Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 07:12 PM BST

PDB ID	:	5IXO
Title	:	Crystal structure of the Arabidopsis receptor kinase HAESA LRR ectdomain (apo form).
Authors	:	Santiago, J.; Hothorn, M.
Deposited on	:	2016-03-23
Resolution	:	1.74 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 following versions of software and data (see references ⓘ) were used in the production of this report:

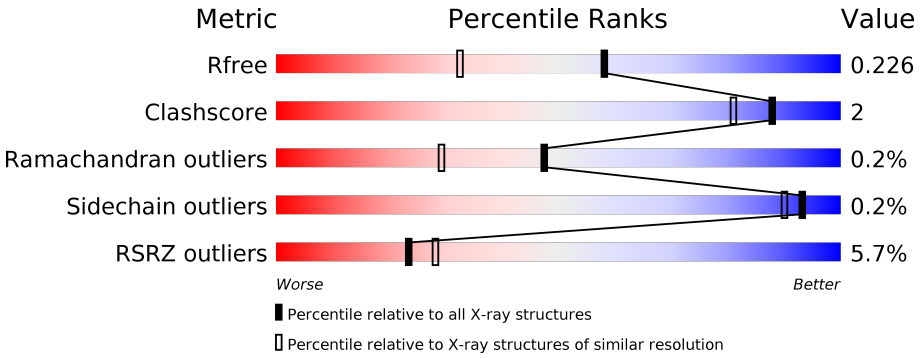
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	616	6%, 89%, 7%, .
2	B	2	100%
2	C	2	100%
2	D	2	50%, 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4740 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 Receptor-like protein kinase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	4	0
			4527	2871	760	882	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP P47735
A	16	SER	-	expression tag	UNP P47735
A	17	SER	-	expression tag	UNP P47735
A	18	MET	-	expression tag	UNP P47735
A	19	GLY	-	expression tag	UNP P47735
A	621	LEU	-	expression tag	UNP P47735
A	622	GLU	-	expression tag	UNP P47735
A	623	GLY	-	expression tag	UNP P47735
A	624	SER	-	expression tag	UNP P47735
A	625	GLU	-	expression tag	UNP P47735
A	626	ASN	-	expression tag	UNP P47735
A	627	LEU	-	expression tag	UNP P47735
A	628	TYR	-	expression tag	UNP P47735
A	629	PHE	-	expression tag	UNP P47735
A	630	GLN	-	expression tag	UNP P47735

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

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

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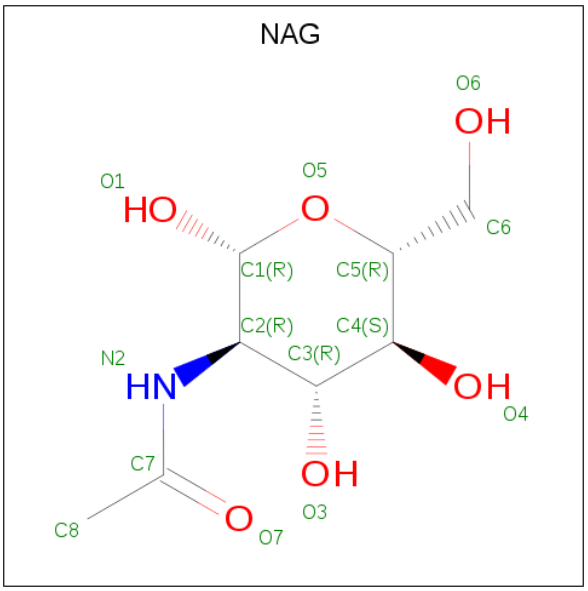
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	2	Total C N O 28 16 2 10	0	0	0
2	D	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

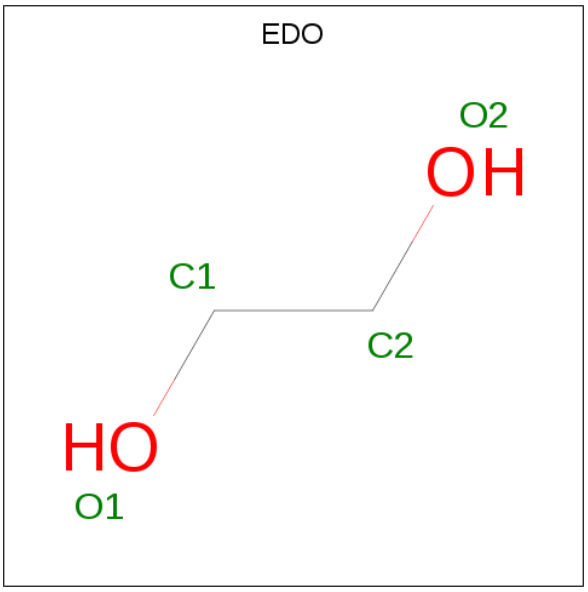


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

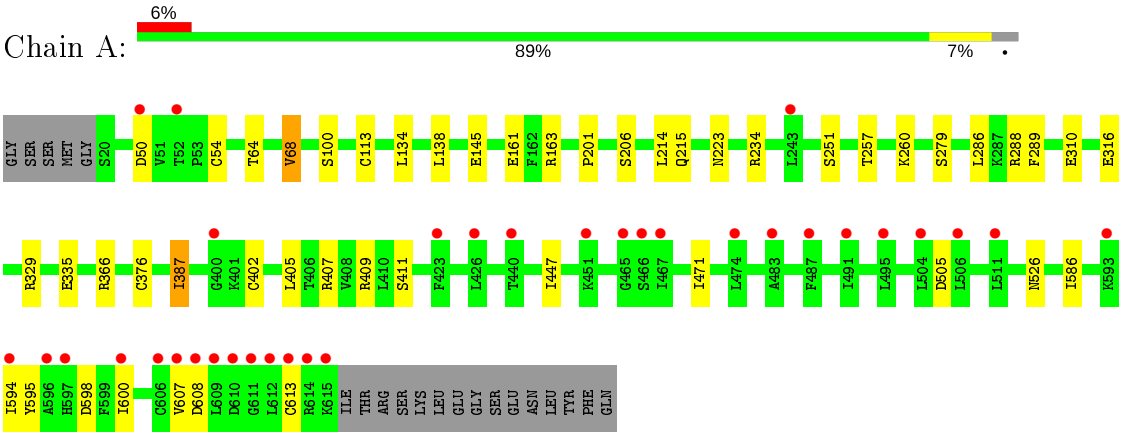
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	78	Total O 78 78	0	0

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.

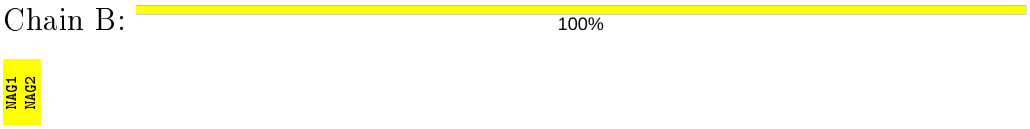
• Molecule 1: Receptor-like protein kinase 5

Chain A:



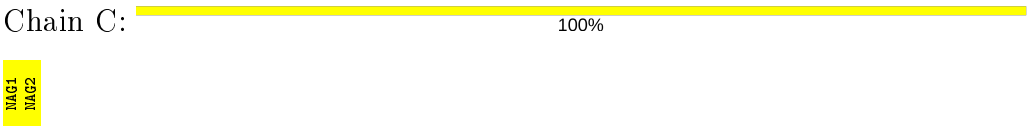
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



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

Chain C:



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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.68Å 148.68Å 58.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	128.76 – 1.74 45.75 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.6 (128.76-1.74) 99.7 (45.75-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.180 , 0.222 0.186 , 0.226	Depositor DCC
R_{free} test set	3713 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	73.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4740	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG, 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	1.26	10/4625 (0.2%)	1.14	18/6288 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	SER	CB-OG	-12.03	1.26	1.42
1	A	206	SER	CB-OG	-6.21	1.34	1.42
1	A	145	GLU	CD-OE1	6.18	1.32	1.25
1	A	161	GLU	CD-OE1	5.99	1.32	1.25
1	A	100	SER	CB-OG	-5.86	1.34	1.42
1	A	310	GLU	CD-OE2	-5.54	1.19	1.25
1	A	335	GLU	CD-OE1	-5.32	1.19	1.25
1	A	215	GLN	CD-OE1	-5.11	1.12	1.24
1	A	214	LEU	C-O	5.10	1.33	1.23
1	A	316	GLU	CG-CD	5.06	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	ARG	NE-CZ-NH2	-16.13	112.23	120.30
1	A	288	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	A	366	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	288	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	407	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	329	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	387	ILE	CB-CA-C	-6.45	98.71	111.60
1	A	163	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	251	SER	CB-CA-C	-5.74	99.20	110.10
1	A	505	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	68	VAL	CG1-CB-CG2	-5.55	102.01	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	260	LYS	CB-CG-CD	-5.29	97.85	111.60
1	A	54	CYS	CA-CB-SG	-5.18	104.67	114.00
1	A	64	THR	OG1-CB-CG2	-5.15	98.16	110.00
1	A	608	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	234	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	598	ASP	CB-CG-OD2	-5.04	113.76	118.30

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	4527	0	4512	19	4
2	B	28	0	25	0	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	42	0	39	0	0
4	A	1	0	0	0	0
5	A	8	0	12	0	0
6	A	78	0	0	4	0
All	All	4740	0	4638	19	4

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 (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ILE:HD11	1:A:409:ARG:HB3	1.39	1.01
1:A:257:THR:HG21	1:A:279:SER:OG	1.68	0.93
1:A:586:ILE:HD12	1:A:607:VAL:HG22	1.54	0.90
1:A:600:ILE:HD11	6:A:874:HOH:O	1.84	0.77
1:A:447:ILE:HD13	1:A:471:ILE:CD1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ILE:HD13	1:A:471:ILE:HD11	1.83	0.61
1:A:600:ILE:CD1	6:A:874:HOH:O	2.43	0.59
1:A:387:ILE:HD11	1:A:409:ARG:CB	2.26	0.56
1:A:113:CYS:HB2	1:A:138:LEU:HD21	1.93	0.49
1:A:68:VAL:CG1	6:A:865:HOH:O	2.61	0.48
1:A:402:CYS:SG	1:A:405:LEU:HG	2.57	0.45
1:A:387:ILE:CD1	1:A:409:ARG:HB3	2.27	0.45
1:A:68:VAL:HG11	6:A:865:HOH:O	2.17	0.44
1:A:201:PRO:HA	1:A:223:ASN:O	2.18	0.43
1:A:286:LEU:HD21	1:A:289:PHE:HB2	2.00	0.43
1:A:594:ILE:HD11	1:A:595:TYR:CE2	2.54	0.43
1:A:387:ILE:HD12	1:A:411:SER:OG	2.20	0.41
1:A:134:LEU:HD11	1:A:138:LEU:HD12	2.01	0.41
1:A:376:CYS:SG	1:A:376:CYS:O	2.79	0.41

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ASN:ND2	1:A:526:ASN:ND2[6_555]	1.56	0.64
1:A:526:ASN:CG	1:A:526:ASN:ND2[6_555]	1.81	0.39
1:A:526:ASN:OD1	1:A:526:ASN:ND2[6_555]	1.90	0.30
1:A:526:ASN:CG	1:A:526:ASN:CG[6_555]	2.19	0.01

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	598/616 (97%)	557 (93%)	40 (7%)	1 (0%)	47 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ASP

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	521/552 (94%)	520 (100%)	1 (0%)	93 90

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

Mol	Chain	Res	Type
1	A	613	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	526	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	NAG	B	1	1,2	14,14,15	0.77	0	17,19,21	1.84	4 (23%)
2	NAG	B	2	2	14,14,15	0.86	1 (7%)	17,19,21	1.87	2 (11%)
2	NAG	C	1	1,2	14,14,15	1.00	1 (7%)	17,19,21	2.27	4 (23%)
2	NAG	C	2	2	14,14,15	1.01	0	17,19,21	2.11	5 (29%)
2	NAG	D	1	1,2	14,14,15	0.61	0	17,19,21	0.70	0
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	0.98	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	5/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	2.56	1.56	1.52
2	C	1	NAG	O5-C5	2.07	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	O5-C1-C2	-6.31	101.32	111.29
2	B	2	NAG	C1-O5-C5	6.27	120.68	112.19
2	C	2	NAG	C4-C3-C2	4.31	117.34	111.02
2	C	2	NAG	C2-N2-C7	4.30	129.03	122.90
2	B	1	NAG	C1-O5-C5	4.20	117.88	112.19
2	C	2	NAG	C8-C7-N2	3.67	122.31	116.10
2	C	1	NAG	O5-C5-C6	3.63	112.89	107.20
2	D	2	NAG	C1-O5-C5	3.29	116.65	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C4-C3-C2	3.29	115.84	111.02
2	B	1	NAG	C6-C5-C4	-2.96	106.07	113.00
2	C	2	NAG	O7-C7-C8	-2.72	117.01	122.06
2	C	2	NAG	C3-C4-C5	2.55	114.79	110.24
2	B	1	NAG	O5-C1-C2	-2.34	107.59	111.29
2	B	1	NAG	O6-C6-C5	-2.34	103.25	111.29
2	B	2	NAG	O7-C7-C8	-2.18	118.01	122.06
2	C	1	NAG	C8-C7-N2	-2.13	112.50	116.10

There are no chirality outliers.

All (9) torsion outliers are listed below:

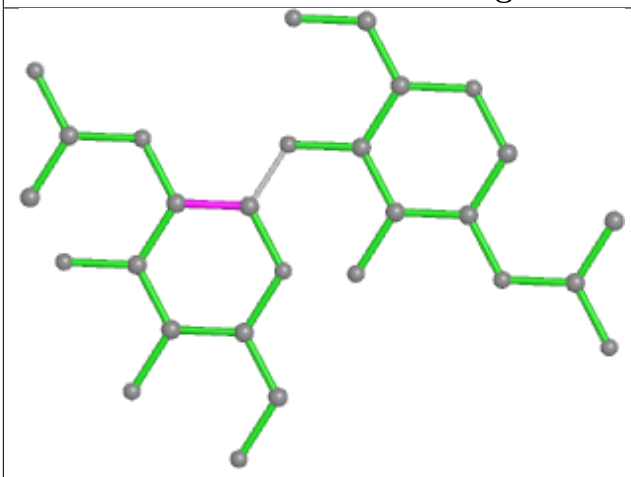
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7

There are no ring outliers.

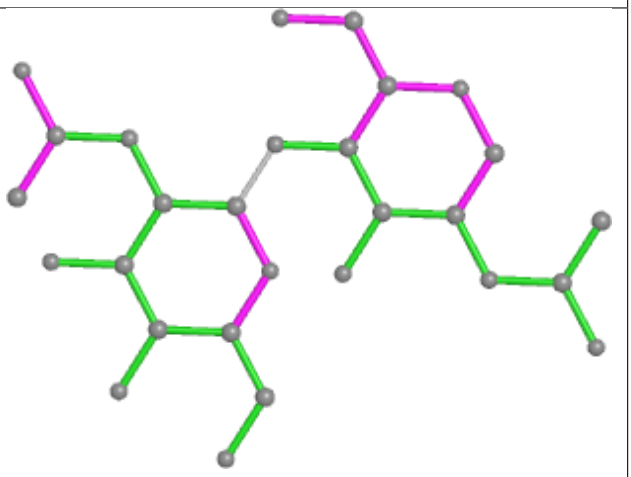
No monomer is involved in short contacts.

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

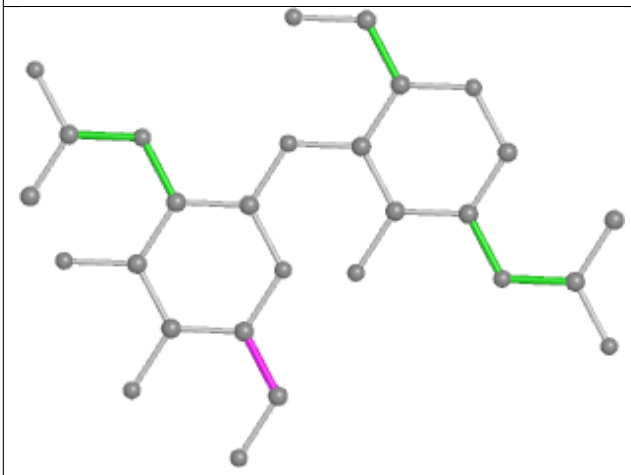
Oligosaccharide Chain B



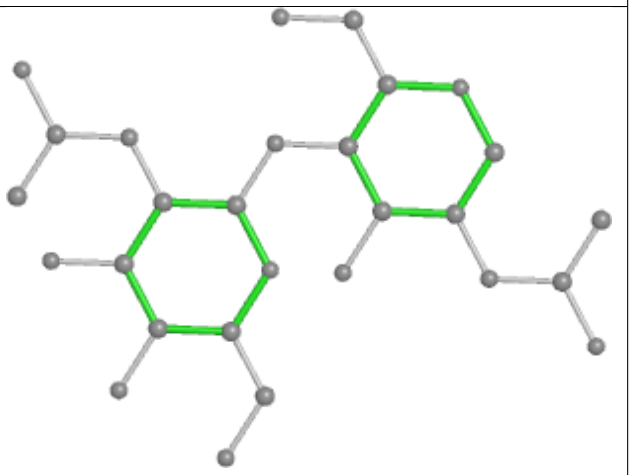
Bond lengths



Bond angles

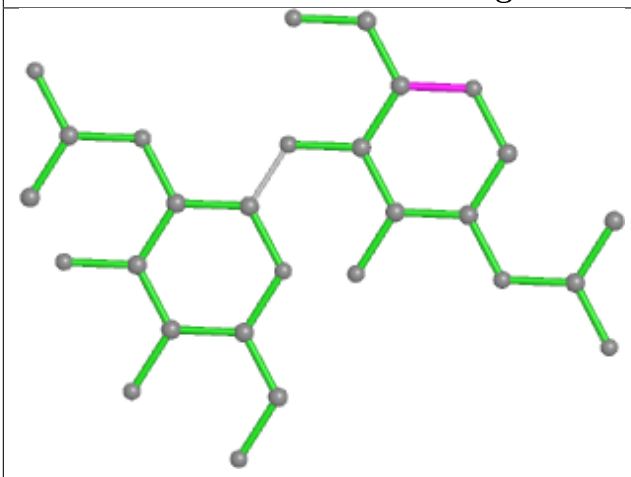


Torsions

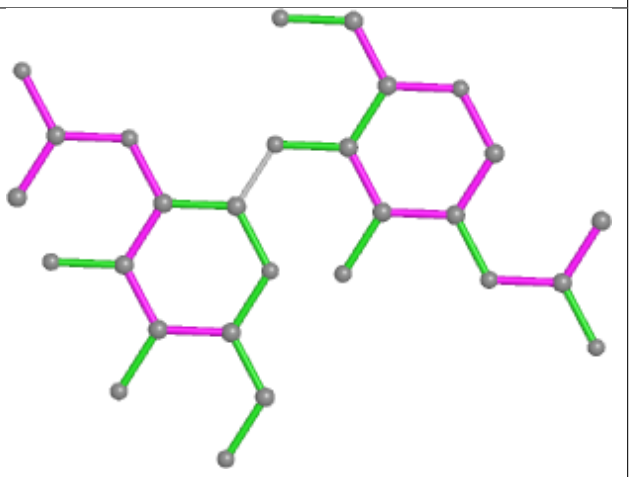


Rings

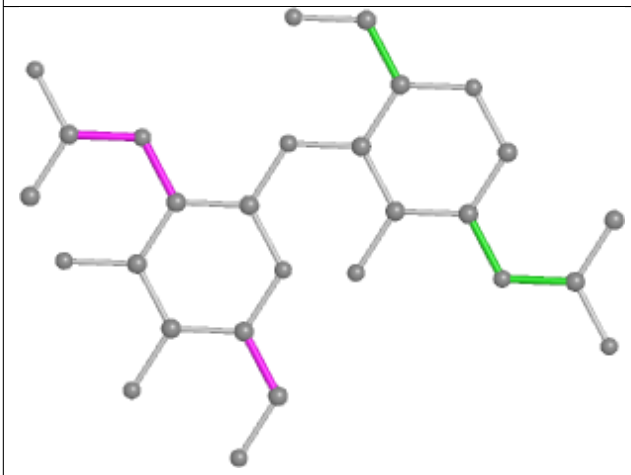
Oligosaccharide Chain C



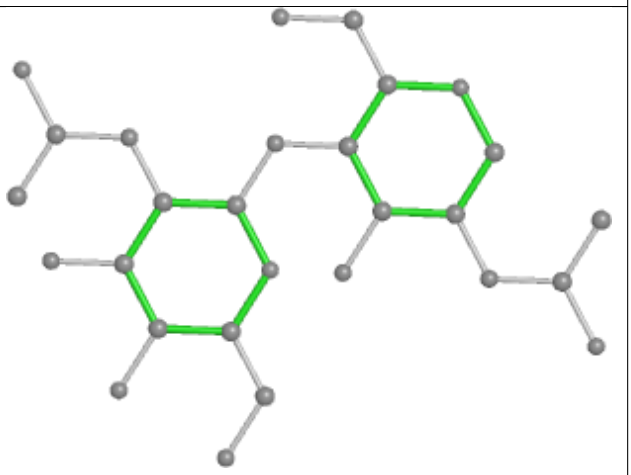
Bond lengths



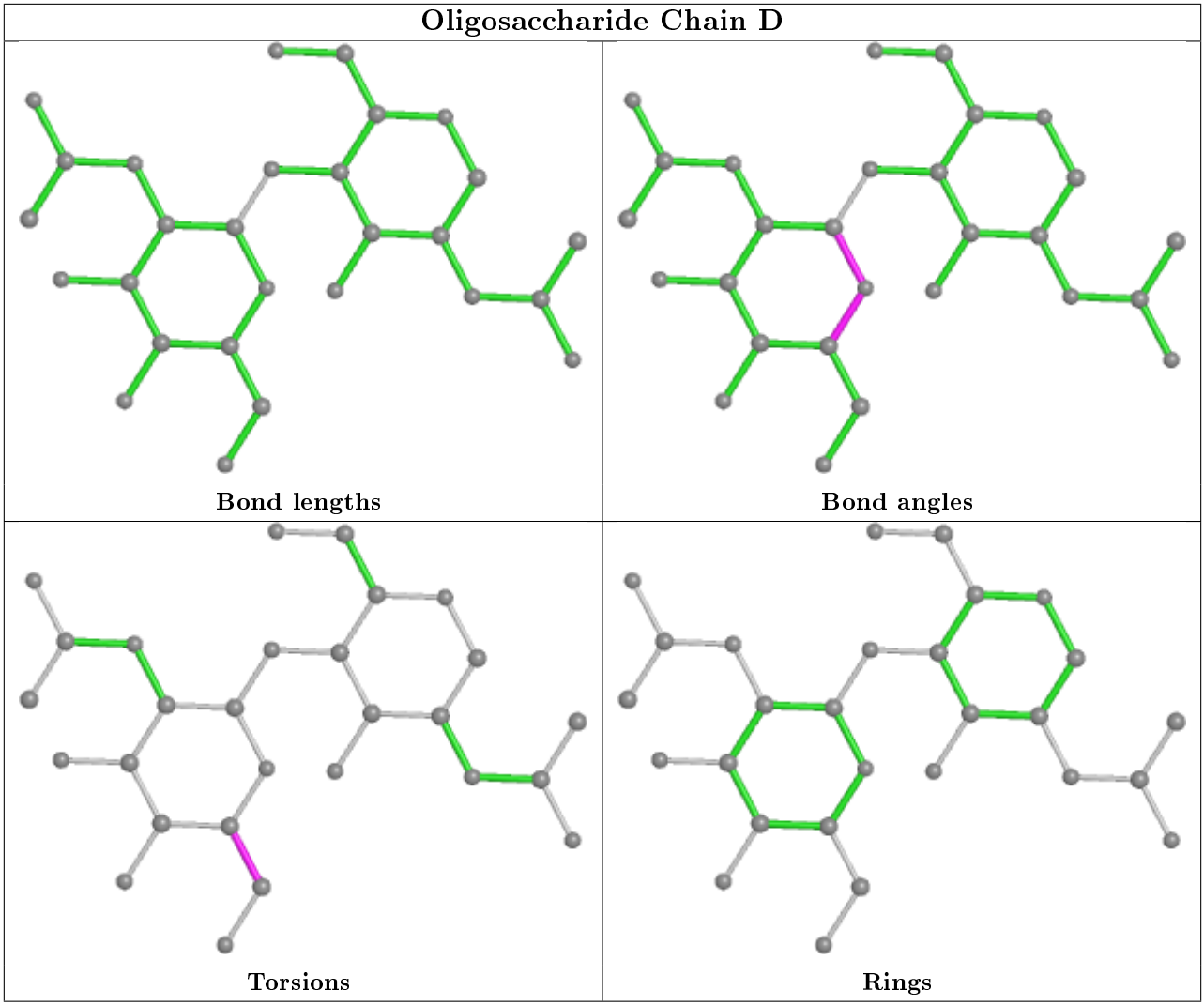
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	EDO	A	711	-	3,3,3	0.86	0	2,2,2	0.45	0
5	EDO	A	712	-	3,3,3	0.90	0	2,2,2	0.39	0
3	NAG	A	703	1	14,14,15	0.97	1 (7%)	17,19,21	1.65	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	706	1	14,14,15	0.87	1 (7%)	17,19,21	0.95	0
3	NAG	A	707	1	14,14,15	0.69	0	17,19,21	1.30	2 (11%)

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	711	-	-	0/1/1/1	-
5	EDO	A	712	-	-	0/1/1/1	-
3	NAG	A	703	1	-	2/6/23/26	0/1/1/1
3	NAG	A	706	1	-	0/6/23/26	0/1/1/1
3	NAG	A	707	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	NAG	C1-C2	2.34	1.55	1.52
3	A	703	NAG	O5-C5	2.29	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	703	NAG	O5-C5-C6	3.40	112.53	107.20
3	A	703	NAG	O5-C1-C2	-2.81	106.85	111.29
3	A	707	NAG	C8-C7-N2	2.59	120.48	116.10
3	A	703	NAG	C3-C4-C5	-2.32	106.10	110.24
3	A	703	NAG	C1-C2-N2	2.22	114.29	110.49
3	A	703	NAG	C4-C3-C2	-2.11	107.92	111.02
3	A	707	NAG	C4-C3-C2	-2.11	107.92	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	NAG	C4-C5-C6-O6
3	A	703	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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^{th} 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	596/616 (96%)	0.29	34 (5%)	23	28	64, 78, 109, 151	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	613	CYS	7.4
1	A	611	GLY	6.2
1	A	607	VAL	5.8
1	A	612	LEU	5.7
1	A	610	ASP	4.8
1	A	50	ASP	4.0
1	A	614	ARG	3.8
1	A	609	LEU	3.8
1	A	593	LYS	3.3
1	A	487	PHE	3.2
1	A	594	ILE	3.1
1	A	615	LYS	3.1
1	A	511	LEU	3.1
1	A	474	LEU	3.0
1	A	608	ASP	2.9
1	A	426	LEU	2.9
1	A	423	PHE	2.7
1	A	506	LEU	2.7
1	A	465	GLY	2.6
1	A	596	ALA	2.6
1	A	597	HIS	2.5
1	A	600	ILE	2.5
1	A	243	LEU	2.5
1	A	606	CYS	2.4
1	A	504	LEU	2.4
1	A	495	LEU	2.3
1	A	466	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	451	LYS	2.3
1	A	483	ALA	2.3
1	A	491	ILE	2.2
1	A	400	GLY	2.1
1	A	467	ILE	2.1
1	A	52	THR	2.1
1	A	440	THR	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)

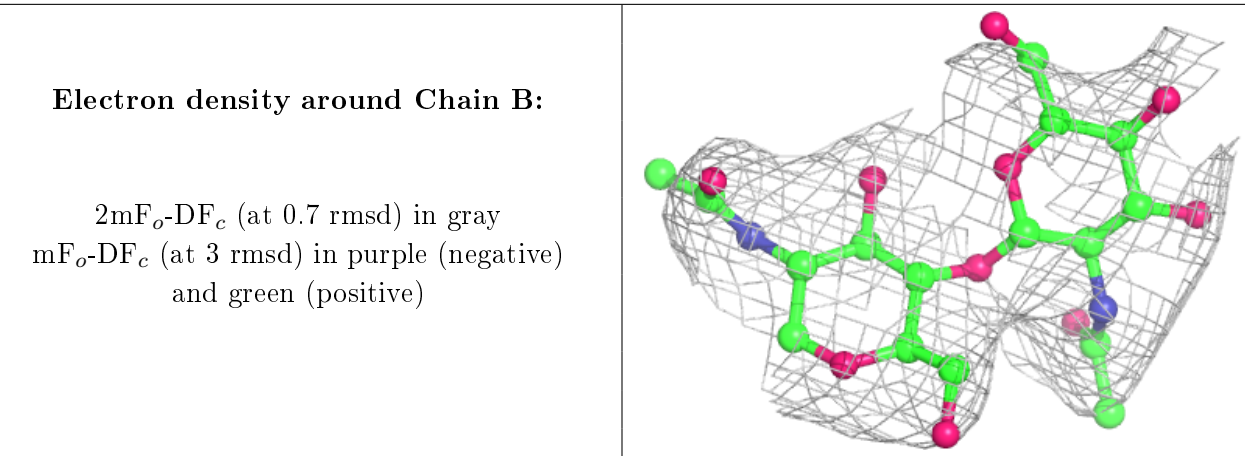
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

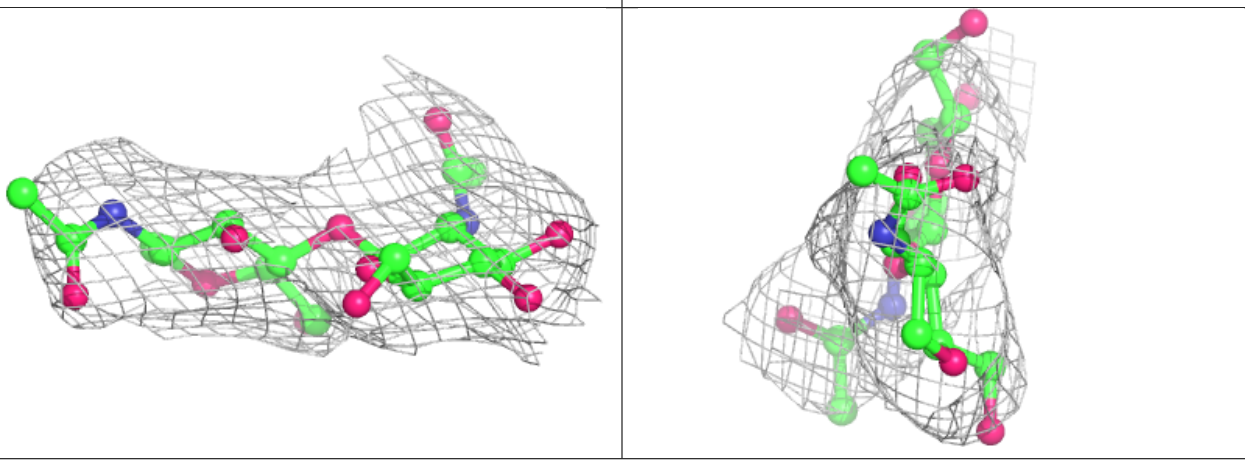
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.72	0.30	100,128,146,154	0
2	NAG	B	2	14/15	0.93	0.24	91,112,135,135	0
2	NAG	D	2	14/15	0.94	0.19	94,100,107,113	0
2	NAG	B	1	14/15	0.94	0.13	82,96,103,105	0
2	NAG	C	1	14/15	0.94	0.10	75,89,98,108	0
2	NAG	D	1	14/15	0.95	0.09	77,88,94,98	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 B:

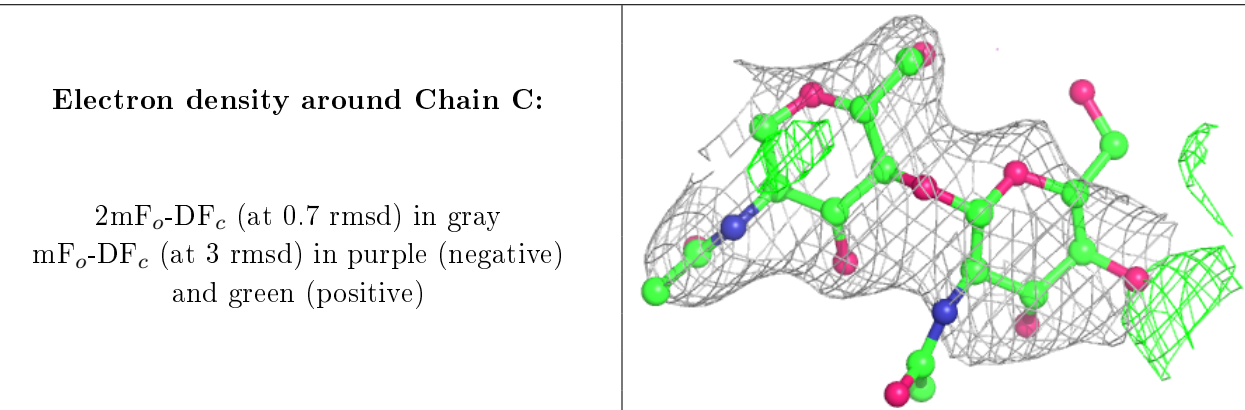
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

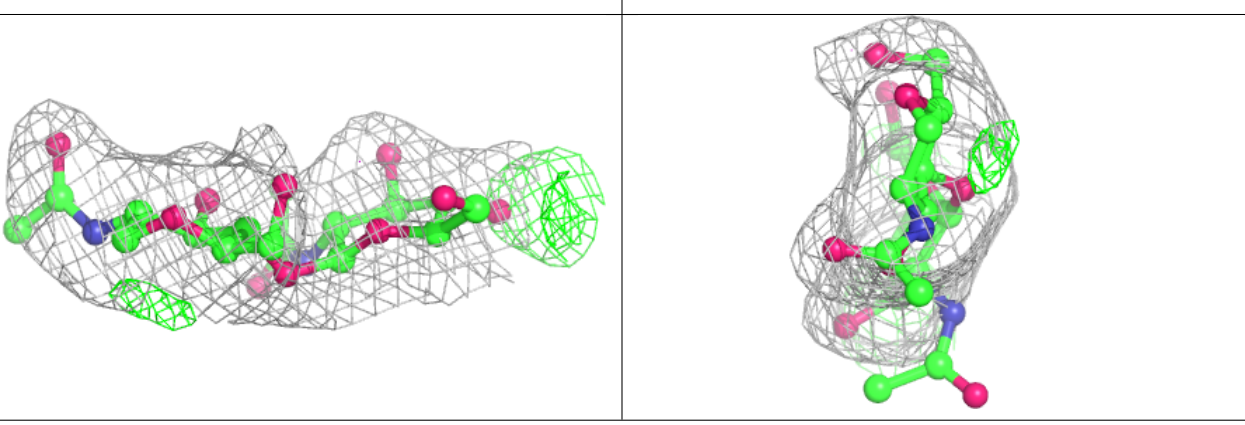




Electron density around Chain C:

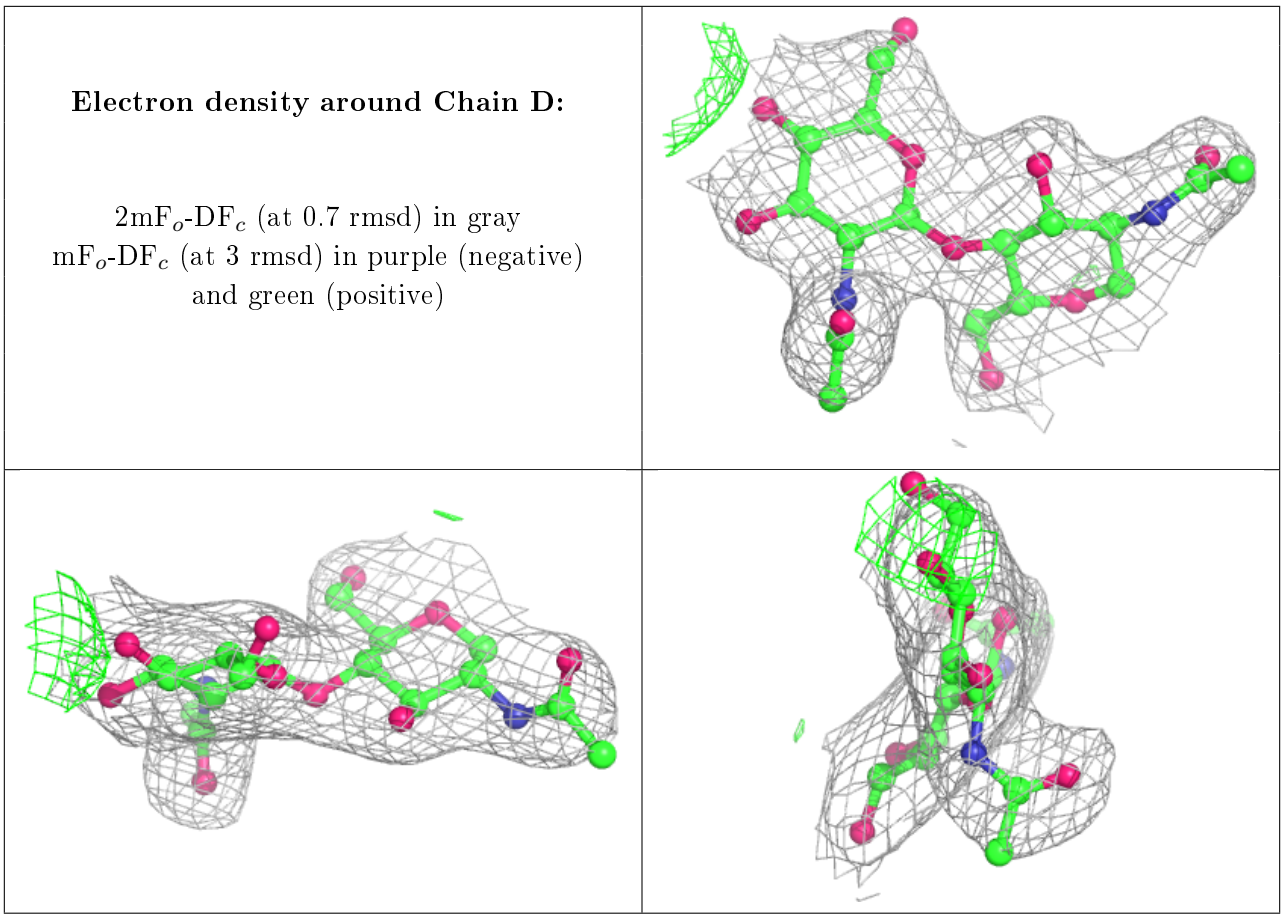
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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)



6.4 Ligands

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^{th} 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
5	EDO	A	712	4/4	0.63	0.24	89,91,92,98	0
5	EDO	A	711	4/4	0.75	0.22	86,91,92,98	0
3	NAG	A	706	14/15	0.89	0.34	89,103,111,116	0
3	NAG	A	707	14/15	0.92	0.09	76,91,106,115	0
3	NAG	A	703	14/15	0.92	0.08	86,94,106,106	0
4	MG	A	710	1/1	0.96	0.30	74,74,74,74	0

6.5 Other polymers

There are no such residues in this entry.