Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 10:45 PM EDT

PDB ID	:	4NEN
Title	:	An internal ligand-bound, metastable state of a leukocyte integrin, aXb2
Authors	:	Sen, M.; Yuki, K.; Springer, T.A.
Deposited on	:	2013-10-29
Resolution	:	2.90 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:

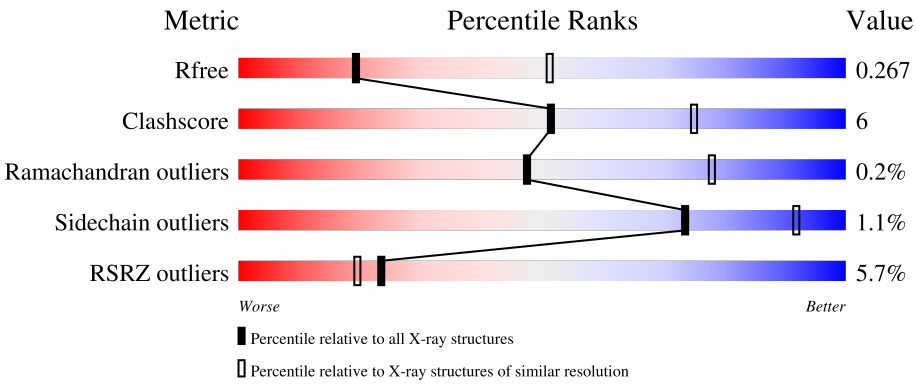
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	1094	4% 82% 15% •
2	B	686	8% 82% 14% •
3	C	2	50% 50%
3	D	2	50% 50%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
3	H	2	100%
4	E	6	33% 50% 17%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13731 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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1063	8265	5239	1422	1567	37	0	4	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASP	ASN	engineered mutation	UNP P20702
A	368	ASP	SER	engineered mutation	UNP P20702
A	678	THR	ASN	engineered mutation	UNP P20702
A	885	SER	ASN	engineered mutation	UNP P20702
A	920	CYS	ASN	engineered mutation	UNP P20702
A	1083	PRO	-	expression tag	UNP P20702
A	1084	GLY	-	expression tag	UNP P20702
A	1085	PRO	-	expression tag	UNP P20702
A	1086	ALA	-	expression tag	UNP P20702
A	1087	ALA	-	expression tag	UNP P20702
A	1088	LEU	-	expression tag	UNP P20702
A	1089	GLN	-	expression tag	UNP P20702
A	1090	THR	-	expression tag	UNP P20702
A	1091	LEU	-	expression tag	UNP P20702
A	1092	PHE	-	expression tag	UNP P20702
A	1093	GLN	-	expression tag	UNP P20702
A	1094	GLY	-	expression tag	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	665	5118	3154	912	987	65	0	4	1

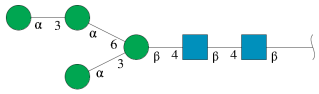
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	ASP	ASN	engineered mutation	UNP P05107
B	232	LYS	ASN	engineered mutation	UNP P05107
B	674	CYS	VAL	engineered mutation	UNP P05107
B	675	GLY	-	expression tag	UNP P05107
B	676	GLY	-	expression tag	UNP P05107
B	677	PRO	-	expression tag	UNP P05107
B	678	ALA	-	expression tag	UNP P05107
B	679	ALA	-	expression tag	UNP P05107
B	680	LEU	-	expression tag	UNP P05107
B	681	GLN	-	expression tag	UNP P05107
B	682	THR	-	expression tag	UNP P05107
B	683	LEU	-	expression tag	UNP P05107
B	684	PHE	-	expression tag	UNP P05107
B	685	GLN	-	expression tag	UNP P05107
B	686	GLY	-	expression tag	UNP P05107

- Molecule 3 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			
3	C	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	G	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	H	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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			
4	E	6	72	40	2	30	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	3	3	3	0	0
5	B	2	2	2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
6	B	1	1	1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	A	1	1	1	0	0

- Molecule 8 is water.

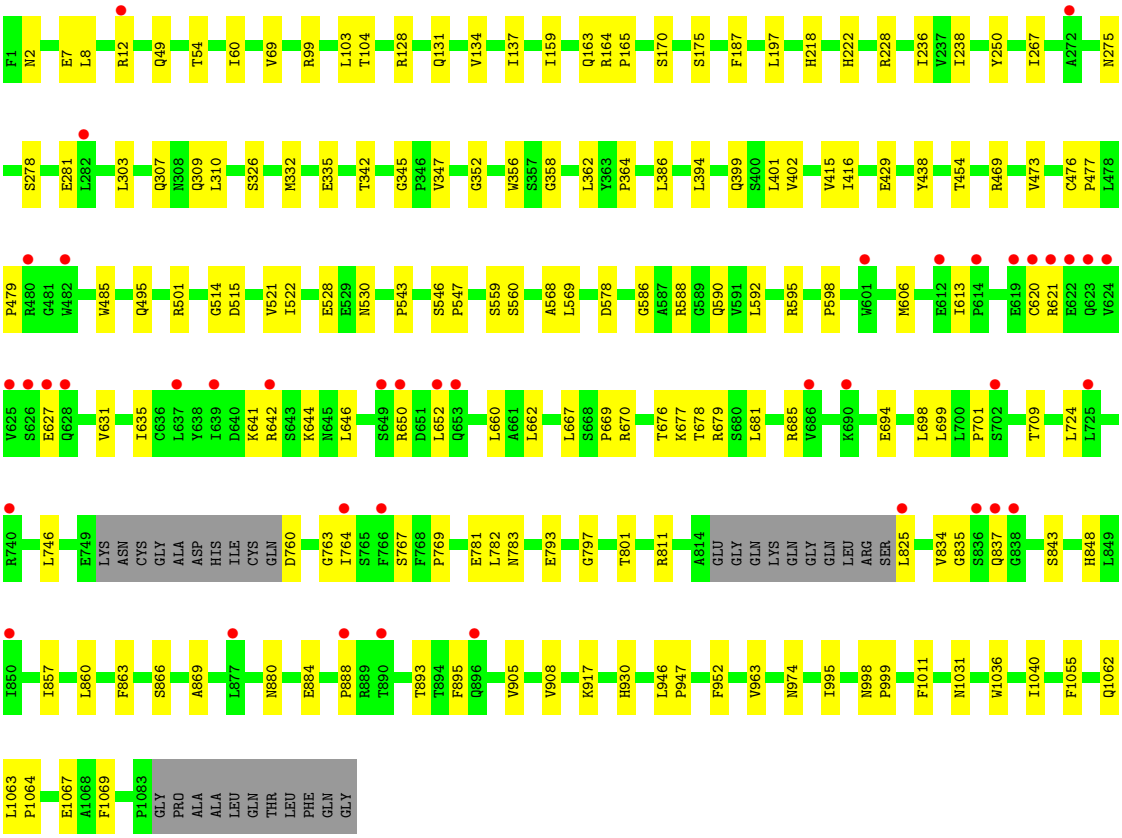
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	74	74	74	0	0
8	B	54	54	54	0	0

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.

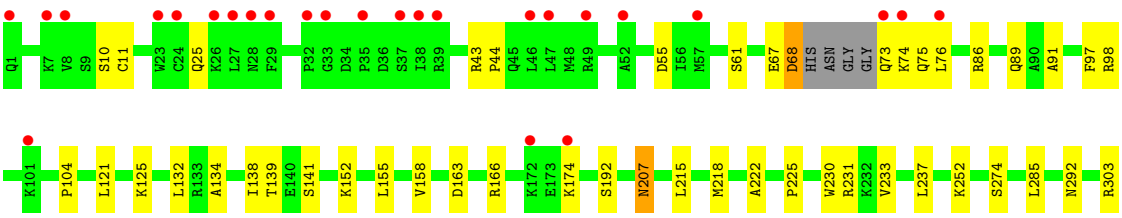
• Molecule 1: Integrin alpha-X

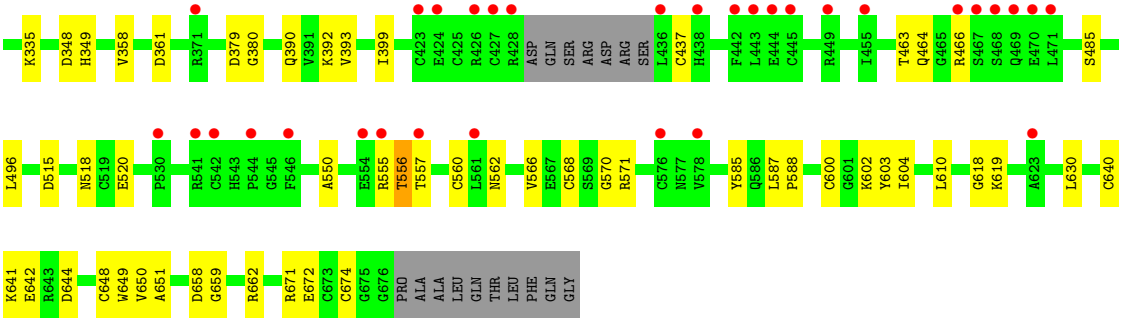
Chain A: 4% 82% 15%



• Molecule 2: Integrin beta-2

Chain B: 8% 82% 14%





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

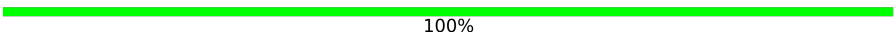
Chain C:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

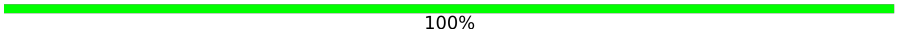
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



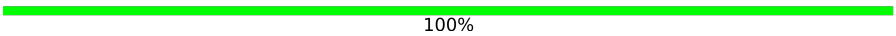
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.09Å 119.85Å 182.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 2.90 47.81 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.81-2.90) 99.3 (47.81-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.224 , 0.264 0.228 , 0.267	Depositor DCC
R_{free} test set	3117 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13731	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 2.89% 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: CA, MG, MAN, CL, NAG, BMA

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	0.22	0/8465	0.43	1/11502 (0.0%)
2	B	0.23	0/5223	0.43	0/7049
All	All	0.22	0/13688	0.43	1/18551 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	888	PRO	N-CA-CB	6.18	110.72	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8265	0	8095	99	0
2	B	5118	0	4920	59	0
3	C	28	0	25	1	0
3	D	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
4	E	72	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	3	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
8	A	74	0	0	3	0
8	B	54	0	0	1	0
All	All	13731	0	13201	150	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.

All (150) 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:952:PHE:HB2	1:A:1011:PHE:HB2	1.68	0.75
1:A:685:ARG:HH12	1:A:694:GLU:HB2	1.53	0.72
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.75	0.68
1:A:995:ILE:HG21	1:A:1040:ILE:HG23	1.78	0.66
1:A:12:ARG:HG2	1:A:590:GLN:HG2	1.76	0.66
1:A:825:LEU:HD22	1:A:857:ILE:HG21	1.78	0.65
2:B:361:ASP:OD2	2:B:392:LYS:NZ	2.29	0.65
1:A:685:ARG:NH1	1:A:694:GLU:OE1	2.28	0.65
1:A:783:ASN:HB3	1:A:860:LEU:HD11	1.78	0.64
2:B:649:TRP:HB2	2:B:672:GLU:HB2	1.79	0.63
2:B:515:ASP:OD2	2:B:518:ASN:ND2	2.29	0.63
1:A:866:SER:HB3	1:A:869:ALA:HB2	1.80	0.63
1:A:685:ARG:NH1	1:A:694:GLU:HB2	2.16	0.61
2:B:158:VAL:HG22	2:B:207:ASN:HB2	1.82	0.61
2:B:463:THR:OG1	2:B:464:GLN:OE1	2.19	0.60
2:B:658:ASP:O	2:B:662:ARG:NH1	2.35	0.59
1:A:501:ARG:NH2	1:A:530:ASN:OD1	2.34	0.59
1:A:781:GLU:OE1	1:A:811:ARG:NH2	2.34	0.59
2:B:141:SER:HB3	2:B:231:ARG:HH12	1.67	0.59
1:A:834:VAL:HG12	1:A:835:GLY:H	1.68	0.59
1:A:69:VAL:HG11	3:D:1:NAG:H82	1.85	0.58
1:A:236:ILE:HG23	1:A:267:ILE:HD13	1.86	0.58
1:A:469:ARG:HD3	1:A:495:GLN:HG2	1.85	0.58
1:A:667:LEU:HD11	2:B:496:LEU:HD23	1.87	0.57
1:A:362:LEU:HG	1:A:364:PRO:HD3	1.87	0.57
2:B:25:GLN:HG2	2:B:55:ASP:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:VAL:HG22	2:B:393:VAL:HG22	1.87	0.56
1:A:402:VAL:HG22	1:A:416:ILE:HG12	1.86	0.56
2:B:74:LYS:O	2:B:98:ARG:HB3	2.06	0.55
1:A:104:THR:OG1	1:A:335:GLU:OE1	2.21	0.55
1:A:128:ARG:HA	1:A:310:LEU:HA	1.88	0.55
1:A:394:LEU:O	1:A:454:THR:N	2.36	0.55
2:B:604:ILE:HD13	2:B:642:GLU:HB2	1.89	0.55
2:B:132:LEU:HD23	2:B:192:SER:HB2	1.88	0.54
2:B:610:LEU:HB3	2:B:630:LEU:HD22	1.89	0.54
1:A:347:VAL:HG11	1:A:401:LEU:HD21	1.89	0.54
1:A:473:VAL:HG21	1:A:522:ILE:HD13	1.90	0.54
2:B:520:GLU:HB2	2:B:550:ALA:HB2	1.90	0.54
2:B:138:ILE:HG22	2:B:139:THR:HG23	1.90	0.53
2:B:587:LEU:HB3	2:B:588:PRO:HA	1.89	0.53
1:A:159:ILE:HD12	1:A:197:LEU:HD11	1.91	0.53
2:B:222:ALA:O	2:B:292:ASN:ND2	2.41	0.53
2:B:618:GLY:O	2:B:619:LYS:HB2	2.08	0.53
1:A:137:ILE:HG22	1:A:238:ILE:HD12	1.89	0.53
1:A:332:MET:HE1	2:B:155:LEU:HD22	1.89	0.53
1:A:415:VAL:HG22	1:A:429:GLU:HG2	1.90	0.53
1:A:598:PRO:HB3	1:A:646:LEU:HD22	1.90	0.52
1:A:760:ASP:N	1:A:793:GLU:OE1	2.42	0.52
2:B:134:ALA:HB1	2:B:335:LYS:HD2	1.92	0.52
1:A:652:LEU:HD23	1:A:724:LEU:HD21	1.92	0.52
2:B:104:PRO:HB3	2:B:141:SER:HB2	1.92	0.52
1:A:905:VAL:HG11	1:A:946:LEU:HD22	1.92	0.51
1:A:236:ILE:HD11	1:A:303:LEU:HD21	1.91	0.51
2:B:61:SER:HB3	2:B:91:ALA:HB2	1.93	0.51
1:A:801:THR:HA	1:A:843:SER:HA	1.92	0.51
1:A:342:THR:OG1	1:A:345:GLY:O	2.23	0.50
1:A:669:PRO:HB3	1:A:679:ARG:HD3	1.93	0.50
1:A:660:LEU:HD12	1:A:681:LEU:HD22	1.94	0.50
1:A:834:VAL:HG12	1:A:835:GLY:N	2.26	0.50
1:A:627:GLU:H	1:A:701:PRO:HA	1.77	0.49
1:A:8:LEU:HD21	1:A:592:LEU:HD23	1.92	0.49
1:A:165:PRO:O	1:A:228:ARG:NH1	2.45	0.49
1:A:128:ARG:NE	1:A:163:GLN:OE1	2.46	0.49
1:A:678:THR:OG1	1:A:679:ARG:N	2.45	0.49
2:B:602:LYS:HE3	2:B:603:TYR:CZ	2.48	0.49
2:B:86:ARG:HD3	2:B:89:GLN:HE21	1.78	0.49
1:A:521:VAL:HG12	1:A:569:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:HG22	1:A:170:SER:HB3	1.94	0.48
1:A:103:LEU:HD22	2:B:155:LEU:HB3	1.95	0.48
1:A:307:GLN:HB2	1:A:309:GLN:HG3	1.96	0.48
1:A:763:GLY:HA2	1:A:893:THR:HB	1.95	0.48
1:A:99:ARG:NH2	2:B:163:ASP:HB3	2.29	0.48
1:A:627:GLU:HB3	1:A:699:LEU:HD13	1.96	0.48
1:A:1036:TRP:CZ3	1:A:1040:ILE:HD11	2.48	0.48
1:A:578:ASP:O	1:A:646:LEU:HD12	2.14	0.48
1:A:946:LEU:HD11	1:A:1055:PHE:HB2	1.96	0.47
2:B:76:LEU:HD23	2:B:76:LEU:HA	1.78	0.47
1:A:797:GLY:HA3	1:A:884:GLU:HG3	1.96	0.47
2:B:67:GLU:O	2:B:68:ASP:HB3	2.14	0.47
2:B:562:ASN:OD1	2:B:566:VAL:N	2.47	0.47
1:A:782:LEU:N	1:A:863:PHE:O	2.48	0.46
1:A:1063:LEU:HD12	1:A:1064:PRO:HD2	1.98	0.46
2:B:104:PRO:HB2	2:B:233:VAL:HG11	1.96	0.46
1:A:801:THR:HB	1:A:880:ASN:HB2	1.97	0.46
2:B:379:ASP:OD1	2:B:380:GLY:N	2.47	0.46
1:A:49:GLN:HB3	1:A:60:ILE:HD11	1.96	0.46
1:A:1062:GLN:HG2	1:A:1067:GLU:HA	1.97	0.46
2:B:252:LYS:NZ	8:B:850:HOH:O	2.49	0.46
2:B:75:GLN:O	2:B:97:PHE:HA	2.14	0.46
1:A:662:LEU:HB2	1:A:679:ARG:HB2	1.97	0.46
1:A:848:HIS:CE1	2:B:485:SER:HB2	2.51	0.46
2:B:121:LEU:HG	2:B:125:LYS:HE3	1.98	0.46
2:B:560:CYS:O	2:B:568:CYS:N	2.46	0.45
2:B:641:LYS:HE2	2:B:651:ALA:HB2	1.98	0.45
1:A:588:ARG:NH1	8:A:1259:HOH:O	2.49	0.45
2:B:571:ARG:HD2	2:B:585:TYR:CE2	2.51	0.45
1:A:358:GLY:HA3	1:A:386:LEU:HB3	1.98	0.45
2:B:348:ASP:OD1	2:B:349:HIS:N	2.46	0.45
1:A:946:LEU:HD12	1:A:947:PRO:HD2	1.99	0.45
2:B:600:CYS:HB3	2:B:640:CYS:HB3	1.93	0.45
1:A:963:VAL:HG22	1:A:1036:TRP:CG	2.52	0.45
1:A:917:LYS:HE2	2:B:641:LYS:O	2.17	0.44
2:B:152:LYS:NZ	2:B:274:SER:O	2.43	0.44
2:B:570:GLY:HA3	2:B:659:GLY:HA2	1.99	0.44
2:B:650:VAL:HG22	2:B:671:ARG:HD2	1.99	0.44
1:A:631:VAL:HB	1:A:698:LEU:HB2	1.99	0.44
1:A:930:HIS:HA	3:C:1:NAG:H61	1.99	0.44
1:A:250:TYR:HE2	1:A:281:GLU:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:TYR:CE2	1:A:281:GLU:HG3	2.52	0.44
1:A:394:LEU:HD23	1:A:399:GLN:HA	2.00	0.44
1:A:99:ARG:HH21	2:B:163:ASP:HB3	1.83	0.43
1:A:606:MET:HG2	1:A:635:ILE:HG12	2.00	0.43
1:A:326:SER:HB3	4:E:6:MAN:H62	1.99	0.43
1:A:559:SER:OG	1:A:560:SER:O	2.34	0.43
1:A:998:ASN:HA	1:A:999:PRO:HD3	1.82	0.43
1:A:479:PRO:HD3	1:A:485:TRP:CD1	2.54	0.43
1:A:848:HIS:ND1	2:B:485:SER:HB2	2.32	0.43
1:A:164:ARG:HD3	1:A:187:PHE:CE2	2.54	0.43
2:B:556:THR:HB	2:B:557:THR:H	1.55	0.43
1:A:131:GLN:NE2	8:A:1242:HOH:O	2.50	0.43
1:A:568:ALA:HB3	1:A:586:GLY:HA3	2.01	0.43
1:A:764:ILE:HG23	1:A:895:PHE:HB2	2.00	0.42
1:A:676:THR:O	1:A:677:LYS:HB2	2.19	0.42
2:B:10:SER:OG	2:B:11:CYS:N	2.52	0.42
1:A:801:THR:HG23	1:A:843:SER:HB3	2.01	0.42
1:A:1036:TRP:HZ3	1:A:1040:ILE:HD11	1.84	0.42
1:A:641:LYS:HG3	1:A:644:LYS:HZ2	1.85	0.42
2:B:218:MET:HG2	2:B:237:LEU:HD21	2.02	0.42
1:A:352:GLY:HA2	1:A:356:TRP:CD1	2.55	0.41
2:B:73:GLN:HG3	2:B:74:LYS:HG3	2.02	0.41
2:B:215:LEU:HG	2:B:285:LEU:HD22	2.02	0.41
2:B:466:ARG:H	2:B:466:ARG:HG2	1.56	0.41
2:B:644:ASP:OD1	2:B:648:CYS:N	2.52	0.41
2:B:43:ARG:N	2:B:44:PRO:HD2	2.36	0.41
2:B:225:PRO:HA	2:B:230:TRP:HD1	1.85	0.41
1:A:963:VAL:HG13	1:A:1036:TRP:CE2	2.55	0.41
1:A:908:VAL:HG12	1:A:1069:PHE:HB3	2.03	0.41
1:A:546:SER:HA	1:A:547:PRO:HD3	1.85	0.41
1:A:476:CYS:HA	1:A:477:PRO:HD2	1.90	0.41
1:A:514:GLY:O	1:A:642:ARG:NH2	2.54	0.41
1:A:515:ASP:CG	8:A:1219:HOH:O	2.59	0.41
1:A:767:SER:O	1:A:769:PRO:HD3	2.21	0.41
2:B:163:ASP:OD1	2:B:166:ARG:NH2	2.52	0.41
1:A:2:ASN:OD1	1:A:2:ASN:N	2.52	0.40
1:A:275:ASN:HB3	1:A:278:SER:HB2	2.03	0.40
1:A:613:ILE:HD11	1:A:746:LEU:HG	2.03	0.40
1:A:7:GLU:HG2	1:A:595:ARG:NH2	2.37	0.40
1:A:670:ARG:NH1	1:A:709:THR:O	2.54	0.40
2:B:399:ILE:H	2:B:399:ILE:HG13	1.68	0.40

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	1061/1094 (97%)	1010 (95%)	48 (4%)	3 (0%)	41	71
2	B	663/686 (97%)	621 (94%)	41 (6%)	1 (0%)	47	78
All	All	1724/1780 (97%)	1631 (95%)	89 (5%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	PRO
1	A	175	SER
1	A	528	GLU
2	B	555	ARG

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	909/932 (98%)	899 (99%)	10 (1%)	73	92
2	B	576/590 (98%)	569 (99%)	7 (1%)	71	91
All	All	1485/1522 (98%)	1468 (99%)	17 (1%)	73	92

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	222[A]	HIS
1	A	222[B]	HIS
1	A	438	TYR
1	A	620	CYS
1	A	621	ARG
1	A	650	ARG
1	A	837	GLN
1	A	974	ASN
1	A	1031	ASN
2	B	68	ASP
2	B	174	LYS
2	B	207	ASN
2	B	303	ARG
2	B	437	CYS
2	B	556	THR
2	B	674	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

16 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	C	1	1,3	14,14,15	0.45	0	17,19,21	0.44	0
3	NAG	C	2	3	14,14,15	0.27	0	17,19,21	0.53	0
3	NAG	D	1	1,3	14,14,15	0.65	0	17,19,21	0.58	0
3	NAG	D	2	3	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	E	1	1,4	14,14,15	0.56	0	17,19,21	0.42	0
4	NAG	E	2	4	14,14,15	0.21	0	17,19,21	0.36	0
4	BMA	E	3	4	11,11,12	0.66	0	15,15,17	1.25	2 (13%)
4	MAN	E	4	4	11,11,12	0.94	0	15,15,17	1.23	3 (20%)
4	MAN	E	5	4	11,11,12	0.83	0	15,15,17	0.98	1 (6%)
4	MAN	E	6	4	11,11,12	1.06	1 (9%)	15,15,17	1.04	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.54	0	17,19,21	0.56	0
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	0.37	0
3	NAG	G	1	3,2	14,14,15	0.50	0	17,19,21	0.40	0
3	NAG	G	2	3	14,14,15	0.31	0	17,19,21	0.39	0
3	NAG	H	1	3,2	14,14,15	0.59	0	17,19,21	0.64	0
3	NAG	H	2	3	14,14,15	0.35	0	17,19,21	0.46	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	1/2/19/22	0/1/1/1
4	MAN	E	6	4	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	6	MAN	C2-C3	2.40	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	3	BMA	C1-O5-C5	2.78	115.96	112.19
4	E	3	BMA	O2-C2-C3	-2.54	105.05	110.14
4	E	6	MAN	O2-C2-C3	-2.53	105.07	110.14
4	E	4	MAN	O3-C3-C2	2.49	114.76	109.99
4	E	4	MAN	C1-O5-C5	2.32	115.34	112.19
4	E	4	MAN	O2-C2-C3	-2.23	105.67	110.14
4	E	5	MAN	O2-C2-C3	-2.15	105.82	110.14

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	E	6	MAN	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6

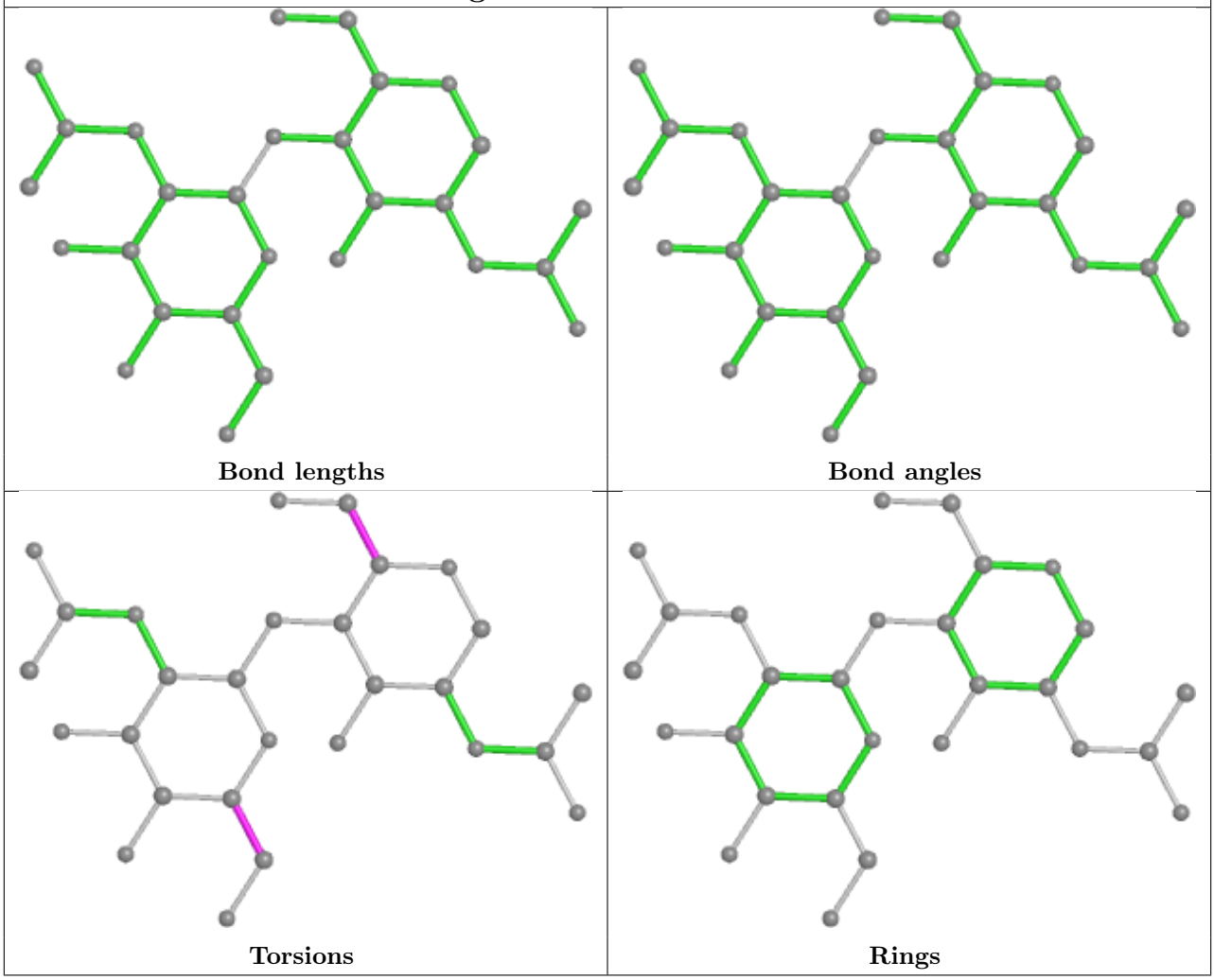
There are no ring outliers.

3 monomers are involved in 3 short contacts:

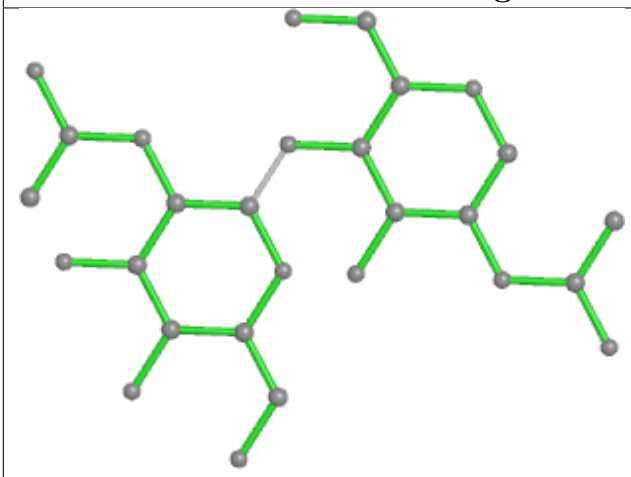
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
3	C	1	NAG	1	0
4	E	6	MAN	1	0

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

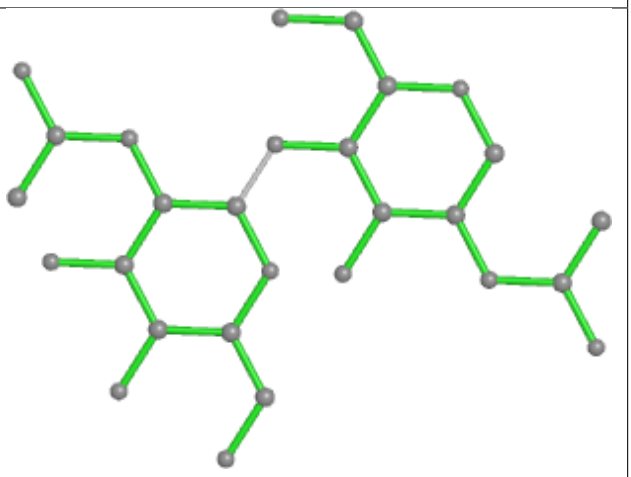
Oligosaccharide Chain C



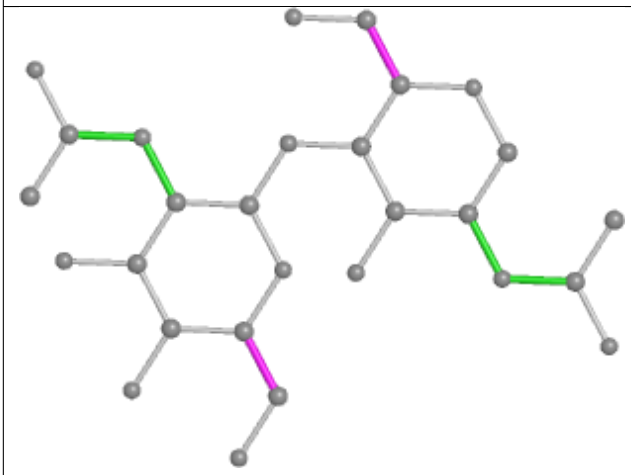
Oligosaccharide Chain D



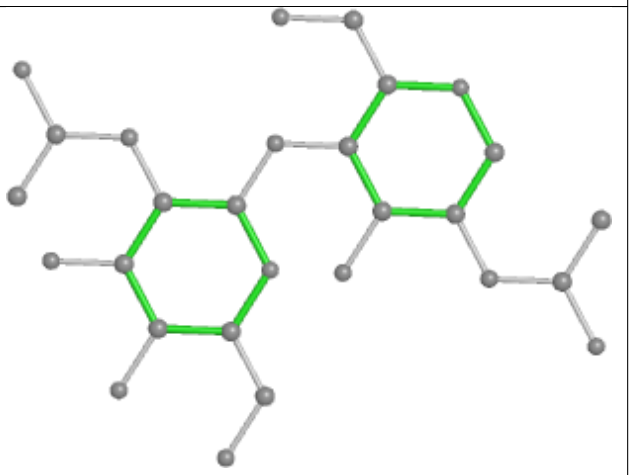
Bond lengths



Bond angles

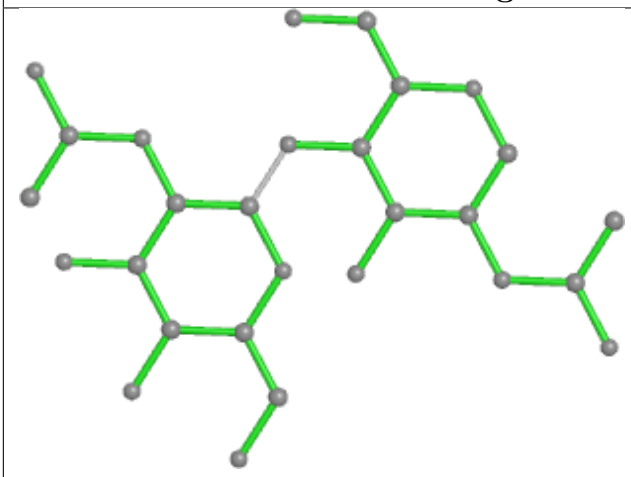


Torsions

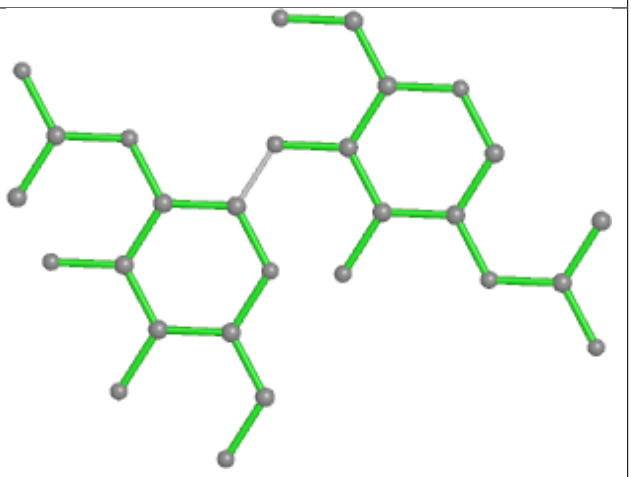


Rings

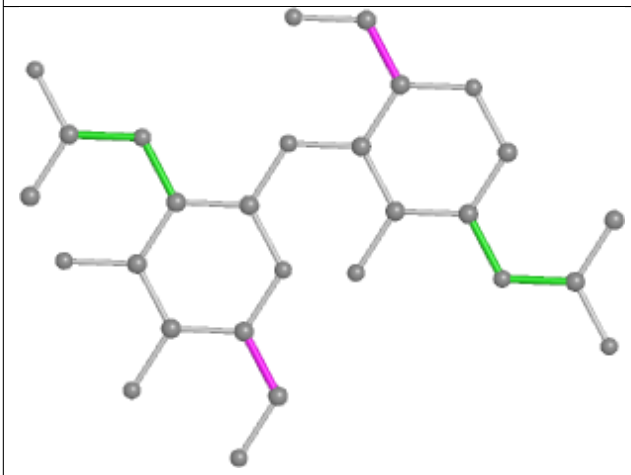
Oligosaccharide Chain F



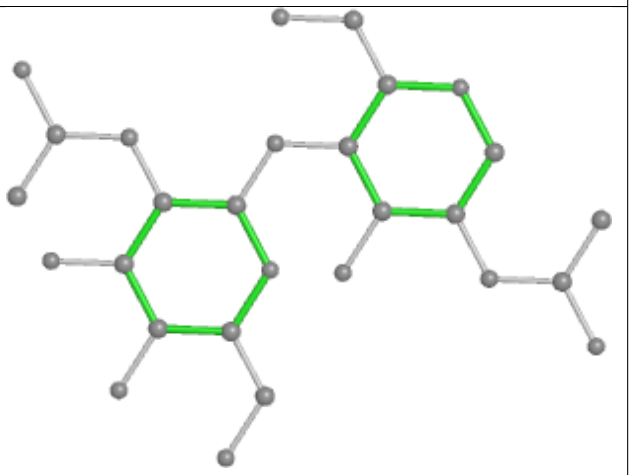
Bond lengths



Bond angles

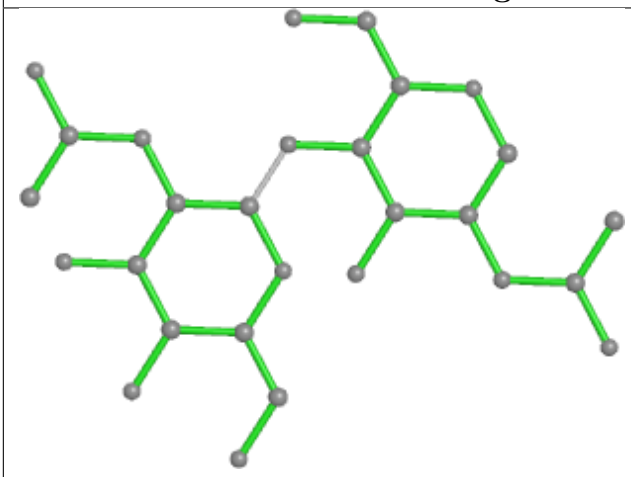


Torsions

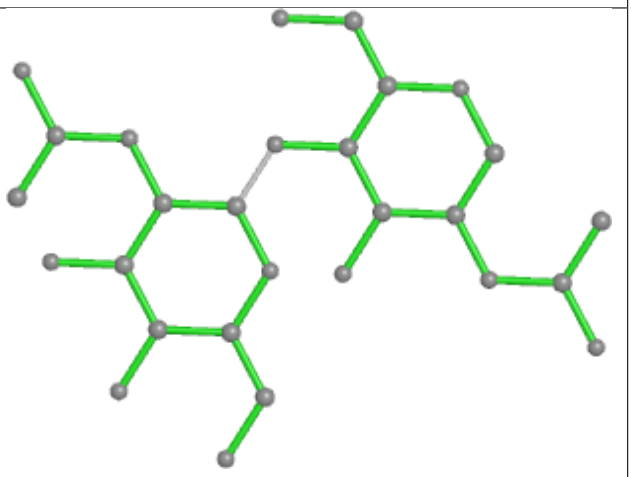


Rings

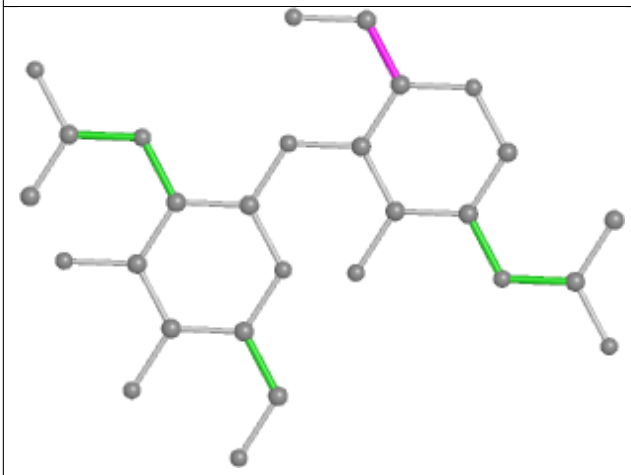
Oligosaccharide Chain G



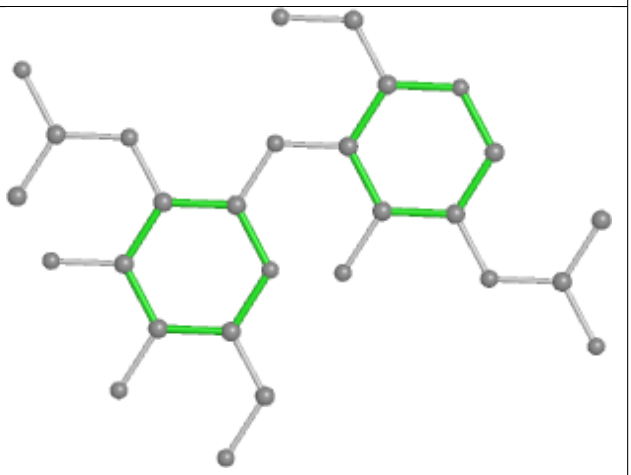
Bond lengths



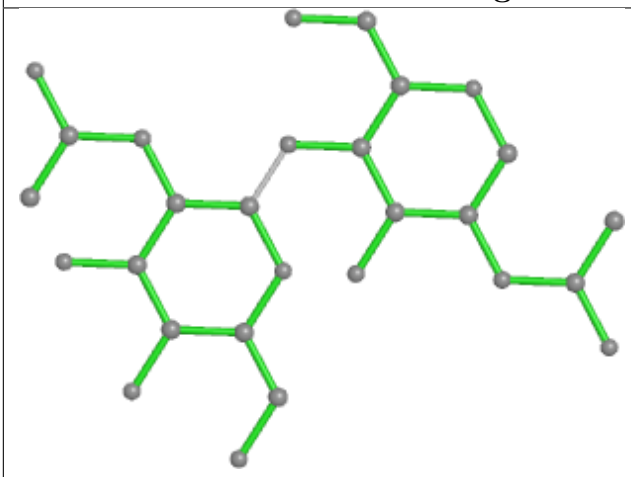
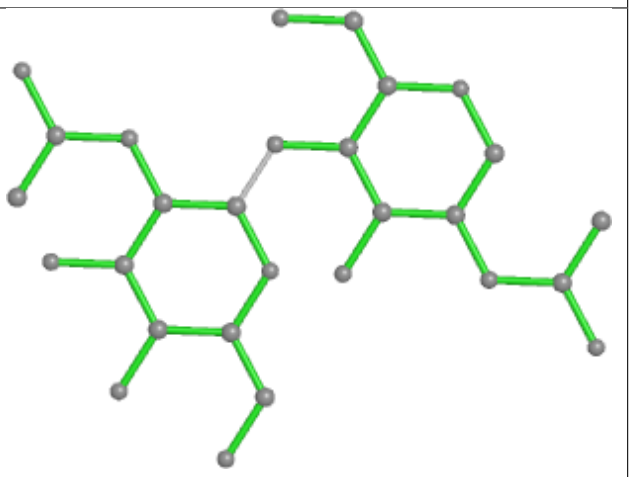
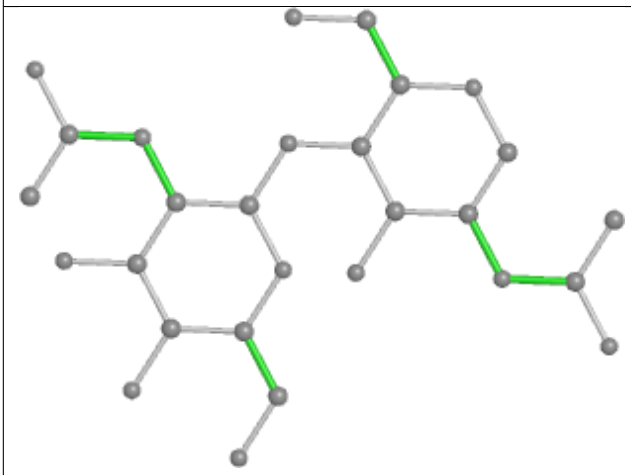
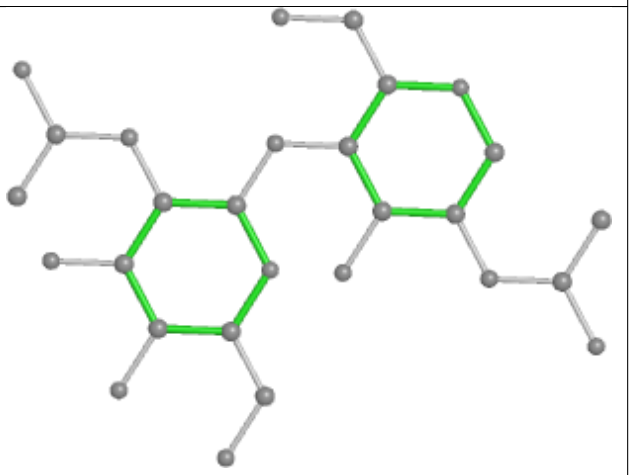
Bond angles



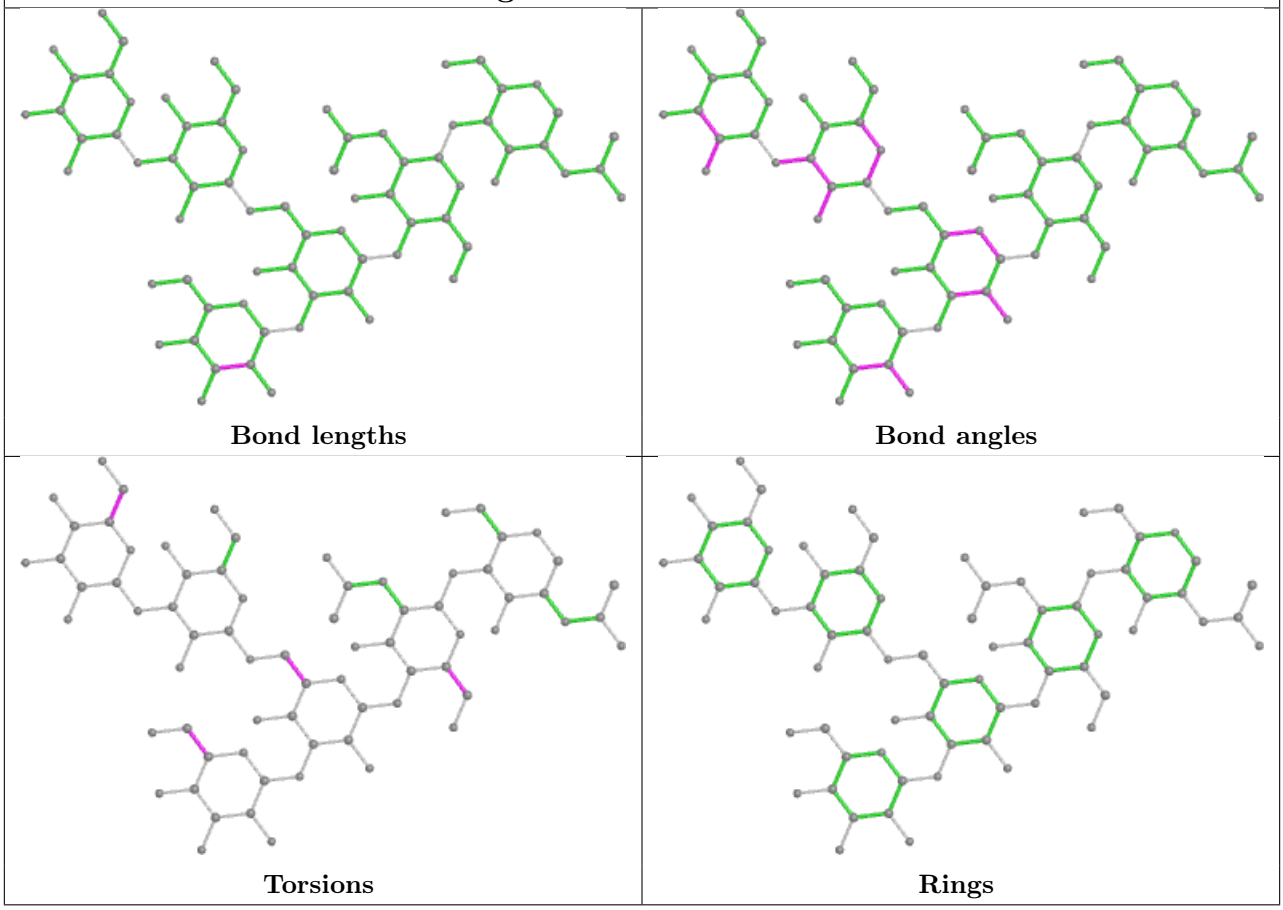
Torsions



Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1063/1094 (97%)	0.18	41 (3%)	39	35	34, 76, 143, 301	0
2	B	665/686 (96%)	0.44	58 (8%)	10	7	34, 94, 175, 250	1 (0%)
All	All	1728/1780 (97%)	0.28	99 (5%)	23	19	34, 81, 165, 301	1 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	626	SER	15.8
2	B	8	VAL	6.1
2	B	468	SER	6.1
1	A	890	THR	5.5
2	B	38	ILE	5.4
2	B	427	CYS	5.3
2	B	469	GLN	4.8
2	B	445	CYS	4.7
2	B	455	ILE	4.6
2	B	24	CYS	4.5
2	B	544	PRO	4.4
1	A	614	PRO	4.3
2	B	554	GLU	4.3
1	A	888	PRO	4.2
2	B	37	SER	4.2
2	B	442	PHE	4.1
2	B	561	LEU	4.1
2	B	443	LEU	4.1
2	B	470	GLU	4.0
1	A	623	GLN	4.0
1	A	619	GLU	3.9
2	B	26	LYS	3.8
1	A	624	VAL	3.8
2	B	23	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	46	LEU	3.8
2	B	424	GLU	3.8
2	B	623	ALA	3.7
1	A	838	GLY	3.6
1	A	612	GLU	3.6
2	B	32	PRO	3.5
1	A	625	VAL	3.5
2	B	426	ARG	3.5
1	A	627	GLU	3.4
2	B	444	GLU	3.4
2	B	101	LYS	3.4
1	A	649	SER	3.3
2	B	436	LEU	3.3
2	B	546	PHE	3.3
2	B	428	ARG	3.2
1	A	766	PHE	3.0
1	A	621	ARG	3.0
1	A	690	LYS	3.0
1	A	480	ARG	3.0
2	B	1	GLN	3.0
2	B	49	ARG	2.9
2	B	466	ARG	2.9
2	B	578	VAL	2.9
1	A	740	ARG	2.8
2	B	467	SER	2.8
2	B	28	ASN	2.8
1	A	622	GLU	2.8
2	B	530	PRO	2.8
2	B	57	MET	2.7
2	B	29	PHE	2.7
1	A	601	TRP	2.7
1	A	639	ILE	2.7
1	A	702	SER	2.7
1	A	725	LEU	2.7
2	B	73	GLN	2.7
1	A	836	SER	2.6
2	B	555	ARG	2.6
2	B	7	LYS	2.6
1	A	764	ILE	2.6
1	A	652	LEU	2.6
1	A	653	GLN	2.6
2	B	423	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	35	PRO	2.6
2	B	174	LYS	2.5
2	B	541	ARG	2.5
1	A	272	ALA	2.4
2	B	27	LEU	2.4
2	B	438	HIS	2.4
1	A	282	LEU	2.4
1	A	686	VAL	2.4
2	B	557	THR	2.3
1	A	850	ILE	2.3
2	B	47	LEU	2.3
2	B	172	LYS	2.3
1	A	642	ARG	2.3
2	B	471	LEU	2.3
1	A	825	LEU	2.3
2	B	52	ALA	2.3
2	B	576	CYS	2.3
2	B	76	LEU	2.2
2	B	542	CYS	2.2
2	B	74	LYS	2.2
1	A	12	ARG	2.2
2	B	449	ARG	2.2
1	A	620	CYS	2.2
2	B	39	ARG	2.1
2	B	371	ARG	2.1
1	A	877	LEU	2.1
1	A	628	GLN	2.1
1	A	896	GLN	2.1
1	A	637	LEU	2.0
1	A	837	GLN	2.0
2	B	33	GLY	2.0
1	A	482	TRP	2.0
1	A	650	ARG	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)

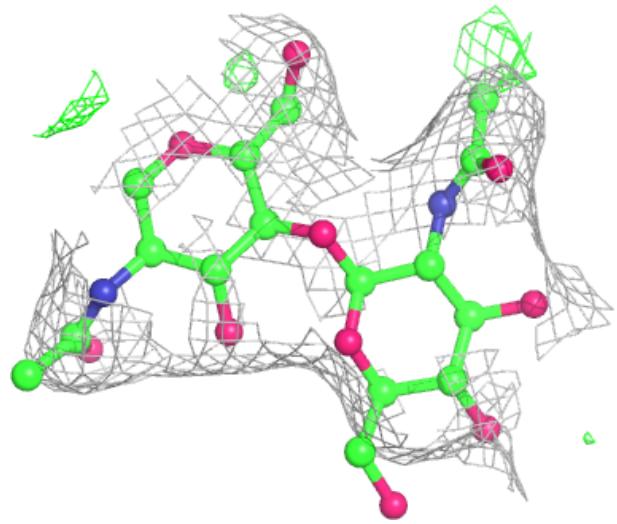
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

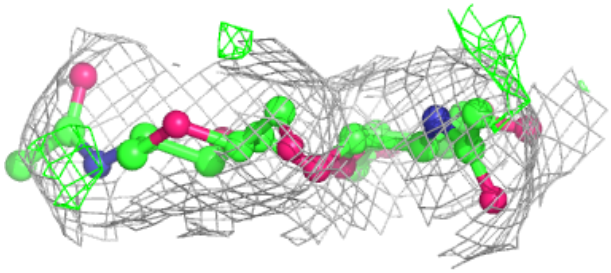
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	E	4	11/12	0.65	0.24	141,148,152,154	0
3	NAG	G	2	14/15	0.79	0.18	161,170,177,179	0
4	BMA	E	3	11/12	0.80	0.12	102,114,137,143	0
4	MAN	E	6	11/12	0.80	0.18	157,165,172,173	0
3	NAG	H	2	14/15	0.81	0.33	139,155,167,175	0
3	NAG	G	1	14/15	0.82	0.14	109,120,133,145	0
3	NAG	C	2	14/15	0.82	0.19	117,134,152,154	0
3	NAG	F	2	14/15	0.83	0.18	141,149,158,159	0
4	MAN	E	5	11/12	0.84	0.24	149,155,160,162	0
3	NAG	H	1	14/15	0.89	0.20	92,105,122,138	0
3	NAG	D	2	14/15	0.89	0.17	69,114,123,127	0
3	NAG	F	1	14/15	0.92	0.16	83,106,111,129	0
3	NAG	C	1	14/15	0.95	0.14	50,81,99,101	0
4	NAG	E	2	14/15	0.95	0.14	66,70,89,94	0
4	NAG	E	1	14/15	0.96	0.17	57,63,70,77	0
3	NAG	D	1	14/15	0.96	0.14	58,77,92,97	0

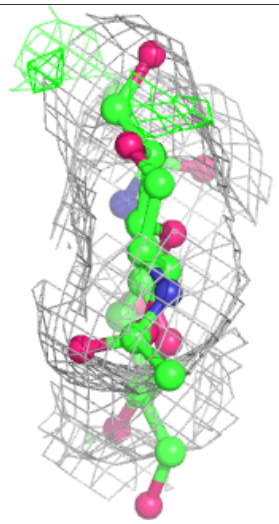
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

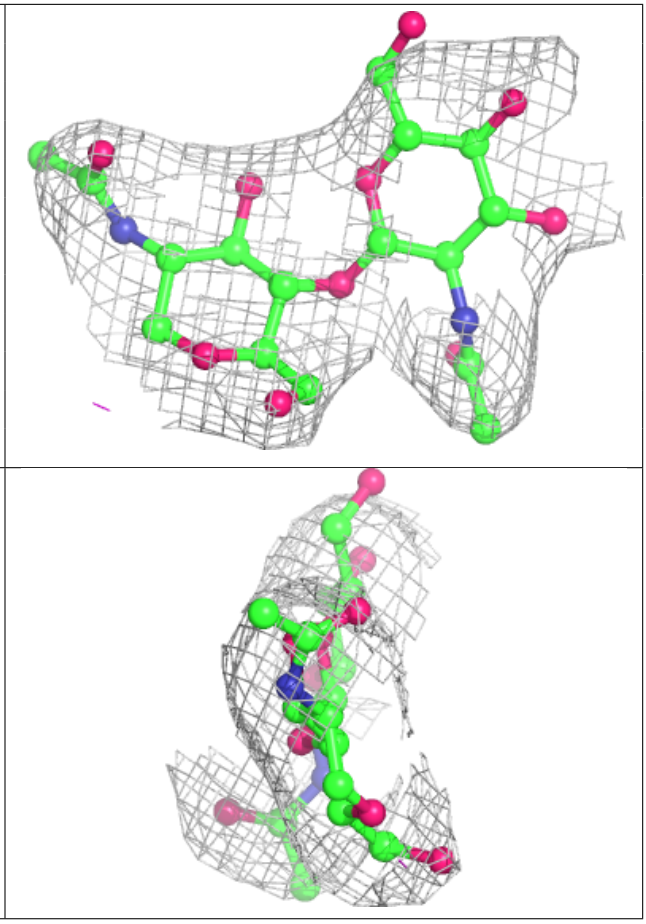






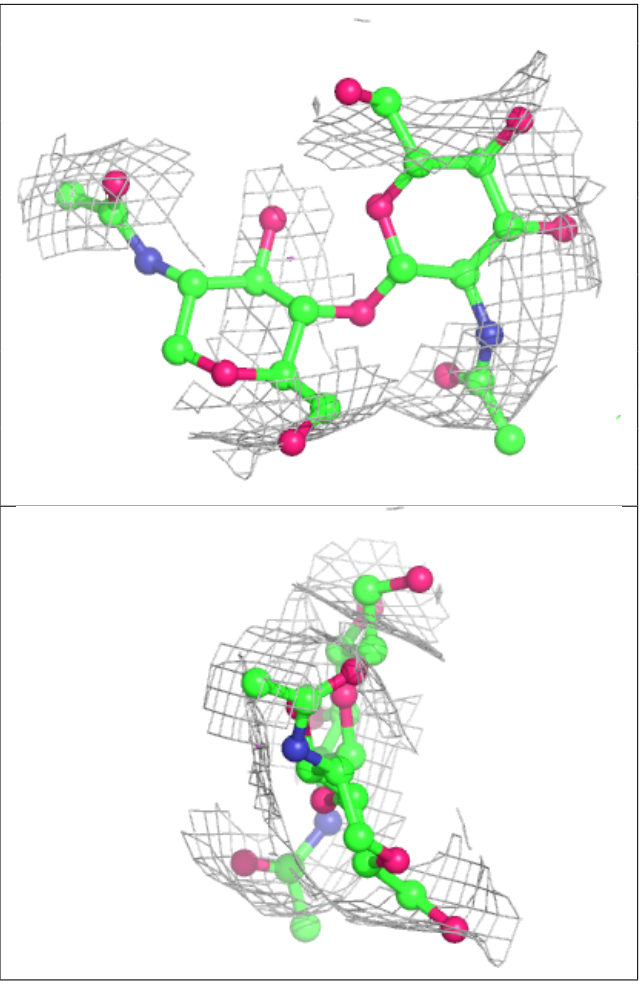
Electron density around Chain D:

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



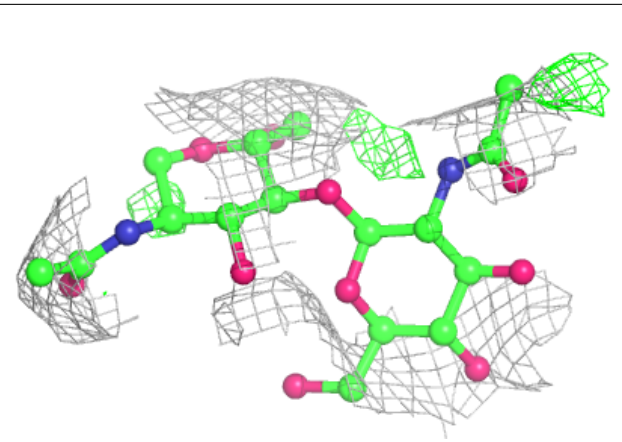
Electron density around Chain F:

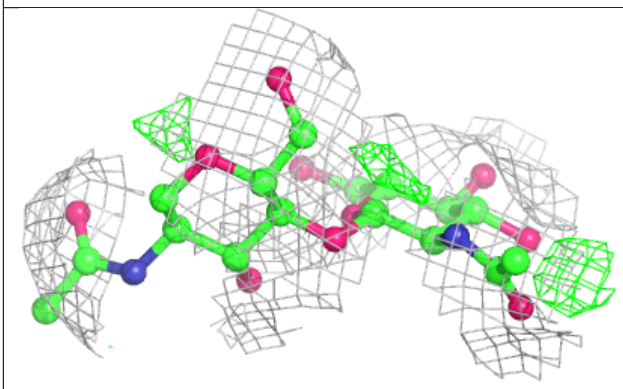
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

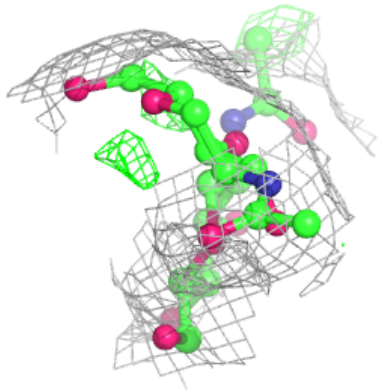


Electron density around Chain G:

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

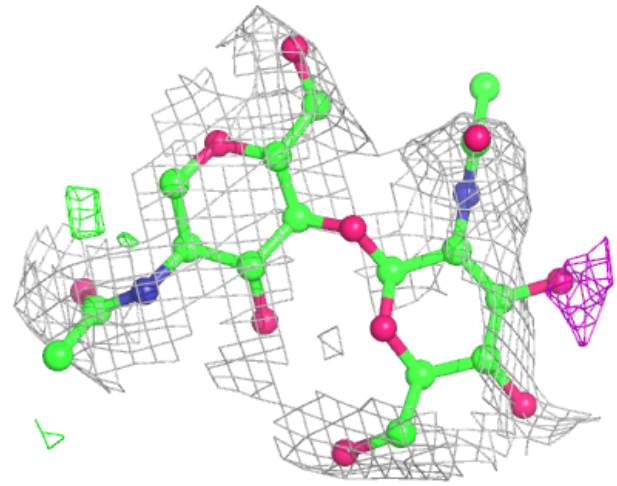


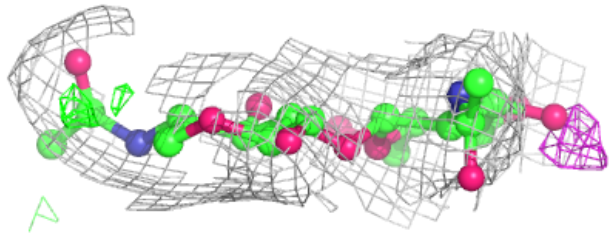


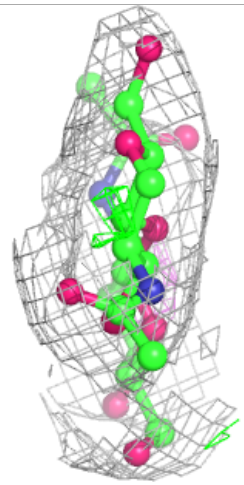


Electron density around Chain H:

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

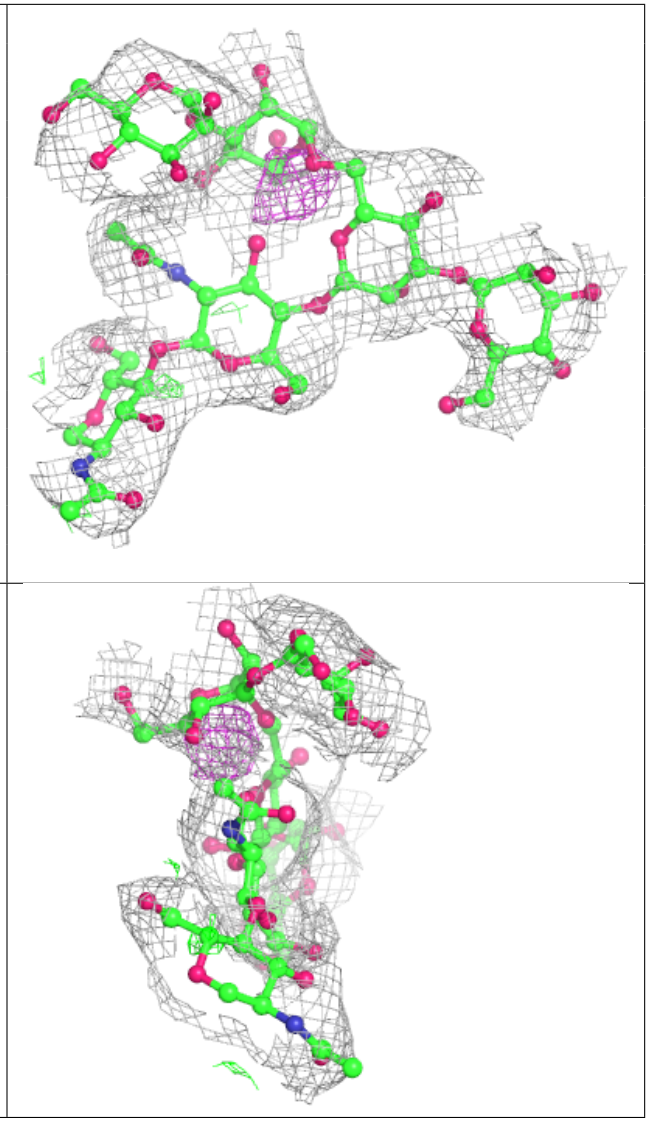






Electron density around Chain E:

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



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
5	CA	A	1115	1/1	0.80	0.13	131,131,131,131	0
5	CA	B	706	1/1	0.88	0.16	92,92,92,92	0
5	CA	B	705	1/1	0.96	0.19	44,44,44,44	0
5	CA	A	1113	1/1	0.96	0.15	54,54,54,54	0
6	MG	A	1116	1/1	0.96	0.09	72,72,72,72	0
5	CA	A	1114	1/1	0.97	0.13	65,65,65,65	0
6	MG	B	707	1/1	0.97	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CL	A	1117	1/1	0.97	0.08	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.