wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 10:41 AM EDT

PDB ID	:	3ULV
Title	:	Structure of quaternary complex of human TLR3ecd with three Fabs (Form2)
Authors	:	Luo, J.; Gilliland, G.L.; Obmolova, O.; Malia, T.; Teplyakov, A.
Deposited on	:	2011-11-11
Resolution	:	3.52 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 (i)) were used in the production of this report:

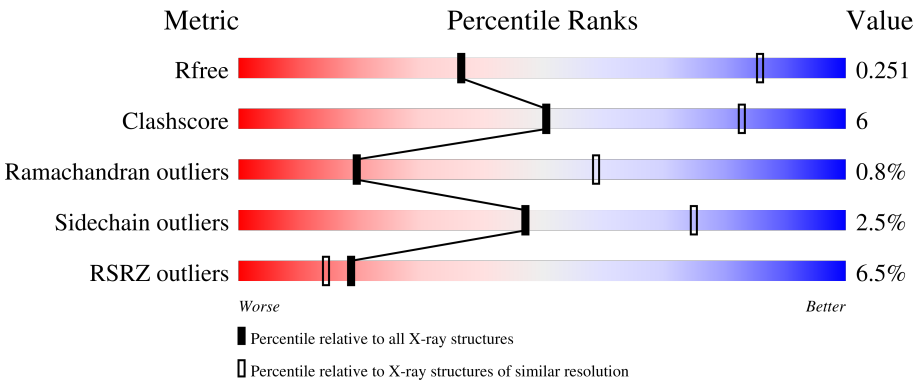
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.52 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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% 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	694	3%, 79%, 17%, •
2	L	214	%, 84%, 15%, •
3	H	225	8%, 84%, 16%
4	C	213	24%, 79%, 18%, ••
5	D	226	17%, 76%, 23%, •

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Mol	Chain	Length	Quality of chain
6	E	215	87% 12%
7	F	223	% 78% 18%
8	B	2	100%
8	G	2	100%
8	I	2	50% 50%
8	K	2	50% 50%
9	J	4	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	A	801	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 15591 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 Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	668	5354	3423	908	1005	18	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ALA	-	cloning artifact	UNP O15455
A	18	ASP	-	cloning artifact	UNP O15455
A	19	LEU	-	cloning artifact	UNP O15455
A	20	GLY	-	cloning artifact	UNP O15455
A	21	SER	-	cloning artifact	UNP O15455
A	703	ALA	-	expression tag	UNP O15455
A	704	SER	-	expression tag	UNP O15455
A	705	HIS	-	expression tag	UNP O15455
A	706	HIS	-	expression tag	UNP O15455
A	707	HIS	-	expression tag	UNP O15455
A	708	HIS	-	expression tag	UNP O15455
A	709	HIS	-	expression tag	UNP O15455
A	710	HIS	-	expression tag	UNP O15455

- Molecule 2 is a protein called Fab15 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1633	1020	273	334	6	0	0	0

- Molecule 3 is a protein called Fab15 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	225	1720	1088	286	337	9	0	0	0

- Molecule 4 is a protein called Fab12 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	210	1579	987	260	328	4	0	0	0

- Molecule 5 is a protein called Fab12 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	224	1712	1080	294	333	5	0	0	0

- Molecule 6 is a protein called Fab1068 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	215	1661	1040	279	336	6	0	0	0

- Molecule 7 is a protein called Fab1068 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	F	217	1656	1050	279	320	7	0	0	0

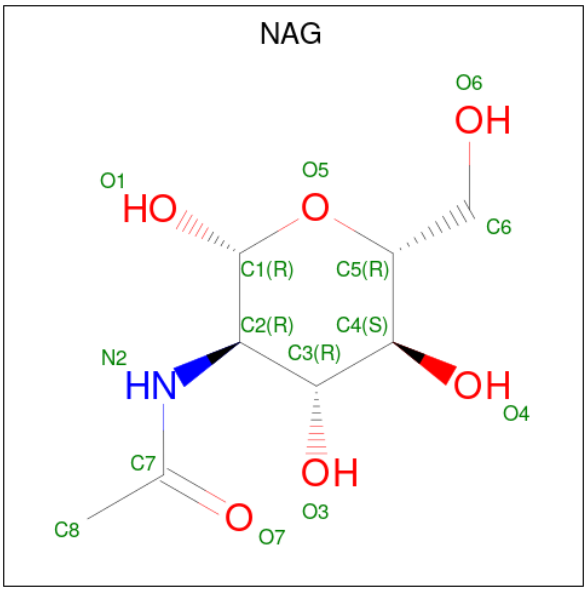
- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 9 is an oligosaccharide called alpha-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.

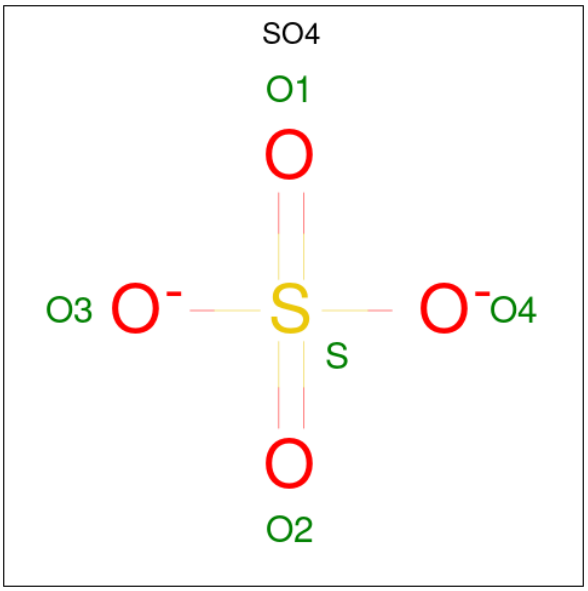
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	J	4	50	28	2	20	0	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



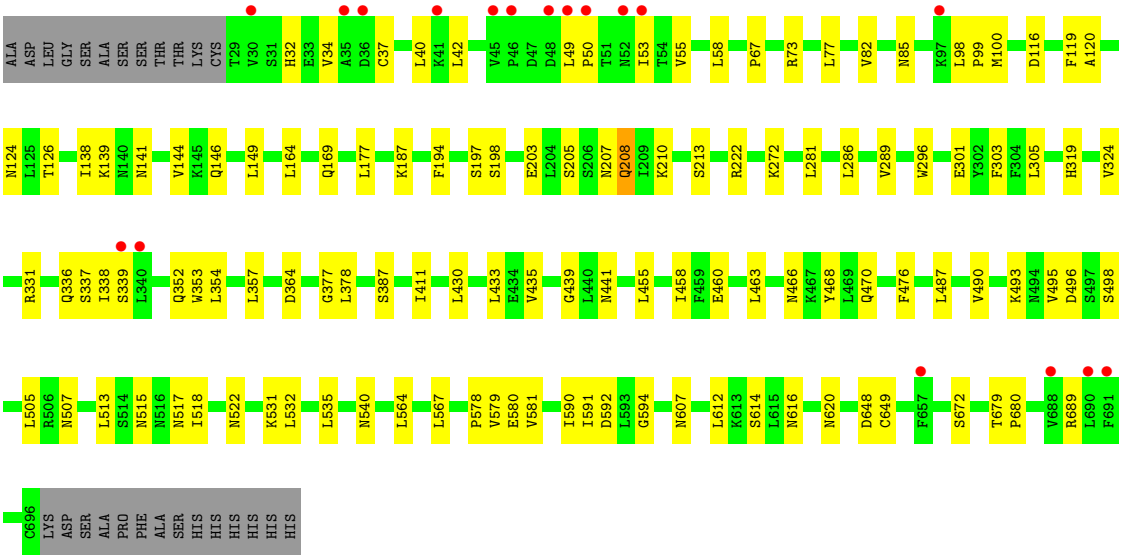
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
11	A	1	5	4	1	0	0
			Total	O	S		
11	A	1	5	4	1	0	0
			Total	O	S		
11	A	1	5	4	1	0	0
			Total	O	S		
11	A	1	5	4	1	0	0
			Total	O	S		
11	E	1	5	4	1	0	0
			Total	O	S		
11	E	1	5	4	1	0	0

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 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.

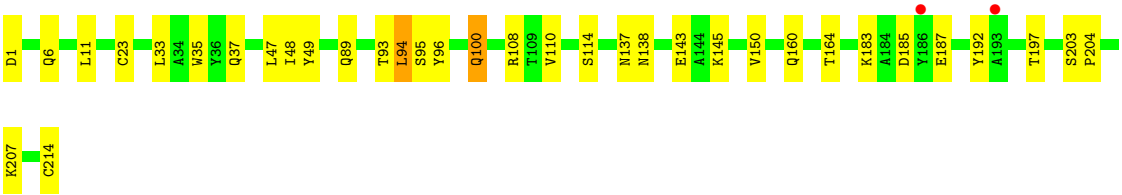
- Molecule 1: Toll-like receptor 3

Chain A:



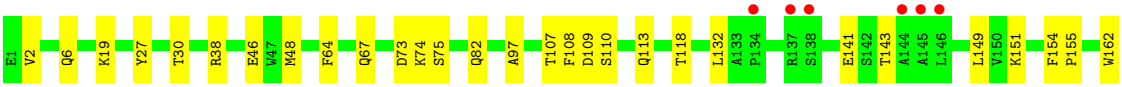
- Molecule 2: Fab15 light chain

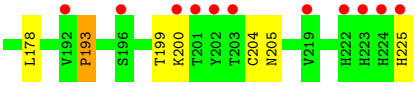
Chain L:



- Molecule 3: Fab15 heavy chain

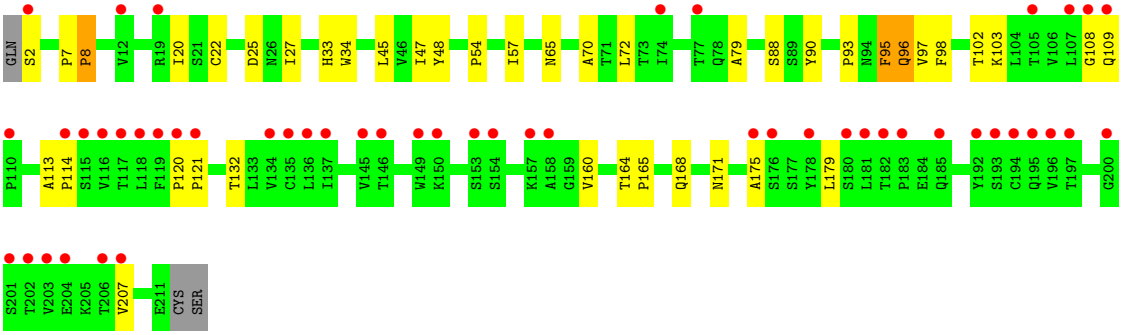
Chain H:





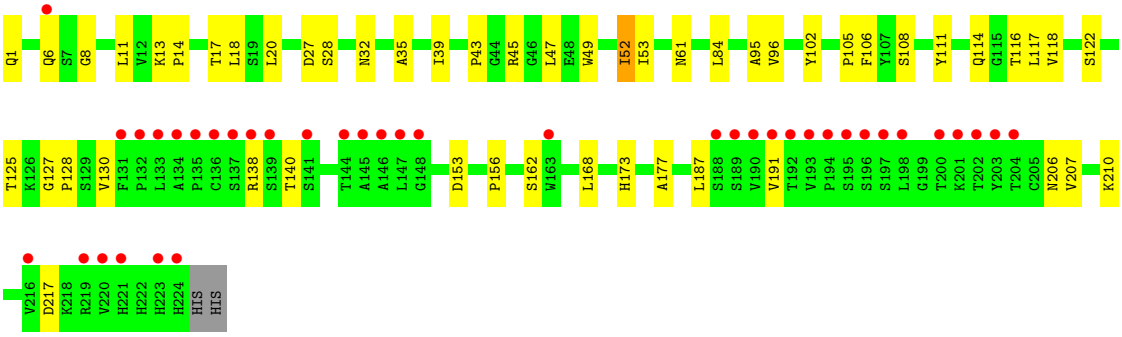
• Molecule 4: Fab12 light chain

Chain C:



• Molecule 5: Fab12 heavy chain

Chain D:

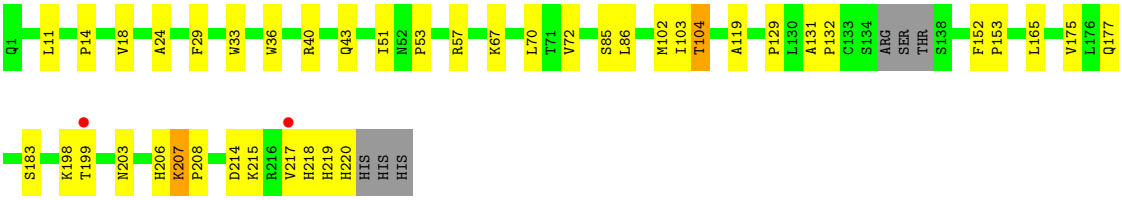


• Molecule 6: Fab1068 light chain

Chain E:

• Molecule 7: Fab1068 heavy chain

Chain F:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

NAG1
NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

NAG1
NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 50% 50%

NAG1
NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 50% 50%

NAG1
NAG2

• Molecule 9: alpha-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 J: 100%

NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	363.30Å 131.66Å 154.20Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	48.45 – 3.52 48.57 – 3.52	Depositor EDS
% Data completeness (in resolution range)	53.5 (48.45-3.52) 53.6 (48.57-3.52)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_896)	Depositor
R, R_{free}	0.231 , 0.253 0.228 , 0.251	Depositor DCC
R_{free} test set	2398 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 78.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	15591	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MAN, BMA, NAG

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	0.21	0/5467	0.37	0/7422
2	L	0.21	0/1666	0.39	0/2259
3	H	0.20	0/1770	0.38	0/2412
4	C	0.21	0/1620	0.41	0/2217
5	D	0.21	0/1759	0.40	0/2405
6	E	0.22	0/1699	0.39	0/2304
7	F	0.21	0/1699	0.41	0/2320
All	All	0.21	0/15680	0.39	0/21339

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5354	0	5352	63	0
2	L	1633	0	1591	16	0
3	H	1720	0	1646	18	0
4	C	1579	0	1501	24	0
5	D	1712	0	1671	29	0
6	E	1661	0	1598	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	1656	0	1626	22	0
8	B	28	0	25	0	0
8	G	28	0	25	0	0
8	I	28	0	25	0	0
8	K	28	0	25	0	0
9	J	50	0	43	3	0
10	A	84	0	78	2	0
11	A	20	0	0	0	0
11	E	10	0	0	0	0
All	All	15591	0	15206	175	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 6.

The worst 5 of 175 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:579:VAL:HG13	1:A:580:GLU:HG2	1.68	0.75
5:D:39:ILE:HG22	5:D:49:TRP:HA	1.74	0.70
1:A:67:PRO:HG2	10:A:802:NAG:HN2	1.59	0.68
1:A:138:ILE:HD12	1:A:164:LEU:HD22	1.75	0.67
1:A:119:PHE:O	1:A:146:GLN:NE2	2.30	0.65

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	666/694 (96%)	609 (91%)	55 (8%)	2 (0%)	41 75
2	L	212/214 (99%)	204 (96%)	6 (3%)	2 (1%)	17 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	223/225 (99%)	207 (93%)	15 (7%)	1 (0%)	34	71
4	C	208/213 (98%)	193 (93%)	12 (6%)	3 (1%)	11	47
5	D	222/226 (98%)	202 (91%)	17 (8%)	3 (1%)	11	47
6	E	213/215 (99%)	198 (93%)	12 (6%)	3 (1%)	11	47
7	F	213/223 (96%)	192 (90%)	20 (9%)	1 (0%)	29	67
All	All	1957/2010 (97%)	1805 (92%)	137 (7%)	15 (1%)	19	59

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
2	L	143	GLU
7	F	218	HIS
2	L	138	ASN
4	C	93	PRO

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	622/644 (97%)	618 (99%)	4 (1%)	86	94
2	L	186/186 (100%)	177 (95%)	9 (5%)	25	60
3	H	194/194 (100%)	190 (98%)	4 (2%)	53	78
4	C	178/181 (98%)	176 (99%)	2 (1%)	73	87
5	D	197/199 (99%)	191 (97%)	6 (3%)	41	71
6	E	188/188 (100%)	178 (95%)	10 (5%)	22	56
7	F	189/195 (97%)	181 (96%)	8 (4%)	30	63
All	All	1754/1787 (98%)	1711 (98%)	43 (2%)	47	75

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	E	33	LEU
7	F	57	ARG
6	E	81	GLU
6	E	108	ARG
7	F	103	ILE

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	208	GLN
1	A	620	ASN
2	L	89	GLN
5	D	173	HIS

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	$\#\|Z\| > 2$
8	NAG	B	1	1,8	14,14,15	0.52	0	17,19,21	0.86	0
8	NAG	B	2	8	14,14,15	0.47	0	17,19,21	0.69	0
8	NAG	G	1	1,8	14,14,15	0.57	0	17,19,21	0.67	0
8	NAG	G	2	8	14,14,15	0.53	0	17,19,21	0.66	0
8	NAG	I	1	1,8	14,14,15	0.54	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	I	2	8	14,14,15	0.55	0	17,19,21	0.67	0
9	NAG	J	1	9,1	14,14,15	0.52	0	17,19,21	0.70	0
9	NAG	J	2	9	14,14,15	0.57	0	17,19,21	0.70	0
9	BMA	J	3	9	11,11,12	0.62	0	15,15,17	0.61	0
9	MAN	J	4	9	11,11,12	0.66	0	15,15,17	1.79	5 (33%)
8	NAG	K	1	1,8	14,14,15	0.47	0	17,19,21	1.32	2 (11%)
8	NAG	K	2	8	14,14,15	0.52	0	17,19,21	0.65	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
8	NAG	B	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	B	2	8	-	2/6/23/26	0/1/1/1
8	NAG	G	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	G	2	8	-	2/6/23/26	0/1/1/1
8	NAG	I	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	I	2	8	-	3/6/23/26	0/1/1/1
9	NAG	J	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	J	2	9	-	2/6/23/26	0/1/1/1
9	BMA	J	3	9	-	1/2/19/22	0/1/1/1
9	MAN	J	4	9	-	1/2/19/22	0/1/1/1
8	NAG	K	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	4	MAN	C1-C2-C3	4.10	114.71	109.67
8	K	1	NAG	O5-C5-C6	3.58	112.82	107.20
9	J	4	MAN	C1-O5-C5	3.29	116.65	112.19
8	K	1	NAG	C1-O5-C5	3.02	116.29	112.19
9	J	4	MAN	O5-C5-C6	2.58	111.25	107.20

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1	NAG	C8-C7-N2-C2
8	B	1	NAG	O7-C7-N2-C2
8	B	2	NAG	C8-C7-N2-C2
8	B	2	NAG	O7-C7-N2-C2
8	G	1	NAG	C8-C7-N2-C2

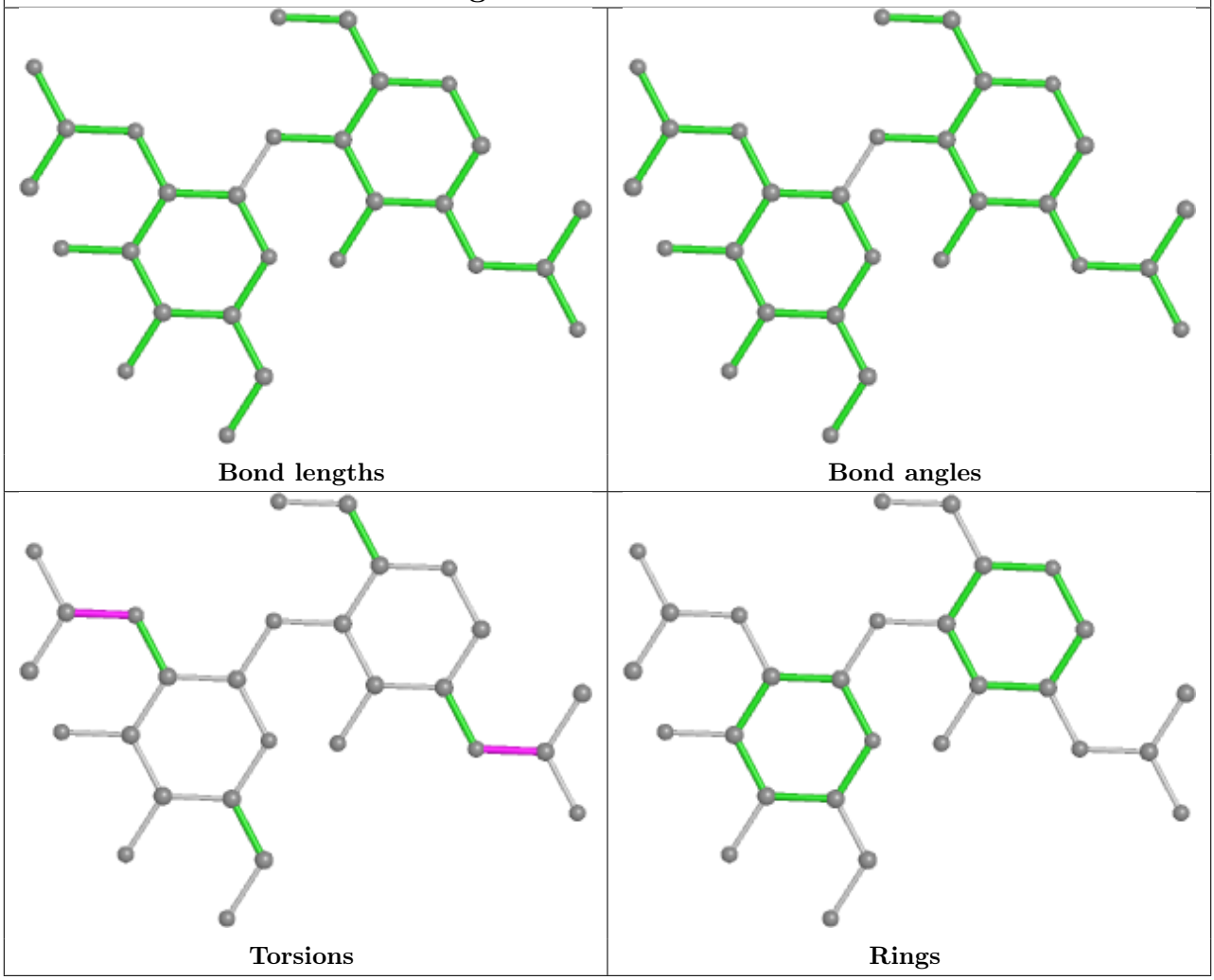
There are no ring outliers.

3 monomers are involved in 3 short contacts:

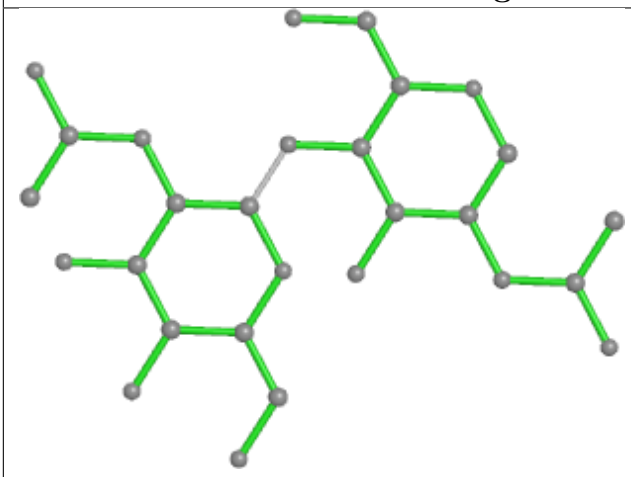
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1	NAG	2	0
9	J	2	NAG	1	0
9	J	3	BMA	1	0

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

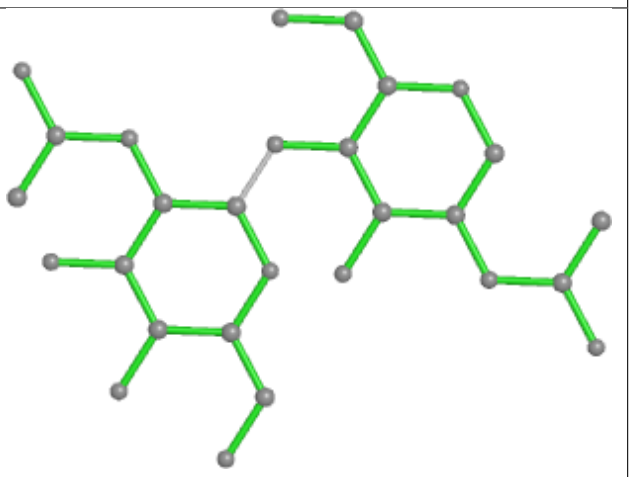
Oligosaccharide Chain B



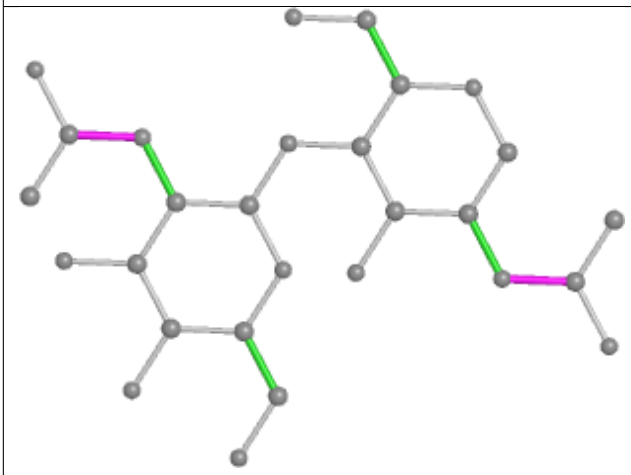
Oligosaccharide Chain G



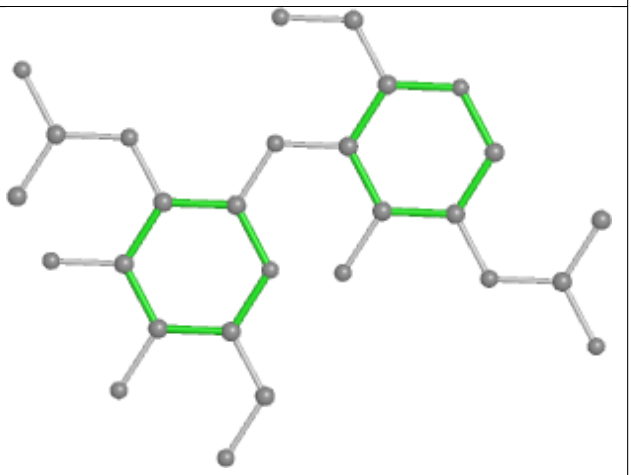
Bond lengths



Bond angles

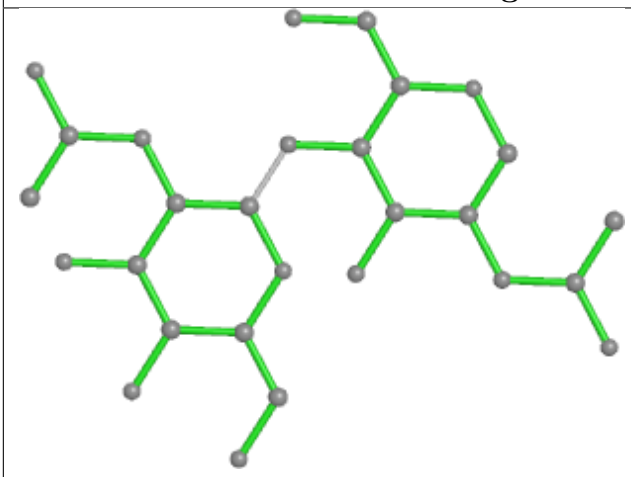


Torsions

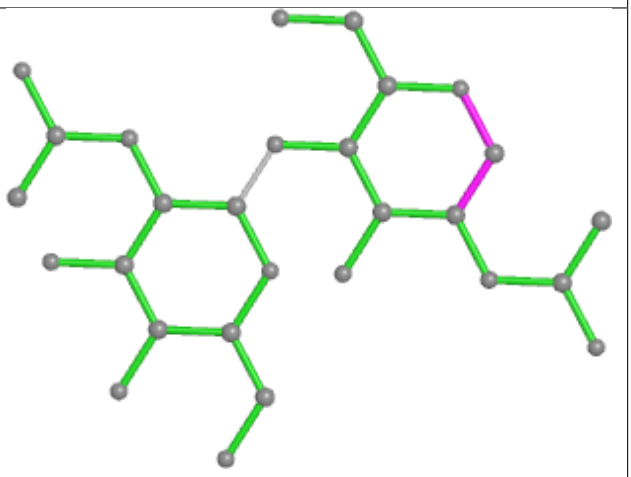


Rings

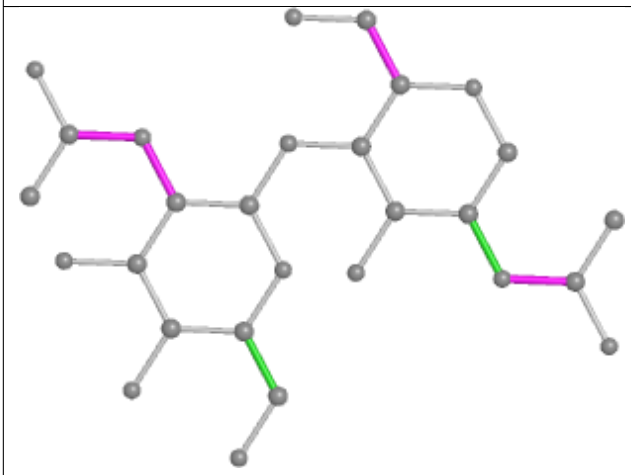
Oligosaccharide Chain I



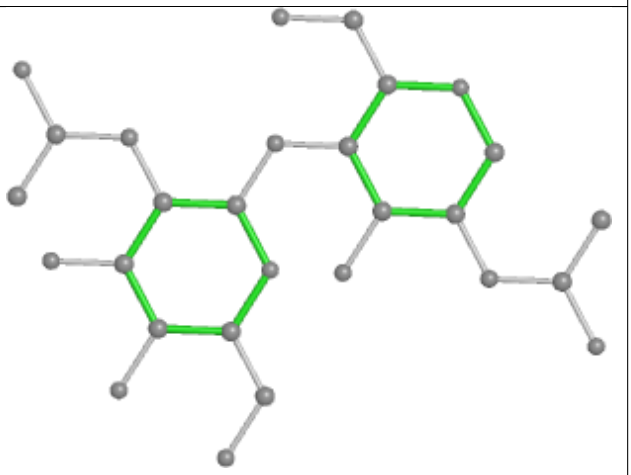
Bond lengths



Bond angles

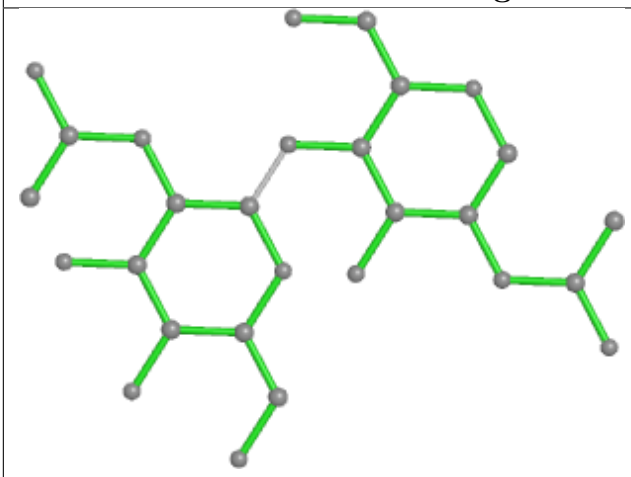


Torsions

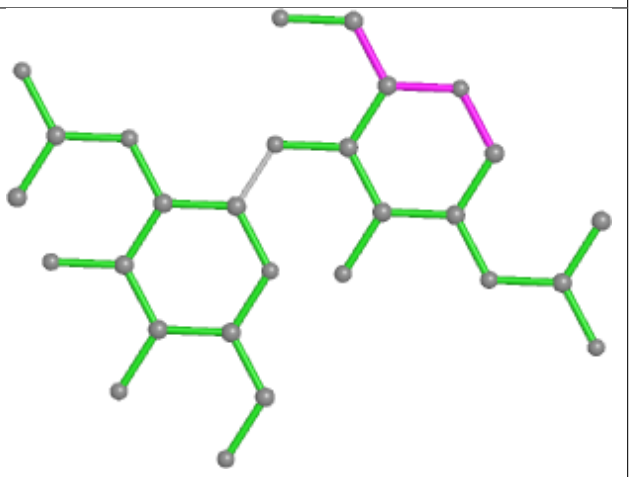


Rings

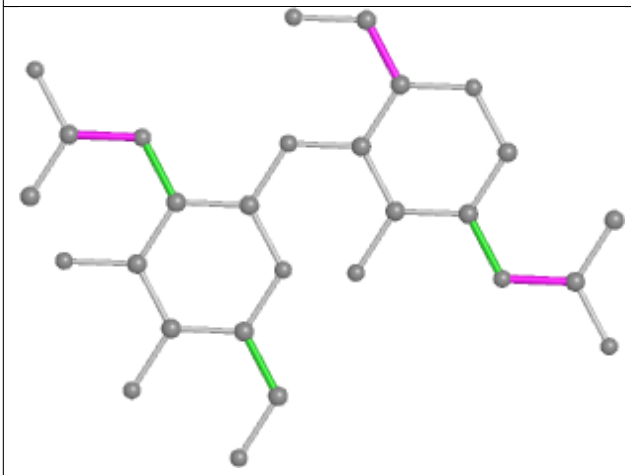
Oligosaccharide Chain K



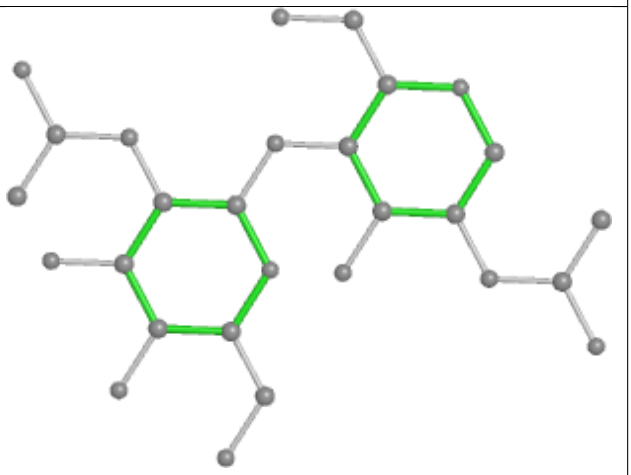
Bond lengths



Bond angles

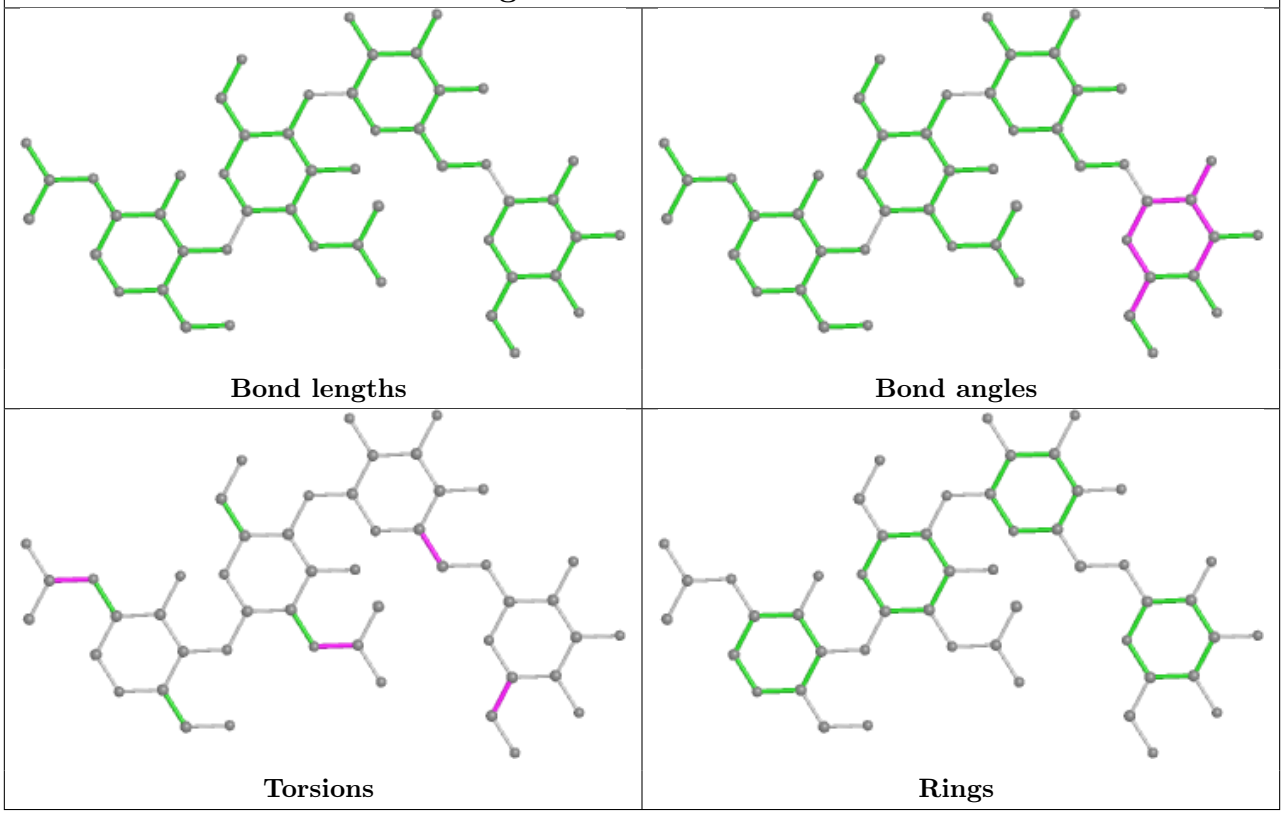


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

12 ligands 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	$\#\|Z\| > 2$
10	NAG	A	804	1	14,14,15	0.51	0	17,19,21	0.72	0
11	SO4	A	819	-	4,4,4	0.14	0	6,6,6	0.05	0
11	SO4	A	821	-	4,4,4	0.14	0	6,6,6	0.04	0
10	NAG	A	805	1	14,14,15	0.55	0	17,19,21	0.66	0
10	NAG	A	801	1	14,14,15	0.55	0	17,19,21	1.14	2 (11%)
11	SO4	A	820	-	4,4,4	0.14	0	6,6,6	0.06	0
11	SO4	E	301	-	4,4,4	0.14	0	6,6,6	0.04	0
10	NAG	A	803	1	14,14,15	0.55	0	17,19,21	0.83	0
11	SO4	E	302	-	4,4,4	0.13	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	NAG	A	808	1	14,14,15	0.47	0	17,19,21	0.78	0
10	NAG	A	802	1	14,14,15	0.52	0	17,19,21	0.72	0
11	SO4	A	822	-	4,4,4	0.14	0	6,6,6	0.04	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
10	NAG	A	804	1	-	2/6/23/26	0/1/1/1
10	NAG	A	805	1	-	4/6/23/26	0/1/1/1
10	NAG	A	801	1	-	3/6/23/26	0/1/1/1
10	NAG	A	803	1	-	0/6/23/26	0/1/1/1
10	NAG	A	808	1	-	2/6/23/26	0/1/1/1
10	NAG	A	802	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	801	NAG	C1-O5-C5	2.88	116.09	112.19
10	A	801	NAG	O5-C1-C2	2.18	114.72	111.29

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	801	NAG	C3-C2-N2-C7
10	A	801	NAG	C8-C7-N2-C2
10	A	801	NAG	O7-C7-N2-C2
10	A	802	NAG	C8-C7-N2-C2
10	A	802	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	803	NAG	1	0
10	A	802	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	A	668/694 (96%)	-0.09	18 (2%) 54 41	3, 49, 124, 179	0
2	L	214/214 (100%)	-0.18	2 (0%) 84 73	13, 55, 122, 149	0
3	H	225/225 (100%)	0.22	17 (7%) 13 11	11, 57, 168, 189	0
4	C	210/213 (98%)	1.23	51 (24%) 0 0	60, 149, 206, 228	0
5	D	224/226 (99%)	0.79	39 (17%) 1 1	39, 86, 225, 262	0
6	E	215/215 (100%)	-0.15	0 100 100	5, 34, 75, 112	0
7	F	217/223 (97%)	-0.12	2 (0%) 84 73	6, 32, 99, 127	0
All	All	1973/2010 (98%)	0.17	129 (6%) 18 14	3, 56, 181, 262	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	134	ALA	12.3
5	D	148	GLY	8.9
4	C	116	VAL	8.2
5	D	147	LEU	8.2
5	D	131	PHE	5.7

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)

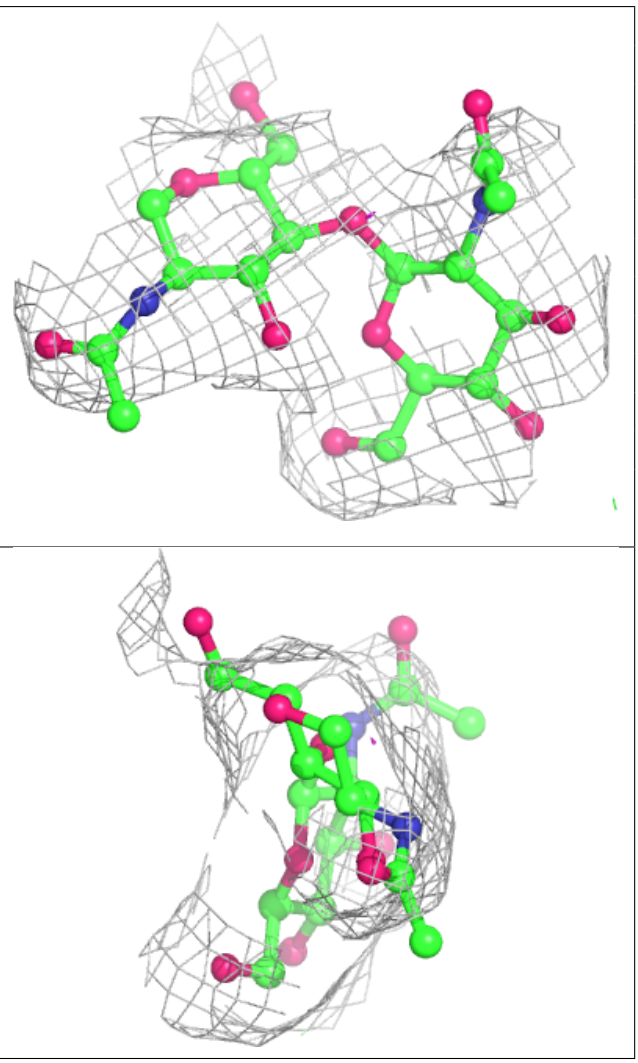
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	G	2	14/15	0.73	0.33	74,124,133,137	0
8	NAG	I	2	14/15	0.81	0.40	105,138,158,163	0
9	BMA	J	3	11/12	0.81	0.20	48,92,120,142	0
9	MAN	J	4	11/12	0.85	0.17	53,101,116,119	0
8	NAG	B	2	14/15	0.87	0.25	94,118,124,125	0
8	NAG	K	1	14/15	0.88	0.19	28,53,88,110	0
9	NAG	J	2	14/15	0.89	0.17	19,62,78,88	0
8	NAG	K	2	14/15	0.91	0.26	77,100,110,112	0
8	NAG	B	1	14/15	0.91	0.30	69,107,119,120	0
8	NAG	G	1	14/15	0.92	0.28	54,68,103,117	0
8	NAG	I	1	14/15	0.92	0.18	57,87,103,134	0
9	NAG	J	1	14/15	0.96	0.17	21,36,53,58	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.

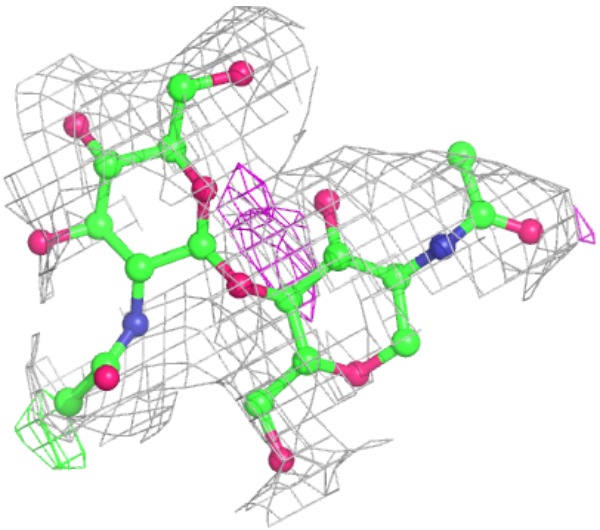
Electron density around Chain B:

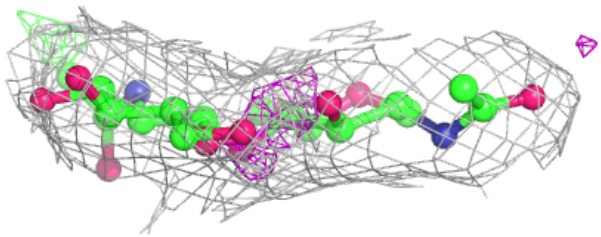
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

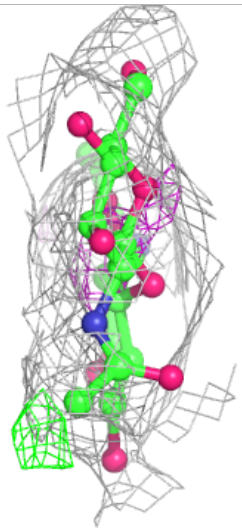


Electron density around Chain G:

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

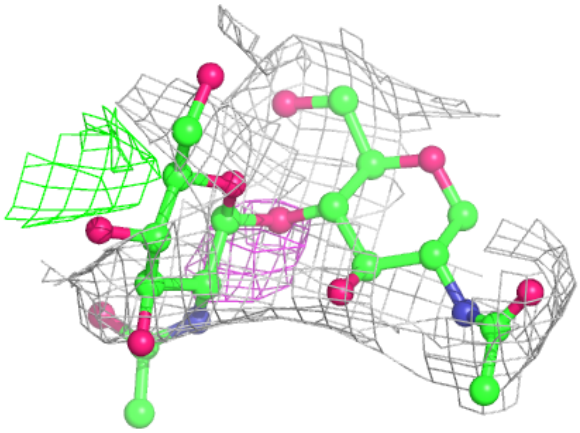


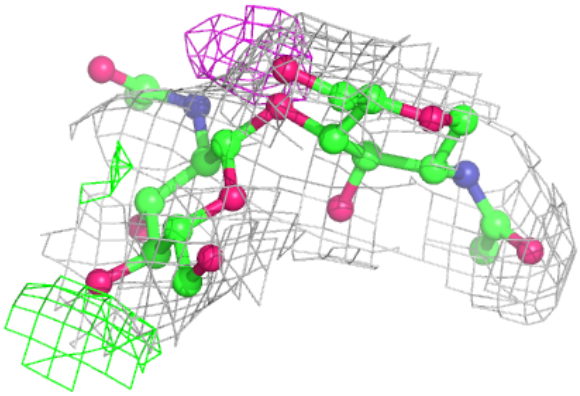


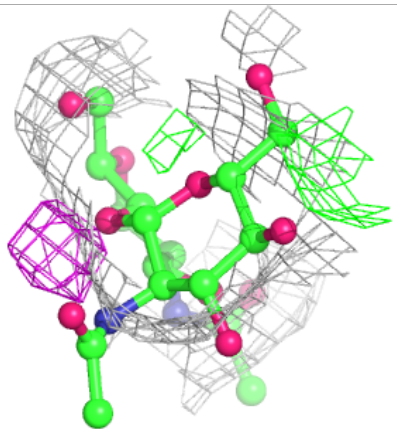


Electron density around Chain I:

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

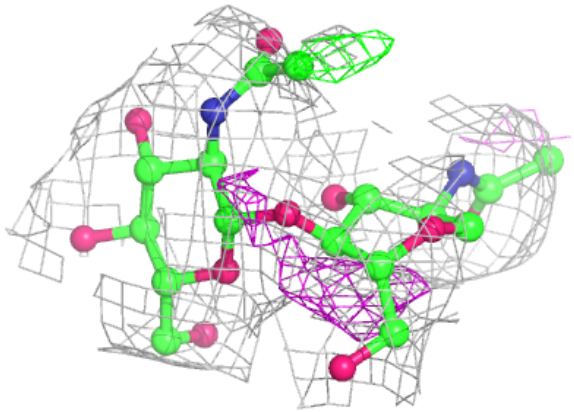


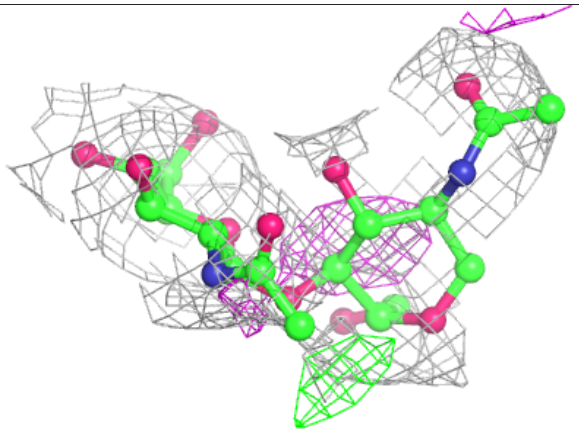


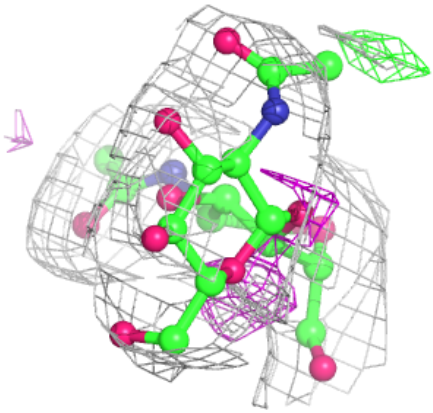


Electron density around Chain K:

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

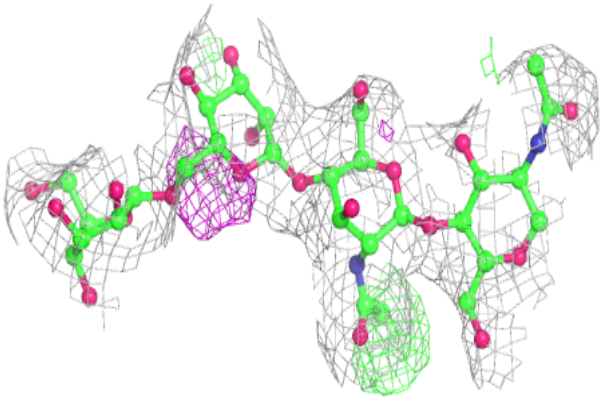


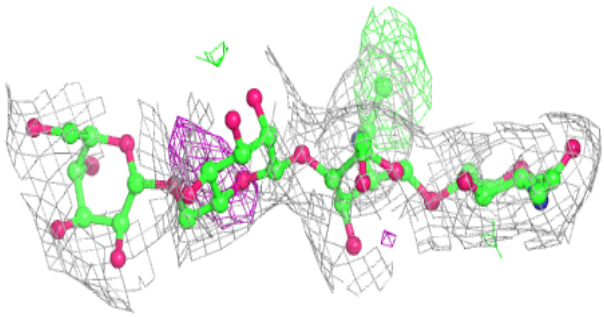


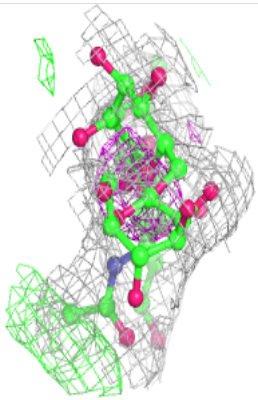


Electron density around Chain J:

$2mF_o$-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
10	NAG	A	801	14/15	0.59	0.50	133,166,191,193	0
10	NAG	A	803	14/15	0.77	0.29	105,151,169,172	0
10	NAG	A	802	14/15	0.78	0.27	94,127,144,145	0
11	SO4	A	822	5/5	0.86	0.29	93,94,115,128	0
10	NAG	A	805	14/15	0.88	0.18	66,87,107,107	0
10	NAG	A	804	14/15	0.89	0.17	57,96,102,111	0
10	NAG	A	808	14/15	0.91	0.17	47,76,88,88	0
11	SO4	E	302	5/5	0.91	0.14	60,84,100,102	0
11	SO4	A	821	5/5	0.93	0.19	69,82,105,113	0
11	SO4	A	820	5/5	0.97	0.16	27,29,36,37	0
11	SO4	E	301	5/5	0.97	0.15	38,47,69,72	0
11	SO4	A	819	5/5	0.97	0.19	26,28,45,50	0

6.5 Other polymers (i)

There are no such residues in this entry.