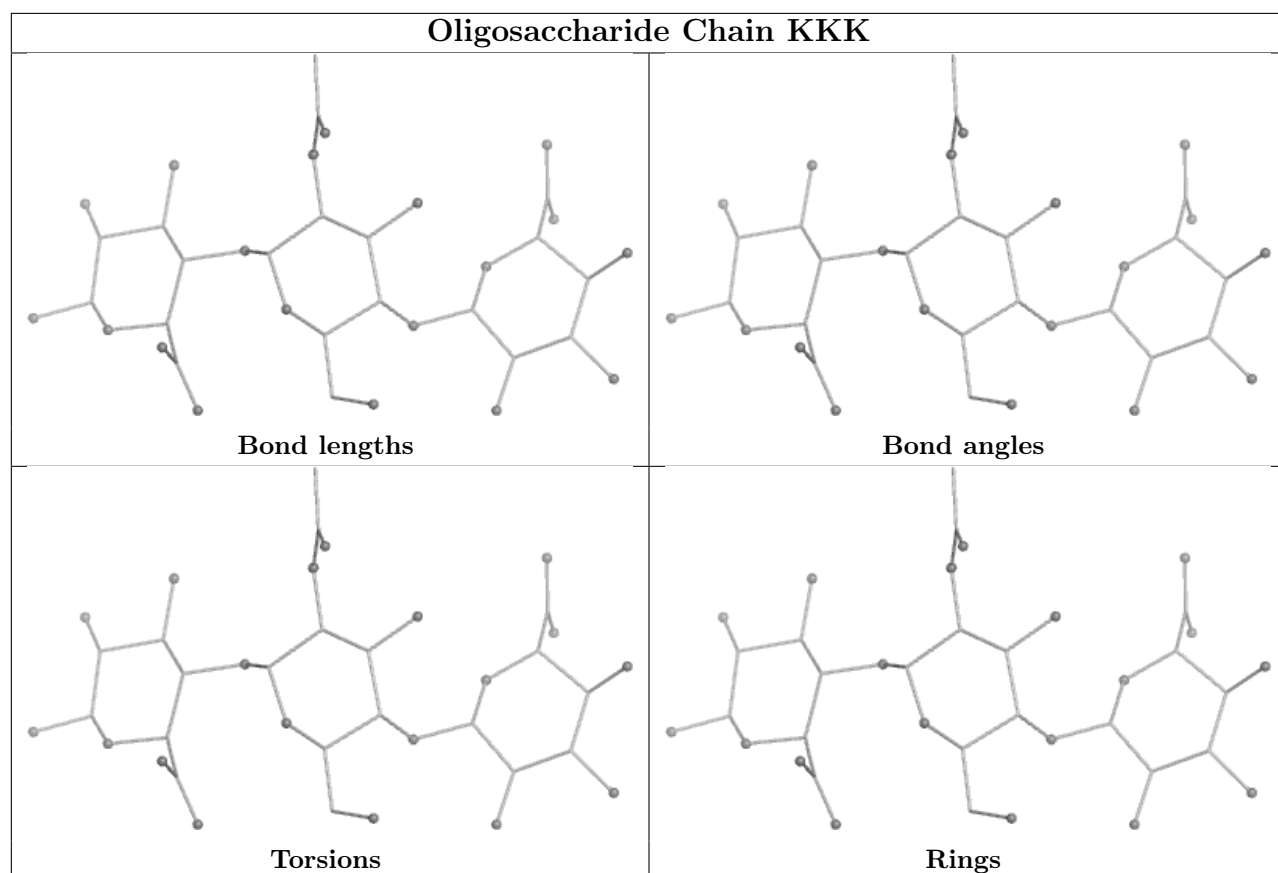
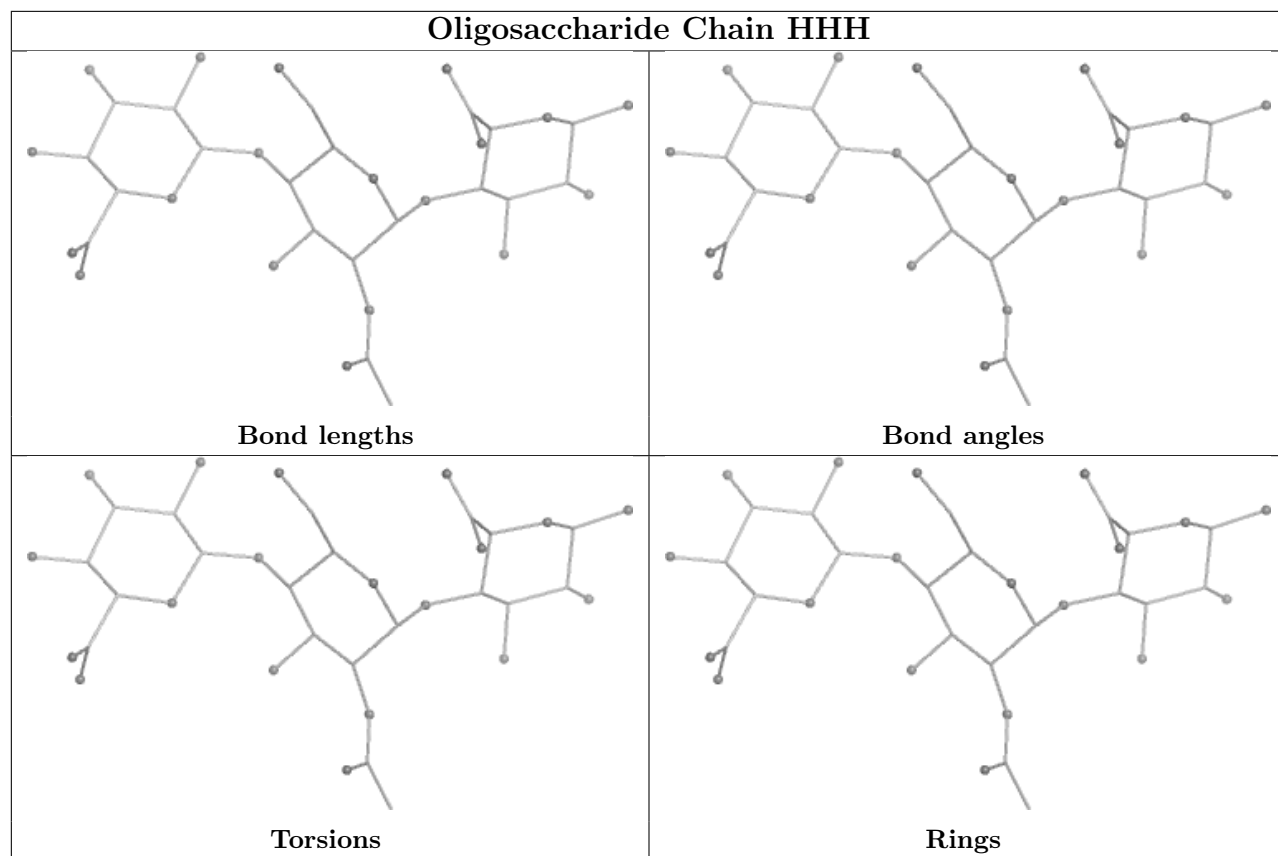
All (5) torsion outliers are listed below:

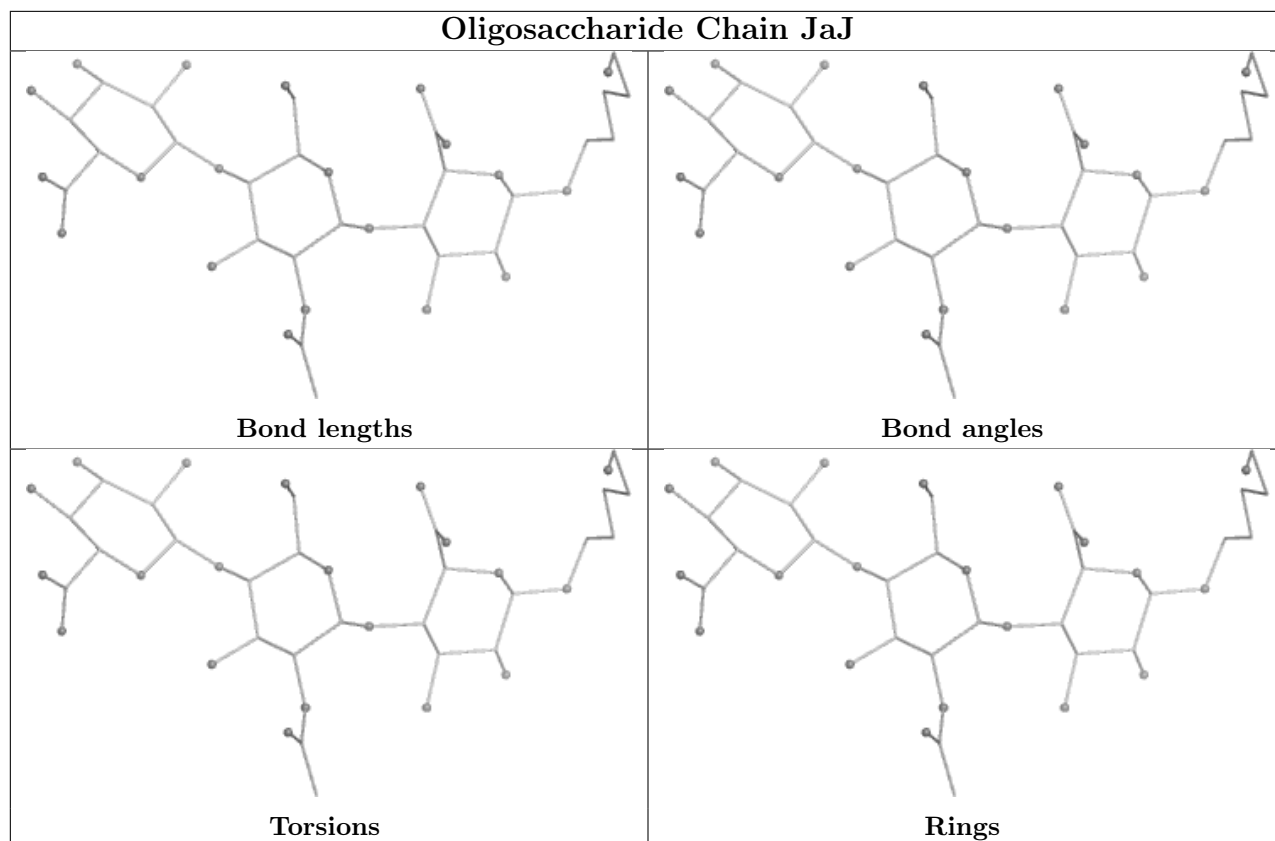
Mol	Chain	Res	Type	Atoms
3	JaJ	1	A1JUC	O1-C13-C14-C15
3	JaJ	1	A1JUC	C14-C13-O1-C1
2	HHH	2	NDG	O5-C5-C6-O6
3	JaJ	2	NDG	O5-C5-C6-O6
3	JaJ	2	NDG	C4-C5-C6-O6

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 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	$\# Z > 2$
4	EDO	AAA	202	-	3,3,3	0.39	0	2,2,2	0.56	0
4	EDO	BBB	202	-	3,3,3	0.08	0	2,2,2	0.25	0
4	EDO	BBB	201	-	3,3,3	0.16	0	2,2,2	0.29	0
4	EDO	DDD	201	-	3,3,3	0.18	0	2,2,2	0.42	0
4	EDO	AAA	201	-	3,3,3	0.18	0	2,2,2	0.37	0
4	EDO	AAA	203	-	3,3,3	0.20	0	2,2,2	0.23	0
4	EDO	CCC	201	-	3,3,3	0.23	0	2,2,2	0.16	0
7	SO4	DDD	204	-	4,4,4	0.33	0	6,6,6	0.10	0
7	SO4	AAA	206	-	4,4,4	0.33	0	6,6,6	0.10	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
4	EDO	AAA	202	-	-	1/1/1/1	-
4	EDO	BBB	202	-	-	1/1/1/1	-
4	EDO	BBB	201	-	-	1/1/1/1	-
4	EDO	DDD	201	-	-	1/1/1/1	-
4	EDO	AAA	201	-	-	1/1/1/1	-
4	EDO	AAA	203	-	-	0/1/1/1	-
4	EDO	CCC	201	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	DDD	201	EDO	O1-C1-C2-O2
4	BBB	202	EDO	O1-C1-C2-O2
4	BBB	201	EDO	O1-C1-C2-O2
4	CCC	201	EDO	O1-C1-C2-O2
4	AAA	202	EDO	O1-C1-C2-O2
4	AAA	201	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DDD	201	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	124/125 (99%)	0.14	4 (3%)	50 50	18, 32, 47, 63	1 (0%)
1	BBB	125/125 (100%)	0.12	2 (1%)	70 71	23, 33, 46, 63	1 (0%)
1	CCC	124/125 (99%)	0.08	2 (1%)	70 71	24, 32, 48, 65	0
1	DDD	125/125 (100%)	0.57	9 (7%)	21 20	27, 37, 53, 68	0
All	All	498/500 (99%)	0.23	17 (3%)	48 48	18, 33, 50, 68	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	124	ILE	4.4
1	BBB	125	ILE	4.0
1	AAA	124	ILE	3.9
1	DDD	125	ILE	3.4
1	BBB	1	MET	2.8
1	DDD	1	MET	2.8
1	CCC	1	MET	2.6
1	DDD	124	ILE	2.6
1	AAA	1	MET	2.6
1	DDD	68	ASN	2.6
1	DDD	99	PHE	2.5
1	DDD	12	LEU	2.4
1	DDD	40	TYR	2.3
1	AAA	40	TYR	2.2
1	AAA	43	ASN	2.1
1	DDD	52	LEU	2.0
1	DDD	92	PHE	2.0

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

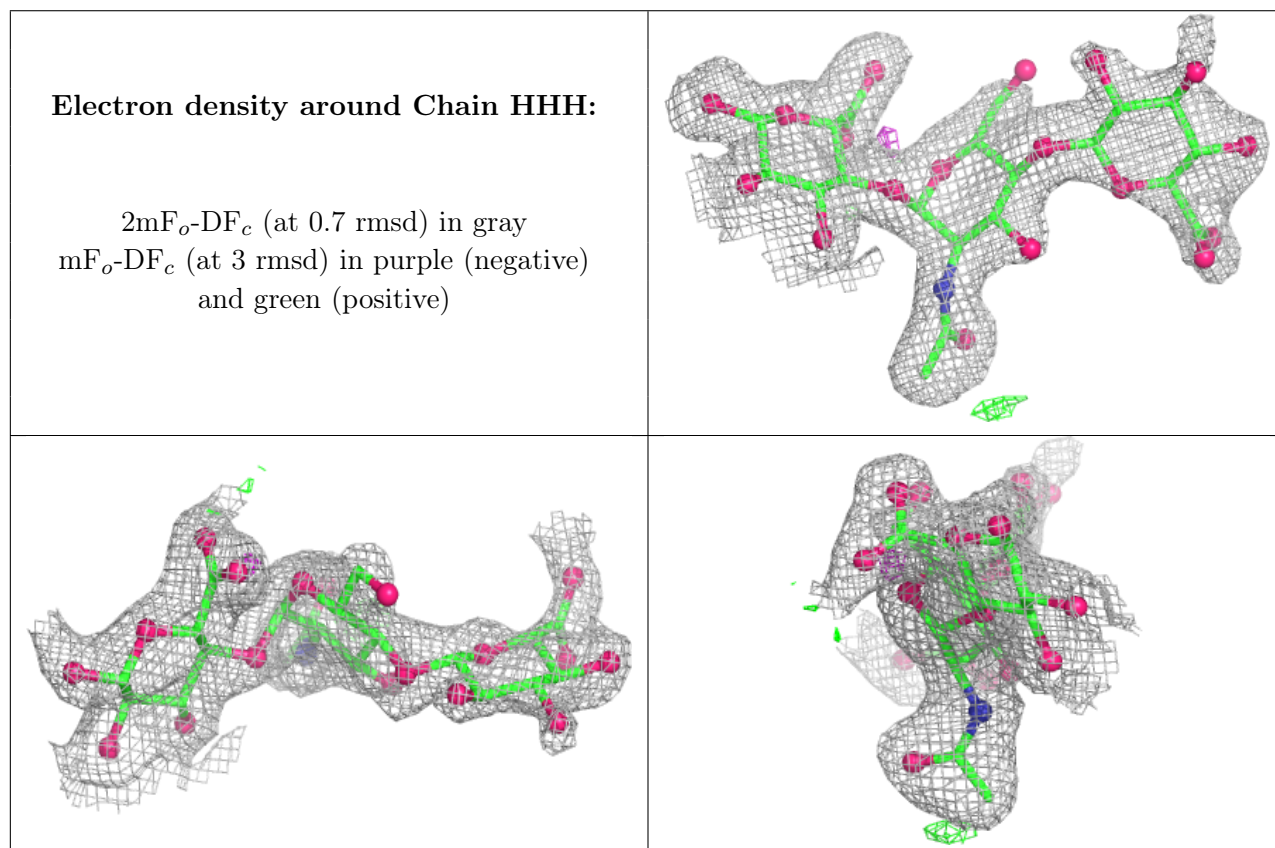
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

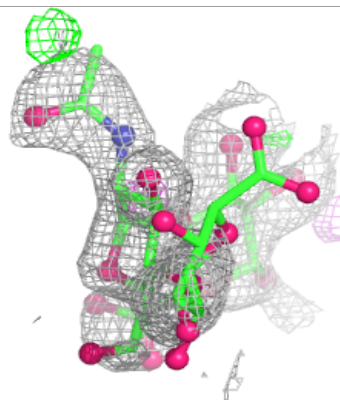
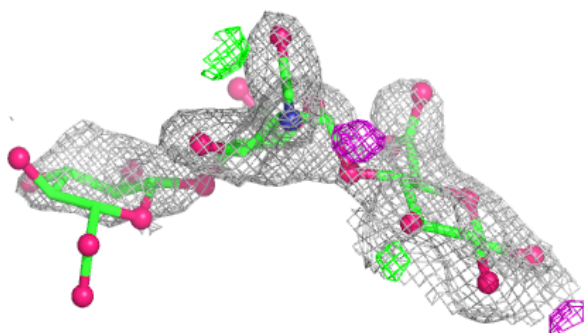
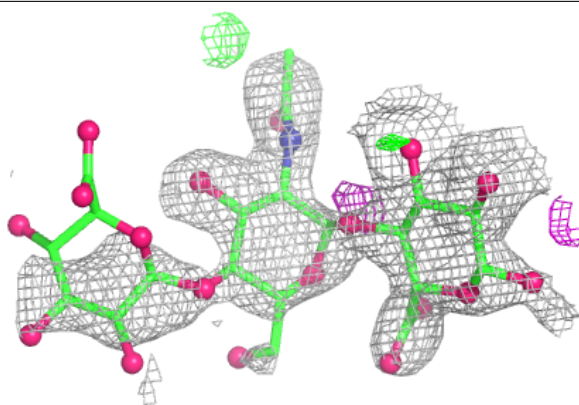
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BDP	HHH	1	13/13	-	-	43,51,58,60	0
2	NDG	HHH	2	14/15	-	-	39,52,65,70	0
2	BDP	HHH	3	12/13	-	-	79,84,88,88	0
2	BDP	KKK	1	13/13	-	-	33,61,72,74	0
2	NDG	KKK	2	14/15	-	-	53,78,88,98	0
2	BDP	KKK	3	12/13	-	-	103,109,128,130	0
3	A1JUC	JaJ	1	19/19	-	-	32,54,71,71	0
3	NDG	JaJ	2	14/15	-	-	41,46,55,59	0
3	BDP	JaJ	3	12/13	-	-	64,67,71,73	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.

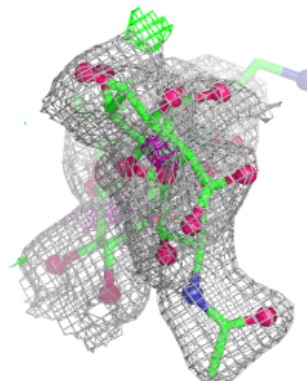
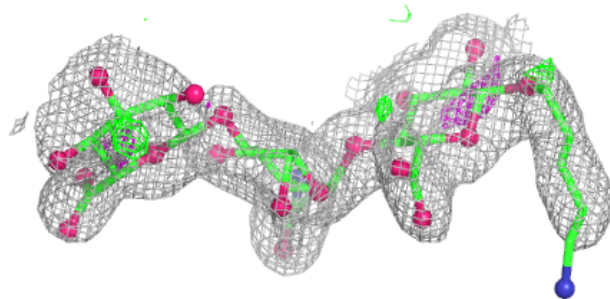
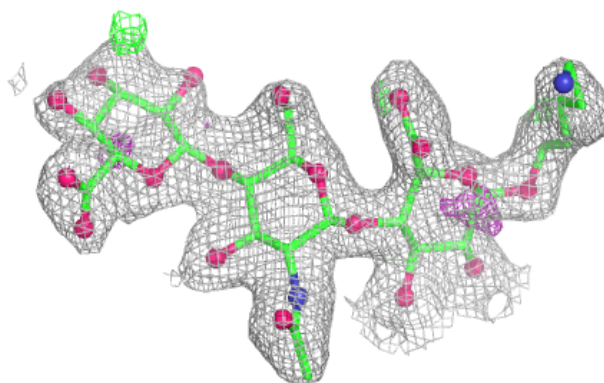


Electron density around Chain KKK:

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

**Electron density around Chain JaJ:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
7	SO4	DDD	204	5/5	0.58	0.17	102,106,120,121	0
4	EDO	BBB	202	4/4	0.75	0.15	56,62,67,70	0
4	EDO	AAA	203	4/4	0.79	0.18	56,57,58,59	0
7	SO4	AAA	206	5/5	0.80	0.11	64,80,88,92	0
4	EDO	BBB	201	4/4	0.83	0.14	67,68,70,71	0
4	EDO	AAA	202	4/4	0.85	0.15	47,48,52,54	0
4	EDO	DDD	201	4/4	0.87	0.13	34,46,47,56	0
4	EDO	AAA	201	4/4	0.89	0.13	44,49,50,54	0
8	NA	AAA	208	1/1	0.93	0.08	50,50,50,50	0
4	EDO	CCC	201	4/4	0.94	0.10	43,47,50,55	0
6	MG	BBB	204	1/1	0.95	0.08	47,47,47,47	0
6	MG	CCC	203	1/1	0.95	0.10	49,49,49,49	0
6	MG	DDD	203	1/1	0.95	0.07	62,62,62,62	0
5	CA	BBB	203	1/1	0.98	0.05	37,37,37,37	0
6	MG	AAA	205	1/1	0.98	0.09	48,48,48,48	0
5	CA	CCC	202	1/1	0.99	0.03	29,29,29,29	0
5	CA	DDD	202	1/1	0.99	0.07	37,37,37,37	0
5	CA	AAA	204	1/1	0.99	0.03	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.