Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2025 – 05:19 PM EST

PDB ID	:	9MHX
Title	:	Human TLR8 ectodomain with small molecule agonist 7
Authors	:	Critton, D.A.
Deposited on	:	2024-12-12
Resolution	:	2.13 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 (i)) were used in the production of this report:

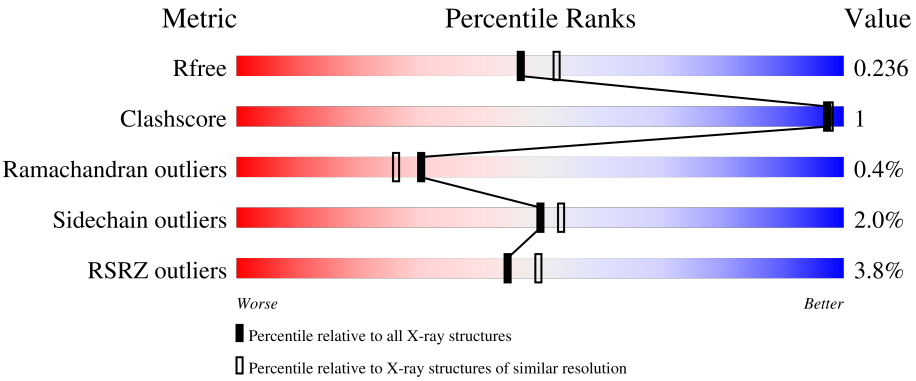
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.13 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	3336 (2.16-2.12)
Clashscore	180529	3585 (2.16-2.12)
Ramachandran outliers	177936	3554 (2.16-2.12)
Sidechain outliers	177891	3553 (2.16-2.12)
RSRZ outliers	164620	3337 (2.16-2.12)

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	807	3% 89% · 7%
1	B	807	4% 87% · 8%
2	C	5	80% 20%
2	F	5	60% 40%
3	D	5	40% 40% 20%

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Mol	Chain	Length	Quality of chain
4	E	5	60% 40%
4	G	5	40% 40% 20%
5	H	4	75% 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25530 atoms, of which 12215 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 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	748	Total	C	H	N	O	S	5811	2	0
			11741	3799	5811	1001	1111	19			
1	B	741	Total	C	H	N	O	S	5737	1	0
			11594	3757	5737	985	1096	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(2-6)]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
2	C	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			
2	F	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyran

ose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	H	N	O	53	0	0
			114	34	53	2	25			

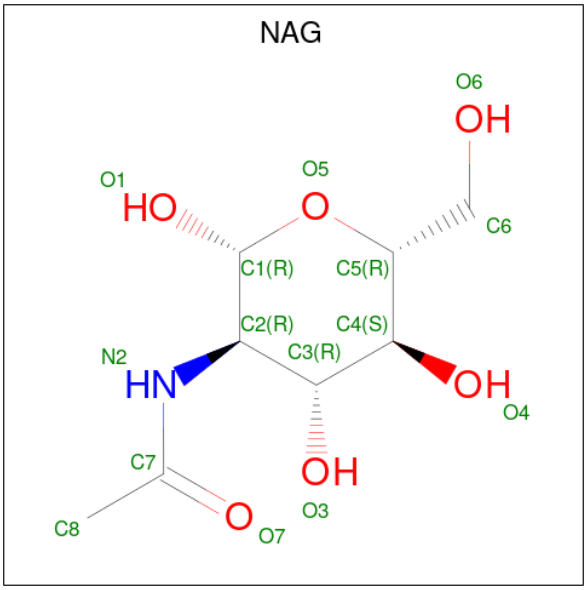
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			
4	G	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.

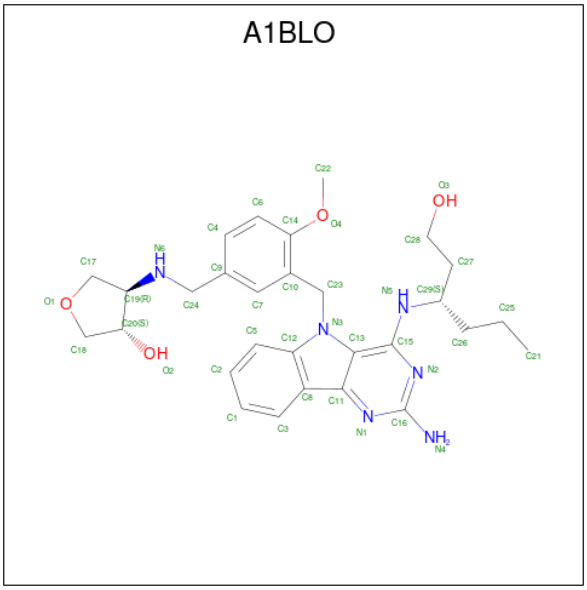
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	4	Total	C	H	N	O	44	0	0
			94	28	44	2	20			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		

- Molecule 7 is (3S,4R)-4-[({3-[(2-amino-4-{[(3S)-1-hydroxyhexan-3-yl]amino}-5H-pyrimido[5,4-b]indol-5-yl)methyl]-4-methoxyphenyl}methyl)amino]oxolan-3-ol (three-letter code: A1BLO) (formula: $C_{29}H_{38}N_6O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	38	0
			77	29	38	6	4		
7	B	1	Total	C	H	N	O	38	0
			77	29	38	6	4		

- Molecule 8 is water.

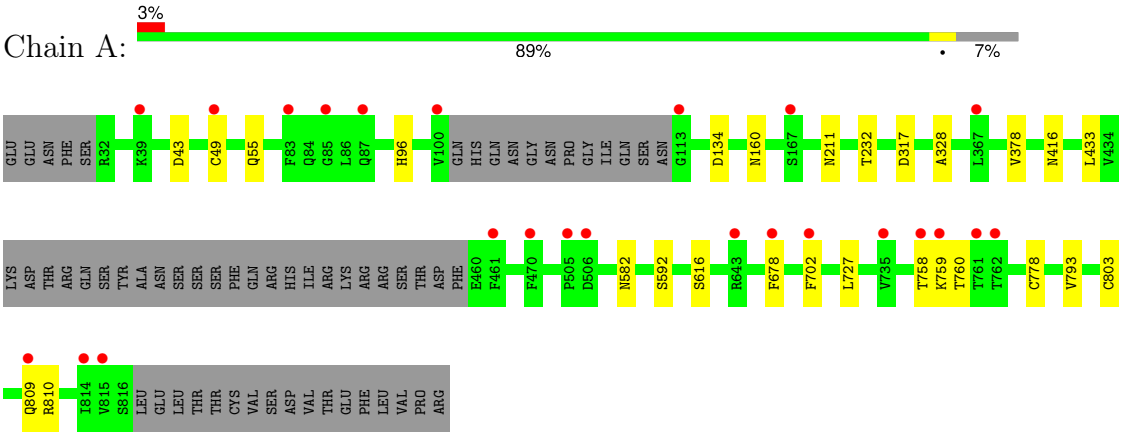
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	412	Total	O	0	0
			412	412		
8	B	375	Total	O	0	0
			375	375		

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.

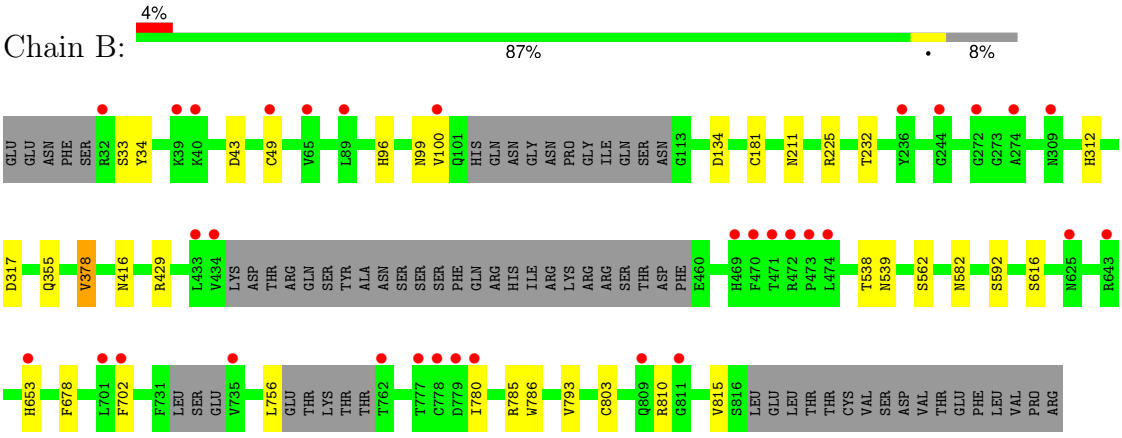
• Molecule 1: Toll-like receptor 8

Chain A:



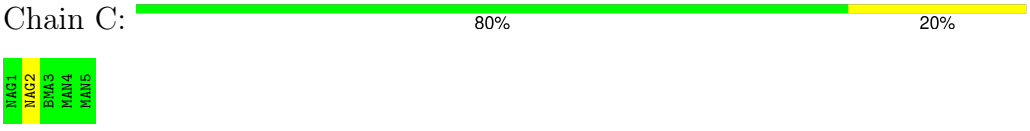
• Molecule 1: Toll-like receptor 8

Chain B:



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

Chain C:

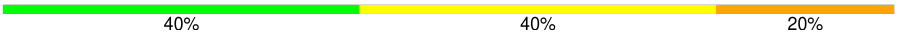


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(2-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 3: alpha-D-mannopyranose-(1-3)-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 D:

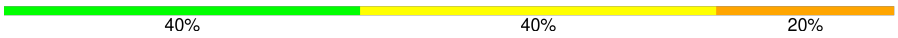


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[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 G:



• Molecule 5: 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 H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	86.24Å 86.24Å 217.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 2.13 19.92 – 2.13	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.92-2.13) 86.7 (19.92-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.13Å)	Xtriage
Refinement program	BUSTER 2.11.8 (20-APR-2021)	Depositor
R, R_{free}	0.220 , 0.242 0.212 , 0.236	Depositor DCC
R_{free} test set	17670 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,l 0.034 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25530	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN, A1BLO

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	0.39	0/6061	0.58	0/8243
1	B	0.39	0/5981	0.58	0/8132
All	All	0.39	0/12042	0.58	0/16375

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	5930	5811	5800	8	1
1	B	5857	5737	5728	10	1
2	C	61	52	52	0	0
2	F	61	52	52	0	0
3	D	61	53	52	1	0
4	E	61	52	52	0	0
4	G	61	52	52	1	0
5	H	50	44	43	0	0
6	A	168	156	156	2	0
6	B	140	130	130	0	0
7	A	39	38	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	39	38	0	0	0
8	A	412	0	0	0	0
8	B	375	0	0	2	0
All	All	13315	12215	12117	20	1

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 1.

All (20) 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)
4:G:3:BMA:H61	4:G:5:MAN:O2	2.05	0.57
1:B:538:THR:HG22	1:B:539:ASN:ND2	2.21	0.56
1:B:96:HIS:HD2	1:B:134:ASP:OD2	1.91	0.54
1:A:96:HIS:HD2	1:A:134:ASP:OD2	1.91	0.53
1:B:312:HIS:HD2	8:B:1362:HOH:O	1.91	0.53
1:B:211:ASN:O	1:B:232:THR:HA	2.11	0.51
1:A:211:ASN:O	1:A:232:THR:HA	2.10	0.51
1:A:758:THR:HG22	1:A:760:THR:H	1.76	0.51
1:A:803:CYS:O	1:A:810:ARG:O	2.29	0.49
1:B:803:CYS:O	1:B:810:ARG:O	2.30	0.48
7:A:913:A1BLO:O4	1:B:378:VAL:HG11	2.14	0.46
1:A:328:ALA:HB1	6:A:911:NAG:O5	2.17	0.44
1:B:756:LEU:HD22	1:B:786:TRP:CG	2.54	0.43
1:A:592:SER:HA	1:A:616:SER:O	2.20	0.41
3:D:3:BMA:H62	3:D:4:MAN:H3	2.02	0.41
1:B:538:THR:HG23	1:B:562:SER:HB2	2.02	0.41
1:A:160:ASN:HB2	6:A:910:NAG:H2	2.03	0.41
1:B:592:SER:HA	1:B:616:SER:O	2.20	0.41
1:B:181:CYS:HB3	8:B:1033:HOH:O	2.20	0.40
1:A:803:CYS:HB2	1:A:809:GLN:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:LYS:O	1:B:225:ARG:HH22[3_555]	1.50	0.10

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	744/807 (92%)	702 (94%)	41 (6%)	1 (0%)	48	49
1	B	732/807 (91%)	683 (93%)	44 (6%)	5 (1%)	19	13
All	All	1476/1614 (91%)	1385 (94%)	85 (6%)	6 (0%)	30	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	TYR
1	B	100	VAL
1	B	33	SER
1	A	378	VAL
1	B	378	VAL
1	B	815	VAL

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	667/751 (89%)	655 (98%)	12 (2%)	54	57
1	B	657/751 (88%)	643 (98%)	14 (2%)	48	51
All	All	1324/1502 (88%)	1298 (98%)	26 (2%)	50	53

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	49	CYS
1	A	55	GLN
1	A	317	ASP
1	A	416	ASN
1	A	433	LEU
1	A	582	ASN
1	A	678	PHE
1	A	702	PHE
1	A	727	LEU
1	A	778	CYS
1	A	793	VAL
1	B	43	ASP
1	B	49	CYS
1	B	99	ASN
1	B	317	ASP
1	B	355	GLN
1	B	416	ASN
1	B	429	ARG
1	B	582	ASN
1	B	653	HIS
1	B	678	PHE
1	B	702	PHE
1	B	780	ILE
1	B	785	ARG
1	B	793	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	288	GLN
1	A	585	ASN
1	B	96	HIS
1	B	288	GLN
1	B	355	GLN
1	B	539	ASN
1	B	585	ASN

5.3.3 RNA

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)

29 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	C	1	1,2	14,14,15	0.38	0	17,19,21	0.79	0
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
2	BMA	C	3	2	11,11,12	0.21	0	15,15,17	0.44	0
2	MAN	C	4	2	11,11,12	0.26	0	15,15,17	0.58	0
2	MAN	C	5	2	11,11,12	0.24	0	13,15,17	0.43	0
3	NAG	D	1	1,3	14,14,15	0.26	0	17,19,21	0.71	0
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.49	0
3	BMA	D	3	3	11,11,12	0.23	0	15,15,17	0.55	0
3	MAN	D	4	3	11,11,12	0.51	0	15,15,17	2.30	3 (20%)
3	MAN	D	5	3	11,11,12	0.23	0	15,15,17	0.63	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.41	0	17,19,21	0.62	0
4	NAG	E	2	4	14,14,15	0.26	0	17,19,21	0.49	0
4	BMA	E	3	4	11,11,12	0.24	0	15,15,17	0.71	0
4	MAN	E	4	4	11,11,12	0.30	0	15,15,17	0.66	1 (6%)
4	MAN	E	5	4	11,11,12	0.47	0	15,15,17	1.66	2 (13%)
2	NAG	F	1	1,2	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
2	NAG	F	2	2	14,14,15	0.32	0	17,19,21	0.73	1 (5%)
2	BMA	F	3	2	11,11,12	0.24	0	15,15,17	0.45	0
2	MAN	F	4	2	11,11,12	0.25	0	15,15,17	0.58	0
2	MAN	F	5	2	11,11,12	0.26	0	13,15,17	0.45	0
4	NAG	G	1	1,4	14,14,15	0.24	0	17,19,21	0.68	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.52	0
4	BMA	G	3	4	11,11,12	0.25	0	15,15,17	0.41	0
4	MAN	G	4	4	11,11,12	0.20	0	15,15,17	0.58	1 (6%)
4	MAN	G	5	4	11,11,12	0.71	0	15,15,17	2.05	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	H	1	1,5	14,14,15	0.41	0	17,19,21	0.60	0
5	NAG	H	2	5	14,14,15	0.24	0	17,19,21	0.51	0
5	BMA	H	3	5	11,11,12	0.24	0	15,15,17	0.50	0
5	MAN	H	4	5	11,11,12	0.39	0	15,15,17	1.76	3 (20%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/18/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	MAN	F	5	2	-	0/2/18/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	1/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4	MAN	C1-O5-C5	6.11	120.37	112.19
5	H	4	MAN	O2-C2-C3	5.70	121.96	110.15
4	G	5	MAN	C1-O5-C5	5.56	119.63	112.19
4	E	5	MAN	O2-C2-C3	4.83	120.15	110.15
3	D	4	MAN	O2-C2-C3	4.52	119.51	110.15
4	G	5	MAN	O2-C2-C3	3.50	117.41	110.15
3	D	4	MAN	C1-C2-C3	3.50	114.74	109.64
4	G	5	MAN	C1-C2-C3	3.08	114.14	109.64
4	E	5	MAN	C1-C2-C3	2.69	113.56	109.64
2	F	2	NAG	O5-C1-C2	-2.61	107.26	111.29
2	C	2	NAG	O5-C1-C2	-2.43	107.53	111.29
5	H	4	MAN	O2-C2-C1	2.41	114.74	109.22
4	G	5	MAN	O2-C2-C1	2.29	114.46	109.22
5	H	4	MAN	C1-O5-C5	2.22	115.17	112.19
3	D	5	MAN	C1-O5-C5	2.05	114.94	112.19
2	F	1	NAG	O5-C1-C2	-2.04	108.13	111.29
4	G	4	MAN	C1-O5-C5	2.04	114.92	112.19
4	E	4	MAN	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3	BMA	C4-C5-C6-O6

All (1) ring outliers are listed below:

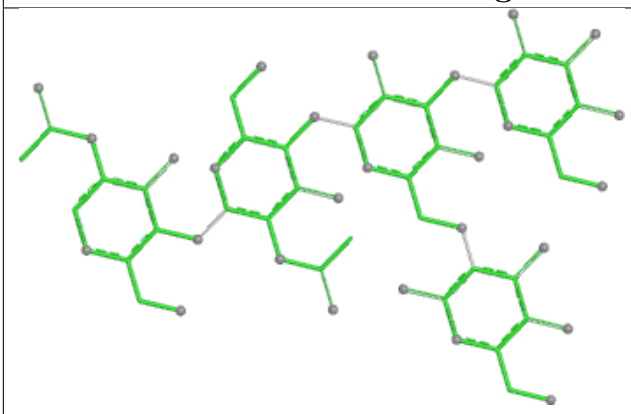
Mol	Chain	Res	Type	Atoms
4	G	5	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 2 short contacts:

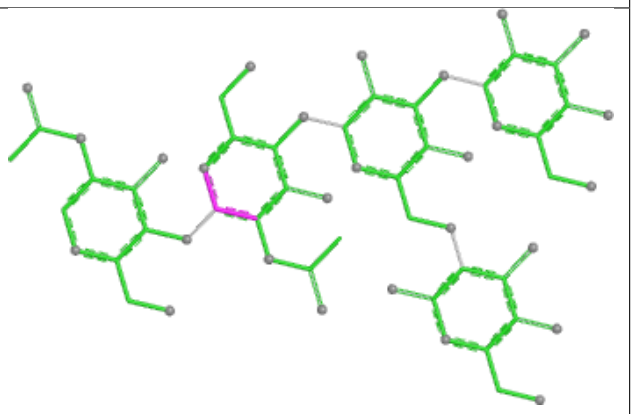
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	BMA	1	0
4	G	3	BMA	1	0
3	D	4	MAN	1	0
4	G	5	MAN	1	0

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

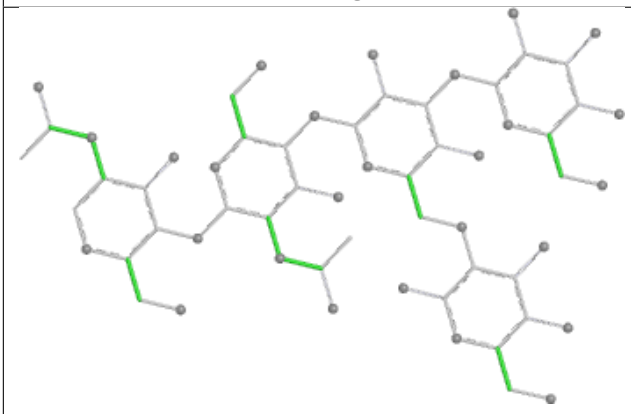
Oligosaccharide Chain C



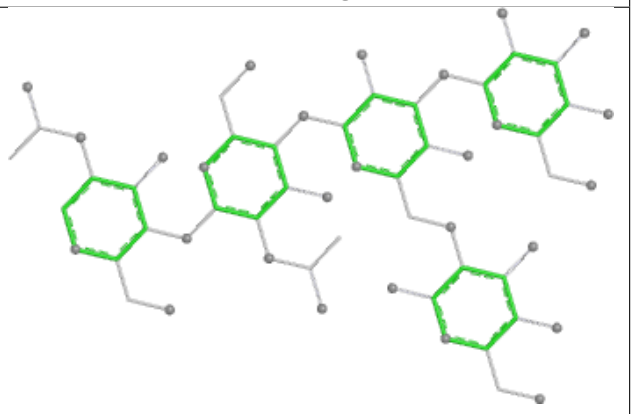
Bond lengths



Bond angles

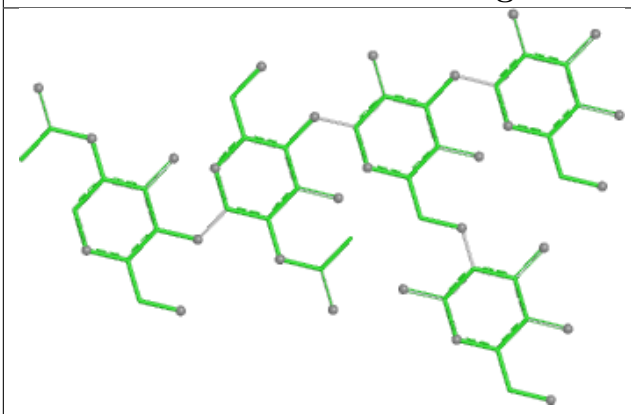


Torsions

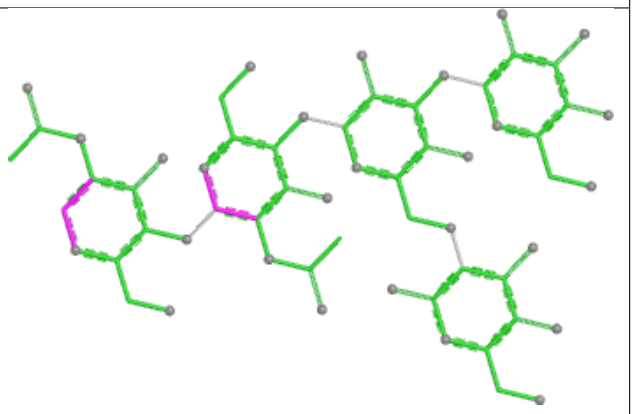


Rings

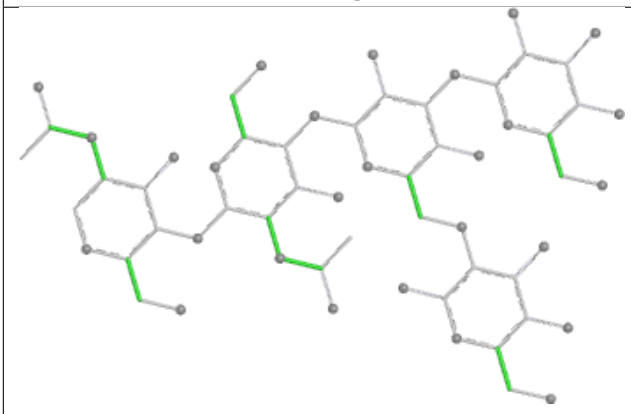
Oligosaccharide Chain F



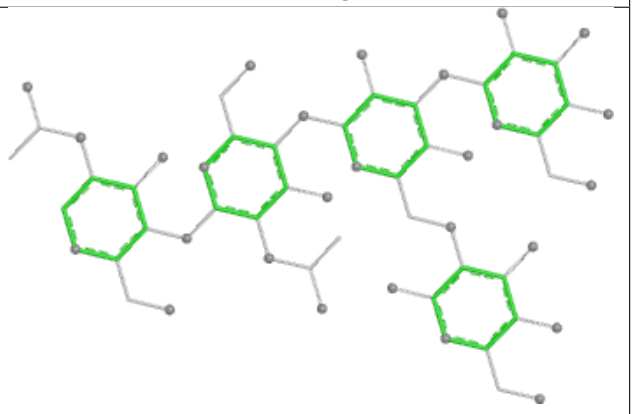
Bond lengths



Bond angles

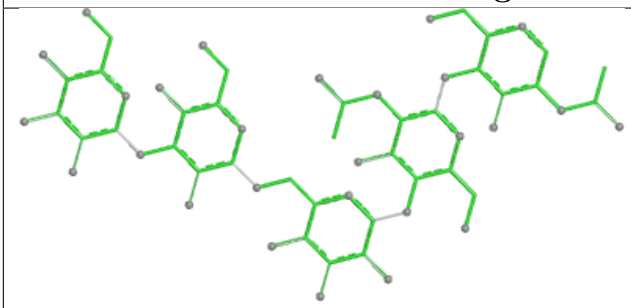


Torsions

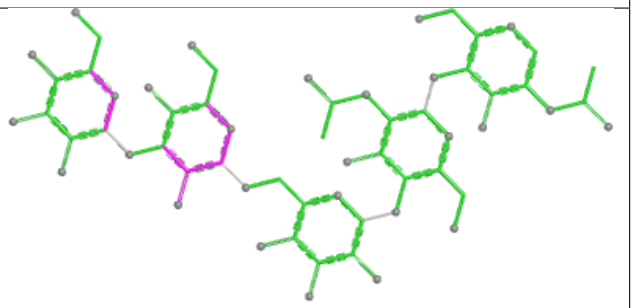


Rings

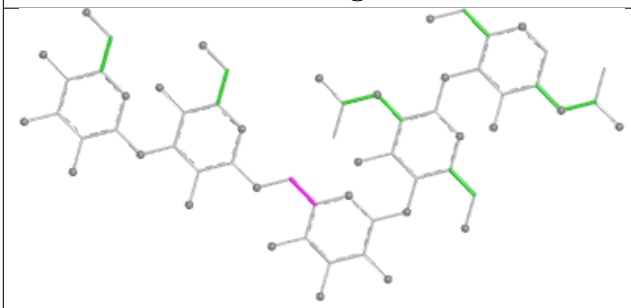
Oligosaccharide Chain D



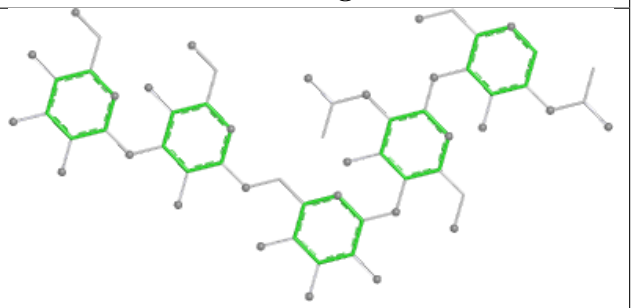
Bond lengths



Bond angles

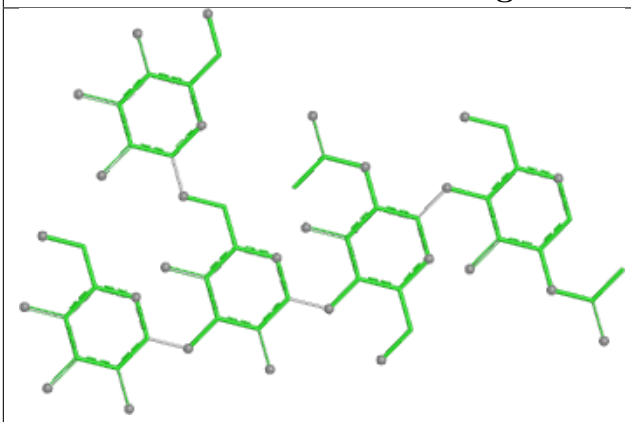


Torsions

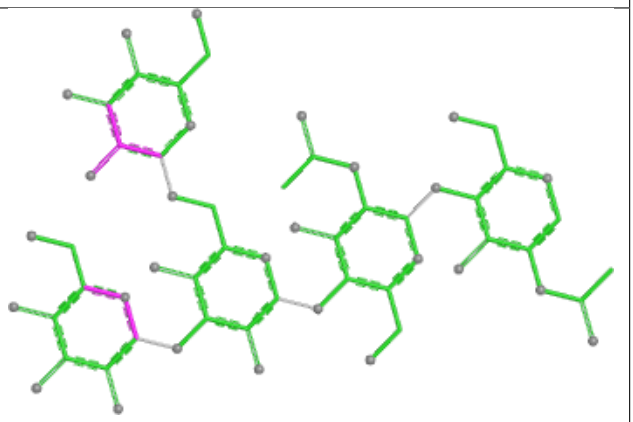


Rings

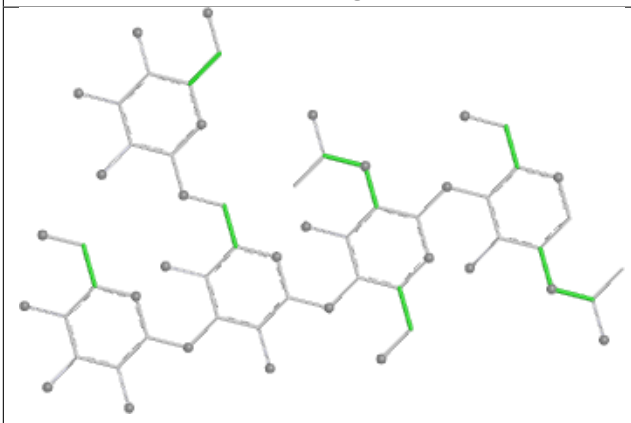
Oligosaccharide Chain E



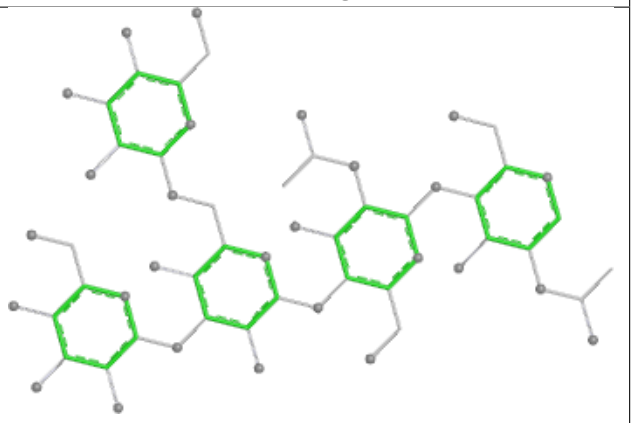
Bond lengths



Bond angles

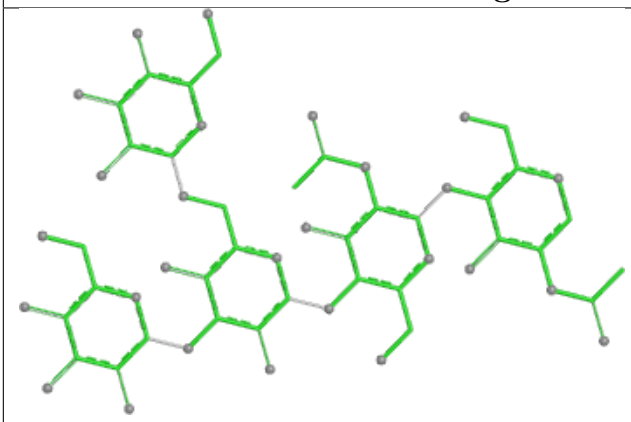


Torsions

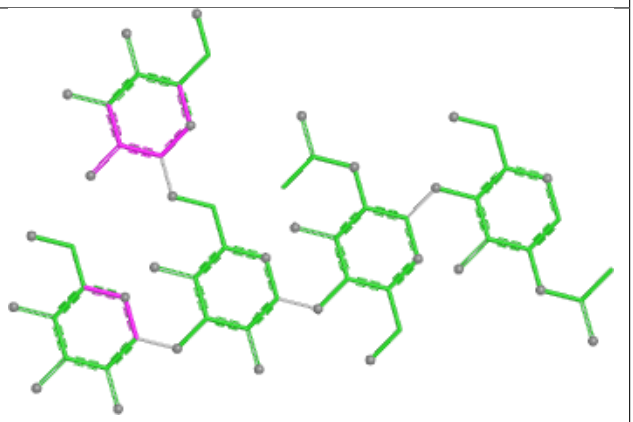


Rings

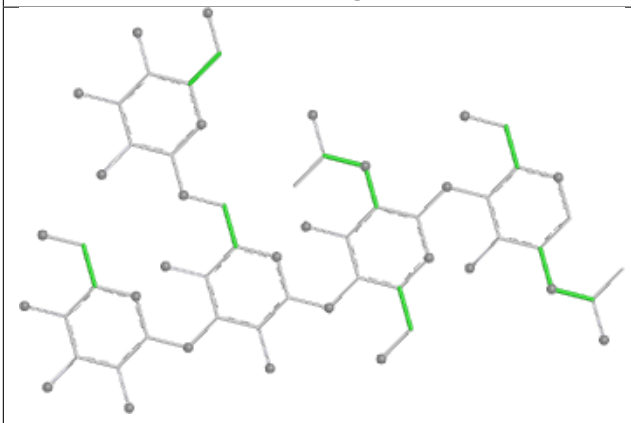
Oligosaccharide Chain G



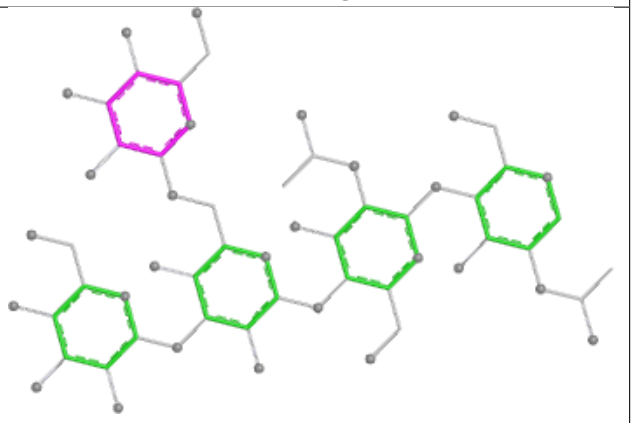
Bond lengths



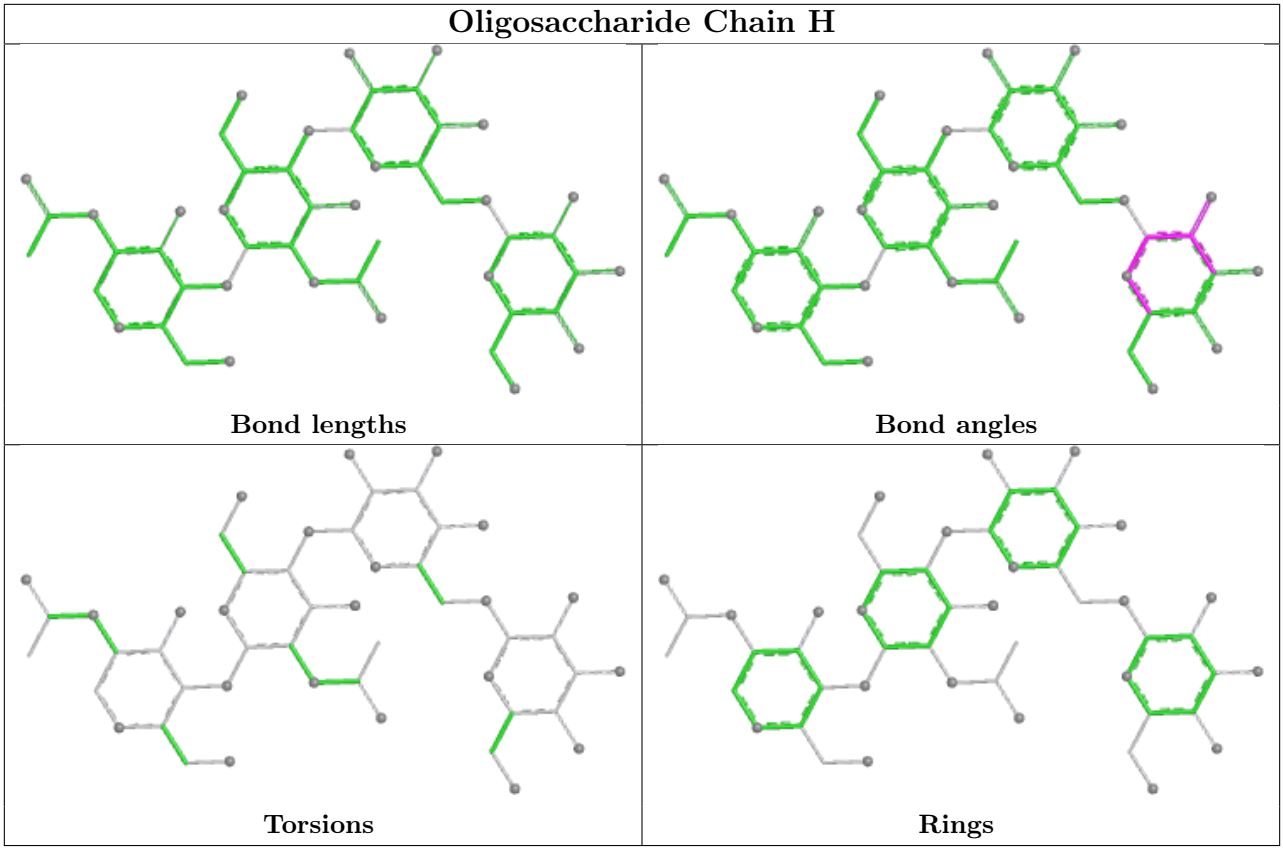
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
7	A1BLO	B	911	-	38,43,43	0.88	1 (2%)	45,60,60	1.39	1 (2%)
6	NAG	B	906	1	14,14,15	0.31	0	17,19,21	0.62	0
6	NAG	B	910	1	14,14,15	0.30	0	17,19,21	0.82	1 (5%)
6	NAG	A	911	1	14,14,15	0.30	0	17,19,21	0.63	0
7	A1BLO	A	913	-	38,43,43	0.68	1 (2%)	45,60,60	1.41	1 (2%)
6	NAG	A	905	1	14,14,15	0.30	0	17,19,21	0.62	0
6	NAG	A	906	1	14,14,15	0.26	0	17,19,21	0.90	1 (5%)
6	NAG	A	908	1	14,14,15	0.29	0	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	B	902	1	14,14,15	0.43	0	17,19,21	1.47	2 (11%)
6	NAG	B	909	1	14,14,15	0.28	0	17,19,21	0.88	1 (5%)
6	NAG	A	902	1	14,14,15	0.44	0	17,19,21	1.48	2 (11%)
6	NAG	A	909	1	14,14,15	0.27	0	17,19,21	0.60	0
6	NAG	A	912	1	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
6	NAG	A	904	1	14,14,15	0.32	0	17,19,21	1.33	2 (11%)
6	NAG	A	907	1	14,14,15	0.28	0	17,19,21	0.79	1 (5%)
6	NAG	A	903	1	14,14,15	0.30	0	17,19,21	0.62	0
6	NAG	B	901	1	14,14,15	0.33	0	17,19,21	1.12	1 (5%)
6	NAG	B	908	1	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
6	NAG	A	910	1	14,14,15	0.60	0	17,19,21	0.84	1 (5%)
6	NAG	B	907	1	14,14,15	0.27	0	17,19,21	0.91	1 (5%)
6	NAG	A	901	1	14,14,15	0.29	0	17,19,21	0.77	1 (5%)
6	NAG	B	904	1	14,14,15	0.30	0	17,19,21	0.62	0
6	NAG	B	905	1	14,14,15	0.30	0	17,19,21	1.32	2 (11%)
6	NAG	B	903	1	14,14,15	0.30	0	17,19,21	0.60	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
7	A1BLO	B	911	-	-	5/21/31/31	0/5/5/5
6	NAG	B	906	1	-	0/6/23/26	0/1/1/1
6	NAG	B	910	1	-	0/6/23/26	0/1/1/1
6	NAG	A	911	1	-	1/6/23/26	0/1/1/1
7	A1BLO	A	913	-	-	3/21/31/31	0/5/5/5
6	NAG	A	905	1	-	0/6/23/26	0/1/1/1
6	NAG	A	906	1	-	0/6/23/26	0/1/1/1
6	NAG	A	908	1	-	0/6/23/26	0/1/1/1
6	NAG	B	902	1	-	0/6/23/26	0/1/1/1
6	NAG	B	909	1	-	0/6/23/26	0/1/1/1
6	NAG	A	902	1	-	0/6/23/26	0/1/1/1
6	NAG	A	909	1	-	1/6/23/26	0/1/1/1
6	NAG	A	912	1	-	0/6/23/26	0/1/1/1
6	NAG	A	904	1	-	1/6/23/26	0/1/1/1
6	NAG	A	907	1	-	0/6/23/26	0/1/1/1
6	NAG	A	903	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	901	1	-	0/6/23/26	0/1/1/1
6	NAG	B	908	1	-	0/6/23/26	0/1/1/1
6	NAG	A	910	1	-	0/6/23/26	0/1/1/1
6	NAG	B	907	1	-	0/6/23/26	0/1/1/1
6	NAG	A	901	1	-	0/6/23/26	0/1/1/1
6	NAG	B	904	1	-	0/6/23/26	0/1/1/1
6	NAG	B	905	1	-	1/6/23/26	0/1/1/1
6	NAG	B	903	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	911	A1BLO	C20-C19	4.31	1.58	1.54
7	A	913	A1BLO	C20-C19	2.71	1.56	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	913	A1BLO	C25-C26-C29	8.14	122.28	114.95
7	B	911	A1BLO	C25-C26-C29	8.02	122.17	114.95
6	A	902	NAG	O5-C1-C2	-5.58	102.66	111.29
6	B	902	NAG	O5-C1-C2	-5.54	102.72	111.29
6	A	904	NAG	O5-C1-C2	-4.61	104.16	111.29
6	B	905	NAG	O5-C1-C2	-4.55	104.26	111.29
6	B	901	NAG	O5-C1-C2	-3.98	105.13	111.29
6	A	906	NAG	O5-C1-C2	-3.07	106.53	111.29
6	B	907	NAG	O5-C1-C2	-3.07	106.54	111.29
6	A	901	NAG	O5-C1-C2	-2.94	106.73	111.29
6	A	904	NAG	C1-C2-N2	2.58	114.50	110.43
6	A	910	NAG	O5-C1-C2	-2.56	107.33	111.29
6	B	905	NAG	C1-C2-N2	2.56	114.46	110.43
6	B	909	NAG	C1-O5-C5	2.50	115.53	112.19
6	A	908	NAG	C1-O5-C5	2.44	115.45	112.19
6	B	910	NAG	C1-O5-C5	2.39	115.38	112.19
6	A	907	NAG	C1-C2-N2	-2.38	106.68	110.43
6	B	908	NAG	O5-C1-C2	-2.22	107.85	111.29
6	B	902	NAG	C1-C2-N2	2.18	113.87	110.43
6	A	902	NAG	C1-C2-N2	2.16	113.84	110.43
6	B	903	NAG	O5-C1-C2	-2.05	108.13	111.29
6	A	912	NAG	C1-O5-C5	2.04	114.91	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	913	A1BLO	C25-C26-C29-C27
7	B	911	A1BLO	C25-C26-C29-C27
7	B	911	A1BLO	C25-C26-C29-N5
7	B	911	A1BLO	C29-C27-C28-O3
7	A	913	A1BLO	C25-C26-C29-N5
7	A	913	A1BLO	C14-C10-C23-N3
7	B	911	A1BLO	C17-C19-N6-C24
7	B	911	A1BLO	C14-C10-C23-N3
6	A	909	NAG	C1-C2-N2-C7
6	A	911	NAG	C1-C2-N2-C7
6	B	905	NAG	C8-C7-N2-C2
6	A	904	NAG	C8-C7-N2-C2

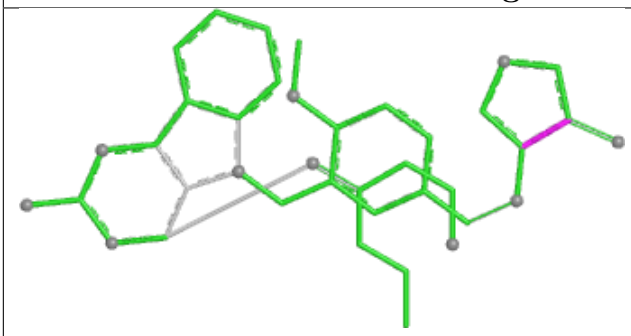
There are no ring outliers.

3 monomers are involved in 3 short contacts:

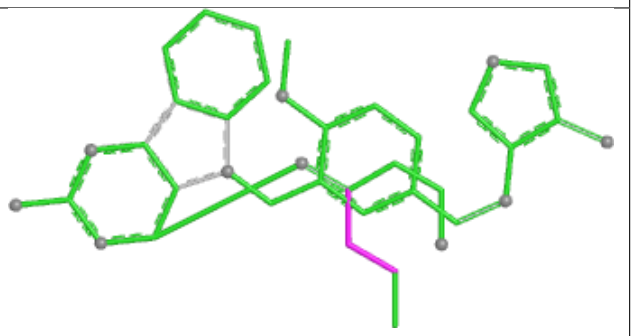
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	911	NAG	1	0
7	A	913	A1BLO	1	0
6	A	910	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

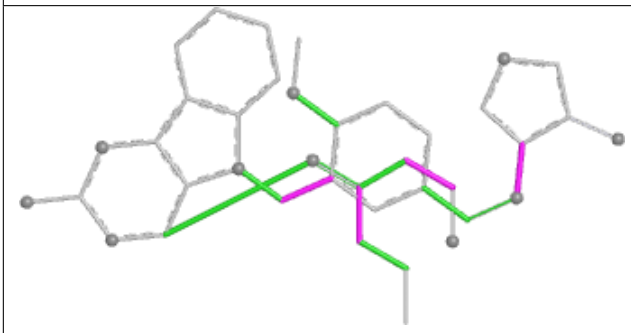
Ligand A1BLO B 911



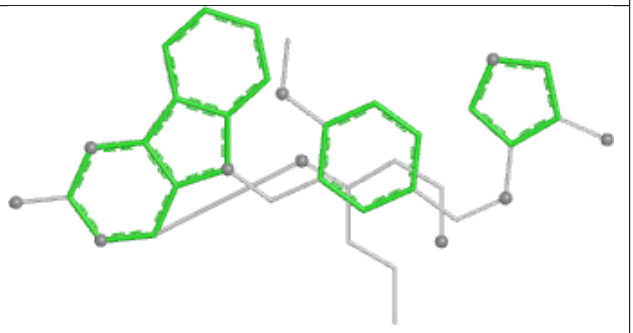
Bond lengths



Bond angles

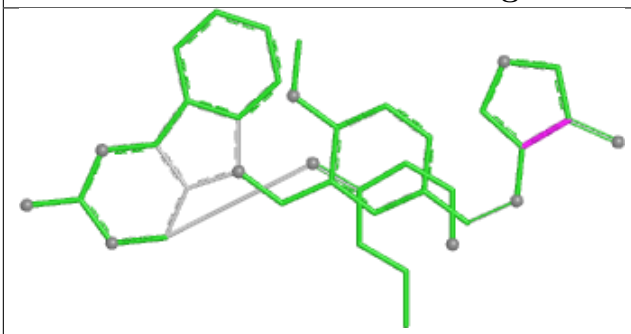


Torsions

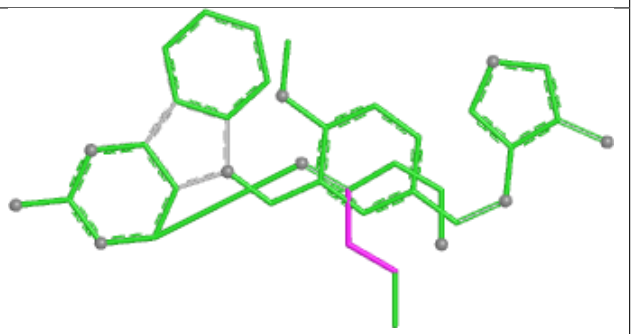


Rings

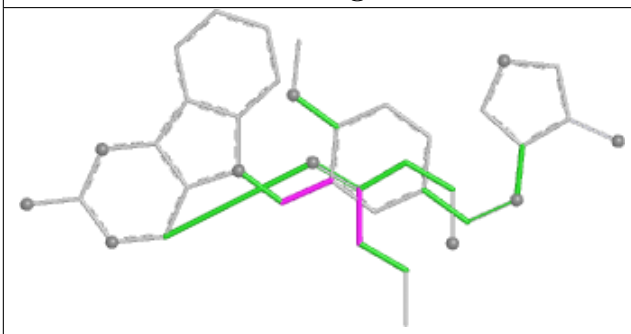
Ligand A1BLO A 913



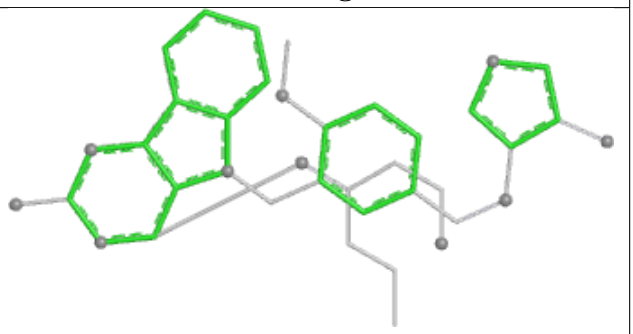
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	748/807 (92%)	0.21	24 (3%)	50	55	14, 25, 45, 66	2 (0%)
1	B	741/807 (91%)	0.35	33 (4%)	39	44	12, 26, 49, 73	1 (0%)
All	All	1489/1614 (92%)	0.28	57 (3%)	44	50	12, 26, 47, 73	3 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	ARG	4.8
1	B	762	THR	4.0
1	A	815	VAL	3.9
1	B	471	THR	3.8
1	A	470	PHE	3.8
1	B	735	VAL	3.8
1	B	49	CYS	3.7
1	B	473	PRO	3.5
1	B	780	ILE	3.4
1	B	434	VAL	3.4
1	A	367	LEU	3.4
1	A	49	CYS	3.3
1	A	759	LYS	3.3
1	A	814	ILE	3.2
1	B	779	ASP	3.1
1	A	505	PRO	3.1
1	B	433	LEU	3.1
1	B	65	VAL	3.0
1	A	758	THR	3.0
1	B	653	HIS	2.9
1	B	778	CYS	2.9
1	A	702	PHE	2.9
1	B	470	PHE	2.9
1	B	244	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	89	LEU	2.8
1	A	809	GLN	2.8
1	A	678	PHE	2.8
1	B	309	ASN	2.8
1	B	236	TYR	2.7
1	A	85	GLY	2.7
1	B	701	LEU	2.7
1	A	100	VAL	2.7
1	B	32	ARG	2.7
1	A	506	ASP	2.7
1	B	809	GLN	2.6
1	A	761	THR	2.6
1	B	100	VAL	2.5
1	B	469	HIS	2.4
1	B	39	LYS	2.4
1	B	643	ARG	2.4
1	A	643	ARG	2.3
1	A	167	SER	2.3
1	A	87	GLN	2.3
1	B	625	ASN	2.3
1	B	777	THR	2.3
1	A	113	GLY	2.3
1	A	461	PHE	2.3
1	B	274	ALA	2.3
1	A	39	LYS	2.1
1	A	735	VAL	2.1
1	B	811	GLY	2.1
1	B	474	LEU	2.1
1	B	702	PHE	2.1
1	B	272	GLY	2.0
1	A	762	THR	2.0
1	A	83	PHE	2.0
1	B	40	LYS	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)

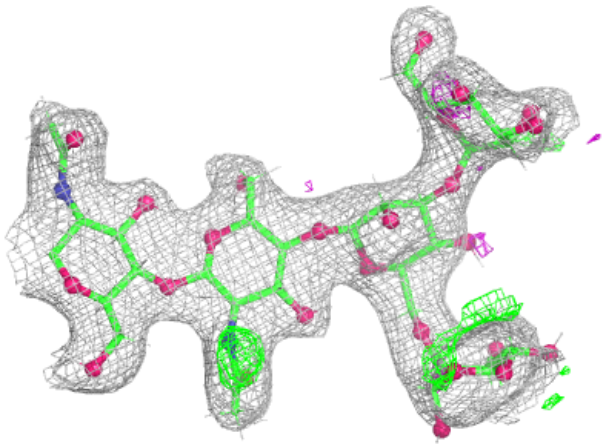
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

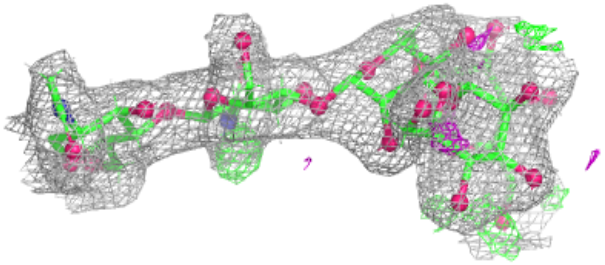
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	E	4	11/12	0.36	0.18	70,74,77,77	10
4	MAN	G	5	11/12	0.48	0.14	70,79,80,80	9
2	MAN	C	5	11/12	0.49	0.14	68,71,73,74	10
5	MAN	H	4	11/12	0.53	0.16	65,68,72,73	10
3	MAN	D	5	11/12	0.55	0.13	73,75,82,82	10
4	MAN	G	4	11/12	0.55	0.12	69,71,78,79	10
4	MAN	E	5	11/12	0.56	0.12	70,74,77,77	10
2	MAN	F	5	11/12	0.56	0.14	67,69,74,75	10
4	BMA	G	3	11/12	0.69	0.11	62,72,76,78	8
3	MAN	D	4	11/12	0.70	0.10	68,76,79,80	9
2	MAN	F	4	11/12	0.70	0.14	61,63,69,69	10
3	BMA	D	3	11/12	0.75	0.10	58,64,71,74	10
5	BMA	H	3	11/12	0.77	0.11	54,60,64,68	10
2	MAN	C	4	11/12	0.77	0.11	57,60,64,64	10
3	NAG	D	2	14/15	0.79	0.12	44,55,61,64	12
4	NAG	G	2	14/15	0.80	0.12	47,56,63,68	13
2	BMA	F	3	11/12	0.80	0.11	56,63,68,70	8
4	BMA	E	3	11/12	0.81	0.10	61,65,72,74	8
2	BMA	C	3	11/12	0.83	0.09	54,60,66,68	8
5	NAG	H	2	14/15	0.84	0.12	39,48,53,56	12
4	NAG	E	2	14/15	0.87	0.11	43,51,56,61	12
2	NAG	C	2	14/15	0.89	0.09	38,45,51,55	12
4	NAG	G	1	14/15	0.94	0.09	35,47,51,55	12
2	NAG	F	2	14/15	0.94	0.09	41,47,51,57	12
2	NAG	C	1	14/15	0.94	0.07	30,36,40,42	12
2	NAG	F	1	14/15	0.94	0.09	29,36,41,44	12
4	NAG	E	1	14/15	0.95	0.07	30,41,43,48	12
5	NAG	H	1	14/15	0.96	0.07	29,41,43,46	12
3	NAG	D	1	14/15	0.96	0.09	31,42,46,51	12

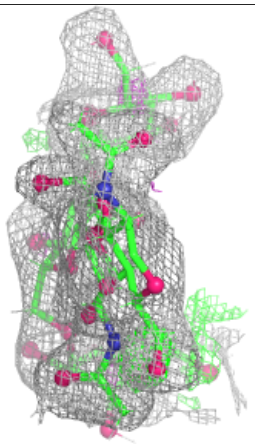
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

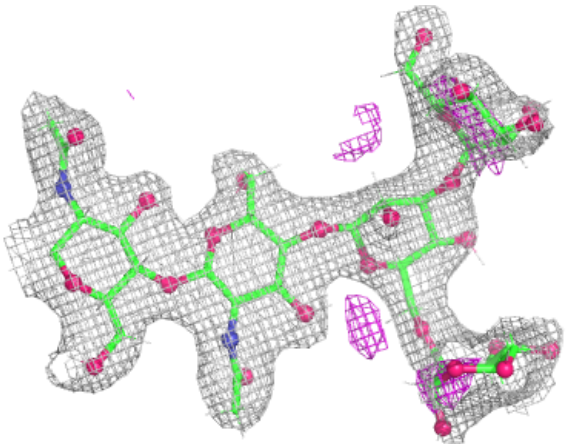


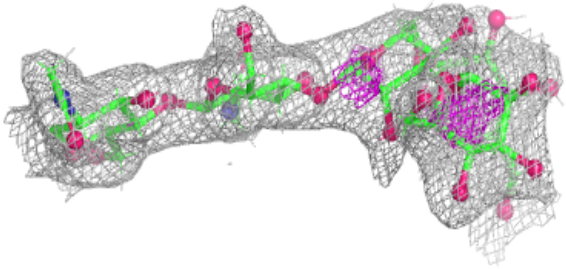


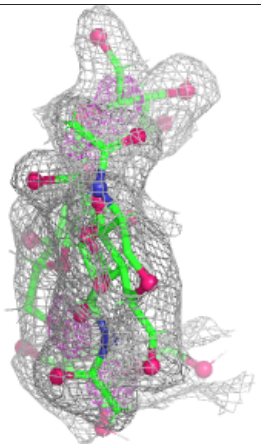


Electron density around Chain F:

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

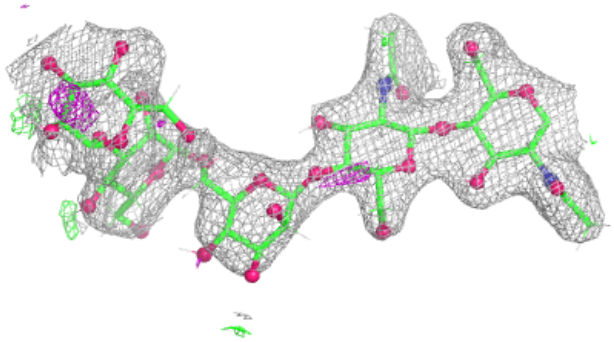


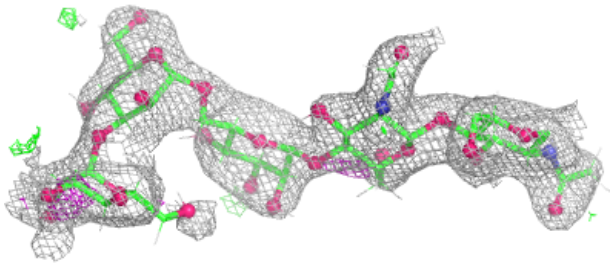


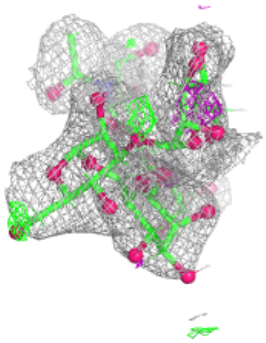


Electron density around Chain D:

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

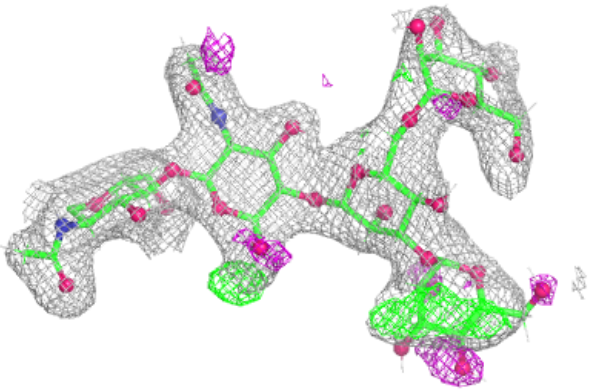


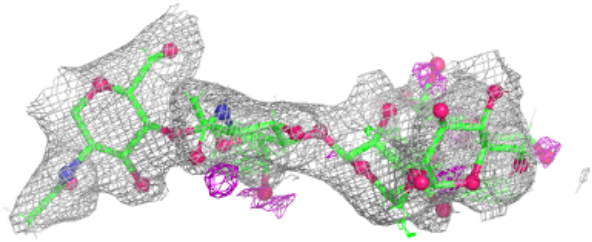


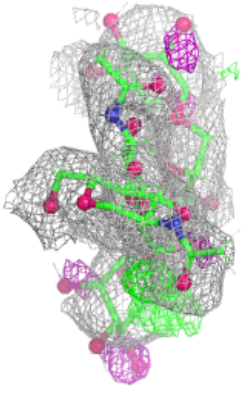


Electron density around Chain E:

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

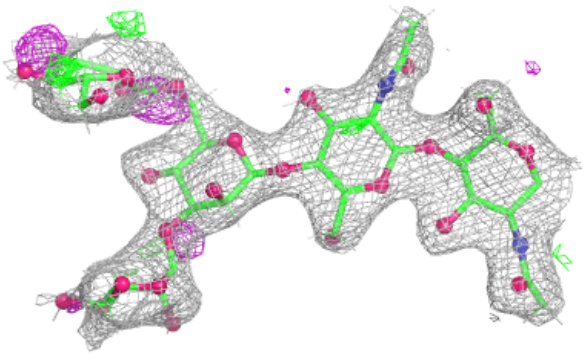


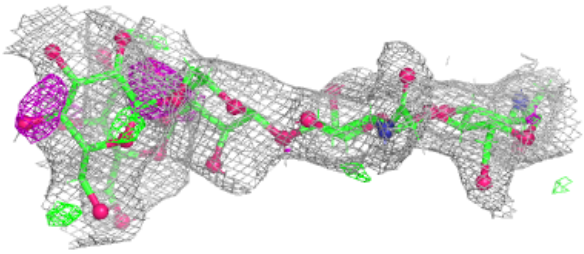


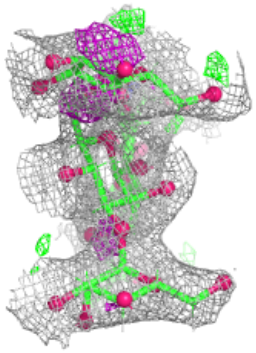


Electron density around Chain G:

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

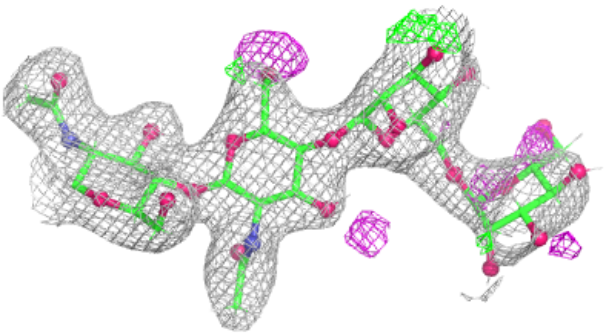


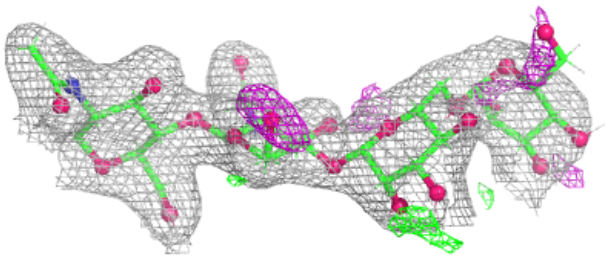


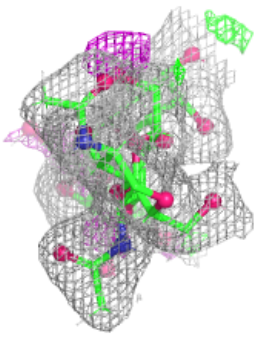


Electron density around Chain H:

$2mF_o$-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)

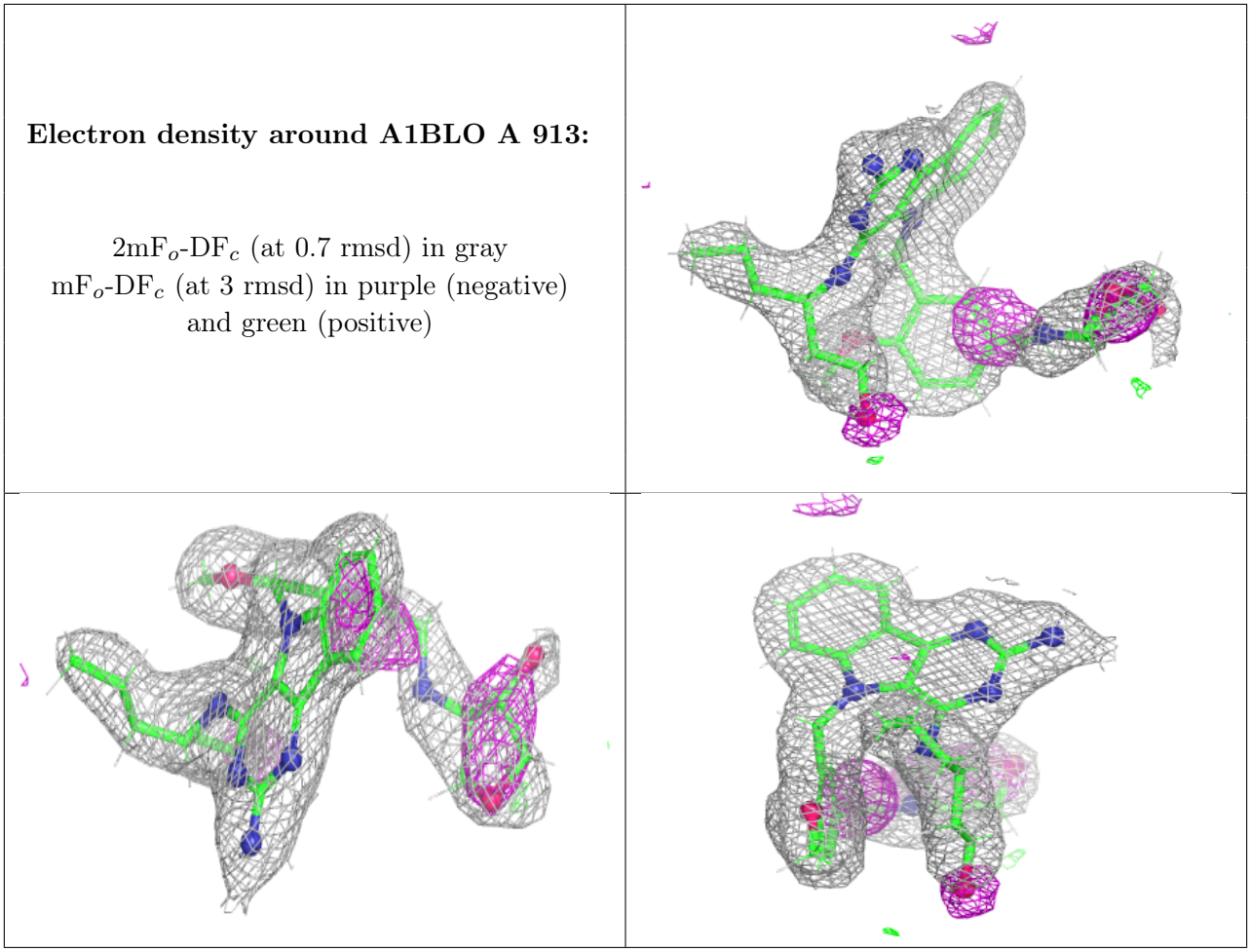
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	NAG	A	902	14/15	0.33	0.21	89,90,117,118	13
6	NAG	A	903	14/15	0.36	0.18	72,74,80,81	13
6	NAG	A	910	14/15	0.36	0.20	83,85,104,105	13
6	NAG	B	908	14/15	0.36	0.19	70,73,77,78	13
6	NAG	A	907	14/15	0.43	0.19	72,75,79,79	13
6	NAG	A	912	14/15	0.46	0.16	69,72,75,75	13
6	NAG	B	902	14/15	0.48	0.18	85,87,106,106	13
6	NAG	A	911	14/15	0.48	0.16	65,68,72,73	13
6	NAG	A	901	14/15	0.50	0.15	91,92,125,127	13
6	NAG	B	904	14/15	0.54	0.15	72,74,79,79	13
6	NAG	B	903	14/15	0.63	0.12	71,72,85,87	13
6	NAG	B	906	14/15	0.70	0.14	67,68,69,70	13
6	NAG	B	909	14/15	0.70	0.13	72,74,82,82	13
6	NAG	B	901	14/15	0.71	0.13	85,87,111,113	13
6	NAG	A	909	14/15	0.75	0.13	86,87,111,113	13
6	NAG	A	904	14/15	0.78	0.11	56,59,60,61	13
6	NAG	A	905	14/15	0.78	0.12	65,66,68,68	13
6	NAG	B	905	14/15	0.80	0.13	51,54,62,62	13
6	NAG	A	906	14/15	0.82	0.13	66,68,77,77	13
6	NAG	A	908	14/15	0.85	0.11	59,61,66,66	13
6	NAG	B	907	14/15	0.85	0.10	72,74,90,92	13
6	NAG	B	910	14/15	0.88	0.09	50,53,57,57	13
7	A1BLO	A	913	39/39	0.88	0.12	37,42,57,57	38
7	A1BLO	B	911	39/39	0.88	0.11	36,41,51,52	38

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

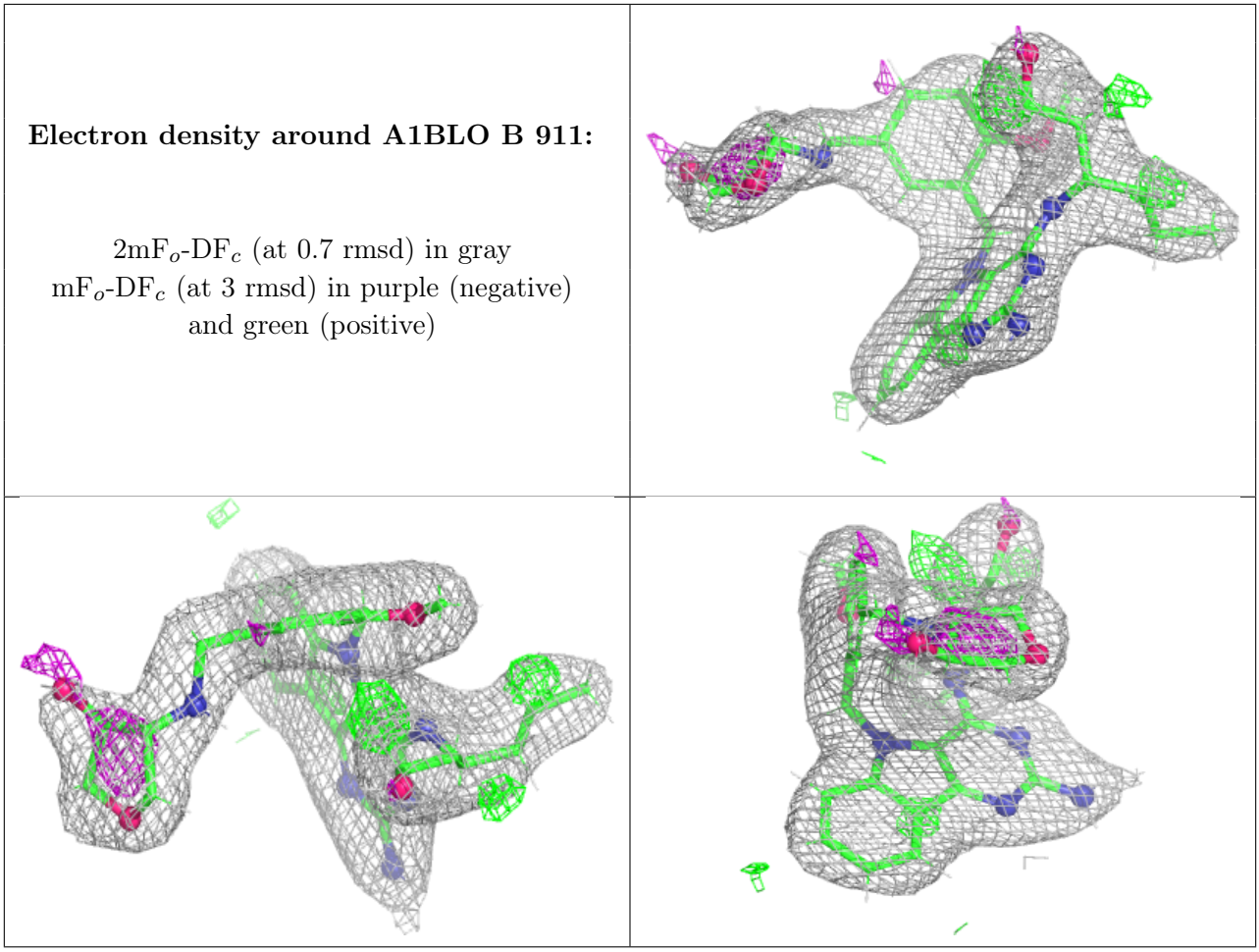
Electron density around A1BLO A 913:

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



Electron density around A1BLO B 911:

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



6.5 Other polymers

There are no such residues in this entry.