wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 02:22 PM JST

PDB ID	:	5Z8Y
Title	:	Crystal structure of human LRRTM2 in complex with Neurexin 1beta
Authors	:	Yamagata, A.; Fukai, S.
Deposited on	:	2018-02-01
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

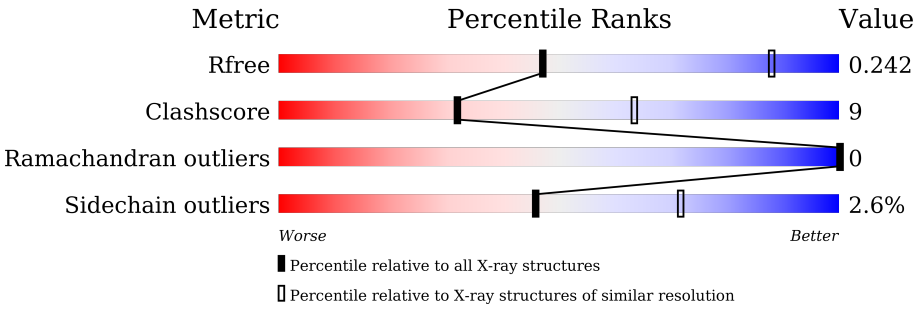
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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	346	71% 23% • 5%
1	C	346	71% 23% • 5%
1	E	346	71% 23% • 5%
1	G	346	73% 21% • 5%
2	B	193	70% 22% • 8%
2	D	193	73% 19% • 8%
2	F	193	70% 21% • 8%

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Mol	Chain	Length	Quality of chain
2	H	193	
3	I	3	
3	J	3	
3	K	3	
3	L	3	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16410 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 Leucine-rich repeat transmembrane neuronal protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2655	1696	465	481	13			
1	C	328	Total	C	N	O	S	0	0	0
			2655	1696	465	481	13			
1	E	328	Total	C	N	O	S	0	0	0
			2655	1696	465	481	13			
1	G	328	Total	C	N	O	S	0	0	0
			2655	1696	465	481	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	ALA	HIS	engineered mutation	UNP O43300
A	372	GLY	-	expression tag	UNP O43300
A	373	SER	-	expression tag	UNP O43300
A	374	HIS	-	expression tag	UNP O43300
A	375	HIS	-	expression tag	UNP O43300
A	376	HIS	-	expression tag	UNP O43300
A	377	HIS	-	expression tag	UNP O43300
A	378	HIS	-	expression tag	UNP O43300
A	379	HIS	-	expression tag	UNP O43300
C	355	ALA	HIS	engineered mutation	UNP O43300
C	372	GLY	-	expression tag	UNP O43300
C	373	SER	-	expression tag	UNP O43300
C	374	HIS	-	expression tag	UNP O43300
C	375	HIS	-	expression tag	UNP O43300
C	376	HIS	-	expression tag	UNP O43300
C	377	HIS	-	expression tag	UNP O43300
C	378	HIS	-	expression tag	UNP O43300
C	379	HIS	-	expression tag	UNP O43300
E	355	ALA	HIS	engineered mutation	UNP O43300
E	372	GLY	-	expression tag	UNP O43300
E	373	SER	-	expression tag	UNP O43300

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Chain	Residue	Modelled	Actual	Comment	Reference
E	374	HIS	-	expression tag	UNP O43300
E	375	HIS	-	expression tag	UNP O43300
E	376	HIS	-	expression tag	UNP O43300
E	377	HIS	-	expression tag	UNP O43300
E	378	HIS	-	expression tag	UNP O43300
E	379	HIS	-	expression tag	UNP O43300
G	355	ALA	HIS	engineered mutation	UNP O43300
G	372	GLY	-	expression tag	UNP O43300
G	373	SER	-	expression tag	UNP O43300
G	374	HIS	-	expression tag	UNP O43300
G	375	HIS	-	expression tag	UNP O43300
G	376	HIS	-	expression tag	UNP O43300
G	377	HIS	-	expression tag	UNP O43300
G	378	HIS	-	expression tag	UNP O43300
G	379	HIS	-	expression tag	UNP O43300

- Molecule 2 is a protein called Neurexin-1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1365	860	244	260	1			
2	D	178	Total	C	N	O	S	0	0	0
			1365	860	244	260	1			
2	F	178	Total	C	N	O	S	0	0	0
			1365	860	244	260	1			
2	H	178	Total	C	N	O	S	0	0	0
			1365	860	244	260	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	ASP	-	expression tag	UNP P58400
B	83	ALA	-	expression tag	UNP P58400
B	84	ALA	-	expression tag	UNP P58400
B	85	SER	-	expression tag	UNP P58400
B	267	GLY	-	expression tag	UNP P58400
B	268	SER	-	expression tag	UNP P58400
B	269	HIS	-	expression tag	UNP P58400
B	270	HIS	-	expression tag	UNP P58400
B	271	HIS	-	expression tag	UNP P58400
B	272	HIS	-	expression tag	UNP P58400
B	273	HIS	-	expression tag	UNP P58400

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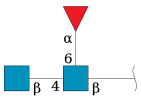
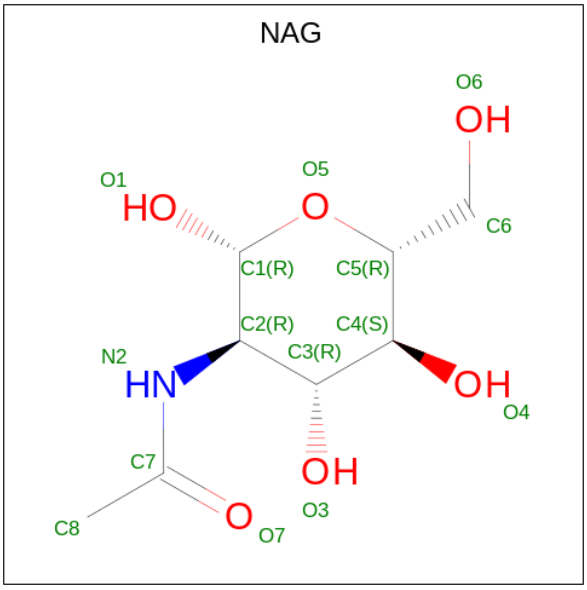
Chain	Residue	Modelled	Actual	Comment	Reference
B	274	HIS	-	expression tag	UNP P58400
D	82	ASP	-	expression tag	UNP P58400
D	83	ALA	-	expression tag	UNP P58400
D	84	ALA	-	expression tag	UNP P58400
D	85	SER	-	expression tag	UNP P58400
D	267	GLY	-	expression tag	UNP P58400
D	268	SER	-	expression tag	UNP P58400
D	269	HIS	-	expression tag	UNP P58400
D	270	HIS	-	expression tag	UNP P58400
D	271	HIS	-	expression tag	UNP P58400
D	272	HIS	-	expression tag	UNP P58400
D	273	HIS	-	expression tag	UNP P58400
D	274	HIS	-	expression tag	UNP P58400
F	82	ASP	-	expression tag	UNP P58400
F	83	ALA	-	expression tag	UNP P58400
F	84	ALA	-	expression tag	UNP P58400
F	85	SER	-	expression tag	UNP P58400
F	267	GLY	-	expression tag	UNP P58400
F	268	SER	-	expression tag	UNP P58400
F	269	HIS	-	expression tag	UNP P58400
F	270	HIS	-	expression tag	UNP P58400
F	271	HIS	-	expression tag	UNP P58400
F	272	HIS	-	expression tag	UNP P58400
F	273	HIS	-	expression tag	UNP P58400
F	274	HIS	-	expression tag	UNP P58400
H	82	ASP	-	expression tag	UNP P58400
H	83	ALA	-	expression tag	UNP P58400
H	84	ALA	-	expression tag	UNP P58400
H	85	SER	-	expression tag	UNP P58400
H	267	GLY	-	expression tag	UNP P58400
H	268	SER	-	expression tag	UNP P58400
H	269	HIS	-	expression tag	UNP P58400
H	270	HIS	-	expression tag	UNP P58400
H	271	HIS	-	expression tag	UNP P58400
H	272	HIS	-	expression tag	UNP P58400
H	273	HIS	-	expression tag	UNP P58400
H	274	HIS	-	expression tag	UNP P58400

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	I	3	Total C N O 38 22 2 14	0	0	0
3	J	3	Total C N O 38 22 2 14	0	0	0
3	K	3	Total C N O 38 22 2 14	0	0	0
3	L	3	Total C N O 38 22 2 14	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0
6	H	1	Total Ca 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0

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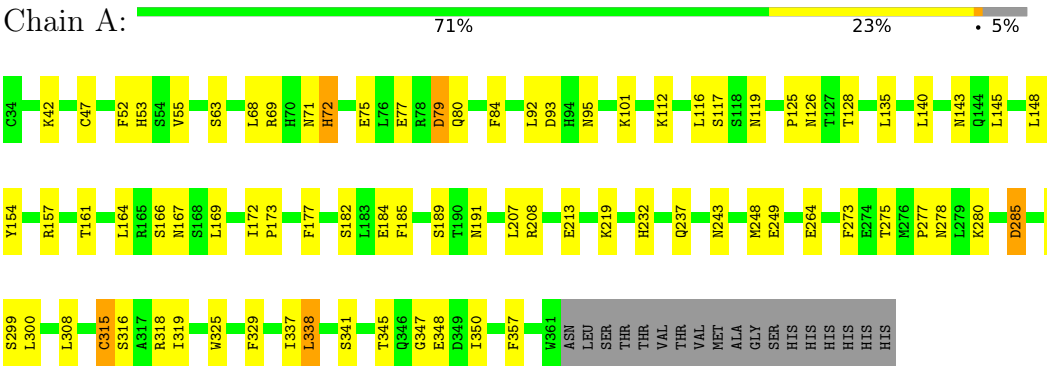
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total O 1 1	0	0
7	H	1	Total O 1 1	0	0

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. 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.

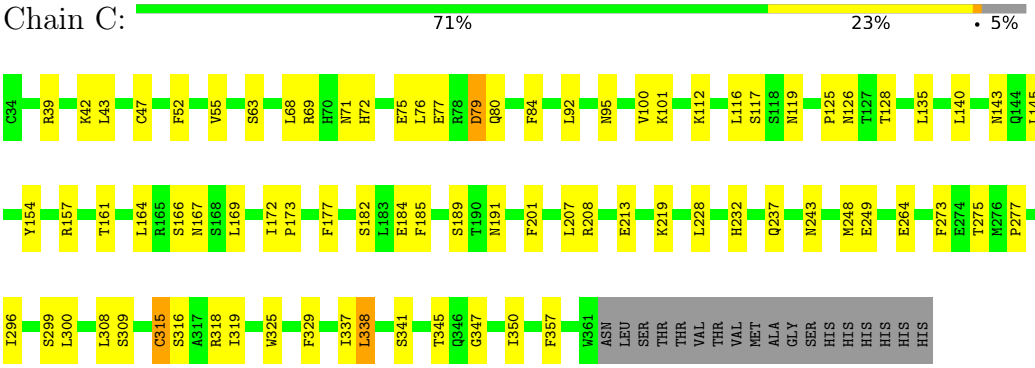
• Molecule 1: Leucine-rich repeat transmembrane neuronal protein 2

Chain A:



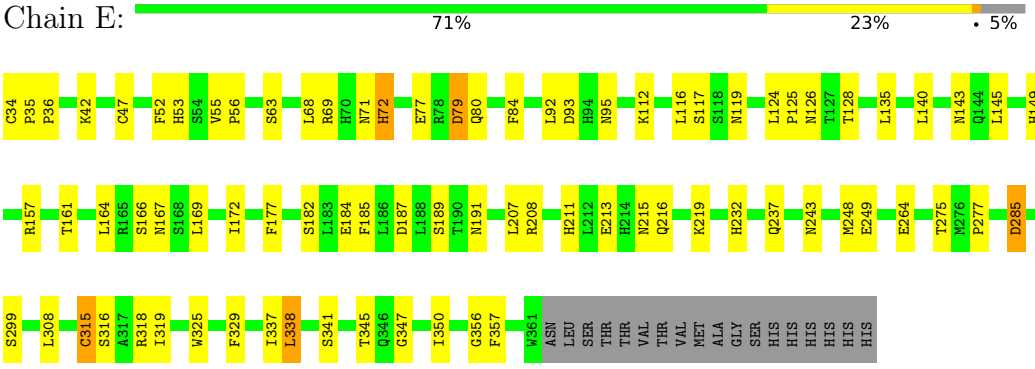
• Molecule 1: Leucine-rich repeat transmembrane neuronal protein 2

Chain C:



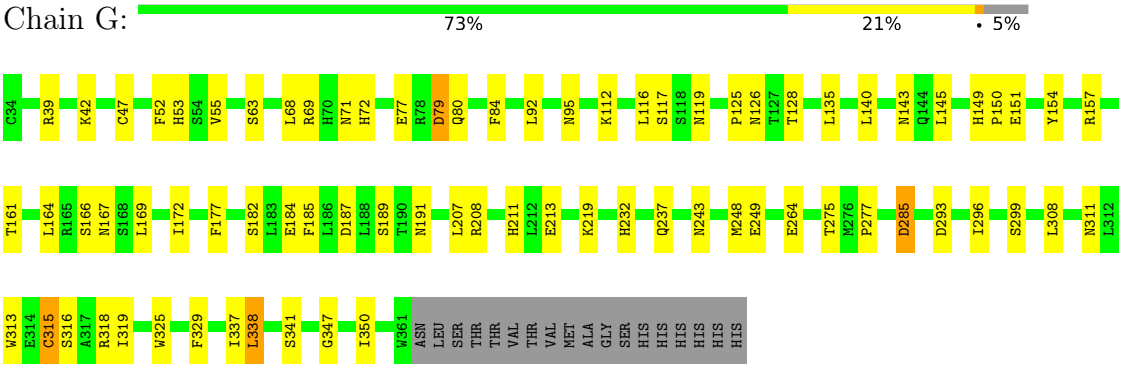
• Molecule 1: Leucine-rich repeat transmembrane neuronal protein 2

Chain E:



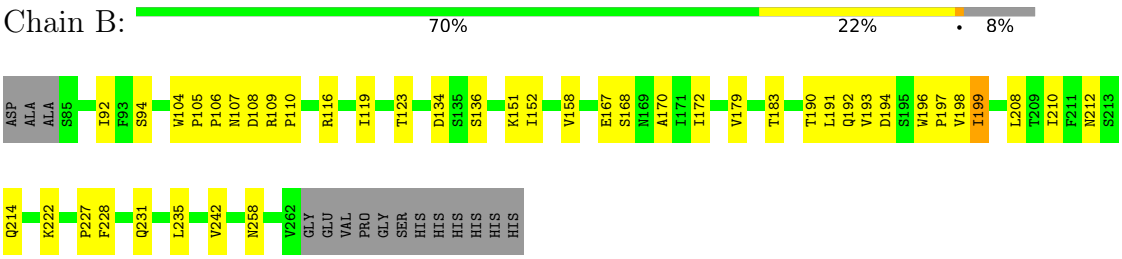
• Molecule 1: Leucine-rich repeat transmembrane neuronal protein 2

Chain G:



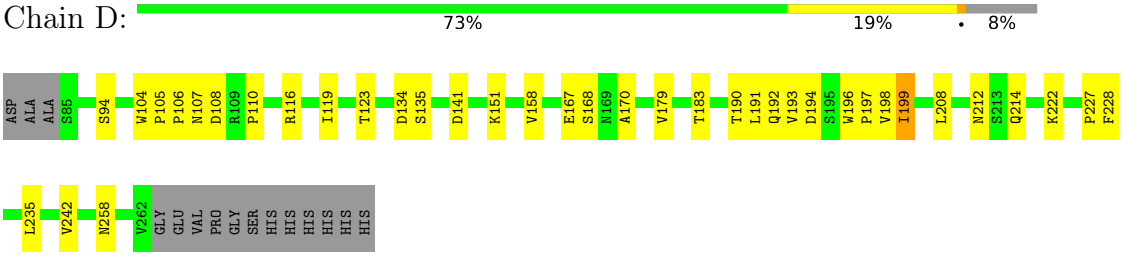
• Molecule 2: Neurexin-1-beta

Chain B:



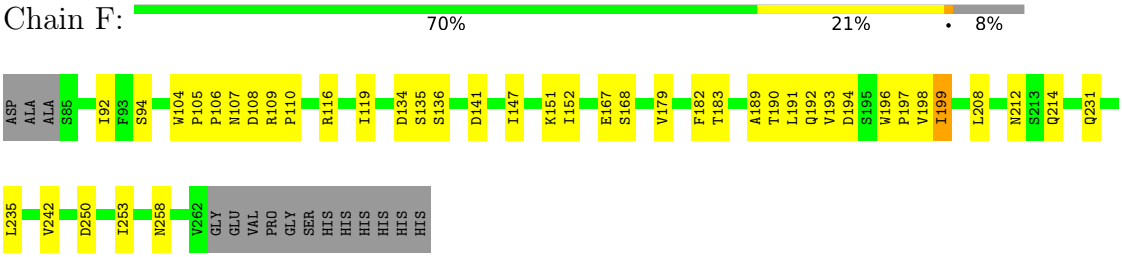
• Molecule 2: Neurexin-1-beta

Chain D:



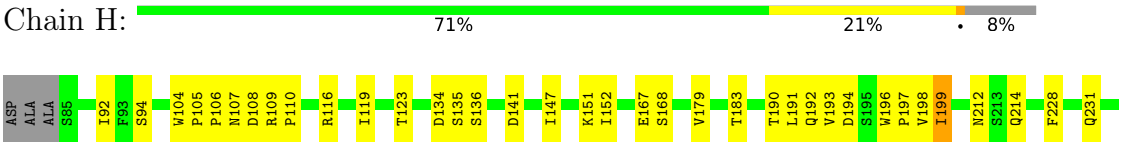
• Molecule 2: Neurexin-1-beta

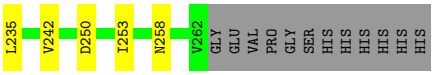
Chain F:



• Molecule 2: Neurexin-1-beta

Chain H:





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

Chain I:

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

Chain J:

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

Chain K:

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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.18Å 99.86Å 109.63Å 91.30° 91.20° 116.47°	Depositor
Resolution (Å)	49.81 – 3.40 49.82 – 3.39	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.81-3.40) 85.6 (49.82-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.209 , 0.241 0.211 , 0.242	Depositor DCC
R_{free} test set	2395 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	75.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 100.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.095 for -h,-k,l 0.096 for k,h,-l 0.417 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	16410	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: ZN, FUC, NAG, CA

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	0.24	0/2716	0.43	0/3679
1	C	0.24	0/2716	0.43	0/3679
1	E	0.24	0/2716	0.43	0/3679
1	G	0.24	0/2716	0.43	0/3679
2	B	0.26	0/1391	0.49	0/1885
2	D	0.26	0/1391	0.50	0/1885
2	F	0.26	0/1391	0.49	0/1885
2	H	0.26	0/1391	0.49	0/1885
All	All	0.25	0/16428	0.45	0/22256

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

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	2655	0	2640	57	0
1	C	2655	0	2640	55	0
1	E	2655	0	2640	56	0
1	G	2655	0	2640	50	0
2	B	1365	0	1351	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1365	0	1351	22	0
2	F	1365	0	1351	23	0
2	H	1365	0	1351	22	0
3	I	38	0	34	0	0
3	J	38	0	34	0	0
3	K	38	0	34	0	0
3	L	38	0	34	0	0
4	A	42	0	39	0	0
4	C	42	0	39	0	0
4	E	42	0	39	0	0
4	G	42	0	39	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
All	All	16410	0	16256	292	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 9.

The worst 5 of 292 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)
2:H:183:THR:HB	2:H:190:THR:HB	1.61	0.82
2:F:183:THR:HB	2:F:190:THR:HB	1.61	0.81
2:B:183:THR:HB	2:B:190:THR:HB	1.64	0.78
2:D:183:THR:HB	2:D:190:THR:HB	1.65	0.78
1:C:184:GLU:HA	1:C:207:LEU:HA	1.71	0.72

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	326/346 (94%)	310 (95%)	16 (5%)	0	100	100
1	C	326/346 (94%)	310 (95%)	16 (5%)	0	100	100
1	E	326/346 (94%)	310 (95%)	16 (5%)	0	100	100
1	G	326/346 (94%)	310 (95%)	16 (5%)	0	100	100
2	B	176/193 (91%)	170 (97%)	6 (3%)	0	100	100
2	D	176/193 (91%)	170 (97%)	6 (3%)	0	100	100
2	F	176/193 (91%)	170 (97%)	6 (3%)	0	100	100
2	H	176/193 (91%)	170 (97%)	6 (3%)	0	100	100
All	All	2008/2156 (93%)	1920 (96%)	88 (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	300/316 (95%)	292 (97%)	8 (3%)	44	70
1	C	300/316 (95%)	293 (98%)	7 (2%)	50	74
1	E	300/316 (95%)	292 (97%)	8 (3%)	44	70
1	G	300/316 (95%)	292 (97%)	8 (3%)	44	70
2	B	144/155 (93%)	140 (97%)	4 (3%)	43	70
2	D	144/155 (93%)	140 (97%)	4 (3%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	144/155 (93%)	140 (97%)	4 (3%)	43 70
2	H	144/155 (93%)	140 (97%)	4 (3%)	43 70
All	All	1776/1884 (94%)	1729 (97%)	47 (3%)	46 72

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	293	ASP
1	G	72	HIS
1	E	315	CYS
2	F	134	ASP
1	G	248	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	335	HIS
1	G	330	GLN
1	E	346	GLN
1	G	191	ASN
1	G	346	GLN

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)

12 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	$\#\|Z\| > 2$
3	NAG	I	1	2,3	14,14,15	0.54	0	17,19,21	0.63	0
3	NAG	I	2	3	14,14,15	0.18	0	17,19,21	0.40	0
3	FUC	I	3	3	10,10,11	0.90	0	14,14,16	1.68	2 (14%)
3	NAG	J	1	2,3	14,14,15	0.61	0	17,19,21	0.59	0
3	NAG	J	2	3	14,14,15	0.18	0	17,19,21	0.42	0
3	FUC	J	3	3	10,10,11	0.78	1 (10%)	14,14,16	1.62	2 (14%)
3	NAG	K	1	2,3	14,14,15	0.47	0	17,19,21	0.55	0
3	NAG	K	2	3	14,14,15	0.14	0	17,19,21	0.44	0
3	FUC	K	3	3	10,10,11	0.82	1 (10%)	14,14,16	1.41	2 (14%)
3	NAG	L	1	2,3	14,14,15	0.51	0	17,19,21	0.58	0
3	NAG	L	2	3	14,14,15	0.17	0	17,19,21	0.40	0
3	FUC	L	3	3	10,10,11	0.74	0	14,14,16	1.40	2 (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
3	NAG	I	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
3	NAG	J	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	FUC	J	3	3	-	-	0/1/1/1
3	NAG	K	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	FUC	K	3	3	-	-	0/1/1/1
3	NAG	L	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	FUC	L	3	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	3	FUC	C1-C2	2.06	1.56	1.52
3	K	3	FUC	C1-C2	2.00	1.56	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	3	FUC	C1-O5-C5	3.98	121.80	112.78
3	J	3	FUC	C1-O5-C5	3.89	121.59	112.78
3	K	3	FUC	C1-O5-C5	3.41	120.52	112.78
3	I	3	FUC	O5-C5-C4	3.40	115.63	109.52
3	L	3	FUC	C1-O5-C5	3.21	120.05	112.78

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

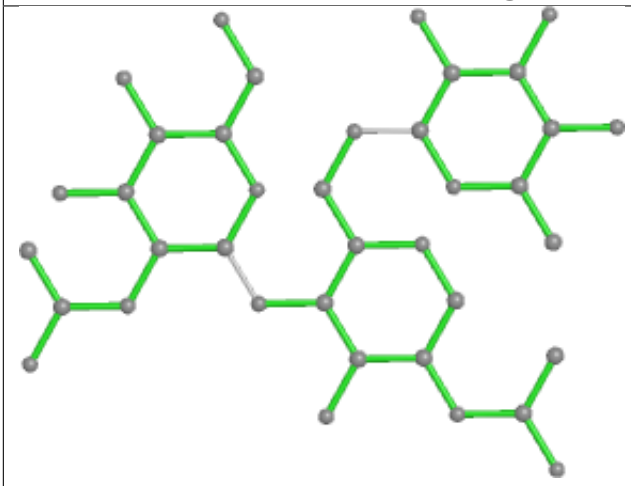
Mol	Chain	Res	Type	Atoms
3	L	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6

There are no ring outliers.

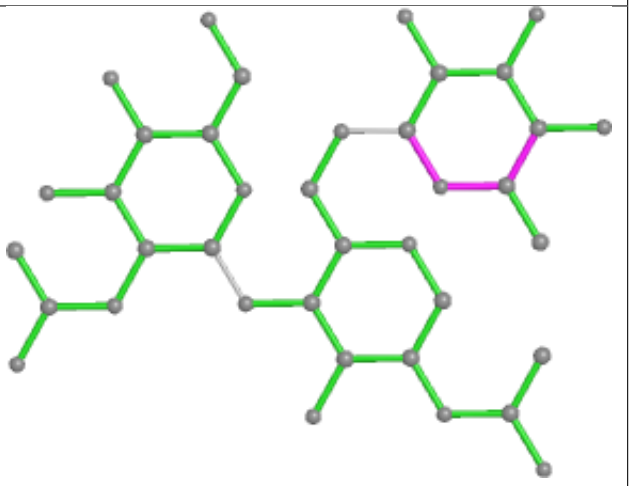
No monomer is involved in short contacts.

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

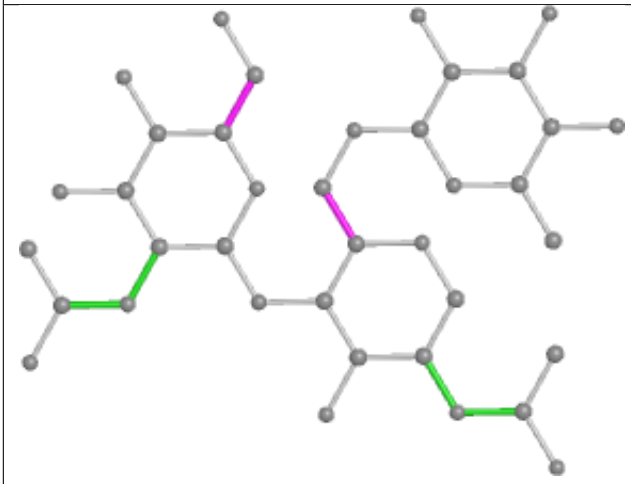
Oligosaccharide Chain I



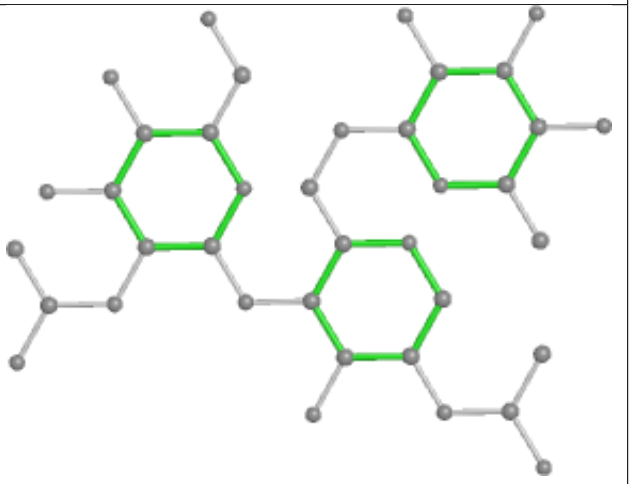
Bond lengths



Bond angles

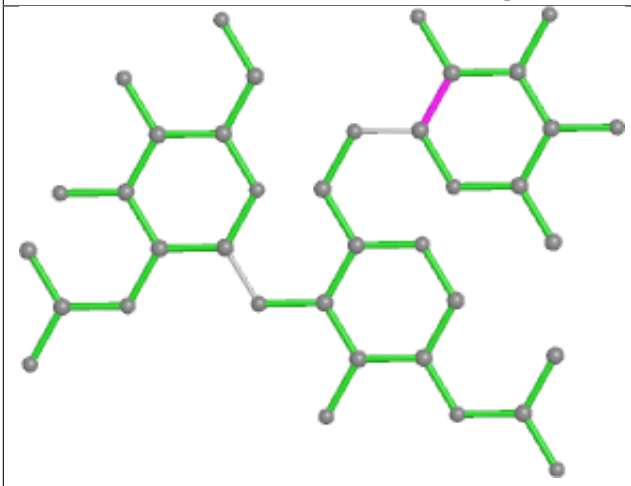


Torsions

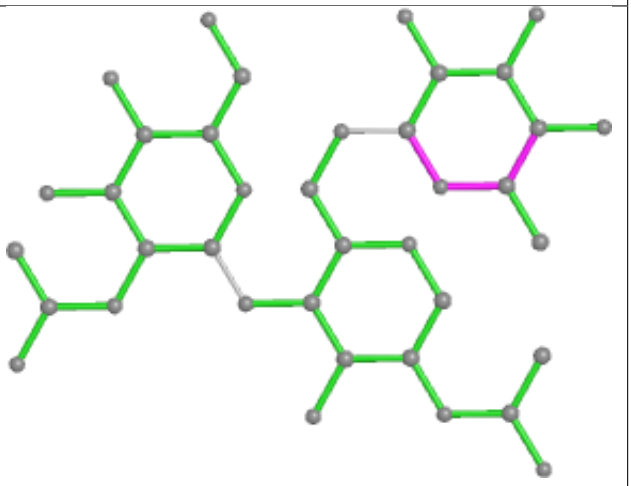


Rings

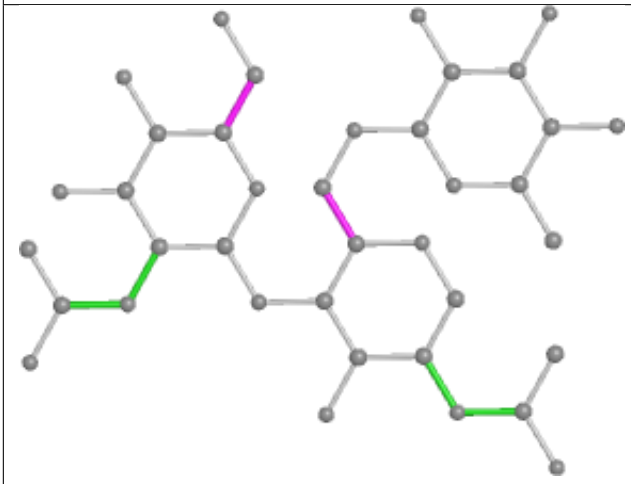
Oligosaccharide Chain J



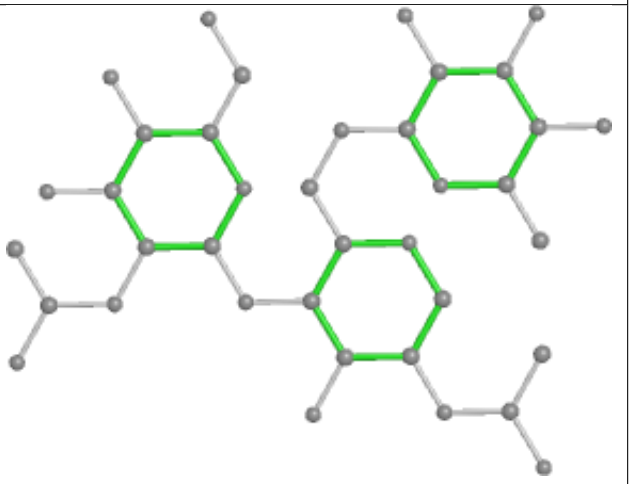
Bond lengths



Bond angles

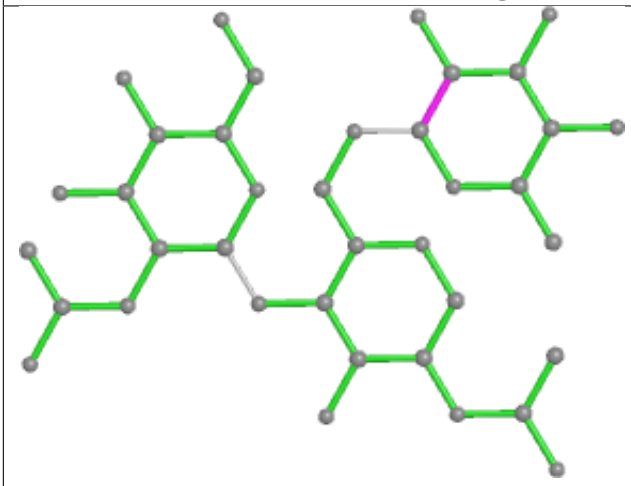


Torsions

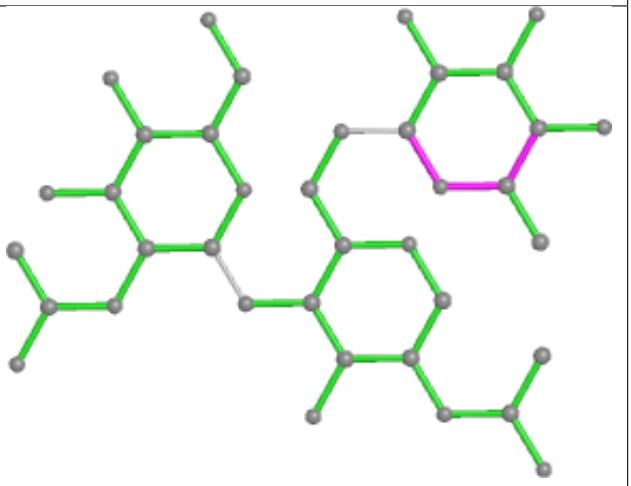


Rings

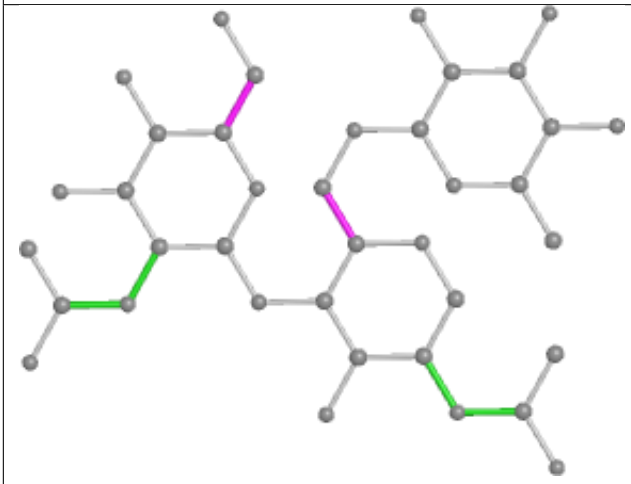
Oligosaccharide Chain K



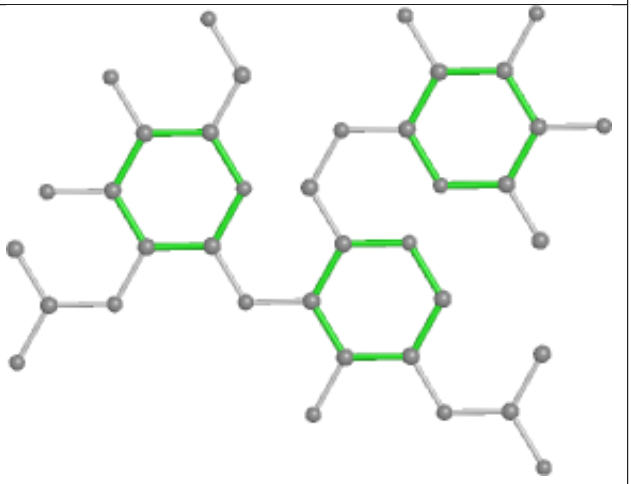
Bond lengths



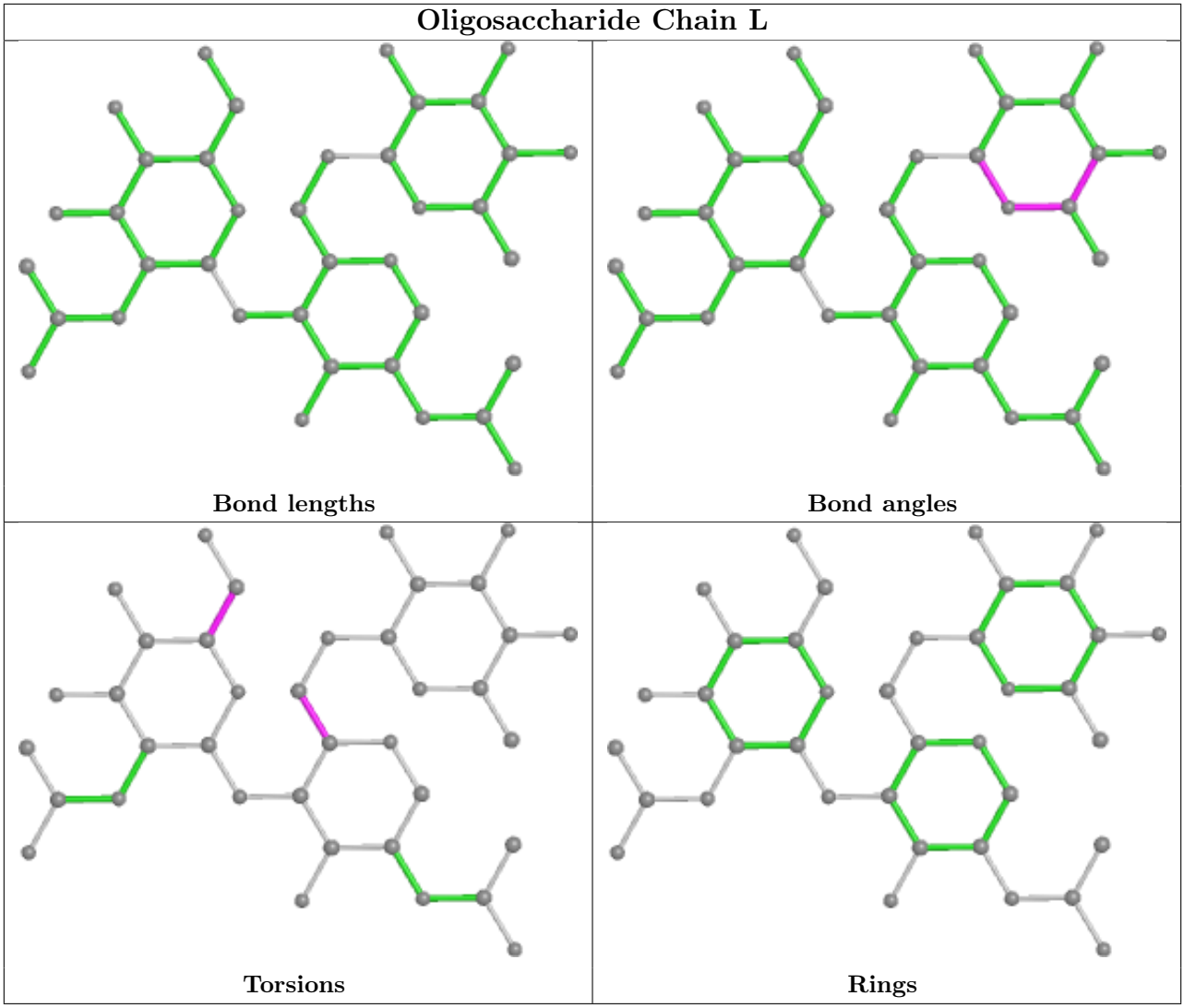
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	NAG	A	403	1	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	E	1002	1	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	G	1000	1	14,14,15	0.29	0	17,19,21	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	1000	1	14,14,15	0.29	0	17,19,21	0.33	0
4	NAG	C	402	1	14,14,15	0.57	0	17,19,21	1.00	1 (5%)
4	NAG	A	401	1	14,14,15	0.28	0	17,19,21	0.33	0
4	NAG	C	401	1	14,14,15	0.26	0	17,19,21	0.32	0
4	NAG	C	403	1	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	A	402	1	14,14,15	0.57	0	17,19,21	1.02	1 (5%)
4	NAG	E	1001	1	14,14,15	0.64	0	17,19,21	0.99	1 (5%)
4	NAG	G	1002	1	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	G	1001	1	14,14,15	0.66	1 (7%)	17,19,21	0.99	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
4	NAG	A	403	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	G	1000	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1000	1	-	2/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	402	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	G	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	G	1001	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1001	NAG	C1-C2	2.06	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	402	NAG	C1-O5-C5	3.76	117.29	112.19
4	C	402	NAG	C1-O5-C5	3.64	117.12	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1001	NAG	C1-O5-C5	3.57	117.03	112.19
4	G	1001	NAG	C1-O5-C5	3.51	116.95	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	NAG	O5-C5-C6-O6
4	A	402	NAG	O5-C5-C6-O6
4	C	402	NAG	O5-C5-C6-O6
4	E	1000	NAG	O5-C5-C6-O6
4	E	1001	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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

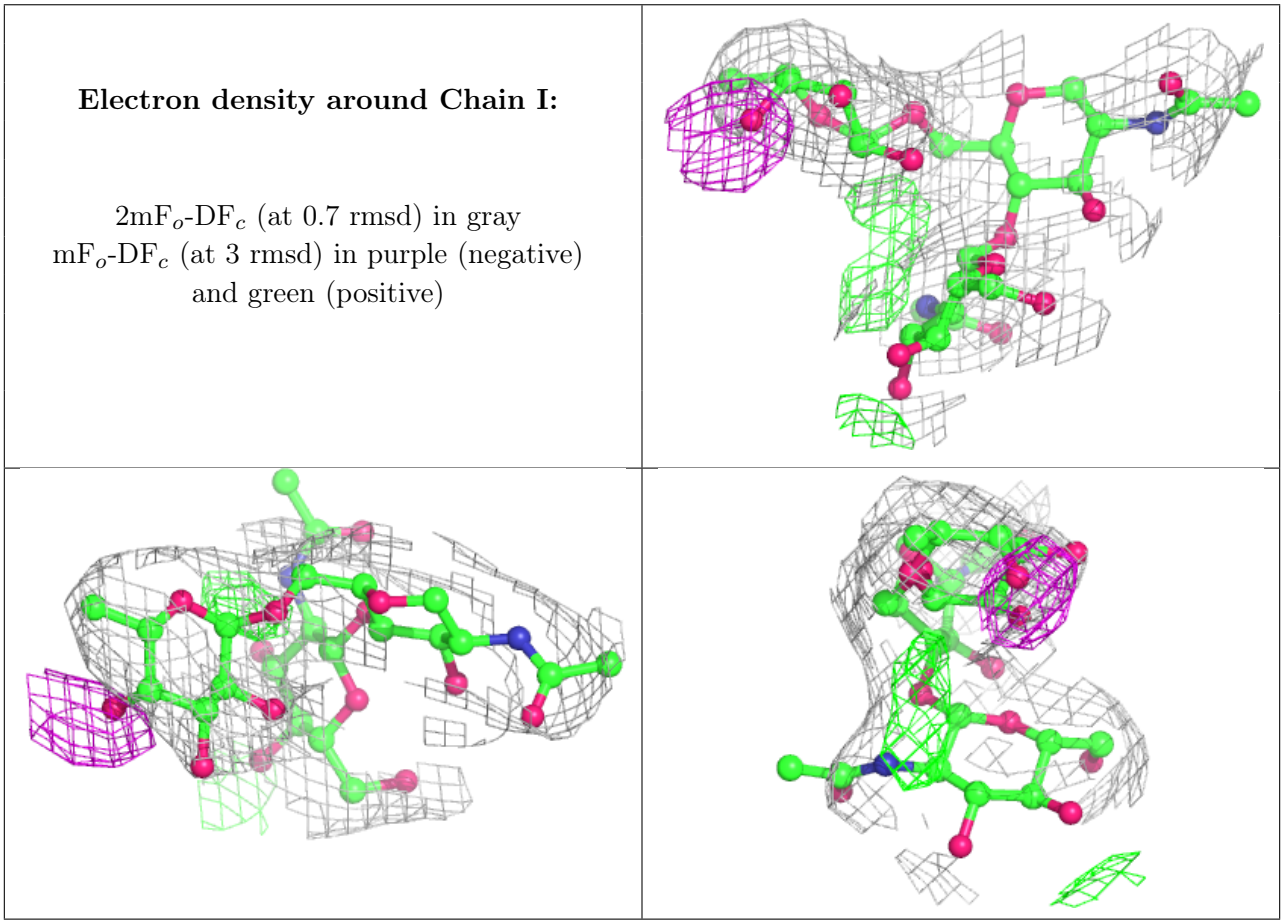
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

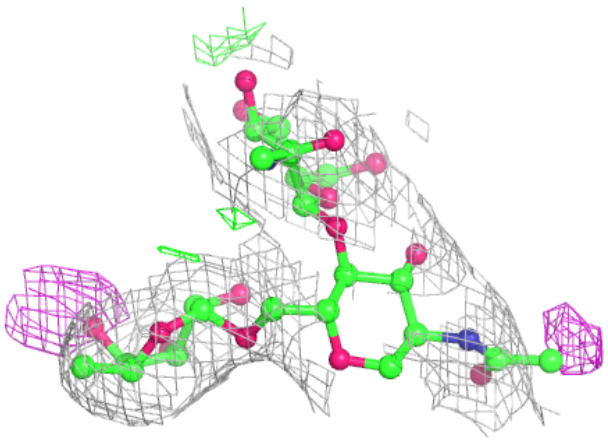
Electron density around Chain I:

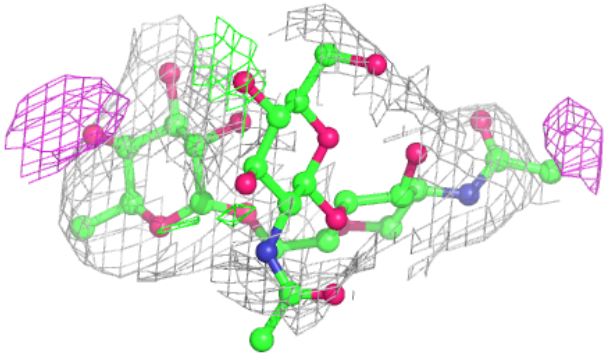
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

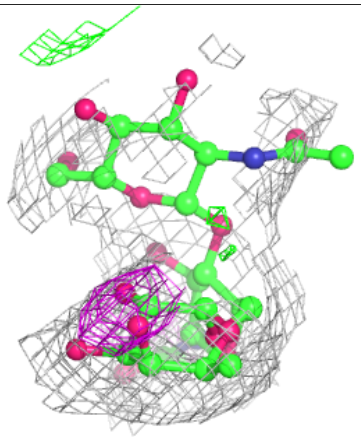


Electron density around Chain J:

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

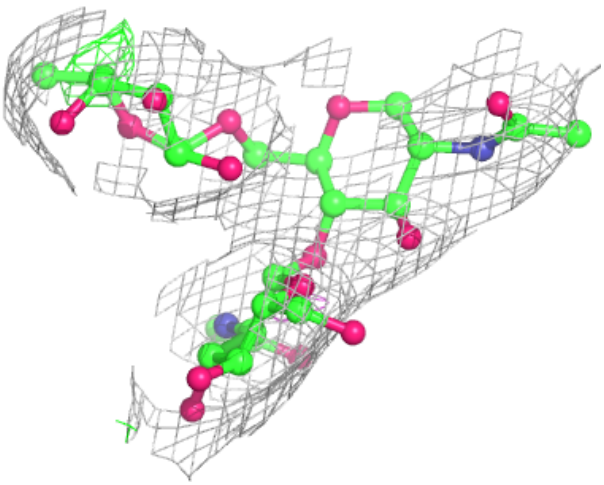


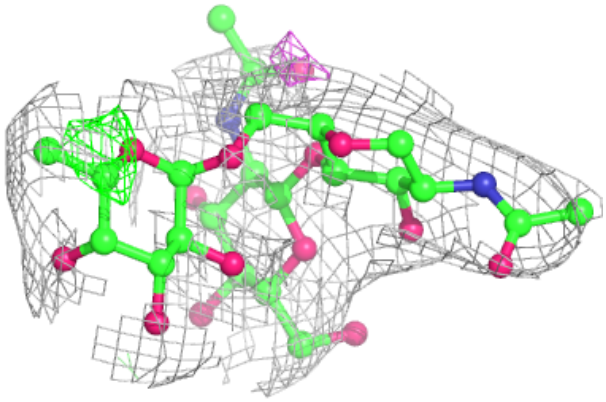


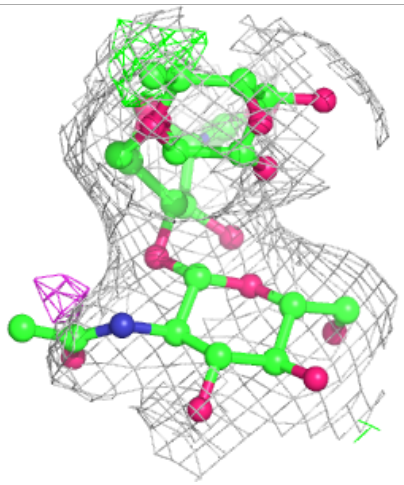


Electron density around Chain K:

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

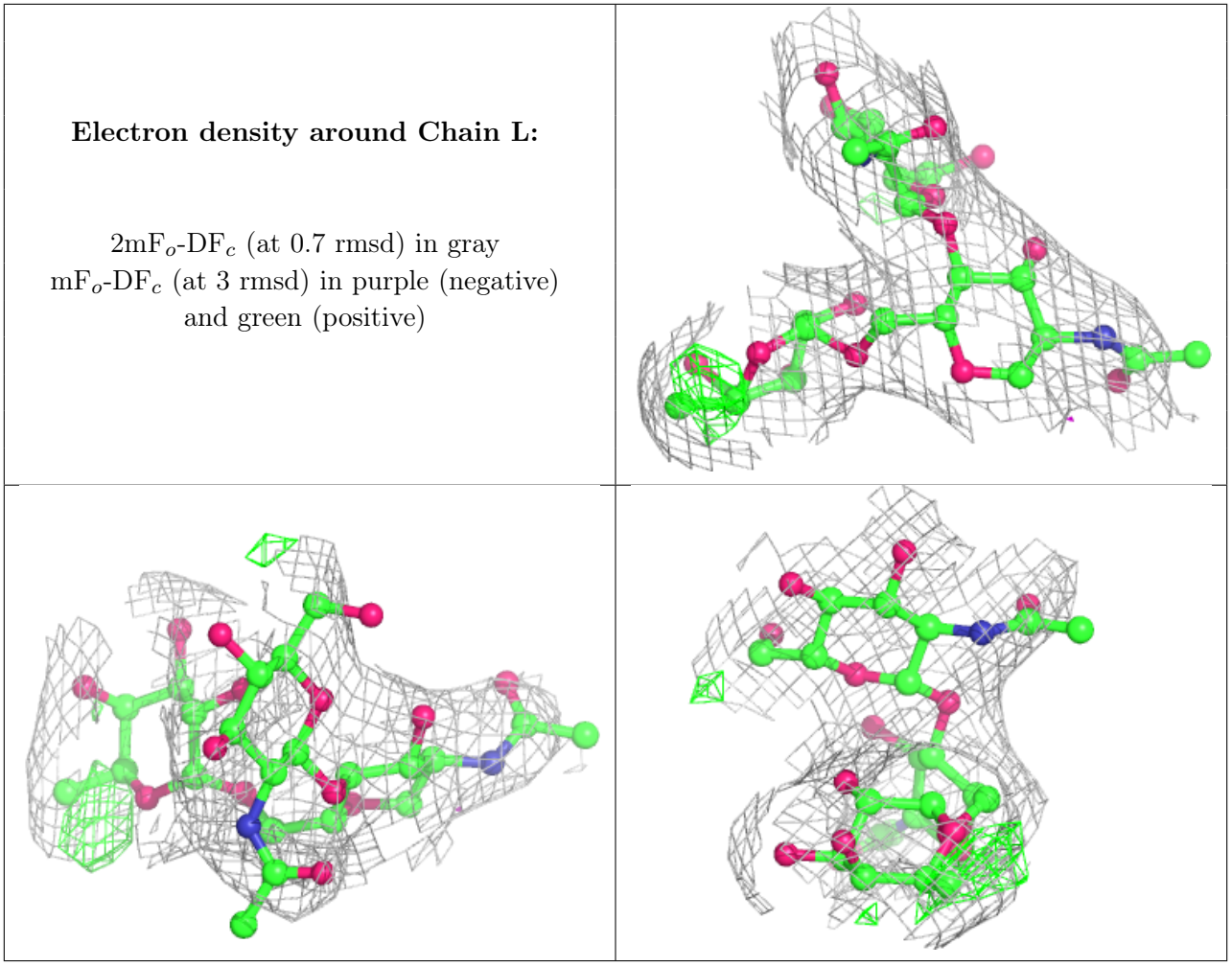






Electron density around Chain L:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.