Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2024 – 06:37 PM EST

PDB ID	:	4EBZ
Title	:	Crystal structure of the ectodomain of a receptor like kinase
Authors	:	Chai, J.; Liu, T.; Han, Z.; She, J; Wang, J.
Deposited on	:	2012-03-26
Resolution	:	1.79 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 (i) 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 (1)) were used in the production of this report:

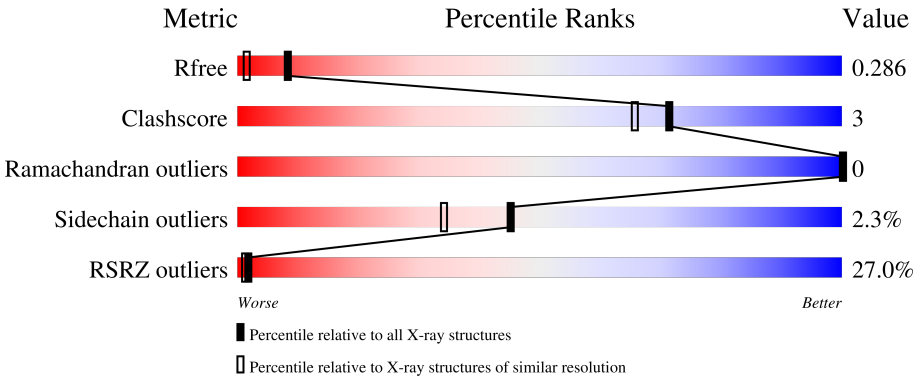
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.79 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	212	25% 86% 8% 6%
2	B	2	100%
2	C	2	50% 50%
2	D	2	50% 50%
3	E	5	80% 20%
4	F	4	75% 25%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2049 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 Chitin elicitor receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1546	969	265	304	8			

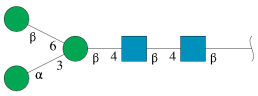
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	HIS	-	expression tag	UNP A8R7E6
A	232	HIS	-	expression tag	UNP A8R7E6
A	233	HIS	-	expression tag	UNP A8R7E6
A	234	HIS	-	expression tag	UNP A8R7E6
A	235	HIS	-	expression tag	UNP A8R7E6
A	236	HIS	-	expression tag	UNP A8R7E6

- 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			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]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
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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	4	Total	C	N	O	0	0	0
			57	32	4	21			

- Molecule 5 is water.

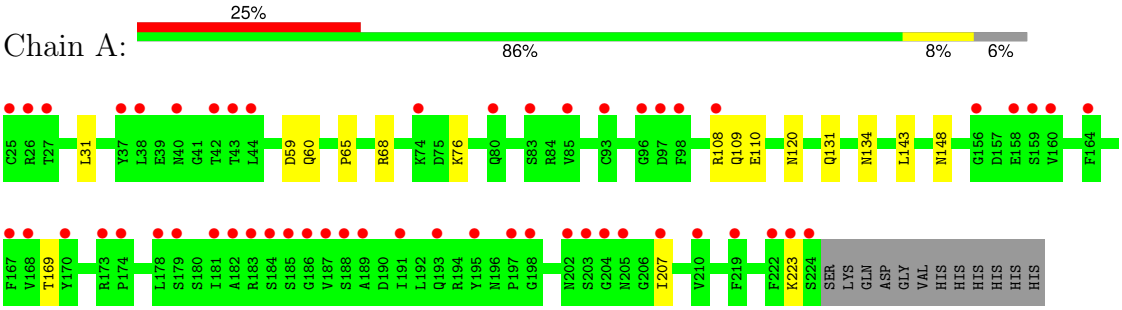
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	301	Total	O	0	0
			301	301		

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. 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. 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.

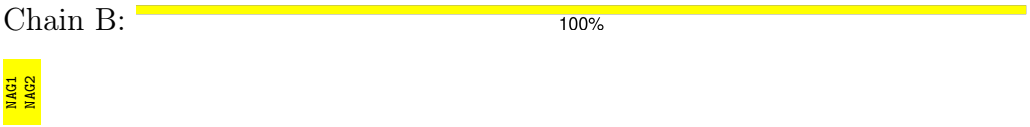
• Molecule 1: Chitin elicitor receptor kinase 1

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:

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

Chain E:

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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.47Å 71.32Å 72.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.94 – 1.79 14.94 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.6 (14.94-1.79) 99.0 (14.94-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.37 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_596)	Depositor
R, R_{free}	0.175 , 0.209 0.254 , 0.286	Depositor DCC
R_{free} test set	1431 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2049	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: BMA, NAG, MAN

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	0/1582	0.63	1/2157 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	ARG	NE-CZ-NH2	-6.22	117.19	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1546	0	1481	11	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	E	61	0	52	0	0
4	F	57	0	51	0	0
5	A	301	0	0	3	0
All	All	2049	0	1659	11	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 (11) 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:134:ASN:HD21	1:A:148:ASN:H	1.16	0.90
1:A:65:PRO:HB3	5:A:1088:HOH:O	2.00	0.61
1:A:109:GLN:HG3	1:A:110:GLU:CG	2.36	0.56
1:A:109:GLN:HG3	1:A:110:GLU:HG2	1.91	0.51
1:A:223:LYS:HE2	5:A:1047:HOH:O	2.10	0.50
1:A:134:ASN:HD21	1:A:148:ASN:N	1.99	0.49
1:A:108:ARG:HH11	1:A:120:ASN:HD21	1.62	0.47
1:A:109:GLN:HG3	1:A:110:GLU:HG3	1.98	0.46
1:A:59:ASP:O	1:A:60:GLN:HB2	2.17	0.45
1:A:169:THR:HG23	1:A:207:ILE:HD13	2.02	0.41
1:A:223:LYS:HG2	5:A:1051:HOH:O	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	198/212 (93%)	191 (96%)	7 (4%)	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	177/188 (94%)	173 (98%)	4 (2%)	45 34

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	76	LYS
1	A	131	GLN
1	A	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	109	GLN
1	A	120	ASN
1	A	134	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)

15 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	2,1	14,14,15	0.61	0	17,19,21	1.40	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	2	2	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
2	NAG	C	1	2,1	14,14,15	0.52	0	17,19,21	1.30	1 (5%)
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	0.91	0
2	NAG	D	1	2,1	14,14,15	0.62	0	17,19,21	1.19	1 (5%)
2	NAG	D	2	2	14,14,15	0.52	0	17,19,21	0.67	0
3	NAG	E	1	3,1	14,14,15	0.65	0	17,19,21	1.35	2 (11%)
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	0.74	0
3	BMA	E	3	3	11,11,12	0.65	0	15,15,17	0.75	0
3	MAN	E	4	3	11,11,12	0.66	0	15,15,17	0.59	0
3	BMA	E	5	3	11,11,12	0.65	0	15,15,17	0.85	0
4	NAG	F	1	4	15,15,15	0.46	0	21,21,21	0.80	0
4	NAG	F	2	4	14,14,15	0.45	0	17,19,21	0.84	0
4	NAG	F	3	4	14,14,15	0.55	0	17,19,21	1.19	2 (11%)
4	NAG	F	4	4	14,14,15	0.53	0	17,19,21	0.61	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
2	NAG	B	1	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	BMA	E	5	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4	-	0/6/26/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	3	4	-	0/6/23/26	0/1/1/1
4	NAG	F	4	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	O5-C1-C2	-3.74	105.50	111.29
2	C	1	NAG	O5-C1-C2	-3.44	105.96	111.29
3	E	1	NAG	O5-C1-C2	-3.29	106.20	111.29
2	D	1	NAG	O5-C1-C2	-2.99	106.66	111.29
2	B	2	NAG	C1-O5-C5	2.26	115.22	112.19
4	F	3	NAG	C6-C5-C4	-2.14	107.76	113.02
3	E	1	NAG	O7-C7-C8	-2.08	118.35	122.05
4	F	3	NAG	C2-N2-C7	-2.02	120.19	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

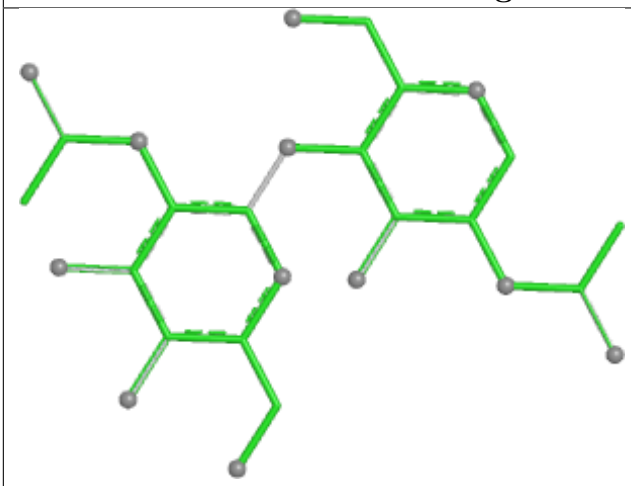
Mol	Chain	Res	Type	Atoms
3	E	5	BMA	O5-C5-C6-O6
3	E	5	BMA	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

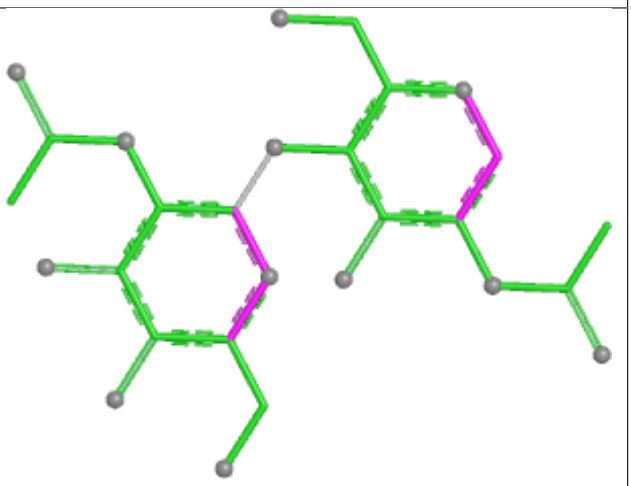
No monomer is involved in short contacts.

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

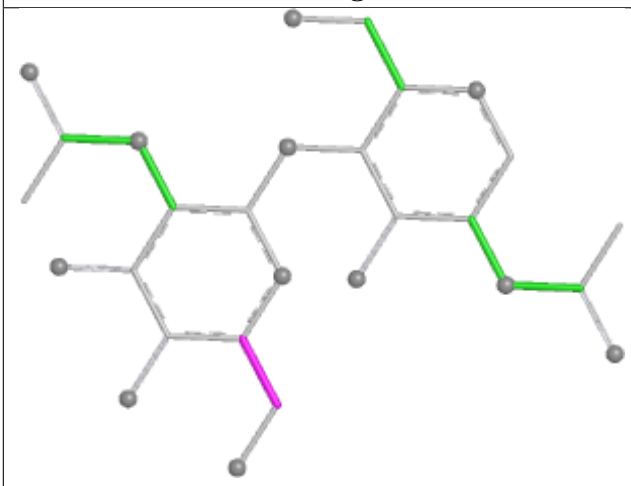
Oligosaccharide Chain B



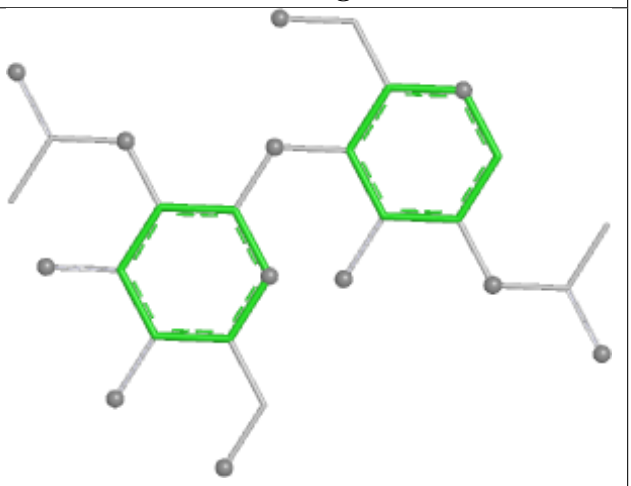
Bond lengths



Bond angles

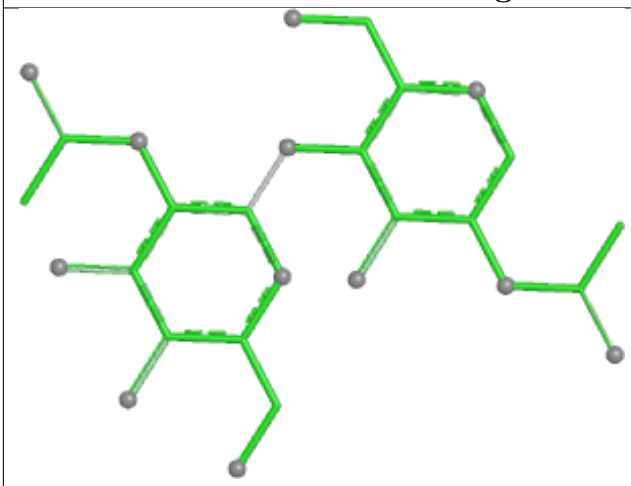


Torsions

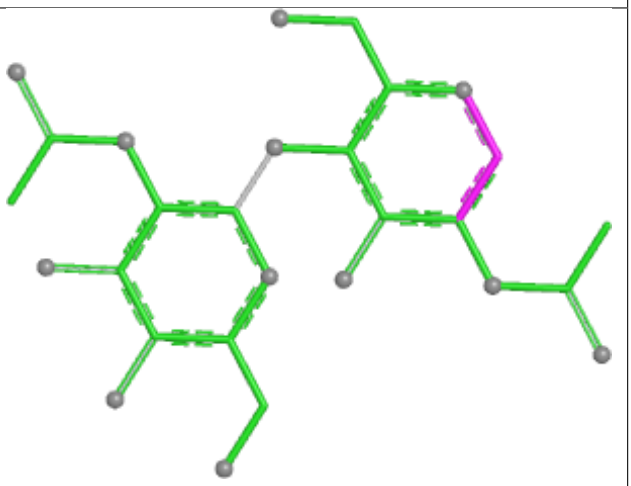


Rings

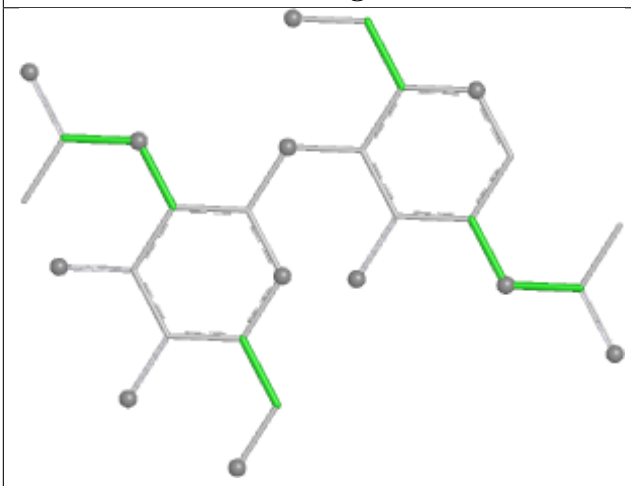
Oligosaccharide Chain C



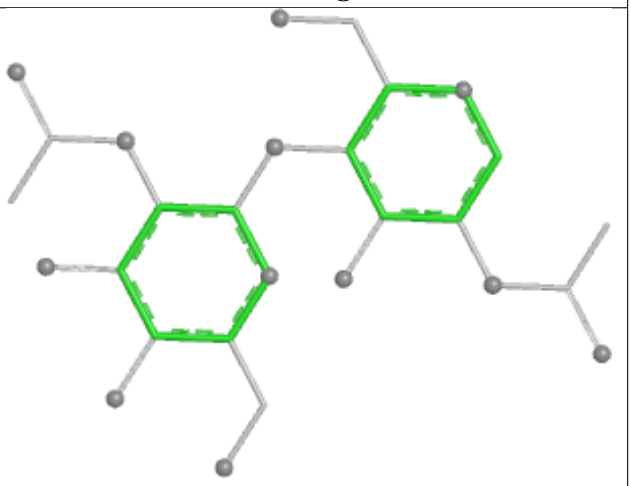
Bond lengths



Bond angles

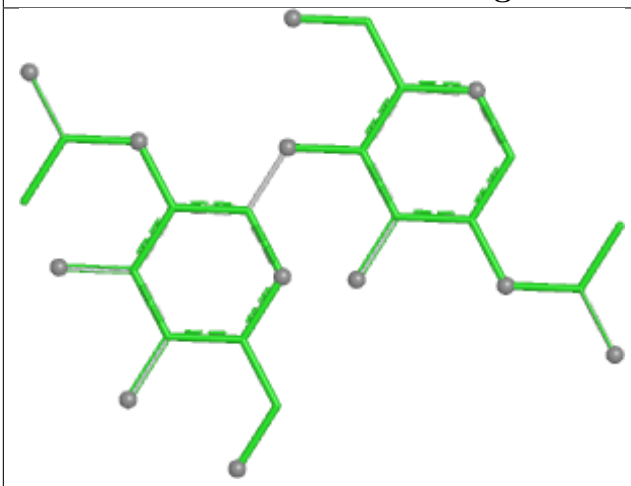


Torsions

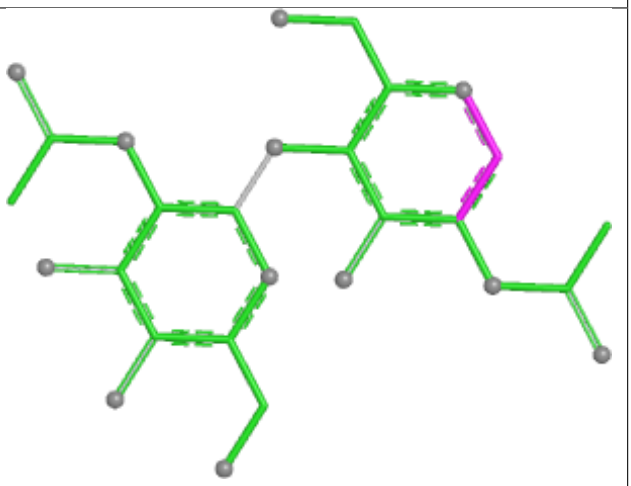


Rings

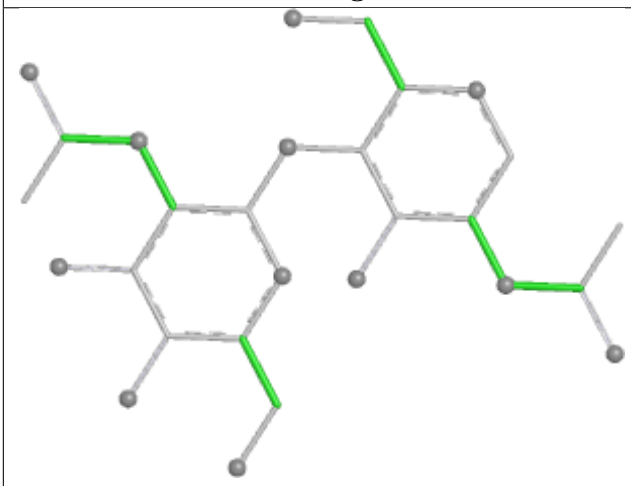
Oligosaccharide Chain D



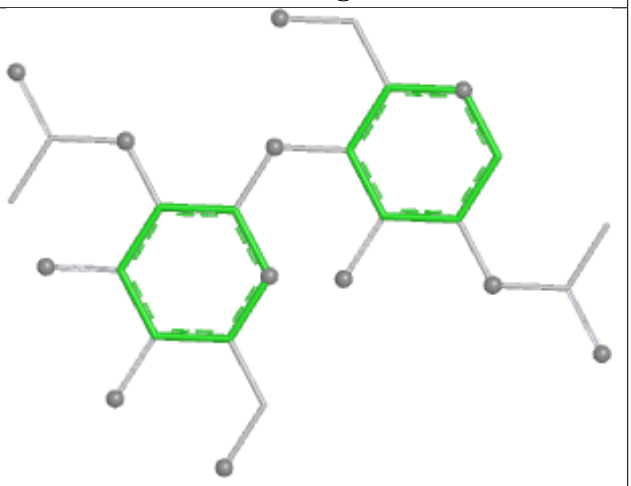
Bond lengths



Bond angles

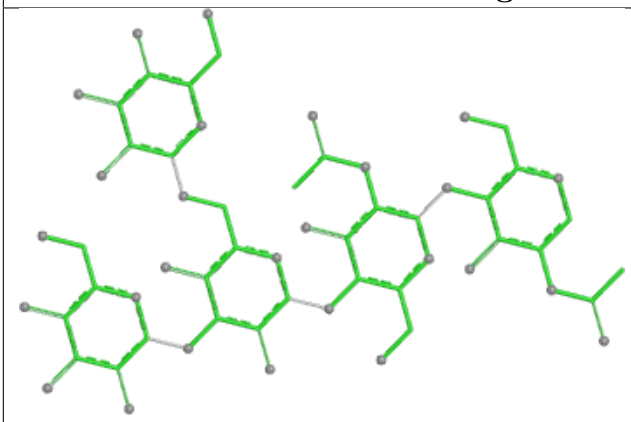


Torsions

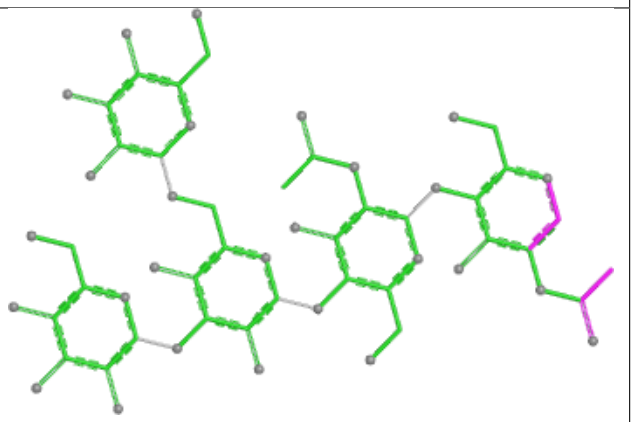


Rings

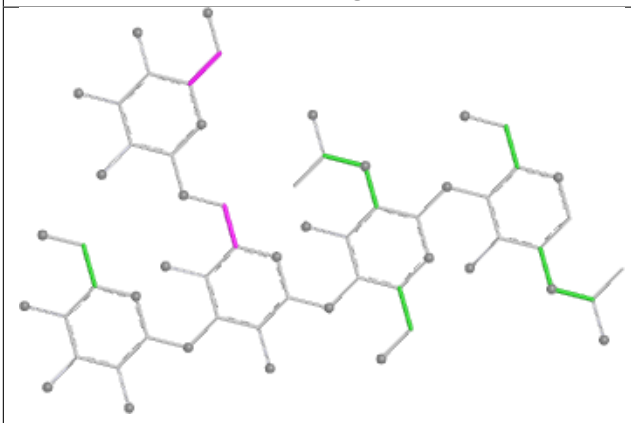
Oligosaccharide Chain E



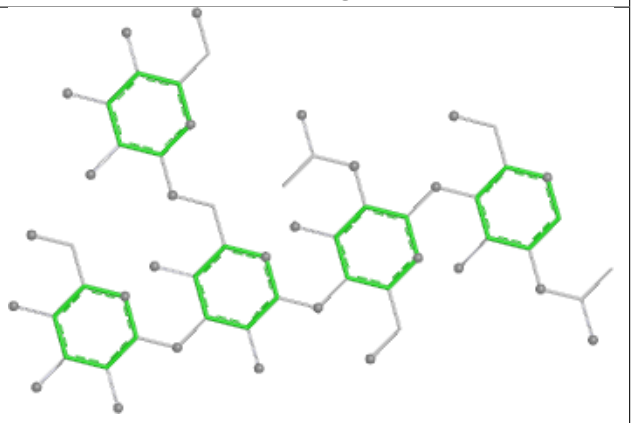
Bond lengths



Bond angles

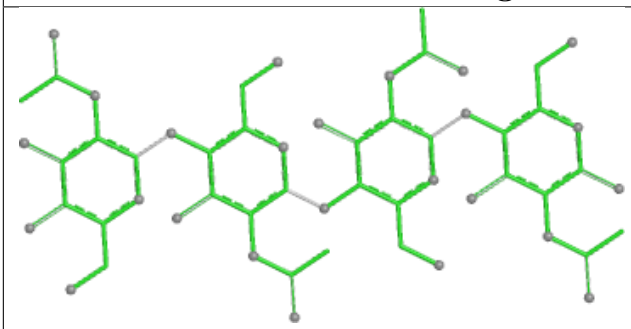


Torsions

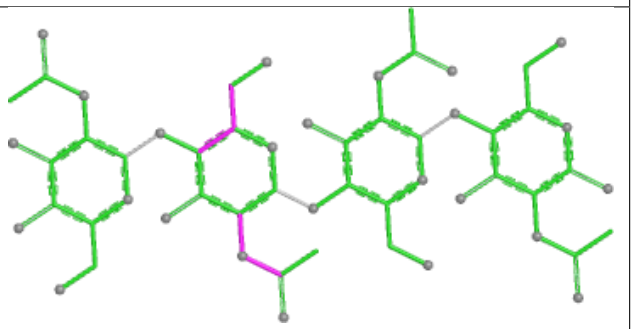


Rings

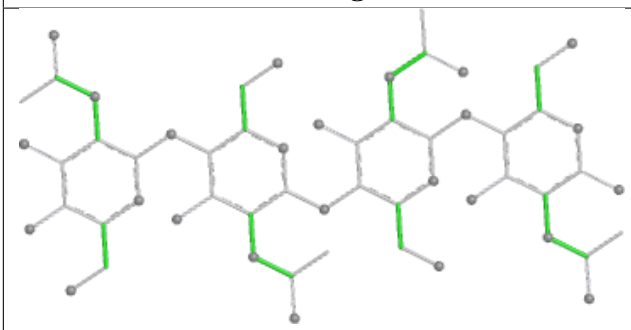
Oligosaccharide Chain F



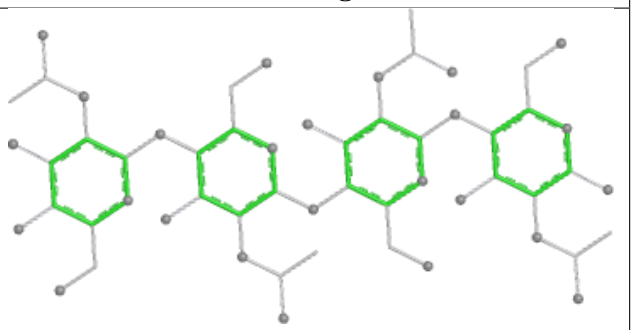
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

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

Warning: The R factor obtained from EDS is 0.2578, which does not match the depositor's R factor of 0.1746. Please interpret the results in this section carefully.

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	200/212 (94%)	1.42	54 (27%) 2 1	18, 27, 48, 71	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	PRO	4.5
1	A	181	ILE	4.1
1	A	74	LYS	4.0
1	A	179	SER	3.6
1	A	187	VAL	3.5
1	A	224	SER	3.5
1	A	25	CYS	3.5
1	A	183	ARG	3.3
1	A	182	ALA	3.2
1	A	27	THR	3.1
1	A	203	SER	3.1
1	A	160	VAL	3.1
1	A	191	ILE	3.0
1	A	195	TYR	3.0
1	A	198	GLY	3.0
1	A	178	LEU	2.9
1	A	197	PRO	2.9
1	A	185	SER	2.8
1	A	26	ARG	2.8
1	A	37	TYR	2.8
1	A	189	ALA	2.7
1	A	156	GLY	2.7
1	A	85	VAL	2.6
1	A	167	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	207	ILE	2.6
1	A	43	THR	2.6
1	A	83	SER	2.6
1	A	202	ASN	2.5
1	A	80	GLN	2.5
1	A	159	SER	2.4
1	A	96	GLY	2.4
1	A	205	ASN	2.4
1	A	164	PHE	2.4
1	A	98	PHE	2.3
1	A	223	LYS	2.3
1	A	108	ARG	2.3
1	A	188	SER	2.3
1	A	42	THR	2.3
1	A	222	PHE	2.2
1	A	204	GLY	2.2
1	A	173	ARG	2.2
1	A	158	GLU	2.2
1	A	219	PHE	2.2
1	A	38	LEU	2.2
1	A	184	SER	2.2
1	A	186	GLY	2.1
1	A	170	TYR	2.1
1	A	210	VAL	2.1
1	A	97	ASP	2.1
1	A	44	LEU	2.1
1	A	93	CYS	2.1
1	A	193	GLN	2.0
1	A	168	VAL	2.0
1	A	40	ASN	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)

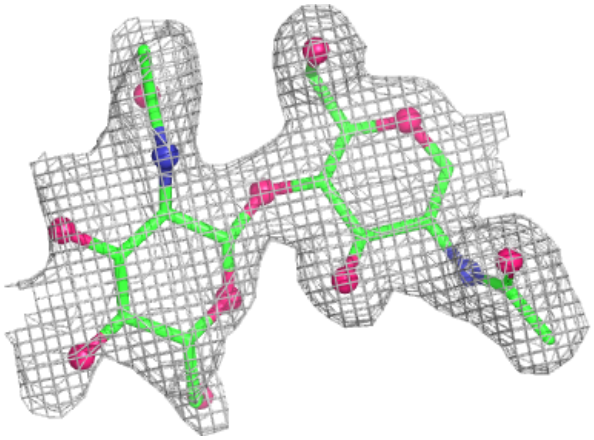
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

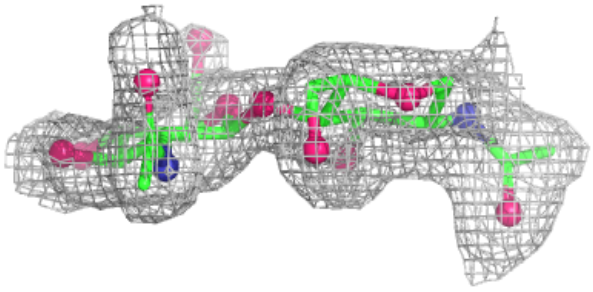
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	E	5	11/12	0.39	0.18	73,80,88,89	0
3	MAN	E	4	11/12	0.43	0.22	76,83,88,91	0
2	NAG	C	2	14/15	0.62	0.17	45,50,65,72	0
2	NAG	B	2	14/15	0.65	0.17	44,57,69,74	0
2	NAG	D	2	14/15	0.76	0.14	38,49,66,68	0
3	BMA	E	3	11/12	0.81	0.14	45,57,65,69	0
4	NAG	F	4	14/15	0.81	0.12	43,47,52,60	0
3	NAG	E	2	14/15	0.82	0.13	33,39,43,48	0
4	NAG	F	3	14/15	0.84	0.12	28,31,40,43	0
2	NAG	D	1	14/15	0.84	0.11	24,32,43,52	0
2	NAG	C	1	14/15	0.85	0.12	21,26,37,40	0
4	NAG	F	1	15/15	0.85	0.12	28,36,52,59	0
3	NAG	E	1	14/15	0.86	0.11	25,29,31,32	0
4	NAG	F	2	14/15	0.89	0.11	26,32,45,45	0
2	NAG	B	1	14/15	0.94	0.09	20,28,32,34	0

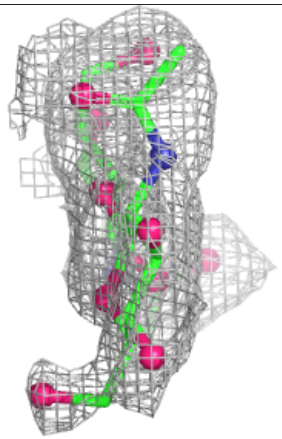
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

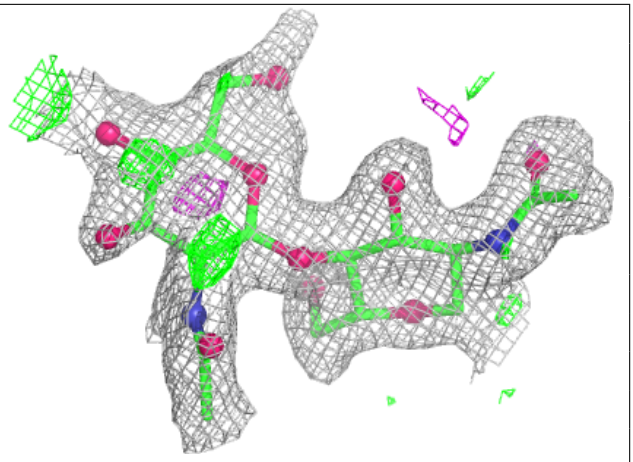


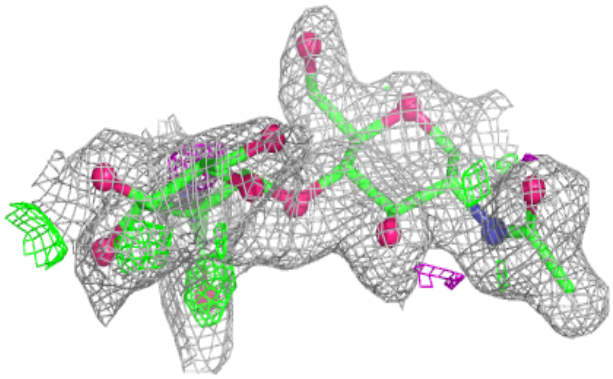


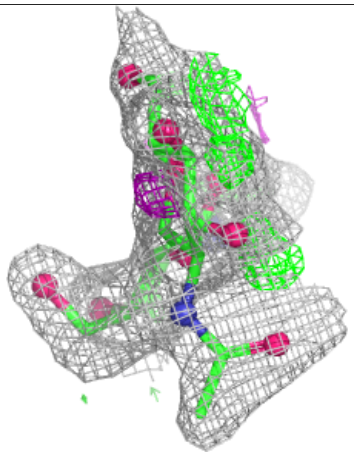


Electron density around Chain C:

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

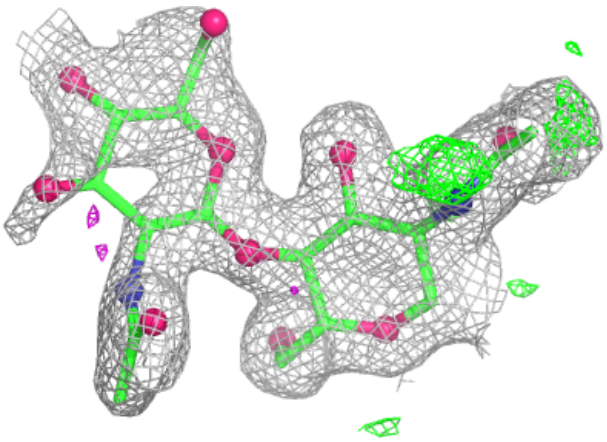


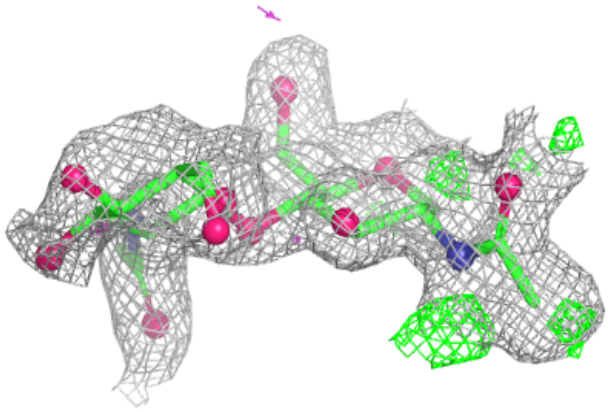


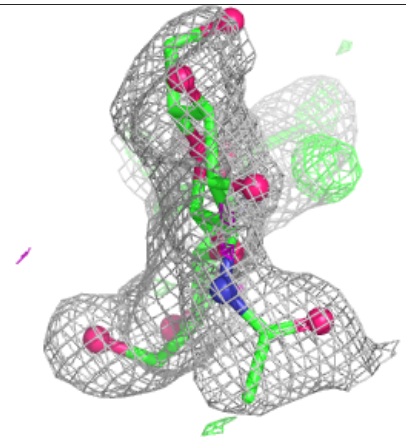


Electron density around Chain D:

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

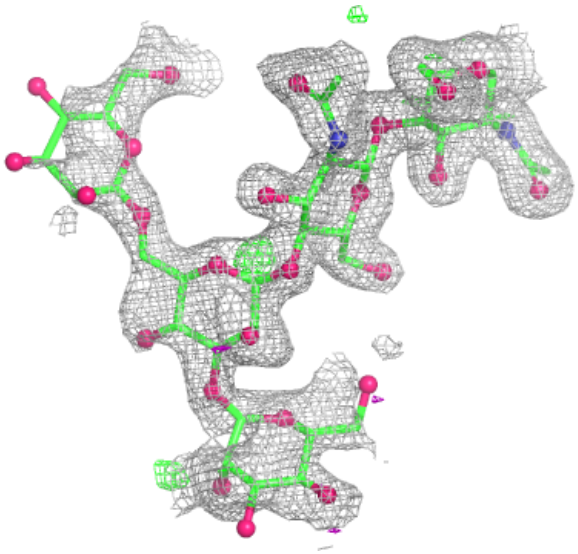


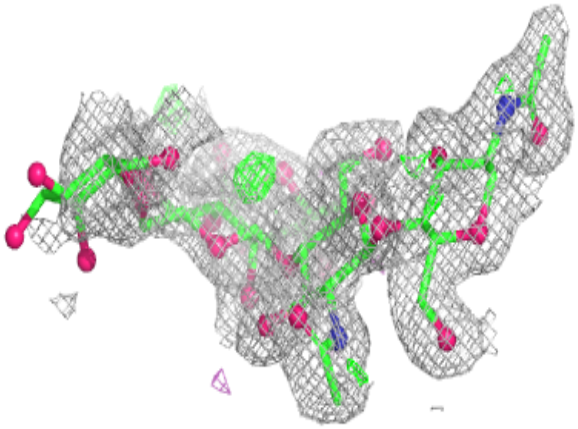


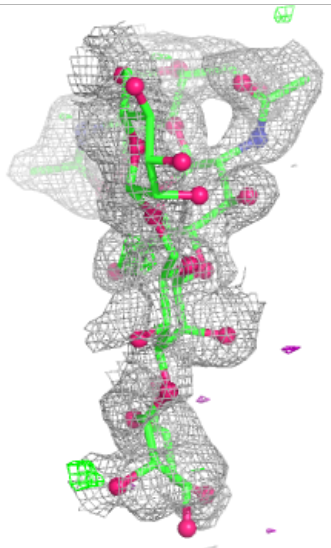


Electron density around Chain E:

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

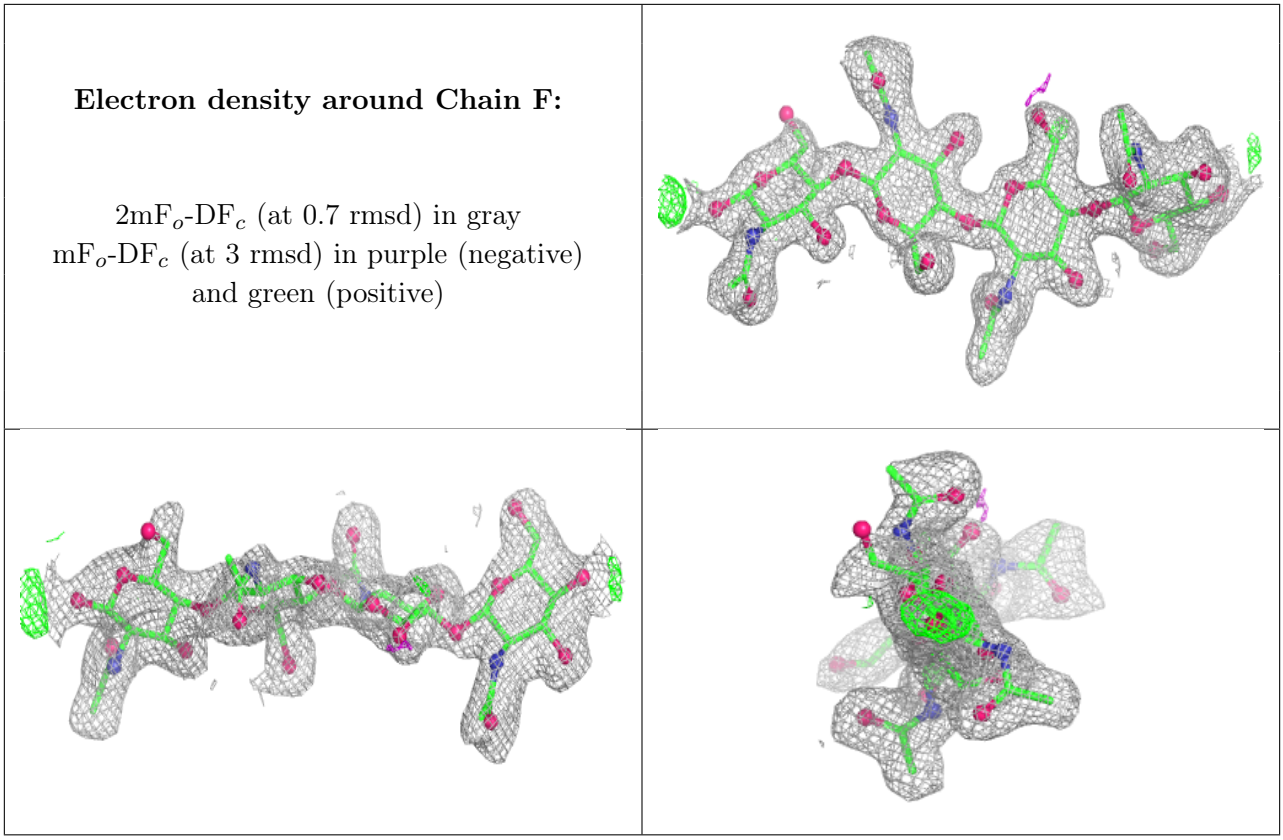






Electron density around Chain F:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.