Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 08:01 PM EDT

PDB ID	:	3D4L
Title	:	Human dipeptidyl peptidase IV/CD26 in complex with a novel inhibitor
Authors	:	Scapin, G.
Deposited on	:	2008-05-14
Resolution	:	2.00 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:

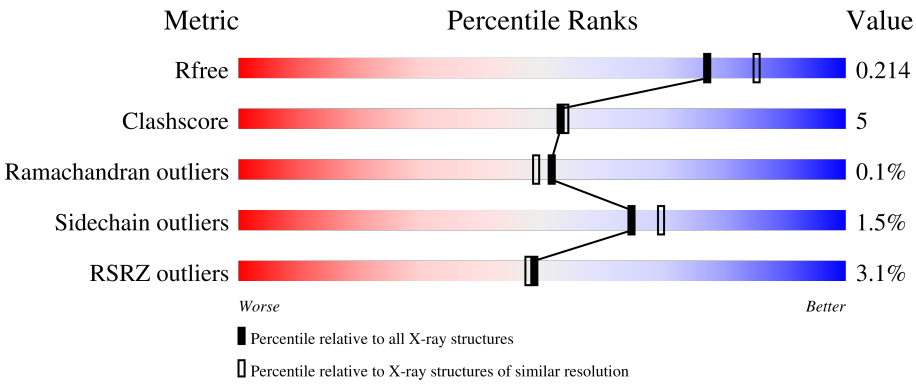
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	728	2% 87% 12%
1	B	728	4% 87% 13%
2	C	2	50% 50%
2	F	2	50% 50%
3	D	2	100%

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Mol	Chain	Length	Quality of chain
3	E	2	50% 50%
3	G	2	50% 50%
3	H	2	50% 50%
3	I	2	100%
3	J	2	100%
3	K	2	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
3	NAG	D	1	X	-	-	X
3	NAG	G	2	-	-	-	X
3	NAG	H	2	-	-	-	X
4	NAG	A	1092	-	-	-	X
4	NAG	A	1520	-	-	-	X
4	NAG	B	2092	-	-	-	X
4	NAG	B	2150	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13340 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 Dipeptidyl peptidase 4 soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5987	3840	987	1134	26	0	3	0
1	B	728	5982	3839	986	1131	26	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	SER	engineered mutation	UNP P27487
B	39	THR	SER	engineered mutation	UNP P27487

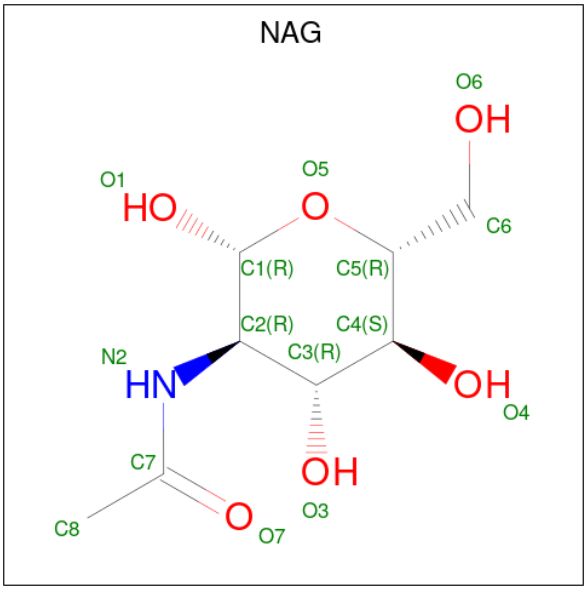
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0

- 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	D	2	28	16	2	10	0	0	0
3	E	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0
3	H	2	28	16	2	10	0	0	0
3	I	2	28	16	2	10	0	0	0
3	J	2	28	16	2	10	0	0	0
3	K	2	28	16	2	10	0	0	0

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



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

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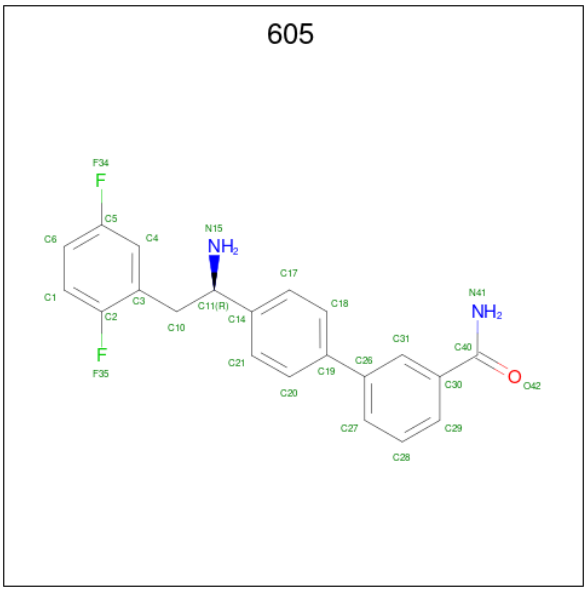
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	1	1	1	0	0

- Molecule 6 is 4'-[(1R)-1-amino-2-(2,5-difluorophenyl)ethyl]biphenyl-3-carboxamide (three-letter code: 605) (formula: $C_{21}H_{18}F_2N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N	O	
6	A	1	26	21	2	2	1	0	0
			Total	C	F	N	O	
6	B	1	26	21	2	2	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	500	500	500	0	0

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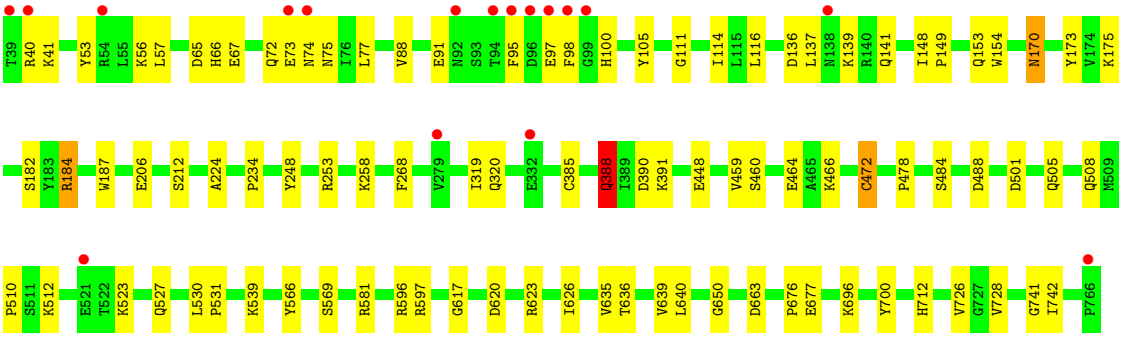
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	482	482	482	0	0

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.

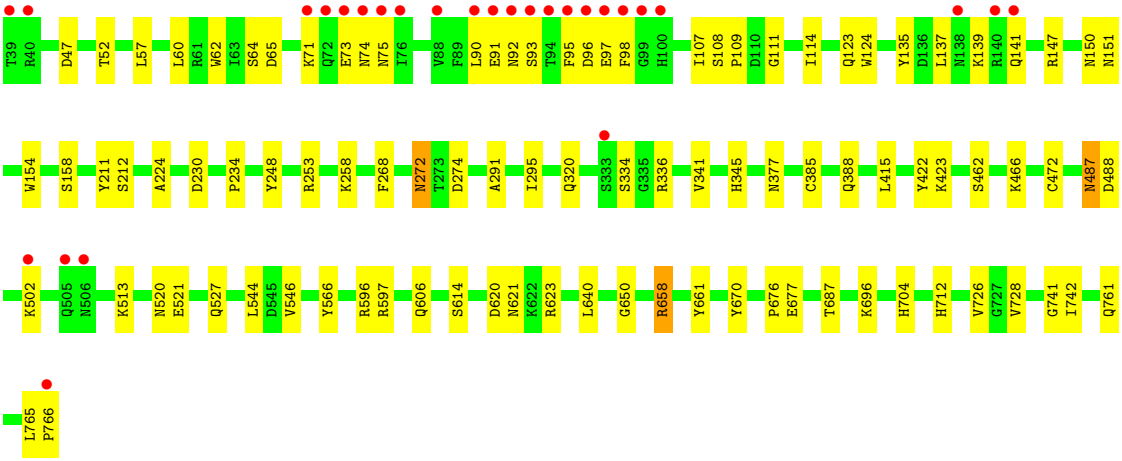
• Molecule 1: Dipeptidyl peptidase 4 soluble form

Chain A:



• Molecule 1: Dipeptidyl peptidase 4 soluble form

Chain B:



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

Chain C:

• Molecule 2: 2-acetamido-2-deoxy-alpha-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 D:

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

Chain E:

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

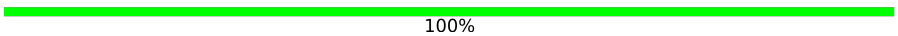
Chain G:

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

Chain H:

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

Chain I:



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

Chain J: 100%

NAG1
NAG2

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

Chain K: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.44Å 125.75Å 137.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 46.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.00) 98.5 (46.35-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.00Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.192 , 0.217 0.190 , 0.214	Depositor DCC
R_{free} test set	6944 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13340	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: NDG, 605, NA, 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	0.50	0/6162	0.69	2/8380 (0.0%)
1	B	0.48	0/6155	0.68	1/8371 (0.0%)
All	All	0.49	0/12317	0.69	3/16751 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	388	GLN	N-CA-C	-5.37	96.51	111.00
1	A	319	ILE	N-CA-C	-5.27	96.77	111.00
1	B	388	GLN	N-CA-C	-5.10	97.23	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	700	TYR	Sidechain
1	B	211	TYR	Sidechain

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	5987	0	5690	63	0
1	B	5982	0	5693	67	0
2	C	28	0	24	1	0
2	F	28	0	24	1	0
3	D	28	0	25	1	0
3	E	28	0	25	0	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
4	A	42	0	39	5	0
4	B	42	0	39	1	0
5	A	1	0	0	0	0
6	A	26	0	18	0	0
6	B	26	0	18	0	0
7	A	500	0	0	1	0
7	B	482	0	0	7	0
All	All	13340	0	11720	131	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 5.

All (131) 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:253:ARG:HH21	1:B:253:ARG:HH21	1.21	0.85
1:A:581:ARG:CZ	4:A:1520:NAG:H62	2.07	0.83
1:A:75:ASN:HD21	4:A:1092:NAG:HN2	1.23	0.82
1:A:66[B]:HIS:CA	1:A:67:GLU:N	2.45	0.80
1:B:147:ARG:HE	4:B:2150:NAG:H83	1.46	0.79
1:A:596:ARG:O	1:A:597:ARG:HD2	1.89	0.72
1:A:696:LYS:HG2	1:A:728:VAL:HG22	1.71	0.72
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.88	0.71
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.27	0.70
1:B:272:ASN:C	1:B:272:ASN:HD22	1.96	0.69
1:B:91:GLU:HG3	1:B:93:SER:H	1.57	0.68
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.74	0.68
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.31	0.66
2:F:2:NDG:O7	2:F:2:NDG:H3	1.95	0.65
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.95	0.63
1:B:596:ARG:O	1:B:597:ARG:HD2	1.98	0.63
1:B:676:PRO:HG2	1:B:677:GLU:OE2	1.98	0.63
1:B:65:ASP:OD2	1:B:466:LYS:HB2	1.99	0.63
1:A:139:LYS:HG3	1:A:141:GLN:HB3	1.82	0.62
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.82	0.61
1:B:597:ARG:HG2	7:B:2772:HOH:O	2.02	0.59
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.85	0.59
1:B:139:LYS:O	1:B:141:GLN:HG3	2.02	0.59
1:B:502:LYS:HD3	1:B:502:LYS:C	2.23	0.58
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.69	0.58
1:A:676:PRO:HG2	1:A:677:GLU:OE2	2.04	0.58
1:B:502:LYS:HD3	1:B:502:LYS:O	2.02	0.58
1:A:581:ARG:NH1	4:A:1520:NAG:H62	2.18	0.57
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.85	0.57
1:B:95:PHE:HB3	1:B:98:PHE:HB2	1.86	0.57
1:A:40:ARG:HG3	1:A:508:GLN:HG3	1.85	0.57
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.35	0.57
1:A:170:ASN:HD22	1:A:170:ASN:N	2.03	0.56
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.87	0.56
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.19	0.56
1:A:77:LEU:HD23	1:A:88:VAL:HA	1.88	0.55
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.42	0.55
1:B:614:SER:HB2	1:B:621:ASN:OD1	2.07	0.54
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.08	0.54
1:A:136:ASP:HB3	1:A:139:LYS:HG2	1.89	0.54
1:A:258:LYS:HZ3	1:A:712:HIS:HD2	1.56	0.54
1:B:75:ASN:ND2	1:B:92:ASN:H	2.06	0.54
3:D:1:NAG:O3	3:D:2:NAG:N2	2.42	0.53
1:A:620:ASP:OD2	1:A:623:ARG:HD3	2.08	0.53
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.07	0.52
1:B:658:ARG:O	1:B:658:ARG:HG3	2.09	0.52
1:A:65[A]:ASP:OD2	1:A:466:LYS:HB2	2.09	0.52
1:A:111:GLY:O	1:A:137:LEU:HD12	2.10	0.52
1:B:341:VAL:HG12	7:B:2773:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:SER:HA	1:B:96:ASP:OD1	2.10	0.51
1:B:60:LEU:HD12	1:B:60:LEU:C	2.32	0.50
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.58	0.50
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.47	0.50
1:B:422:TYR:CE2	1:B:423:LYS:HE2	2.47	0.49
2:C:1:NAG:HO3	2:C:2:NDG:H6	1.60	0.49
1:B:272:ASN:ND2	1:B:274:ASP:H	2.10	0.49
3:G:1:NAG:H61	3:G:2:NAG:O5	2.12	0.49
1:B:544:LEU:HG	1:B:546[A]:VAL:CG2	2.41	0.49
1:A:73:GLU:HB3	4:A:1092:NAG:H3	1.94	0.49
1:B:696:LYS:CG	1:B:728:VAL:HG22	2.43	0.49
1:B:487:ASN:C	1:B:487:ASN:HD22	2.15	0.48
1:B:272:ASN:HD22	1:B:274:ASP:H	1.62	0.48
1:B:334:SER:O	1:B:336:ARG:HG2	2.13	0.48
1:B:109:PRO:HG2	1:B:158:SER:O	2.13	0.48
1:B:741:GLY:O	1:B:742:ILE:C	2.52	0.48
1:A:73:GLU:O	1:A:74:ASN:HB2	2.14	0.48
1:B:150:ASN:O	1:B:151:ASN:HB2	2.14	0.48
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.96	0.48
1:B:73:GLU:O	1:B:74:ASN:HB2	2.13	0.47
1:B:71:LYS:NZ	7:B:2408:HOH:O	2.46	0.47
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.97	0.47
1:B:520:ASN:O	1:B:521:GLU:HB2	2.15	0.47
1:A:539:LYS:HD3	1:A:617:GLY:O	2.15	0.47
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.81	0.46
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.51	0.46
1:A:56:LYS:C	1:A:57:LEU:HD12	2.35	0.46
1:A:88:VAL:HG11	1:A:91:GLU:OE2	2.17	0.45
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.37	0.45
1:A:390:ASP:O	1:A:391:LYS:HD2	2.16	0.45
1:A:459:VAL:HG22	1:A:460:SER:N	2.32	0.45
1:B:107:ILE:HG22	1:B:108:SER:O	2.16	0.45
1:B:415:LEU:C	1:B:415:LEU:HD23	2.36	0.45
1:A:472:CYS:O	1:A:478:PRO:HA	2.17	0.45
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.98	0.45
1:B:345:HIS:HD2	7:B:2452:HOH:O	2.00	0.45
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.99	0.45
1:A:57:LEU:HB3	7:A:1607:HOH:O	2.17	0.44
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.98	0.44
1:A:136:ASP:CB	1:A:139:LYS:HG2	2.47	0.44
1:B:513:LYS:O	1:B:527:GLN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65[A]:ASP:CG	1:A:464:GLU:HB2	2.38	0.44
1:A:258:LYS:HZ3	1:A:712:HIS:CD2	2.35	0.44
1:A:741:GLY:O	1:A:742:ILE:C	2.57	0.43
1:B:60:LEU:HD12	1:B:60:LEU:O	2.18	0.43
1:B:253:ARG:HD3	7:B:2794:HOH:O	2.18	0.43
1:A:484[A]:SER:O	1:A:488:ASP:HA	2.19	0.43
1:A:95:PHE:CE1	1:A:116:LEU:HD11	2.53	0.43
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.54	0.43
1:B:47:ASP:HA	1:B:52:THR:HG23	2.00	0.43
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.53	0.43
1:A:41:LYS:HE2	1:A:53:TYR:OH	2.18	0.43
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.37	0.42
1:B:62:TRP:CG	1:B:462:SER:HA	2.54	0.42
1:B:765:LEU:HA	1:B:766:PRO:HD3	1.90	0.42
1:A:388:GLN:HB2	1:A:391:LYS:HB2	2.00	0.42
1:A:388:GLN:CB	1:A:391:LYS:HB2	2.48	0.42
1:B:64:SER:HB2	7:B:2506:HOH:O	2.19	0.42
1:B:291:ALA:O	1:B:295:ILE:HG23	2.19	0.42
1:B:123:GLN:HG2	1:B:124:TRP:N	2.35	0.42
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.55	0.42
1:A:523:LYS:H	1:A:523:LYS:HG2	1.59	0.42
1:B:272:ASN:C	1:B:272:ASN:ND2	2.69	0.41
1:A:626:ILE:HG23	1:A:636:THR:HG23	2.03	0.41
1:B:111:GLY:O	1:B:137:LEU:HD12	2.20	0.41
1:A:66[B]:HIS:CD2	1:A:67:GLU:HG3	2.56	0.41
1:A:148:ILE:HA	1:A:149:PRO:HD3	1.89	0.41
1:A:635:VAL:O	1:A:639:VAL:HG23	2.20	0.41
1:B:377:ASN:HB2	7:B:2684:HOH:O	2.21	0.41
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.98	0.41
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.56	0.41
1:A:512:LYS:HE3	1:A:527:GLN:CD	2.41	0.41
1:A:581:ARG:NH2	4:A:1520:NAG:H62	2.35	0.40
1:B:658:ARG:HB2	1:B:687:THR:HG22	2.03	0.40
1:A:72:GLN:O	1:A:73:GLU:HB2	2.21	0.40
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.91	0.40
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.56	0.40
1:B:487:ASN:HD22	1:B:488:ASP:N	2.19	0.40
1:B:546[A]:VAL:HG22	1:B:606:GLN:NE2	2.35	0.40
1:A:501:ASP:O	1:A:505:GLN:HG3	2.21	0.40
1:B:596:ARG:N	1:B:670:TYR:O	2.52	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	729/728 (100%)	705 (97%)	23 (3%)	1 (0%)	51	49
1	B	728/728 (100%)	700 (96%)	27 (4%)	1 (0%)	51	49
All	All	1457/1456 (100%)	1405 (96%)	50 (3%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	B	320	GLN

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	656/653 (100%)	648 (99%)	8 (1%)	71	76
1	B	655/653 (100%)	644 (98%)	11 (2%)	60	65
All	All	1311/1306 (100%)	1292 (99%)	19 (1%)	65	72

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	170	ASN
1	A	184	ARG
1	A	385	CYS

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Mol	Chain	Res	Type
1	A	388	GLN
1	A	448	GLU
1	A	472	CYS
1	A	566	TYR
1	B	57	LEU
1	B	97	GLU
1	B	230	ASP
1	B	272	ASN
1	B	385	CYS
1	B	472	CYS
1	B	487	ASN
1	B	566	TYR
1	B	658	ARG
1	B	704	HIS
1	B	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	75	ASN
1	A	123	GLN
1	A	169	ASN
1	A	170	ASN
1	A	435	GLN
1	A	505	GLN
1	A	572	ASN
1	A	712	HIS
1	B	51	ASN
1	B	138	ASN
1	B	141	GLN
1	B	169	ASN
1	B	272	ASN
1	B	345	HIS
1	B	487	ASN
1	B	572	ASN
1	B	606	GLN
1	B	712	HIS
1	B	761	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

18 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	0.71	0	17,19,21	1.20	1 (5%)
2	NDG	C	2	2	14,14,15	0.74	0	17,19,21	0.76	0
3	NAG	D	1	3,1	14,14,15	0.73	1 (7%)	17,19,21	0.70	0
3	NAG	D	2	3	14,14,15	0.81	1 (7%)	17,19,21	0.68	0
3	NAG	E	1	3,1	14,14,15	0.57	0	17,19,21	0.69	1 (5%)
3	NAG	E	2	3	14,14,15	0.61	0	17,19,21	0.71	0
2	NAG	F	1	1,2	14,14,15	0.61	0	17,19,21	0.76	1 (5%)
2	NDG	F	2	2	14,14,15	0.95	1 (7%)	17,19,21	1.05	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.68	0	17,19,21	1.00	1 (5%)
3	NAG	G	2	3	14,14,15	0.63	0	17,19,21	0.70	0
3	NAG	H	1	3,1	14,14,15	0.65	0	17,19,21	0.68	0
3	NAG	H	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.19	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.53	0	17,19,21	0.71	0
3	NAG	I	2	3	14,14,15	0.57	0	17,19,21	0.65	0
3	NAG	J	1	3,1	14,14,15	0.56	0	17,19,21	0.85	0
3	NAG	J	2	3	14,14,15	0.58	0	17,19,21	0.71	0
3	NAG	K	1	3,1	14,14,15	0.42	0	17,19,21	0.88	1 (5%)
3	NAG	K	2	3	14,14,15	0.59	0	17,19,21	0.72	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
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NDG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NDG	F	2	2	-	1/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NDG	C1-C2	2.75	1.56	1.52
3	H	2	NAG	C1-C2	2.37	1.55	1.52
3	D	2	NAG	C1-C2	2.28	1.55	1.52
3	D	1	NAG	C1-C2	2.08	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	2	NAG	C4-C3-C2	3.78	116.56	111.02
2	C	1	NAG	C4-C3-C2	-3.20	106.33	111.02
2	F	2	NDG	C4-C3-C2	2.84	115.18	111.02
3	K	1	NAG	C2-N2-C7	-2.53	119.30	122.90
3	K	2	NAG	C2-N2-C7	-2.14	119.85	122.90
3	G	1	NAG	C2-N2-C7	-2.12	119.89	122.90
3	E	1	NAG	C2-N2-C7	-2.12	119.89	122.90
2	F	1	NAG	C2-N2-C7	-2.10	119.92	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	C1-C2-N2-C7
3	K	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	C	2	NDG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	F	2	NDG	C3-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	I	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C3-C2-N2-C7
2	C	2	NDG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7
3	D	2	NAG	C1-C2-N2-C7

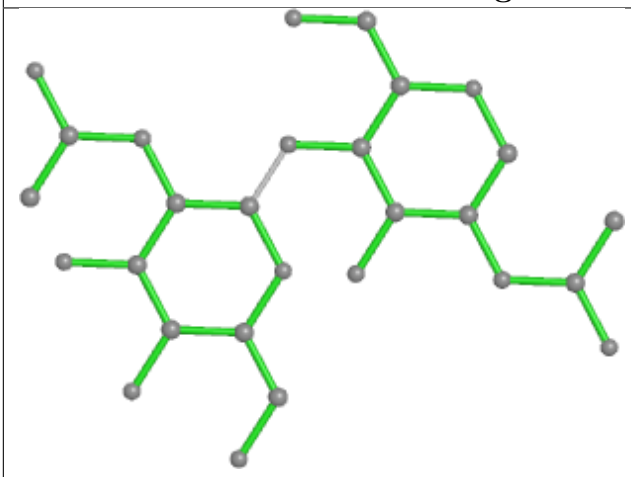
There are no ring outliers.

7 monomers are involved in 4 short contacts:

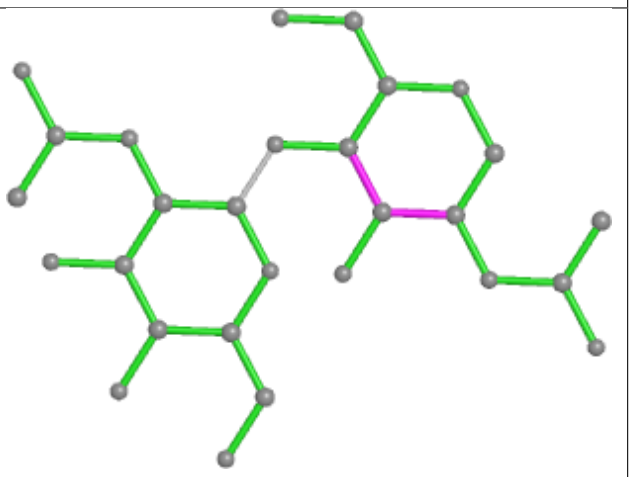
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	G	2	NAG	1	0
3	D	2	NAG	1	0
2	F	2	NDG	1	0
2	C	1	NAG	1	0
2	C	2	NDG	1	0
3	D	1	NAG	1	0

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

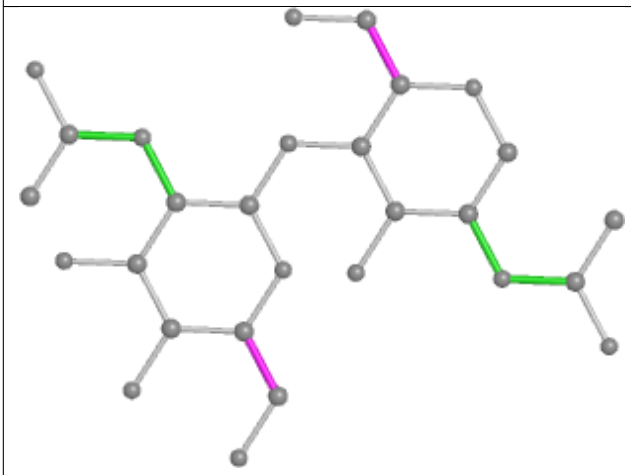
Oligosaccharide Chain C



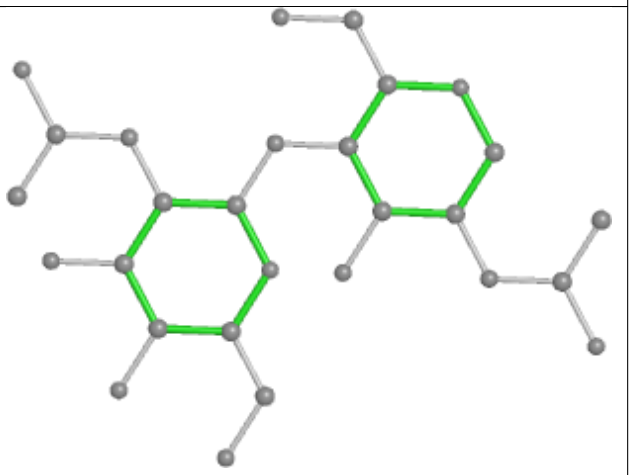
Bond lengths



Bond angles

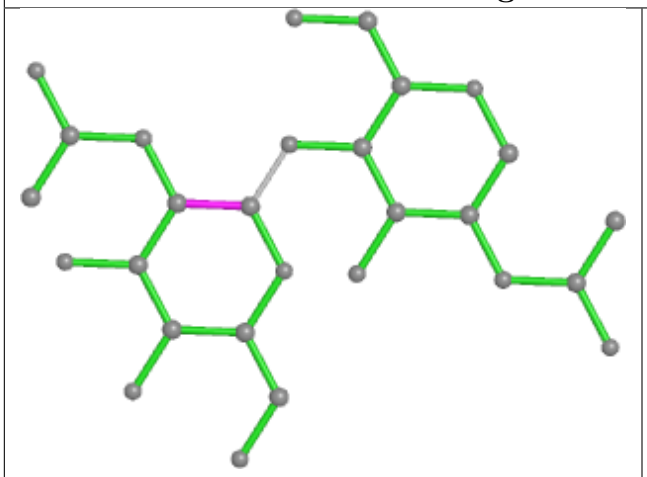


Torsions

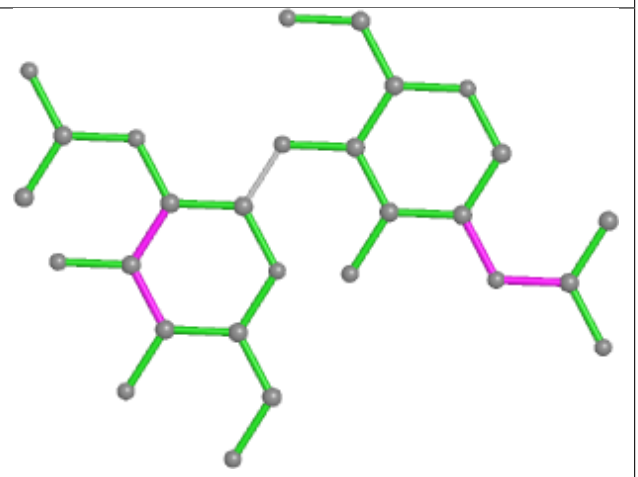


Rings

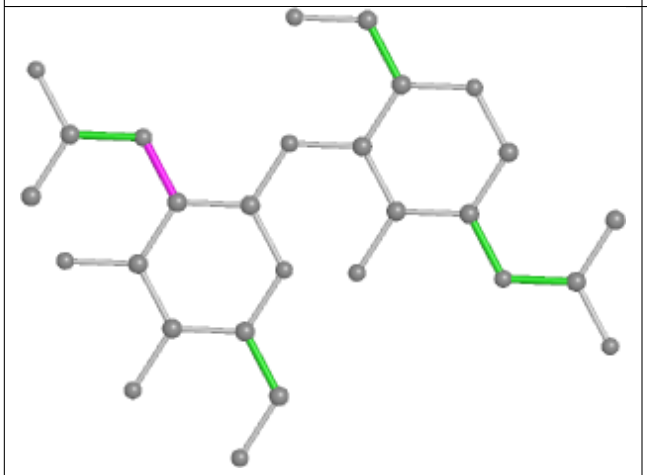
Oligosaccharide Chain F



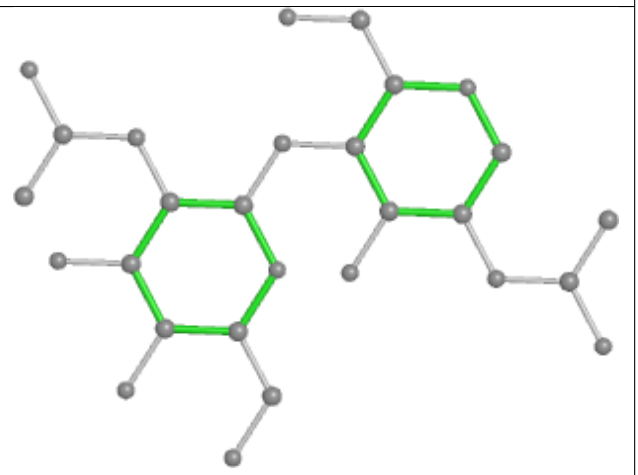
Bond lengths



Bond angles

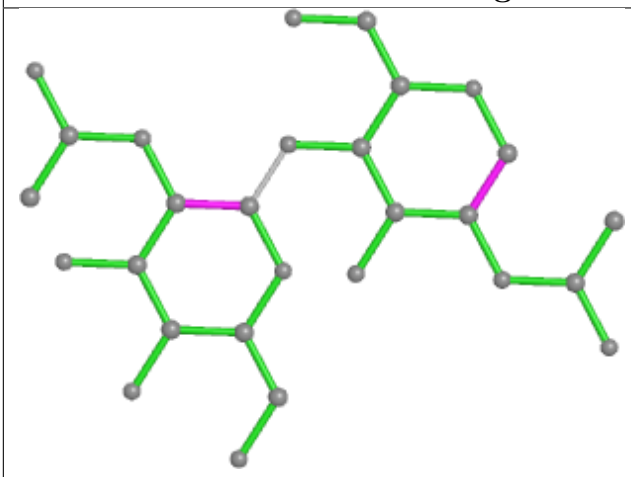


Torsions

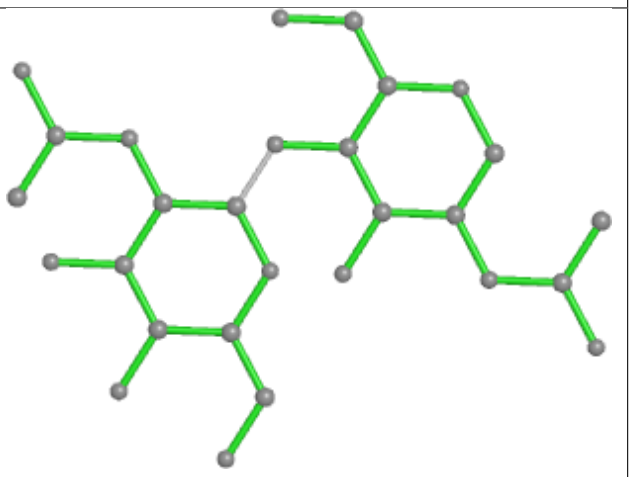


Rings

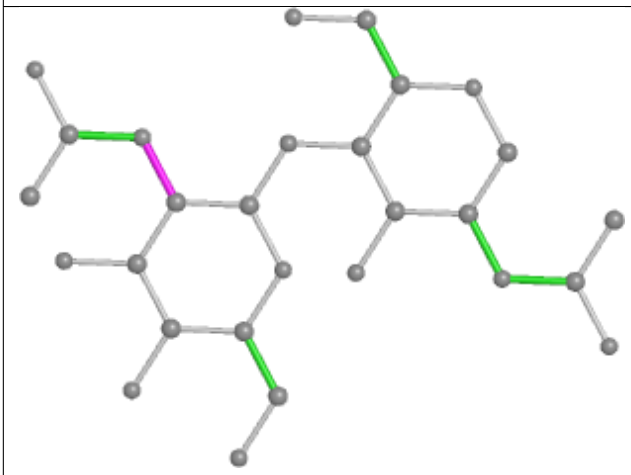
Oligosaccharide Chain D



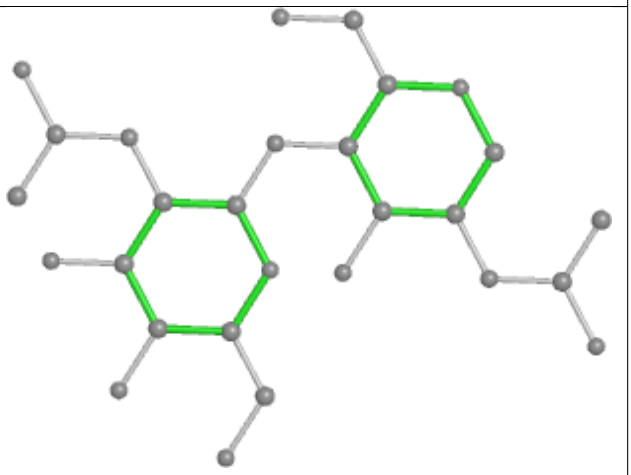
Bond lengths



Bond angles

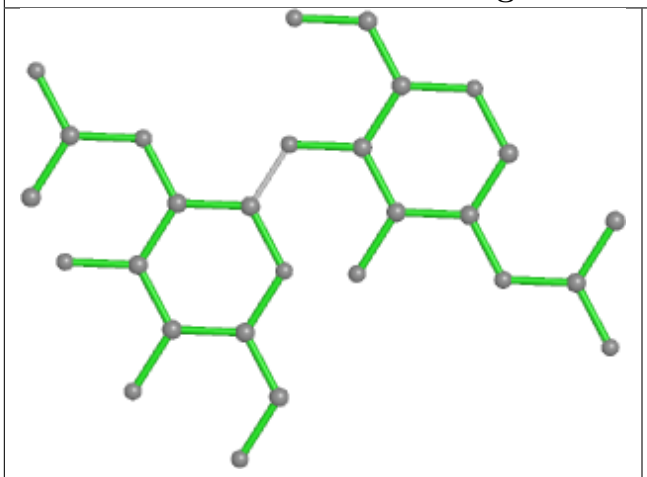


Torsions

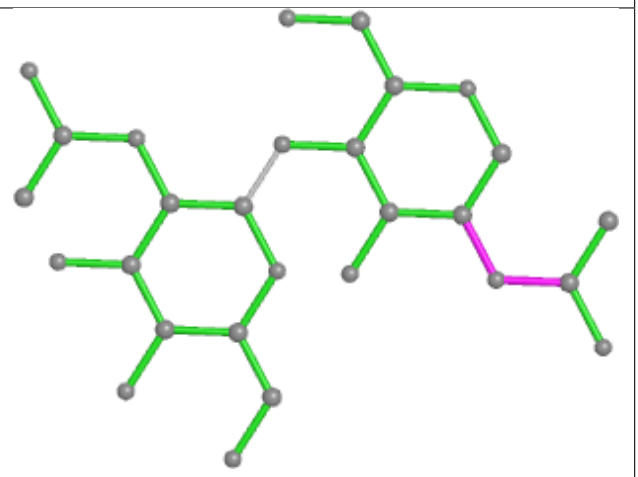


Rings

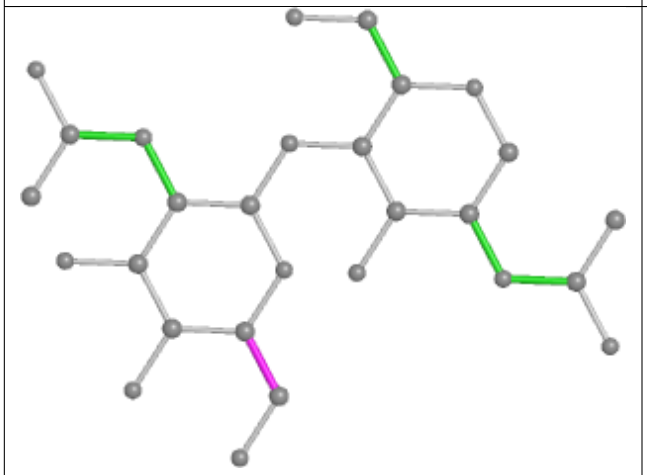
Oligosaccharide Chain E



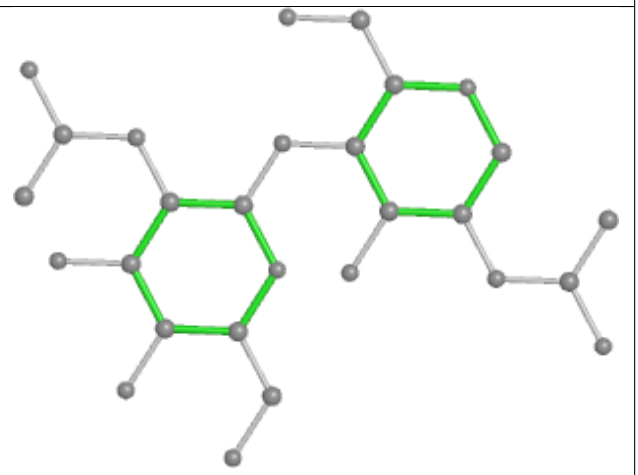
Bond lengths



Bond angles

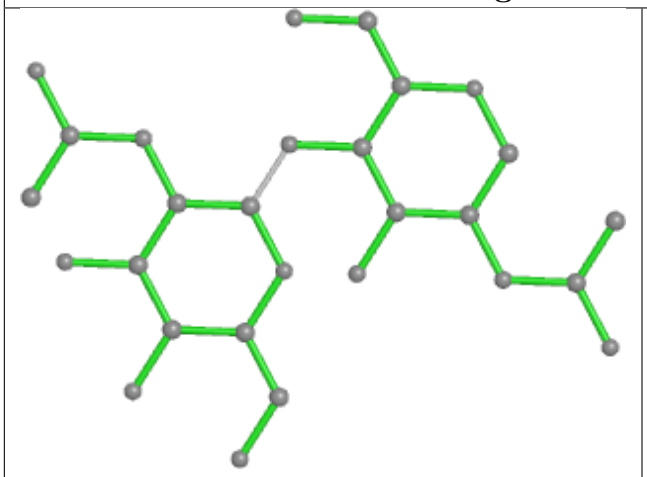


Torsions

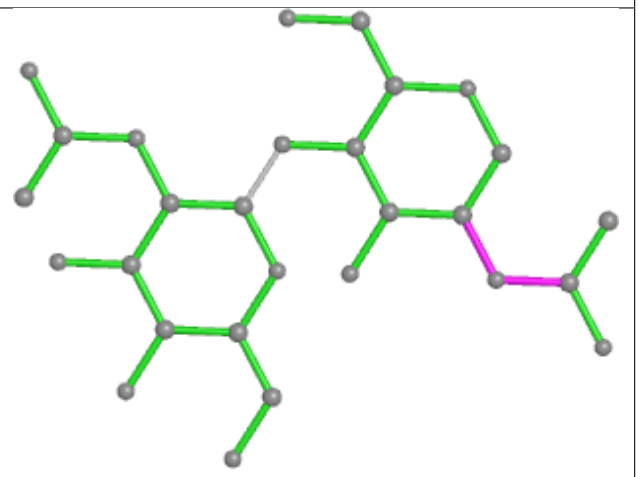


Rings

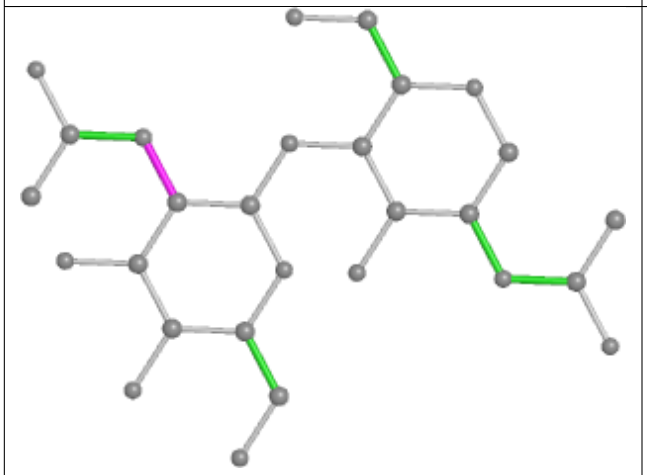
Oligosaccharide Chain G



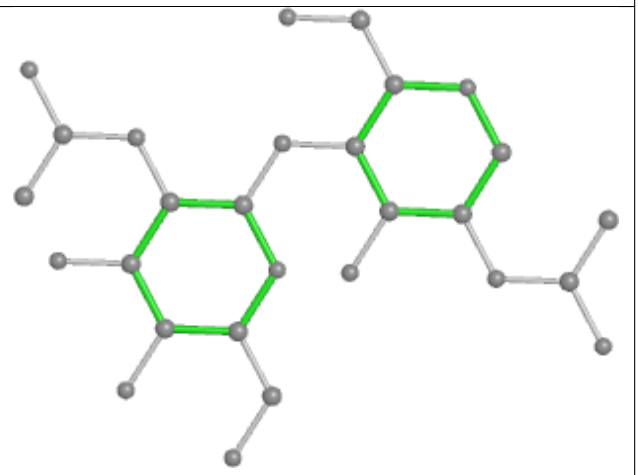
Bond lengths



Bond angles

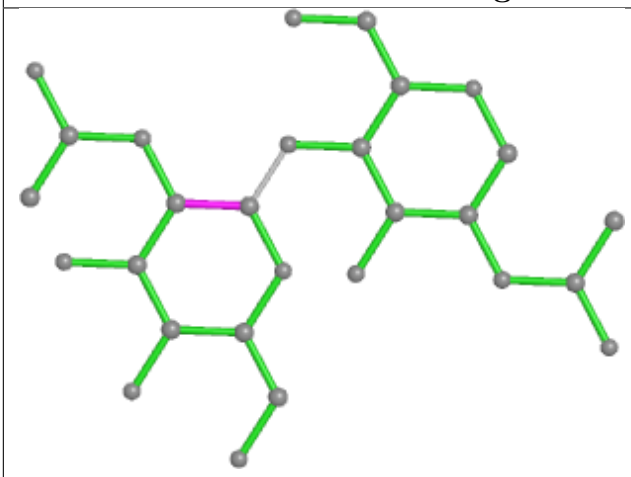


Torsions

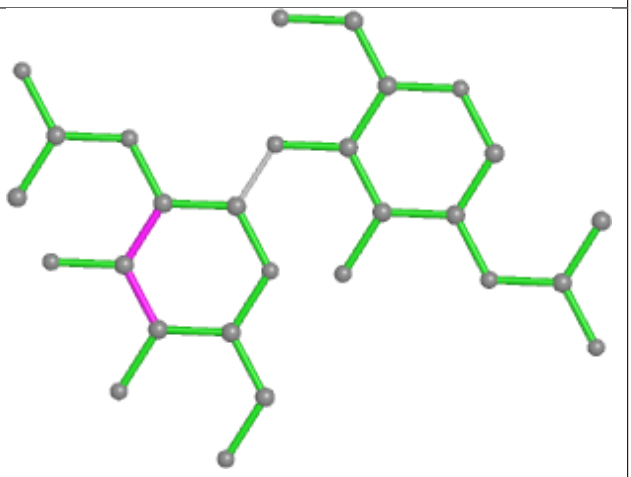


Rings

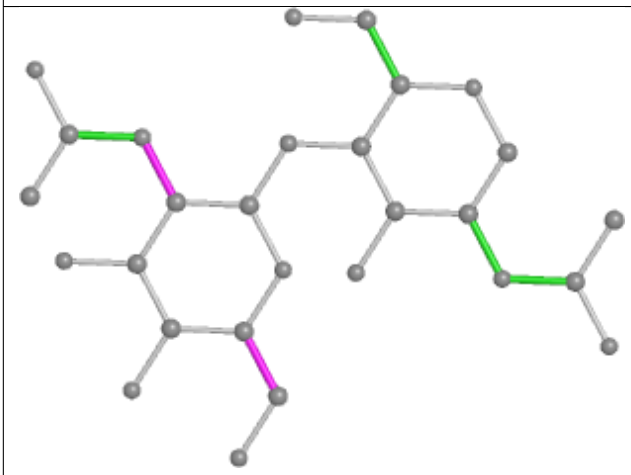
Oligosaccharide Chain H



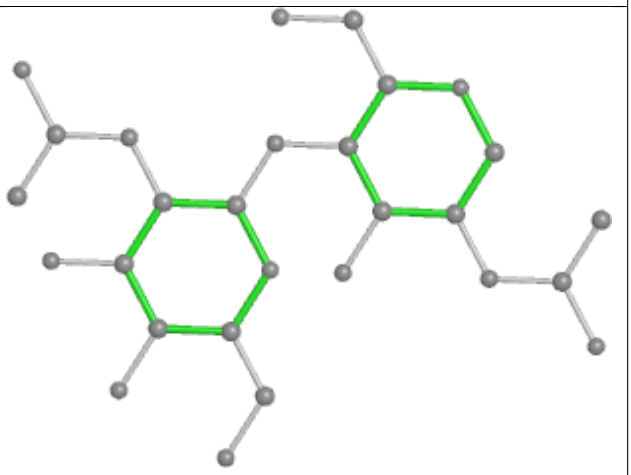
Bond lengths



Bond angles

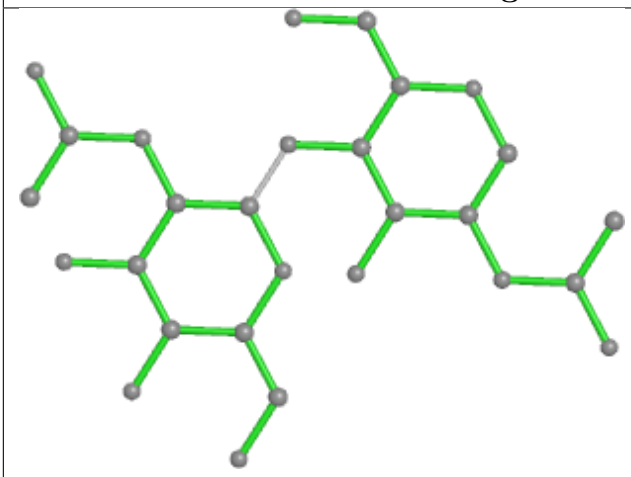


Torsions

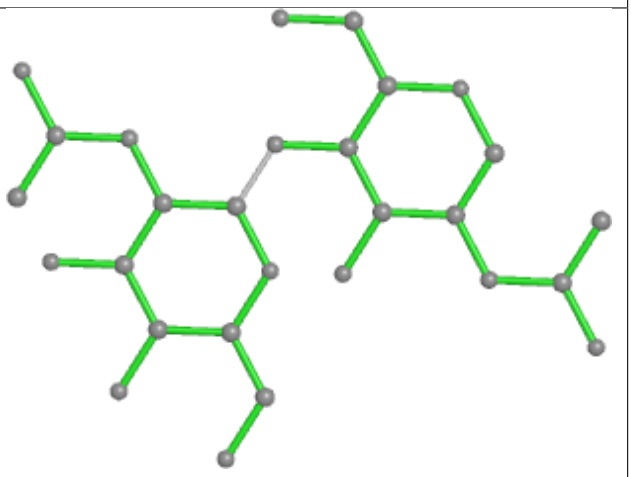


Rings

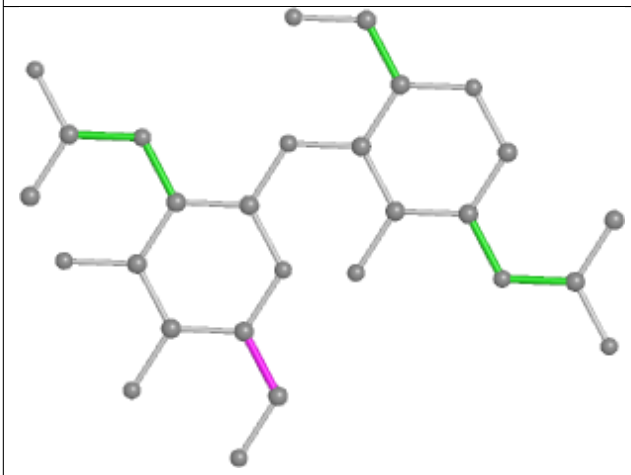
Oligosaccharide Chain I



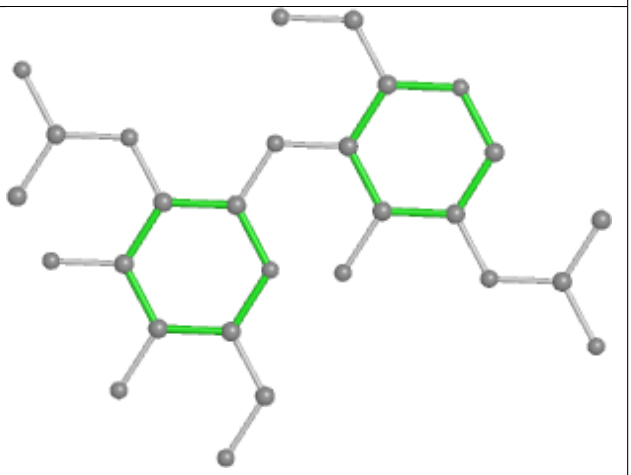
Bond lengths



Bond angles

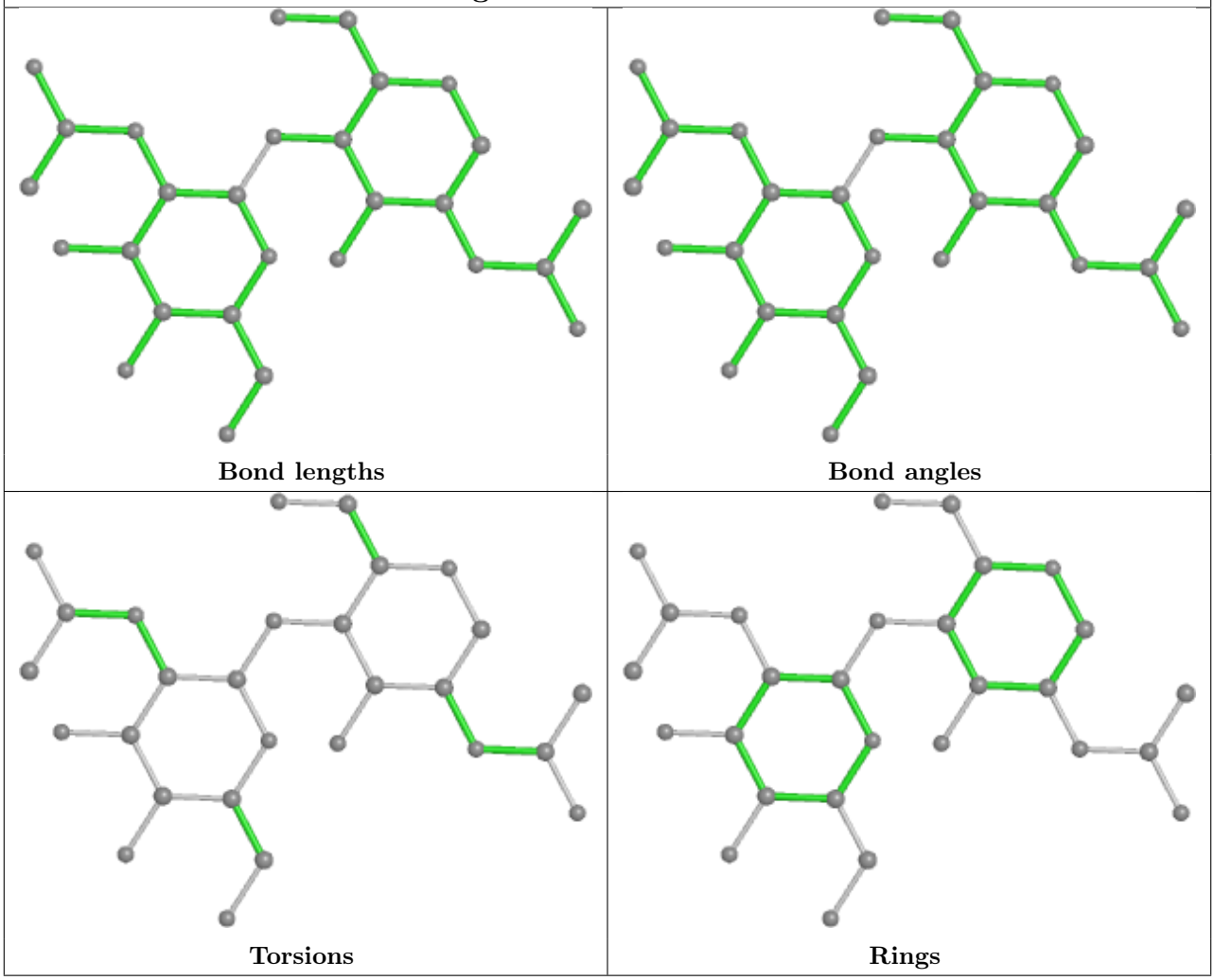


Torsions

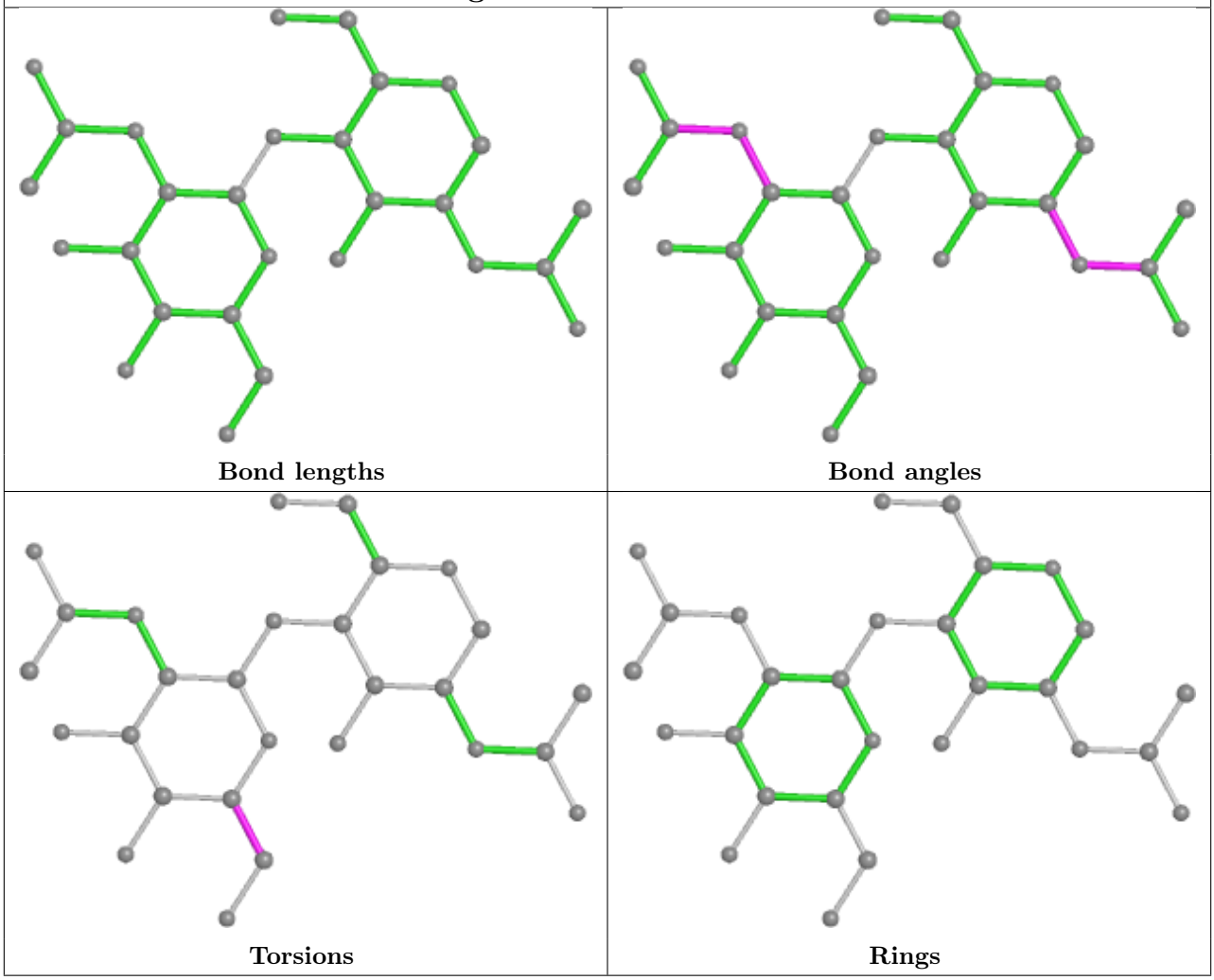


Rings

Oligosaccharide Chain J



Oligosaccharide Chain K



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	2092	1	14,14,15	0.78	1 (7%)	17,19,21	0.68	0
6	605	A	1521	-	27,28,28	3.50	19 (70%)	31,39,39	1.36	4 (12%)
6	605	B	1521	-	27,28,28	3.56	19 (70%)	31,39,39	1.23	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1281	1	14,14,15	0.72	0	17,19,21	0.83	1 (5%)
4	NAG	B	2321	1	14,14,15	0.53	0	17,19,21	0.97	1 (5%)
4	NAG	B	2150	1	14,14,15	0.57	0	17,19,21	0.73	1 (5%)
4	NAG	A	1092	1	14,14,15	0.71	0	17,19,21	0.55	0
4	NAG	A	1520	1	14,14,15	0.79	0	17,19,21	0.74	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
4	NAG	B	2092	1	-	4/6/23/26	0/1/1/1
6	605	A	1521	-	-	6/12/16/16	0/3/3/3
6	605	B	1521	-	-	2/12/16/16	0/3/3/3
4	NAG	A	1281	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2321	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2150	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1092	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1520	1	-	3/6/23/26	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1521	605	C21-C14	6.48	1.49	1.39
6	B	1521	605	C29-C30	6.35	1.50	1.39
6	B	1521	605	C21-C14	6.12	1.48	1.39
6	A	1521	605	C29-C30	5.96	1.49	1.39
6	B	1521	605	C17-C14	5.64	1.48	1.39
6	A	1521	605	C17-C14	5.14	1.47	1.39
6	B	1521	605	C31-C30	4.99	1.46	1.37
6	A	1521	605	C6-C5	4.95	1.46	1.37
6	B	1521	605	C6-C5	4.88	1.46	1.37
6	A	1521	605	C31-C30	4.77	1.45	1.37
6	A	1521	605	C4-C5	4.40	1.45	1.37
6	B	1521	605	C4-C3	4.38	1.47	1.39
6	B	1521	605	C20-C21	4.38	1.45	1.36
6	B	1521	605	C28-C27	4.37	1.46	1.36
6	A	1521	605	C4-C3	4.25	1.46	1.39
6	A	1521	605	C28-C27	4.10	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1521	605	C1-C2	4.03	1.46	1.37
6	A	1521	605	C20-C21	3.89	1.44	1.36
6	A	1521	605	C6-C1	3.88	1.45	1.38
6	B	1521	605	C28-C29	3.83	1.47	1.38
6	A	1521	605	C20-C19	3.75	1.51	1.41
6	A	1521	605	C3-C2	3.67	1.44	1.38
6	B	1521	605	C3-C2	3.58	1.44	1.38
6	B	1521	605	C6-C1	3.51	1.45	1.38
6	A	1521	605	C28-C29	3.46	1.46	1.38
6	B	1521	605	C20-C19	3.37	1.50	1.41
6	B	1521	605	C4-C5	3.35	1.43	1.37
6	A	1521	605	C27-C26	3.09	1.49	1.41
6	B	1521	605	C27-C26	2.96	1.49	1.41
6	B	1521	605	C18-C17	2.80	1.42	1.36
6	B	1521	605	F34-C5	-2.66	1.29	1.36
6	A	1521	605	C1-C2	2.65	1.43	1.37
6	A	1521	605	F34-C5	-2.62	1.30	1.36
6	A	1521	605	C14-C11	-2.53	1.48	1.52
6	B	1521	605	F35-C2	-2.45	1.29	1.35
6	B	1521	605	C31-C26	2.31	1.47	1.42
6	A	1521	605	C11-N15	2.30	1.52	1.47
6	A	1521	605	F35-C2	-2.27	1.29	1.35
4	B	2092	NAG	C1-C2	2.02	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1521	605	C17-C14-C11	-3.99	114.63	120.46
6	A	1521	605	C21-C14-C11	3.83	126.05	120.46
6	B	1521	605	C21-C14-C11	3.29	125.27	120.46
6	B	1521	605	C17-C14-C11	-3.17	115.83	120.46
6	B	1521	605	O42-C40-N41	-2.59	118.90	122.58
4	A	1281	NAG	C2-N2-C7	-2.32	119.59	122.90
4	B	2321	NAG	C2-N2-C7	-2.29	119.64	122.90
6	A	1521	605	C4-C3-C2	2.17	119.10	116.58
4	B	2150	NAG	C2-N2-C7	-2.16	119.83	122.90
6	A	1521	605	O42-C40-C30	2.14	122.19	119.63
6	B	1521	605	O42-C40-C30	2.03	122.06	119.63

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1521	605	N15-C11-C14-C21
6	B	1521	605	N15-C11-C14-C21
4	B	2092	NAG	O5-C5-C6-O6
4	A	1092	NAG	O5-C5-C6-O6
4	B	2092	NAG	C4-C5-C6-O6
4	A	1092	NAG	C4-C5-C6-O6
4	B	2092	NAG	C1-C2-N2-C7
6	A	1521	605	N15-C11-C14-C17
6	B	1521	605	N15-C11-C14-C17
4	A	1520	NAG	C3-C2-N2-C7
4	A	1520	NAG	O5-C5-C6-O6
6	A	1521	605	C29-C30-C40-N41
4	B	2092	NAG	C3-C2-N2-C7
6	A	1521	605	C29-C30-C40-O42
6	A	1521	605	C31-C30-C40-N41
4	A	1520	NAG	C1-C2-N2-C7
6	A	1521	605	C31-C30-C40-O42

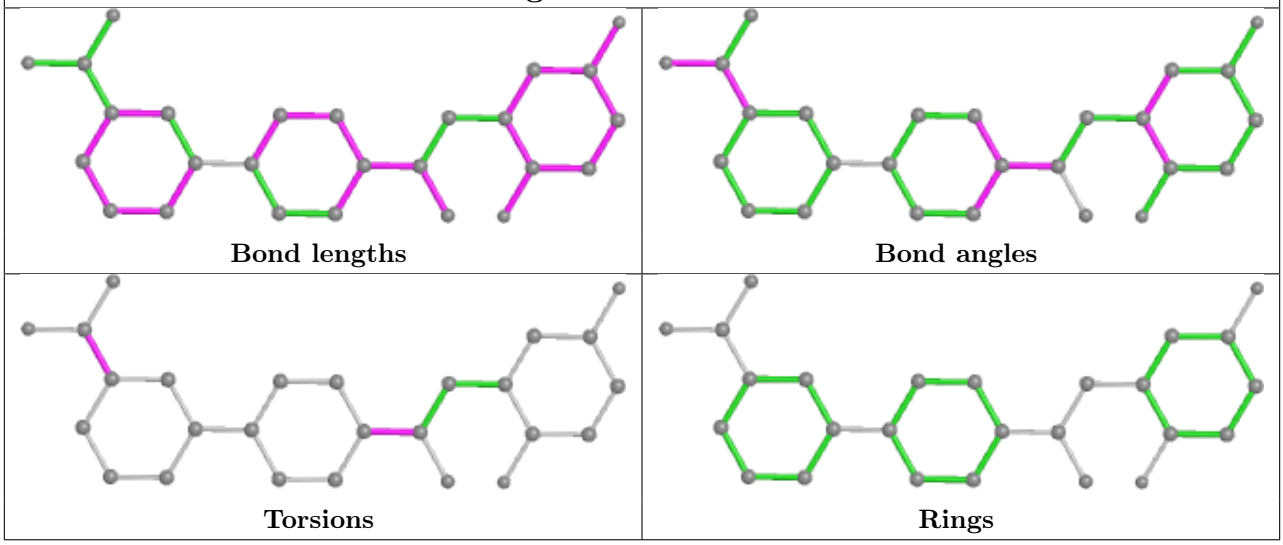
There are no ring outliers.

3 monomers are involved in 6 short contacts:

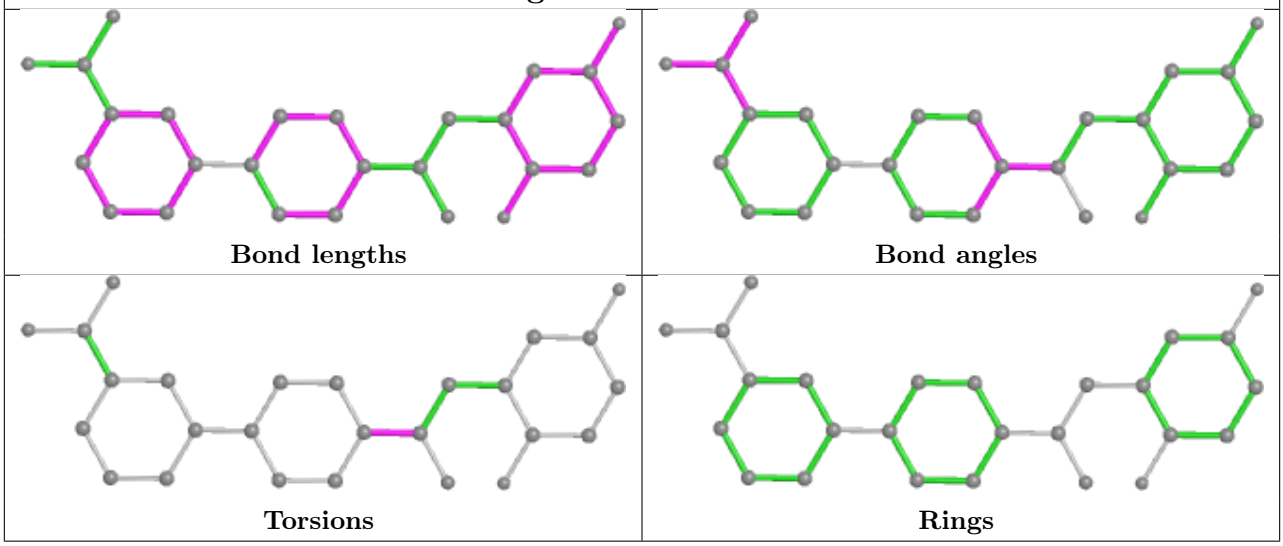
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2150	NAG	1	0
4	A	1092	NAG	2	0
4	A	1520	NAG	3	0

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 605 A 1521



Ligand 605 B 1521



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	728/728 (100%)	0.00	17 (2%)	60	59	21, 29, 48, 59	0
1	B	728/728 (100%)	0.02	28 (3%)	40	39	21, 31, 49, 59	0
All	All	1456/1456 (100%)	0.01	45 (3%)	49	48	21, 30, 49, 59	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	7.3
1	B	39	THR	7.1
1	B	766	PRO	5.6
1	A	766	PRO	5.5
1	B	95	PHE	5.1
1	A	74	ASN	4.9
1	B	98	PHE	4.7
1	A	97	GLU	4.5
1	B	96	ASP	4.5
1	A	73	GLU	4.3
1	B	91	GLU	4.3
1	B	97	GLU	4.2
1	B	88	VAL	4.2
1	B	73	GLU	3.8
1	B	93	SER	3.8
1	B	92	ASN	3.8
1	A	40	ARG	3.6
1	B	99	GLY	3.6
1	B	94	THR	3.6
1	B	74	ASN	3.5
1	A	96	ASP	3.3
1	A	99	GLY	3.3
1	B	40	ARG	3.2
1	A	279	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	92	ASN	3.2
1	B	100	HIS	3.1
1	B	90	LEU	2.9
1	A	98	PHE	2.9
1	A	94	THR	2.8
1	B	505	GLN	2.7
1	B	138	ASN	2.7
1	B	506	ASN	2.6
1	B	140	ARG	2.6
1	A	521	GLU	2.6
1	A	95	PHE	2.4
1	B	502	LYS	2.4
1	B	72	GLN	2.3
1	A	54	ARG	2.2
1	B	71	LYS	2.2
1	B	141	GLN	2.1
1	A	138	ASN	2.1
1	B	76	ILE	2.1
1	B	75	ASN	2.1
1	A	332	GLU	2.0
1	B	333	SER	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
2	NDG	C	2	14/15	0.51	0.38	58,60,61,61	0
3	NAG	G	2	14/15	0.55	0.42	56,58,60,60	0
3	NAG	D	1	14/15	0.59	0.41	55,58,60,61	0
3	NAG	D	2	14/15	0.61	0.40	59,61,62,63	0
3	NAG	H	2	14/15	0.61	0.51	59,60,61,61	0
3	NAG	K	2	14/15	0.64	0.25	50,52,54,54	0
2	NDG	F	2	14/15	0.76	0.37	53,56,58,59	0

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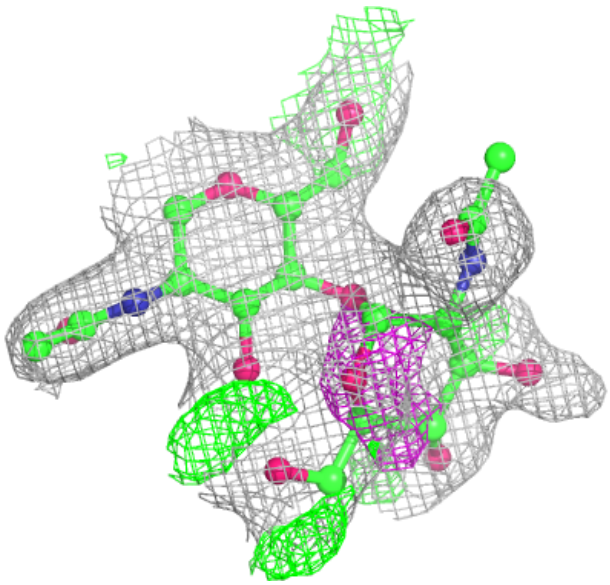
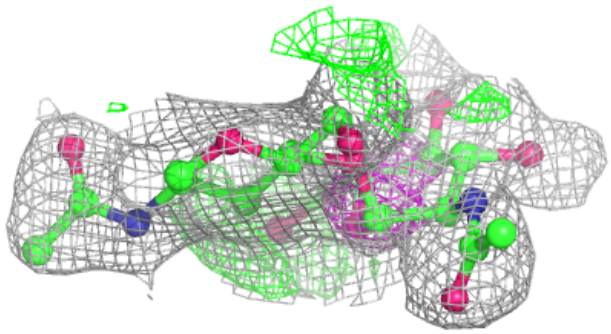
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	H	1	14/15	0.78	0.21	50,53,55,57	0
3	NAG	E	2	14/15	0.80	0.26	52,54,57,57	0
2	NAG	C	1	14/15	0.81	0.16	46,50,53,56	0
3	NAG	G	1	14/15	0.82	0.29	43,48,49,54	0
3	NAG	J	2	14/15	0.83	0.28	48,51,52,53	0
3	NAG	I	2	14/15	0.88	0.17	48,49,51,51	0
3	NAG	K	1	14/15	0.91	0.12	40,41,46,48	0
2	NAG	F	1	14/15	0.92	0.15	39,43,47,49	0
3	NAG	E	1	14/15	0.92	0.15	44,47,49,49	0
3	NAG	J	1	14/15	0.92	0.12	33,35,40,45	0
3	NAG	I	1	14/15	0.93	0.11	41,44,46,46	0

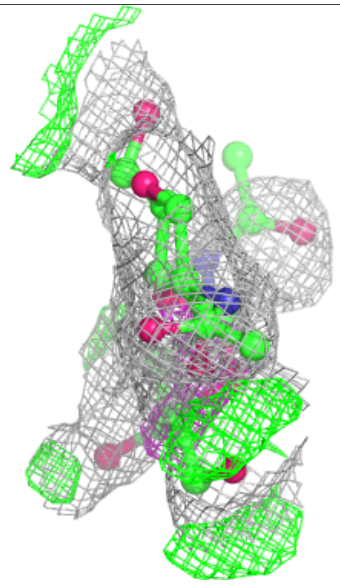
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

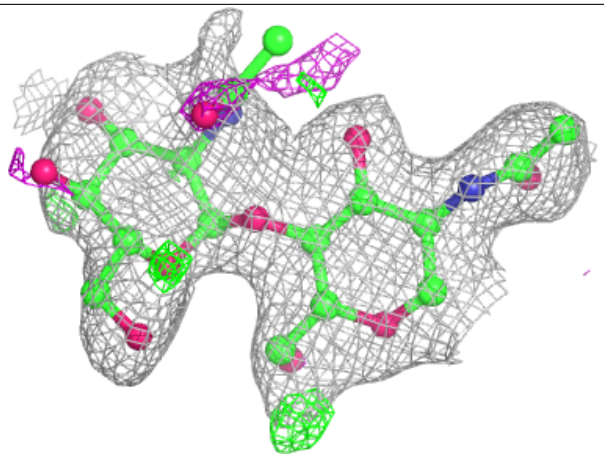


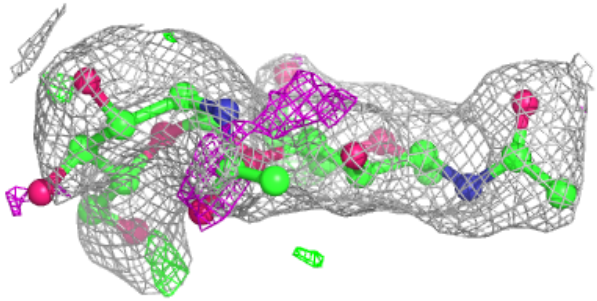


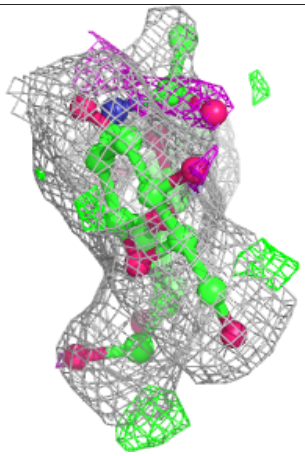


Electron density around Chain F:

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

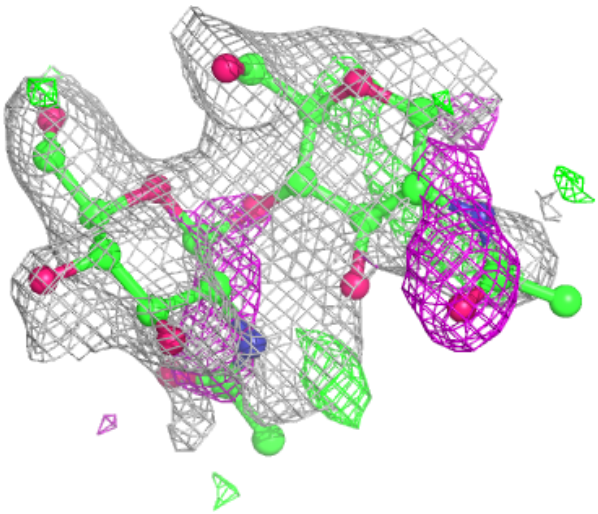


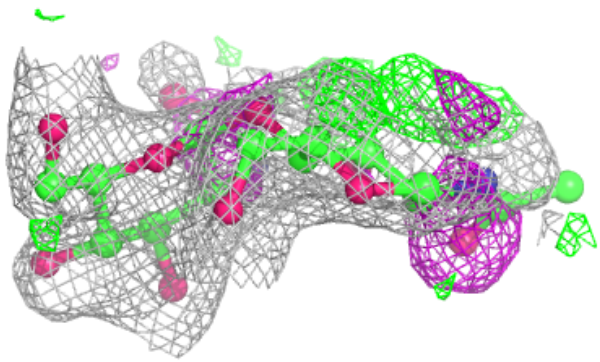


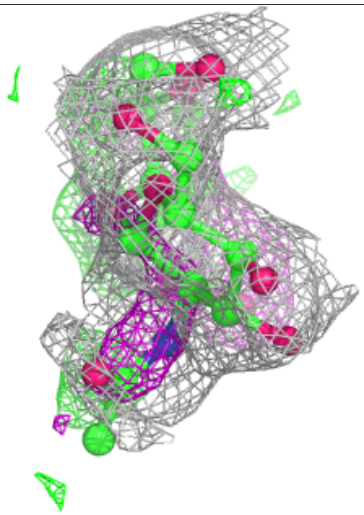


Electron density around Chain D:

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

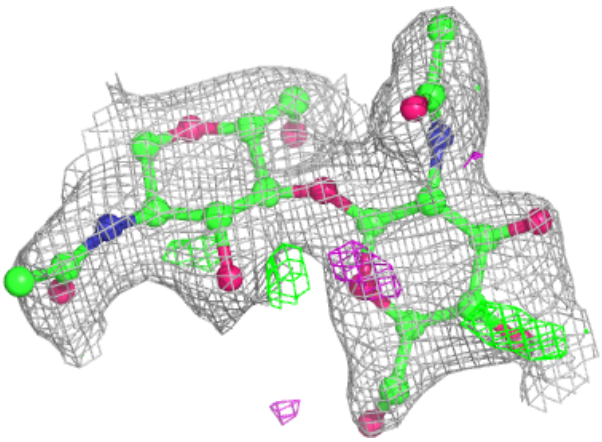


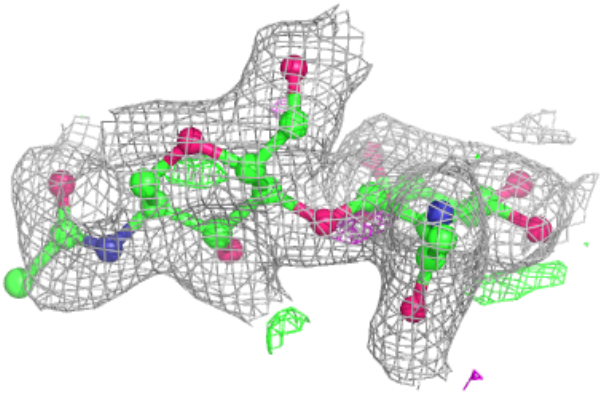


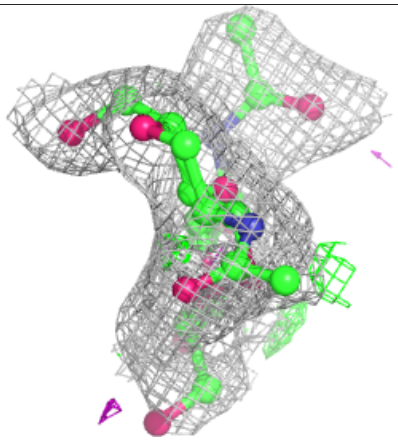


Electron density around Chain E:

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

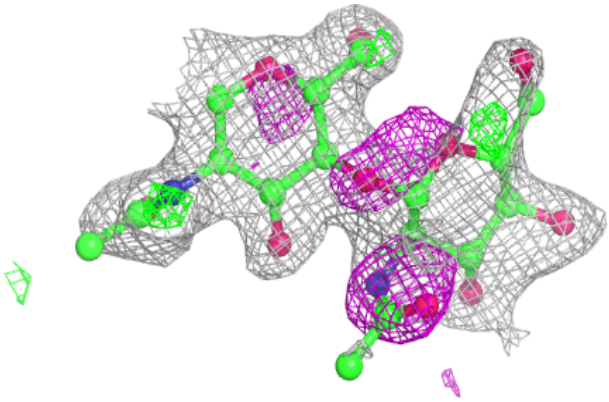


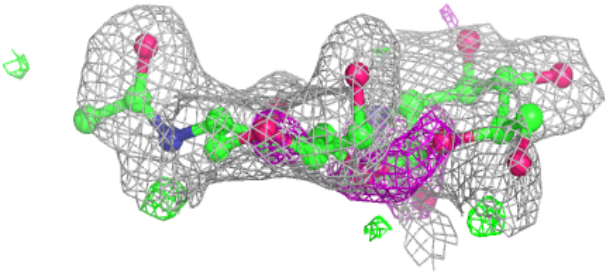


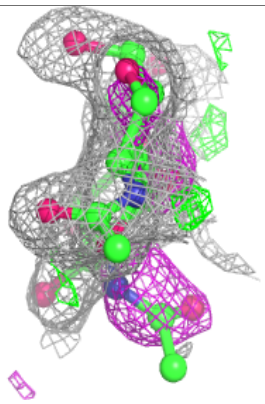


Electron density around Chain G:

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

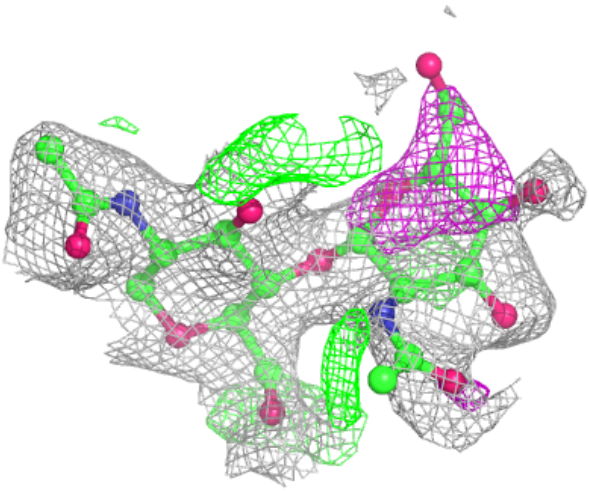


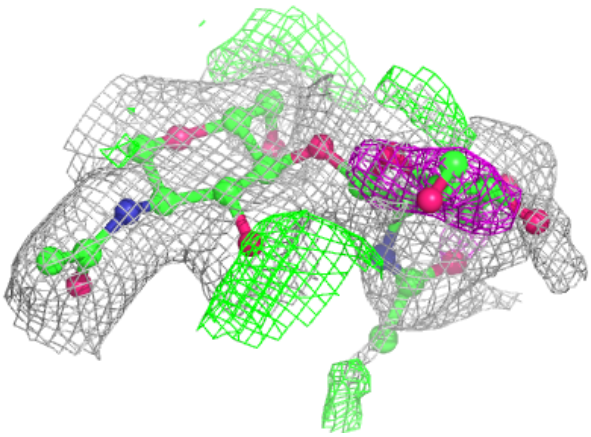


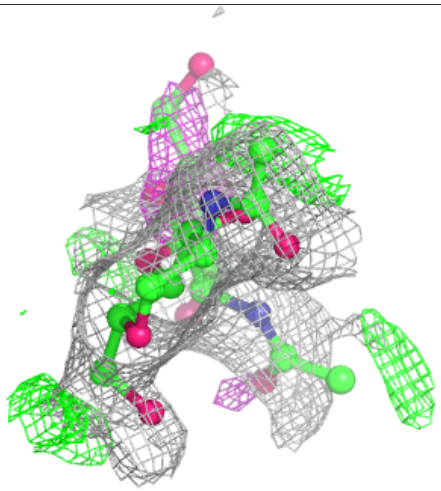


Electron density around Chain H:

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

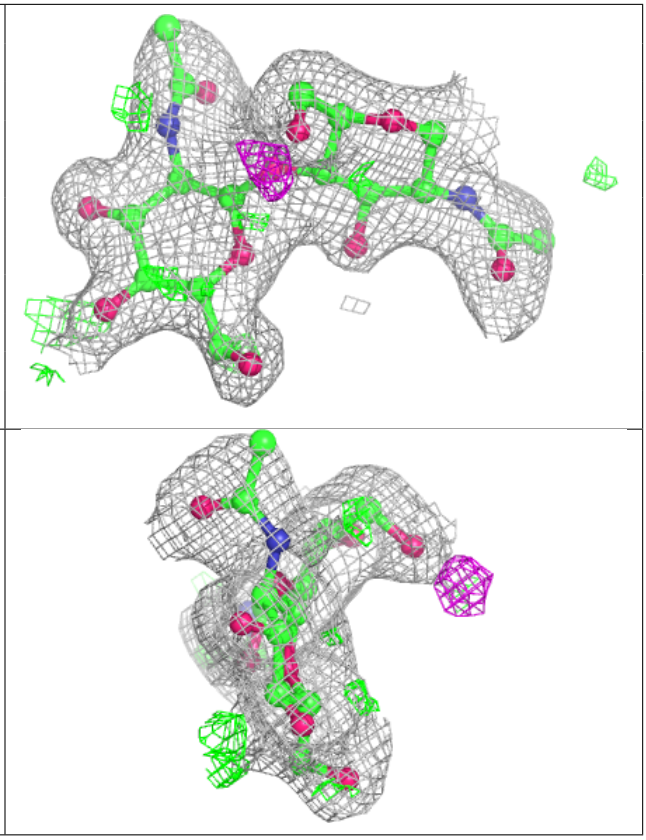


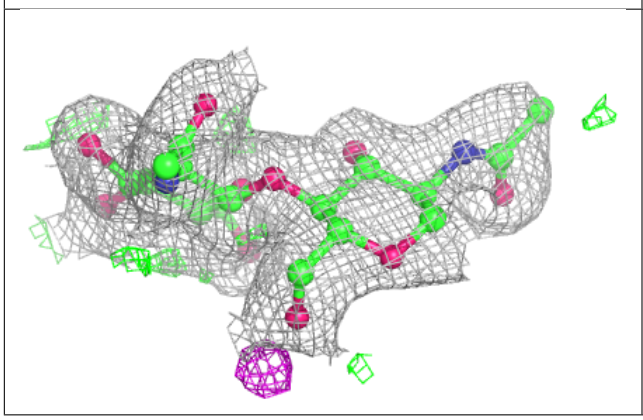




Electron density around Chain I:

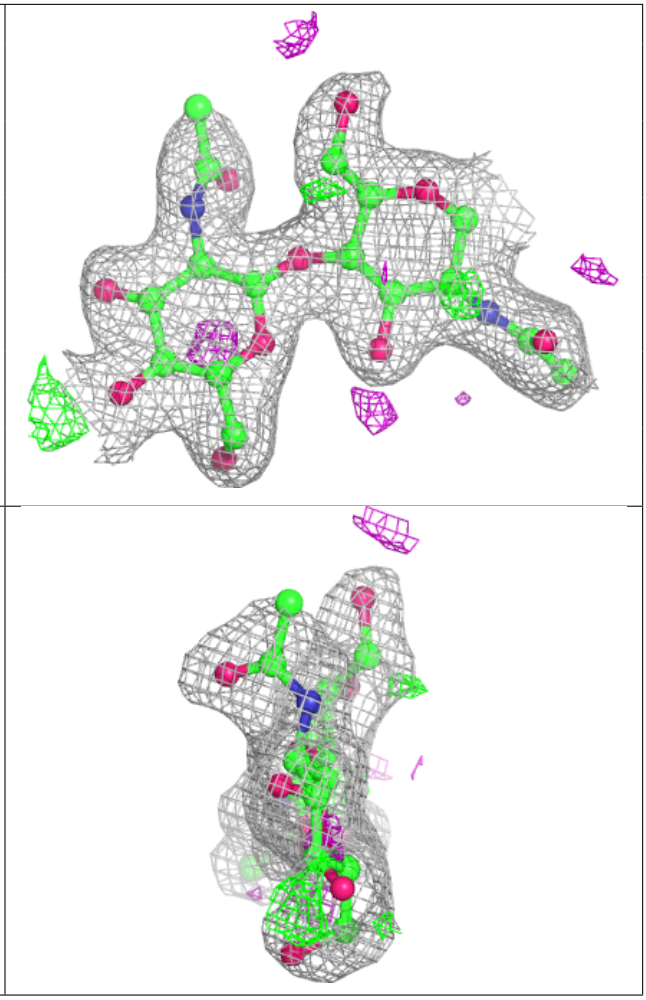
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





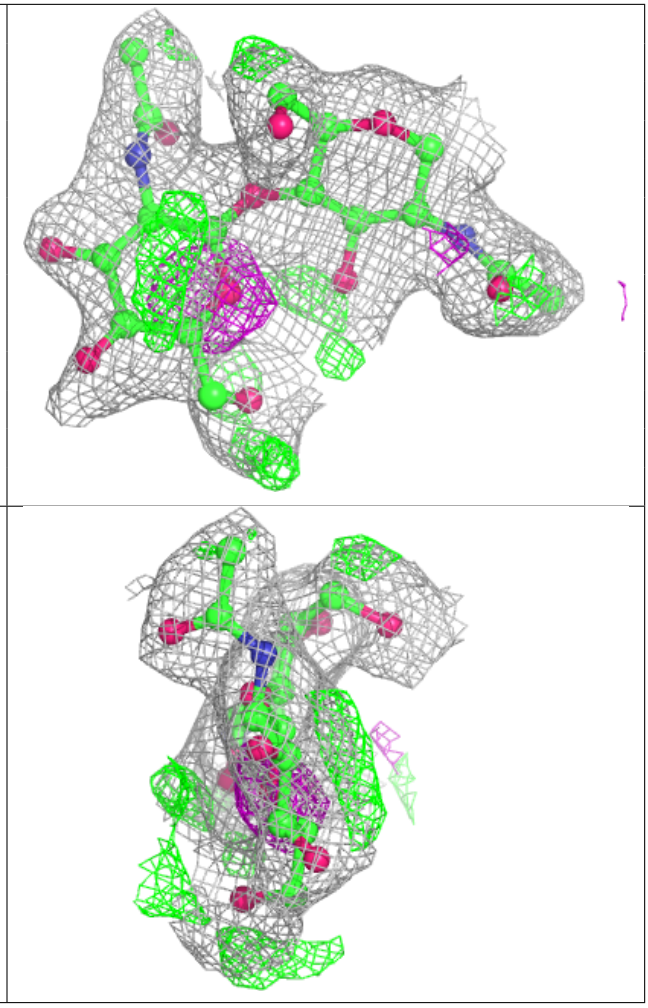
Electron density around Chain J:

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



Electron density around Chain K:

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



6.4 Ligands (i)

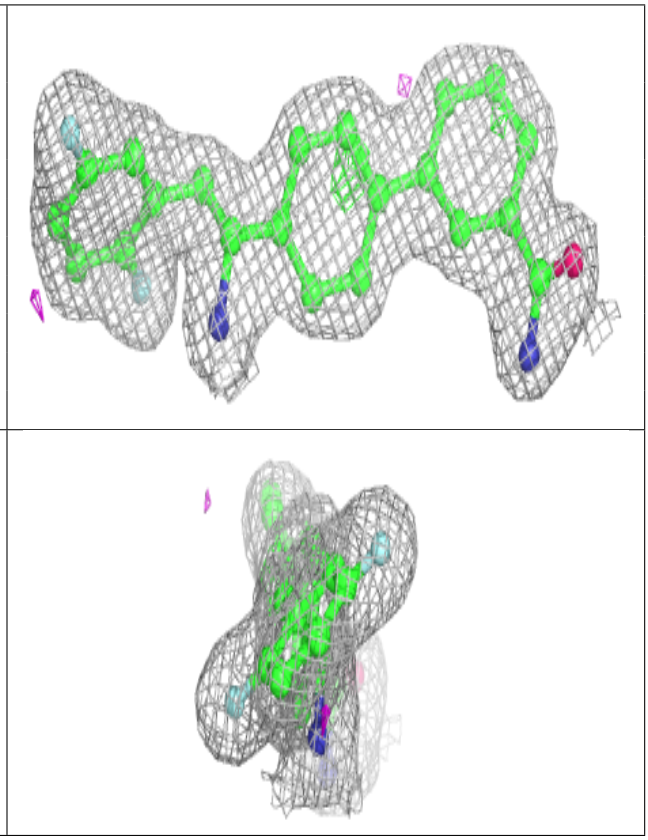
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	1520	14/15	0.53	0.42	59,60,60,60	0
4	NAG	A	1092	14/15	0.62	0.54	61,62,62,62	0
4	NAG	B	2092	14/15	0.68	0.43	60,60,61,62	0
4	NAG	B	2150	14/15	0.77	0.41	53,55,57,57	0
4	NAG	B	2321	14/15	0.82	0.28	42,46,48,49	0
4	NAG	A	1281	14/15	0.86	0.18	47,49,50,51	0
6	605	B	1521	26/26	0.95	0.19	21,26,32,35	0
6	605	A	1521	26/26	0.97	0.18	17,22,29,32	0
5	NA	A	1	1/1	0.97	0.06	35,35,35,35	0

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.

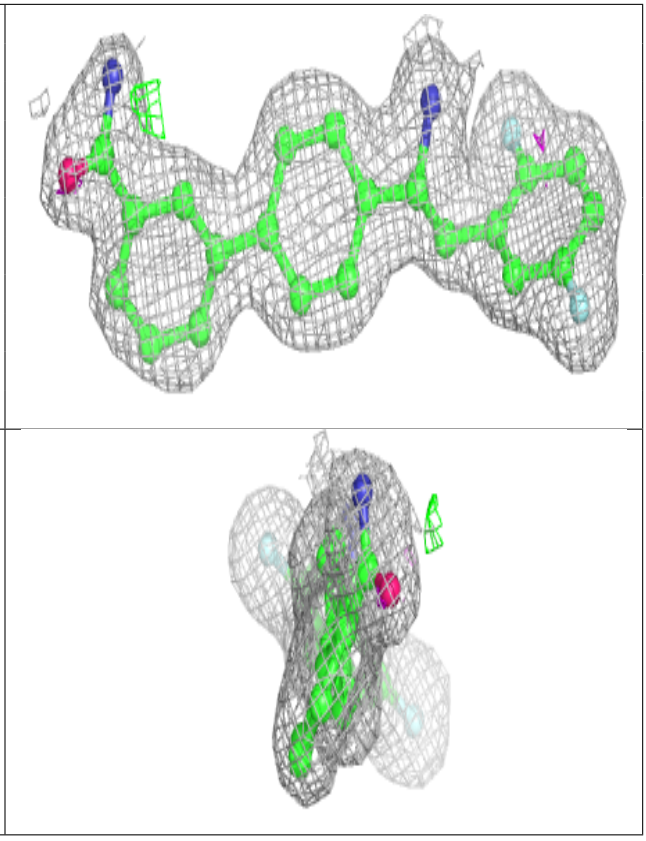
Electron density around 605 B 1521:

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



Electron density around 605 A 1521:

$2mF_o$-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 (i)

There are no such residues in this entry.