Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2020 – 05:01 PM BST

PDB ID	:	4XII
Title	:	X-ray structure of human butyrylcholinesterase in complex with N-((1-(2,3-dihydro-1H-inden-2-yl)piperidin-3-yl)methyl)-8-hydroxy-N-(2-methoxyethyl)-5-nitroquinoline-7-carboxamide
Authors	:	Knez, D.; Boris, B.; Coquelle, N.; Sosic, I.; Sink, R.; Brazzolotto, X.; Mravljak, J.; Colletier, J.P.; Gobec, S.
Deposited on	:	2015-01-07
Resolution	:	2.70 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 following versions of software and data (see references (1)) were used in the production of this report:

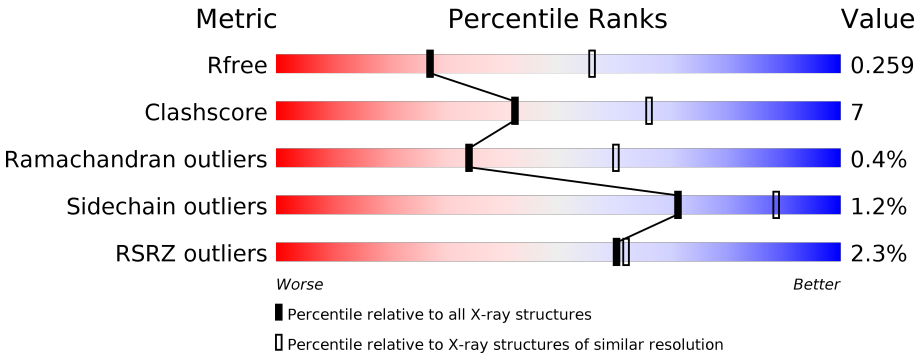
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	544	85% 12%
1	B	544	3% 82% 14%
2	C	3	33% 33% 33%
3	D	2	100%
3	E	2	50% 50%
3	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	2	50% 50%

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
2	NAG	C	1	-	-	X	-
2	FUL	C	3	X	-	-	-
3	NAG	G	1	X	-	-	-
5	NAG	A	1002	X	-	-	-
5	NAG	A	1011	X	-	-	-
5	NAG	B	1008	X	-	-	-
6	FUL	A	1010	-	-	X	-
7	FUC	A	1012	-	-	-	X

2 Entry composition

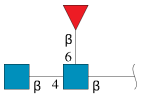
There are 10 unique types of molecules in this entry. The entry contains 8849 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	2	1
			4195	2706	710	764	15			
1	B	525	Total	C	N	O	S	0	1	1
			4168	2693	701	759	15			

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

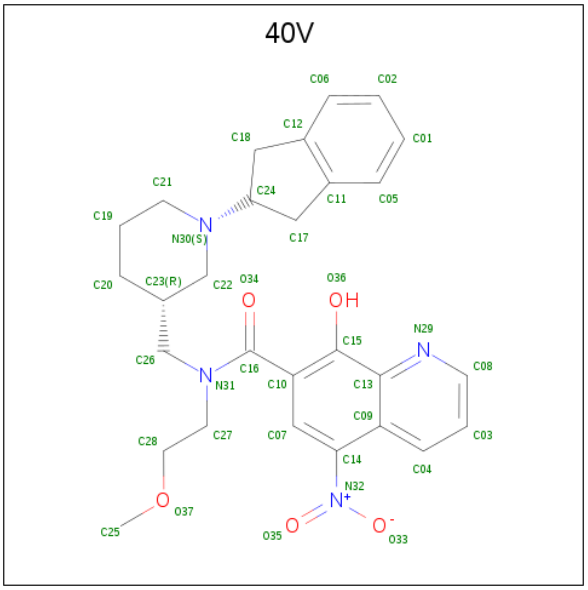


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

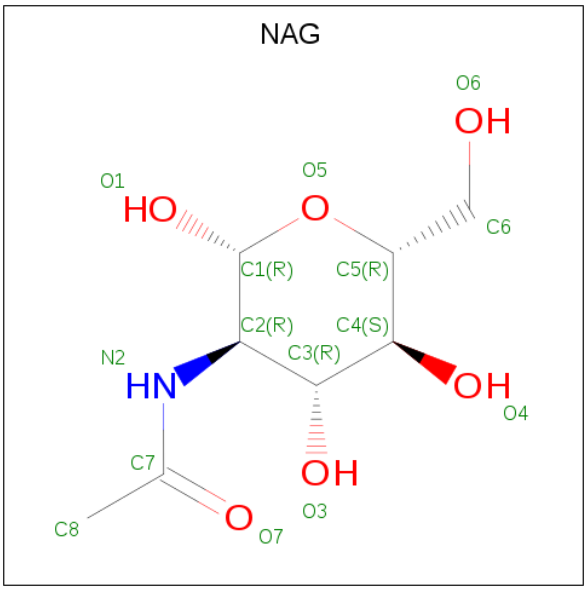
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is N-{[(3R)-1-(2,3-dihydro-1H-inden-2-yl)piperidin-3-yl]methyl}-8-hydroxy-N-(2-methoxyethyl)-5-nitroquinoline-7-carboxamide (three-letter code: 40V) (formula: $C_{28}H_{32}N_4O_5$).



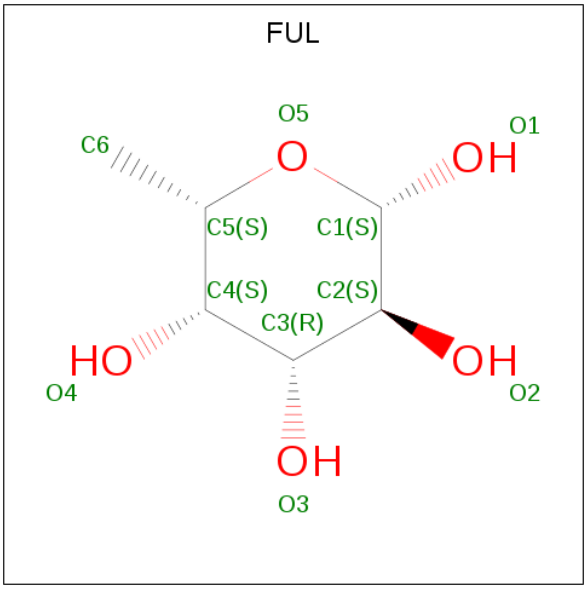
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			37	28	4	5		
4	B	1	Total	C	N	O	0	0
			37	28	4	5		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is beta-L-fucopyranose (three-letter code: FUL) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0

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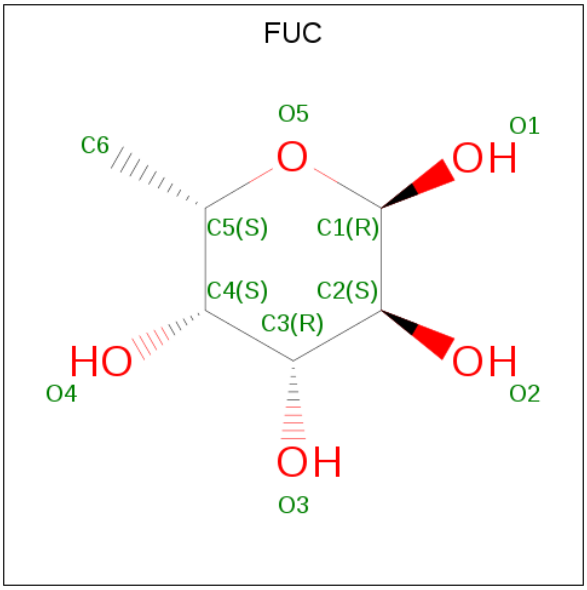
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 10 6 4	0	0

- Molecule 7 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).

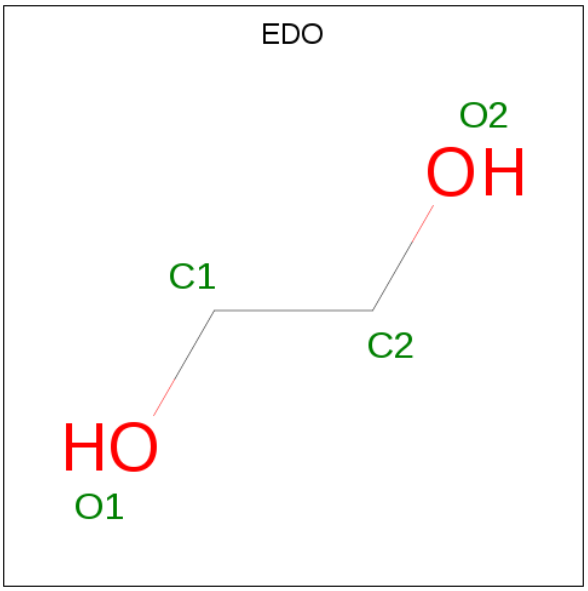


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 10 6 4	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Cl 1 1	0	0
8	A	3	Total Cl 3 3	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

- Molecule 10 is water.

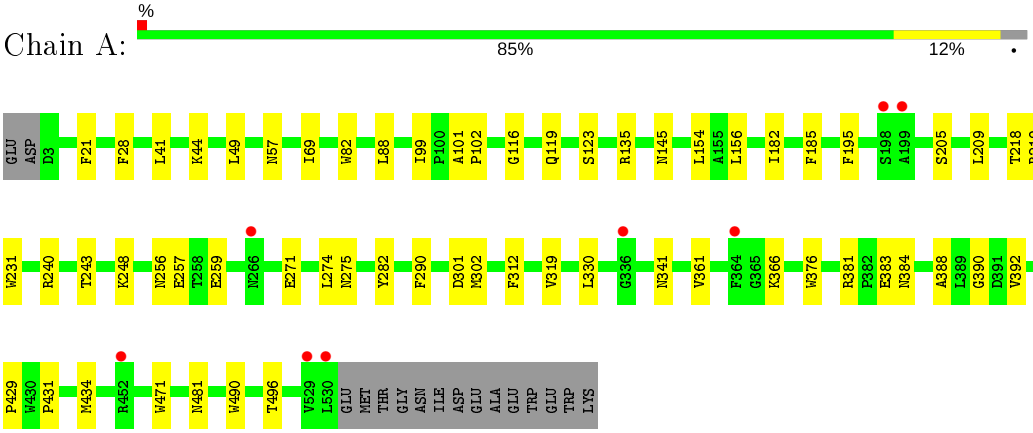
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	35	Total O 35 35	0	0
10	B	27	Total O 27 27	0	0

3 Residue-property plots

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.

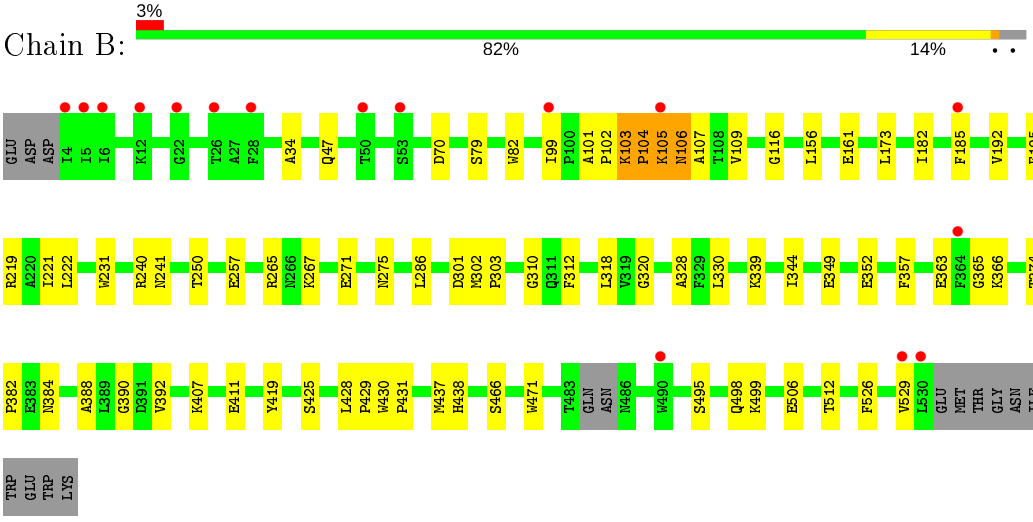
• Molecule 1: Cholinesterase

Chain A:



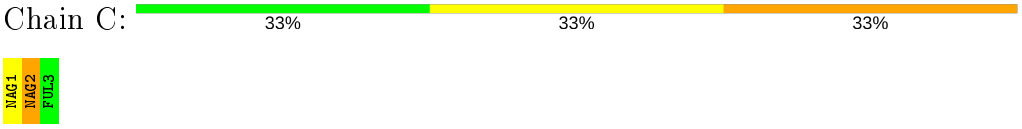
• Molecule 1: Cholinesterase

Chain B:



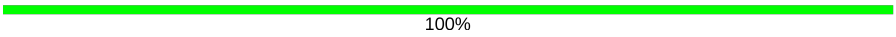
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

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 E:

• 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:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.04Å 79.76Å 230.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 2.70 46.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.19-2.70) 99.0 (46.76-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.257 0.210 , 0.259	Depositor DCC
R_{free} test set	1509 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å^2)	76.8	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8849	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, EDO, 40V, FUC, FUL

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	0.37	0/4317	0.54	0/5864
1	B	0.35	0/4286	0.54	3/5821 (0.1%)
All	All	0.36	0/8603	0.54	3/11685 (0.0%)

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	B	381	ARG	C-N-CD	-8.37	102.19	120.60
1	B	381	ARG	C-N-CA	6.28	148.38	122.00
1	B	103	LYS	C-N-CD	5.07	139.04	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4195	0	4083	41	0
1	B	4168	0	4049	60	0
2	C	38	0	33	7	0
3	D	28	0	25	0	0
3	E	28	0	25	6	0
3	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	28	0	25	2	0
4	A	37	0	32	4	0
4	B	37	0	32	5	0
5	A	28	0	26	3	0
5	B	112	0	103	5	0
6	A	20	0	20	8	0
6	B	10	0	10	0	0
7	A	10	0	10	3	0
8	A	3	0	0	1	0
8	B	1	0	0	0	0
9	A	8	0	12	0	0
9	B	8	0	12	0	0
10	A	35	0	0	1	0
10	B	27	0	0	0	0
All	All	8849	0	8522	119	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 7.

All (119) 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:57:ASN:HD21	2:C:1:NAG:C1	1.01	1.55
1:B:241:ASN:HD21	5:B:1005:NAG:C1	1.14	1.52
1:B:106:ASN:OD1	5:B:1004:NAG:C1	1.64	1.44
6:A:1010:FUL:C1	3:E:1:NAG:O6	1.69	1.40
1:A:57:ASN:ND2	2:C:1:NAG:C1	1.82	1.40
1:B:241:ASN:ND2	5:B:1005:NAG:C1	1.88	1.37
6:A:1017:FUL:C1	3:G:1:NAG:O6	1.88	1.20
2:C:1:NAG:O4	2:C:2:NAG:H62	1.56	1.01
6:A:1017:FUL:C1	3:G:1:NAG:HO6	1.70	1.01
6:A:1010:FUL:C1	3:E:1:NAG:C6	2.45	0.95
6:A:1010:FUL:C1	3:E:1:NAG:HO6	1.79	0.91
1:A:116:GLY:O	10:A:1101:HOH:O	1.94	0.84
1:B:241:ASN:CG	5:B:1005:NAG:C1	2.47	0.82
1:B:240:ARG:NH2	1:B:257:GLU:OE2	2.13	0.81
5:A:1011:NAG:O6	7:A:1012:FUC:O5	2.02	0.77
1:A:156:LEU:HD13	1:A:257:GLU:HB3	1.74	0.70
6:A:1010:FUL:C2	3:E:1:NAG:O6	2.41	0.68
1:B:101:ALA:HA	1:B:102:PRO:C	2.17	0.65
5:A:1011:NAG:C6	7:A:1012:FUC:O5	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ARG:O	1:A:384:ASN:ND2	2.31	0.64
1:B:241:ASN:OD1	5:B:1005:NAG:C1	2.47	0.63
2:C:1:NAG:O4	2:C:2:NAG:C6	2.28	0.62
1:A:123:SER:OG	1:A:145:ASN:OD1	2.10	0.59
5:A:1011:NAG:H62	7:A:1012:FUC:O5	2.04	0.58
1:A:256:ASN:OD1	1:A:259:GLU:N	2.37	0.57
1:A:154:LEU:HD11	1:A:243:THR:HG23	1.85	0.57
1:A:271:GLU:O	1:A:275:ASN:ND2	2.36	0.57
1:B:428:LEU:HD23	1:B:430:TRP:H	1.70	0.57
1:B:330:LEU:HD11	1:B:390:GLY:HA2	1.86	0.57
1:A:381:ARG:HH11	1:A:383:GLU:HB2	1.71	0.56
1:B:376:TRP:CH2	1:B:384:ASN:HB3	2.41	0.56
1:B:526:PHE:O	1:B:529:VAL:HG12	2.05	0.55
1:B:99:ILE:HD11	1:B:185:PHE:HB3	1.89	0.55
1:B:407:LYS:O	1:B:411:GLU:HG2	2.06	0.55
1:A:481:ASN:HA	8:A:1019:CL:CL	2.45	0.54
6:A:1010:FUL:O2	3:E:1:NAG:O6	2.25	0.54
1:B:116:GLY:HA2	4:B:1001:40V:O34	2.07	0.53
1:A:82:TRP:CE2	4:A:1001:40V:H13	2.44	0.52
1:B:376:TRP:CZ3	1:B:384:ASN:HB3	2.45	0.52
2:C:1:NAG:O3	2:C:2:NAG:C1	2.58	0.51
1:A:240:ARG:NH1	1:A:257:GLU:OE2	2.36	0.51
1:A:381:ARG:HB3	1:A:384:ASN:ND2	2.26	0.51
1:B:105:LYS:CD	1:B:105:LYS:N	2.73	0.51
1:A:428:LEU:HD12	1:A:429:PRO:HD2	1.91	0.51
1:A:376:TRP:CZ3	1:A:384:ASN:HB3	2.46	0.50
1:B:156:LEU:HD13	1:B:257:GLU:HB3	1.92	0.50
1:B:438:HIS:CD2	4:B:1001:40V:H28	2.46	0.50
1:B:34:ALA:HB2	1:B:173:LEU:HD23	1.94	0.49
1:B:271:GLU:O	1:B:275:ASN:ND2	2.36	0.49
1:B:82:TRP:CE2	4:B:1001:40V:H13	2.48	0.49
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.95	0.49
1:A:69:ILE:HD11	1:A:88:LEU:HD11	1.94	0.49
1:B:388:ALA:O	1:B:392:VAL:HG23	2.13	0.48
1:B:363:GLU:HA	1:B:366:LYS:HE3	1.94	0.48
1:B:103:LYS:HG3	1:B:104:PRO:HD2	1.96	0.48
2:C:1:NAG:O3	2:C:2:NAG:H2	2.14	0.48
1:A:431:PRO:HG2	1:A:434:MET:HG3	1.96	0.47
1:B:349:GLU:HA	1:B:352:GLU:OE1	2.14	0.46
1:B:374:THR:HG22	1:B:376:TRP:CZ2	2.50	0.46
1:B:104:PRO:C	1:B:105:LYS:HD3	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLY:HA3	1:B:419:TYR:CD2	2.50	0.46
1:A:361:VAL:O	1:A:366:LYS:NZ	2.44	0.46
1:B:381:ARG:HB2	1:B:384:ASN:ND2	2.31	0.46
1:B:105:LYS:HD3	1:B:105:LYS:N	2.31	0.46
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.78	0.45
1:B:301:ASP:OD1	1:B:302:MET:N	2.45	0.45
1:A:419:TYR:HB3	1:A:490:TRP:CZ2	2.51	0.45
1:B:250:THR:HB	1:B:267:LYS:HE2	1.98	0.45
1:A:44:LYS:HB3	1:A:44:LYS:HE3	1.85	0.45
1:B:218:THR:HG22	1:B:219:ARG:HG3	1.99	0.45
1:B:428:LEU:HA	1:B:429:PRO:HD3	1.74	0.44
1:A:209:LEU:HD23	1:A:312:PHE:HB3	2.00	0.44
1:A:388:ALA:O	1:A:392:VAL:HG23	2.17	0.44
1:B:328:ALA:HB2	1:B:437:MET:HE3	1.99	0.44
1:A:182:ILE:HA	1:A:182:ILE:HD12	1.79	0.43
1:A:330:LEU:HD11	1:A:390:GLY:HA2	1.99	0.43
1:A:428:LEU:HA	1:A:429:PRO:HD3	1.82	0.43
1:B:310:GLY:HA2	1:B:312:PHE:CE2	2.53	0.43
1:B:381:ARG:HB3	1:B:382:PRO:CA	2.47	0.43
2:C:1:NAG:O3	2:C:2:NAG:C2	2.67	0.43
1:A:21:PHE:O	1:A:135:ARG:NH2	2.51	0.43
1:A:119:GLN:NE2	1:A:290:PHE:O	2.47	0.43
1:A:28:PHE:HE1	1:A:99:ILE:HD12	1.83	0.43
1:B:101:ALA:HA	1:B:102:PRO:O	2.18	0.43
1:B:231:TRP:CE2	4:B:1001:40V:H21	2.54	0.43
1:B:104:PRO:CG	1:B:107:ALA:HB2	2.49	0.43
1:B:109:VAL:HB	1:B:192:VAL:HG22	2.00	0.43
1:A:218:THR:HG22	1:A:219:ARG:HG3	2.01	0.43
1:B:320:GLY:HA3	1:B:419:TYR:CE2	2.53	0.43
1:B:195:PHE:CB	1:B:221:ILE:HB	2.49	0.43
1:A:301:ASP:OD1	1:A:302:MET:N	2.51	0.42
1:B:106:ASN:HA	1:B:106:ASN:HD22	1.59	0.42
4:B:1001:40V:H5	4:B:1001:40V:H23	1.61	0.42
1:B:495:SER:O	1:B:498:GLN:NE2	2.40	0.42
1:A:82:TRP:CD2	4:A:1001:40V:H13	2.55	0.42
1:A:231:TRP:CE2	4:A:1001:40V:H21	2.55	0.42
1:B:103:LYS:HG3	1:B:104:PRO:CD	2.49	0.42
6:A:1010:FUL:C2	3:E:1:NAG:HO6	2.27	0.42
1:A:101:ALA:HA	1:A:102:PRO:C	2.39	0.42
1:B:161:GLU:OE1	1:B:265:ARG:NH1	2.32	0.41
1:B:286:LEU:HD12	1:B:357:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:LYS:HG2	1:B:512:THR:HG22	2.02	0.41
1:B:425:SER:HB3	1:B:428:LEU:HB2	2.02	0.41
1:B:109:VAL:HG21	1:B:182:ILE:HG12	2.03	0.41
1:B:99:ILE:HD11	1:B:185:PHE:HD2	1.85	0.41
1:B:365:GLY:CA	1:B:529:VAL:HG21	2.51	0.41
1:A:195:PHE:CB	1:A:221:ILE:HB	2.51	0.41
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.80	0.41
1:B:365:GLY:HA3	1:B:529:VAL:HG21	2.03	0.41
1:B:221:ILE:HG23	1:B:318:LEU:HB3	2.03	0.41
1:B:344:ILE:HD13	1:B:382:PRO:HG2	2.03	0.41
4:A:1001:40V:C07	4:A:1001:40V:H7	2.51	0.40
1:A:99:ILE:HD11	1:A:185:PHE:CD2	2.56	0.40
1:B:302:MET:HA	1:B:303:PRO:HD3	1.90	0.40
1:B:339:LYS:HA	1:B:431:PRO:HG3	2.02	0.40
1:B:205:SER:HB3	1:B:222:LEU:HD21	2.02	0.40
1:B:70:ASP:OD2	1:B:79:SER:HB2	2.21	0.40
1:A:381:ARG:HB3	1:A:384:ASN:HD21	1.86	0.40
1:A:319:VAL:O	1:A:418:PHE:HA	2.22	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	528/544 (97%)	503 (95%)	24 (4%)	1 (0%)	47	73
1	B	522/544 (96%)	496 (95%)	23 (4%)	3 (1%)	25	50
All	All	1050/1088 (96%)	999 (95%)	47 (4%)	4 (0%)	34	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	381	ARG
1	B	506	GLU
1	A	282	TYR
1	B	104	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	450/467 (96%)	445 (99%)	5 (1%)	73 90
1	B	445/467 (95%)	439 (99%)	6 (1%)	69 87
All	All	895/934 (96%)	884 (99%)	11 (1%)	71 88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	LYS
1	A	274	LEU
1	A	341	ASN
1	A	471	TRP
1	A	496	THR
1	B	47	GLN
1	B	105	LYS
1	B	106	ASN
1	B	381	ARG
1	B	466	SER
1	B	471	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	384	ASN
1	B	241	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

11 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	2	14,14,15	0.40	0	17,19,21	0.65	0
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	1.45	2 (11%)
2	FUL	C	3	2	10,10,11	0.29	0	14,14,16	0.62	0
3	NAG	D	1	1,3	14,14,15	0.26	0	17,19,21	0.43	0
3	NAG	D	2	3	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	E	1	1,3	14,14,15	0.56	0	17,19,21	0.60	0
3	NAG	E	2	3	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	F	1	1,3	14,14,15	0.39	0	17,19,21	0.72	1 (5%)
3	NAG	F	2	3	14,14,15	0.49	0	17,19,21	0.45	0
3	NAG	G	1	1,3	14,14,15	0.46	0	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.25	0	17,19,21	0.50	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
2	NAG	C	1	2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	FUL	C	3	2	1/1/4/5	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	NAG	G	1	1,3	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	O5-C1-C2	-4.08	104.85	111.29
2	C	2	NAG	C4-C3-C2	2.88	115.24	111.02
3	F	1	NAG	C1-O5-C5	2.27	115.27	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	FUL	C1
3	G	1	NAG	C1

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

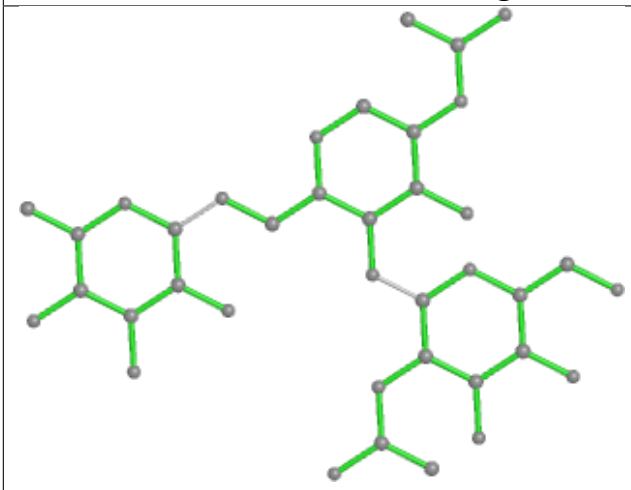
There are no ring outliers.

4 monomers are involved in 15 short contacts:

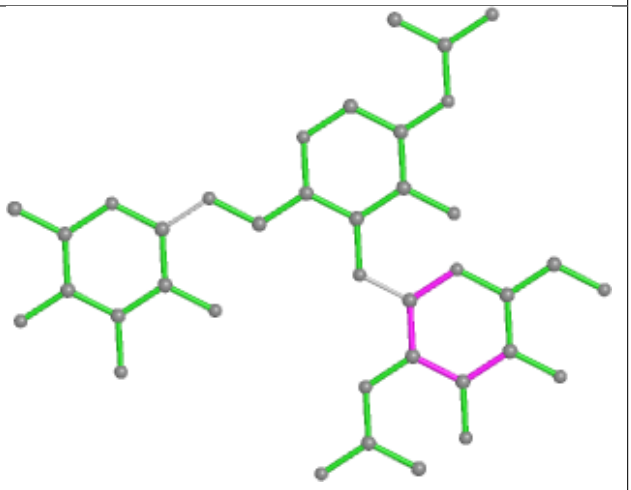
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	6	0
2	C	2	NAG	5	0
3	G	1	NAG	2	0
2	C	1	NAG	7	0

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

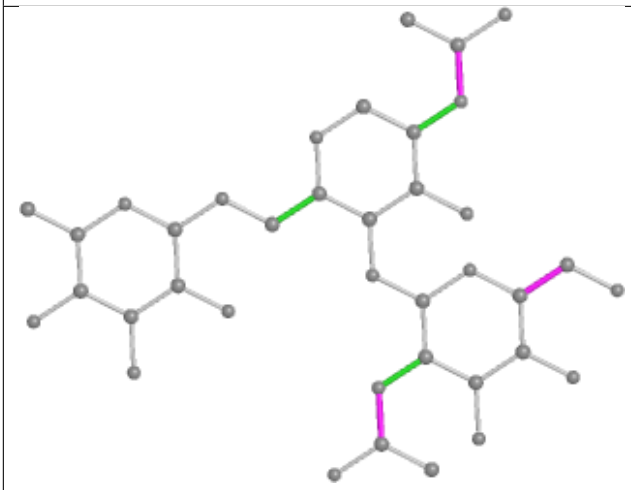
Oligosaccharide Chain C



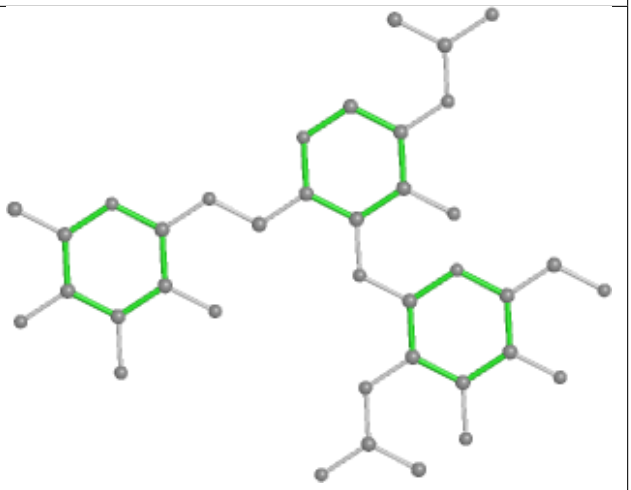
Bond lengths



Bond angles

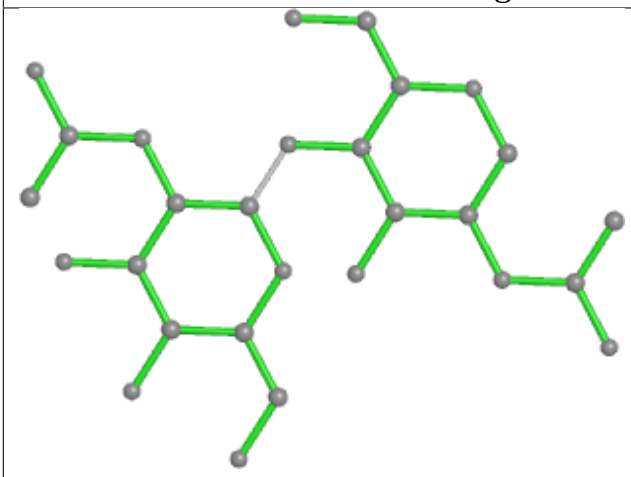


Torsions

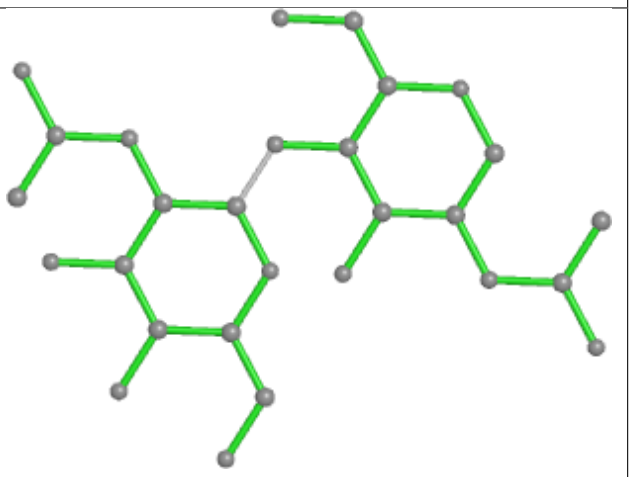


Rings

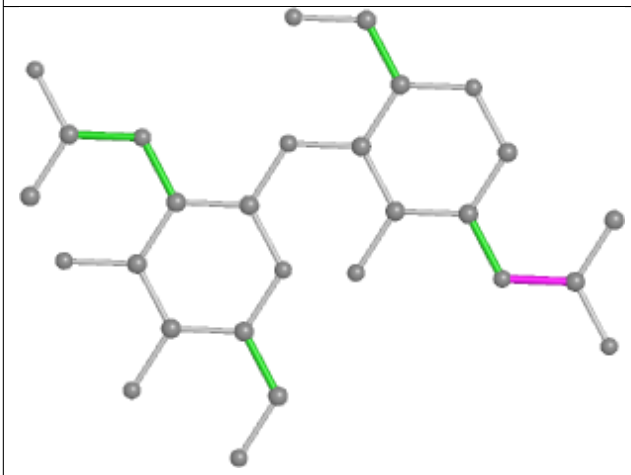
Oligosaccharide Chain D



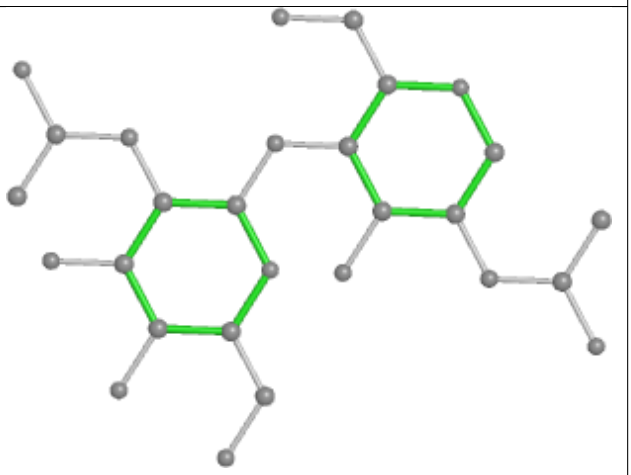
Bond lengths



Bond angles

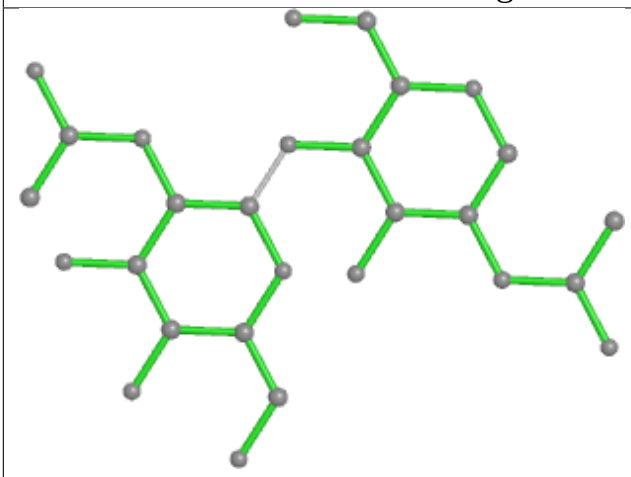


Torsions

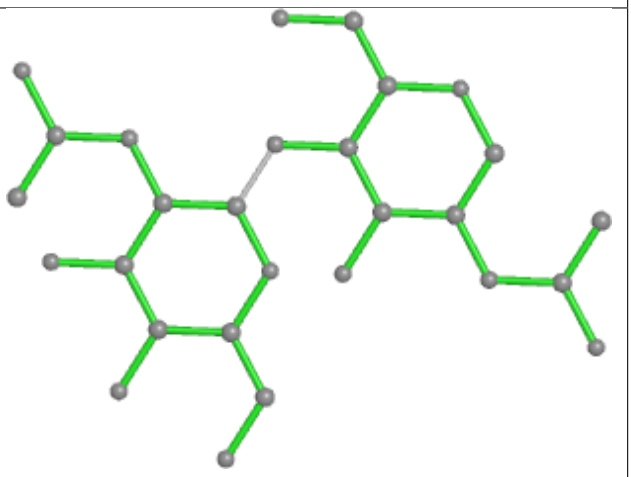


Rings

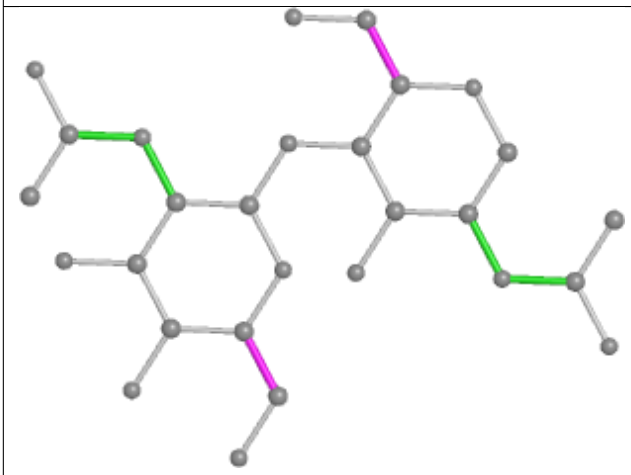
Oligosaccharide Chain E



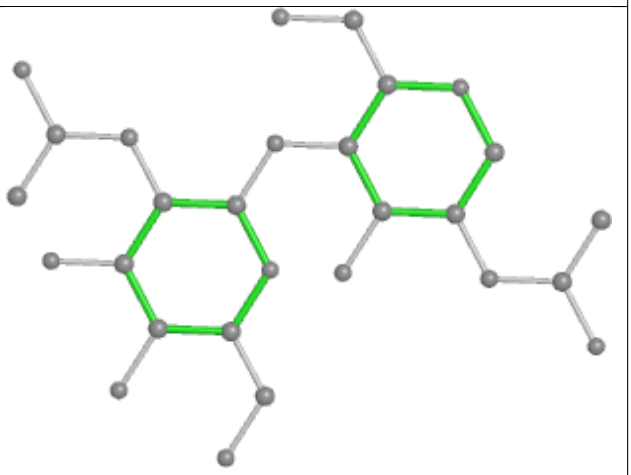
Bond lengths



Bond angles

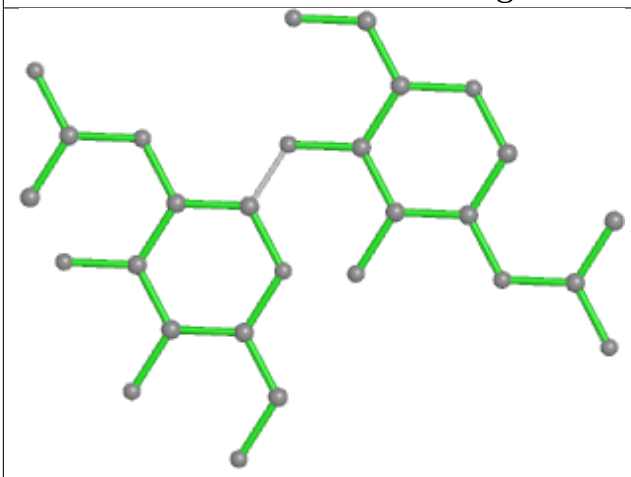


Torsions

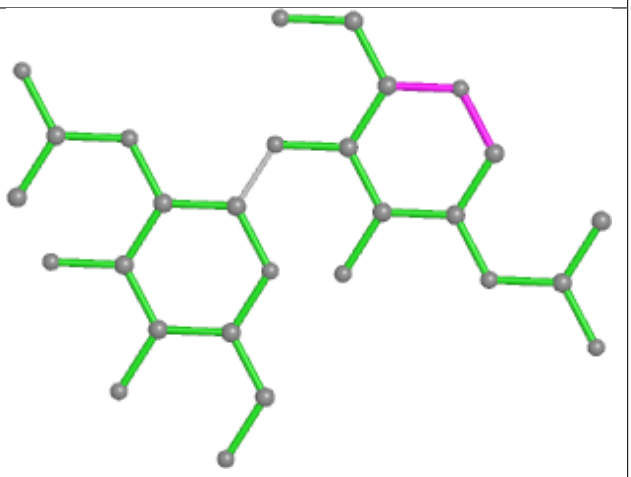


Rings

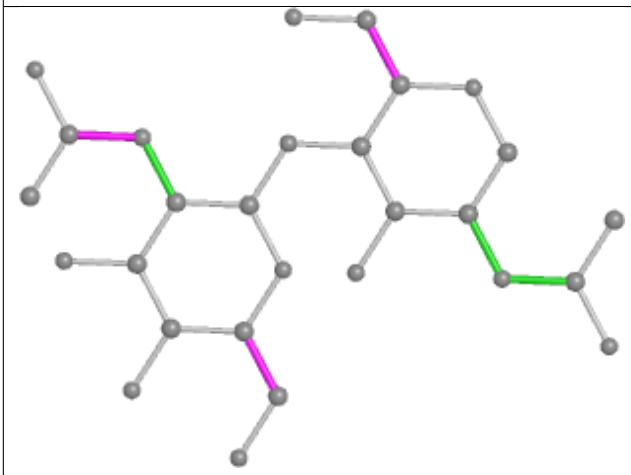
Oligosaccharide Chain F



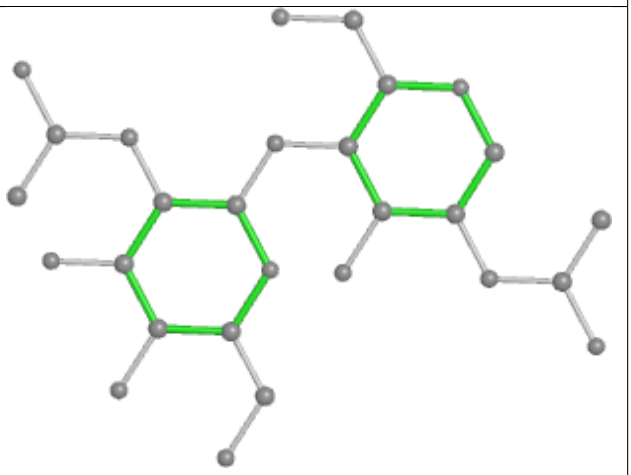
Bond lengths



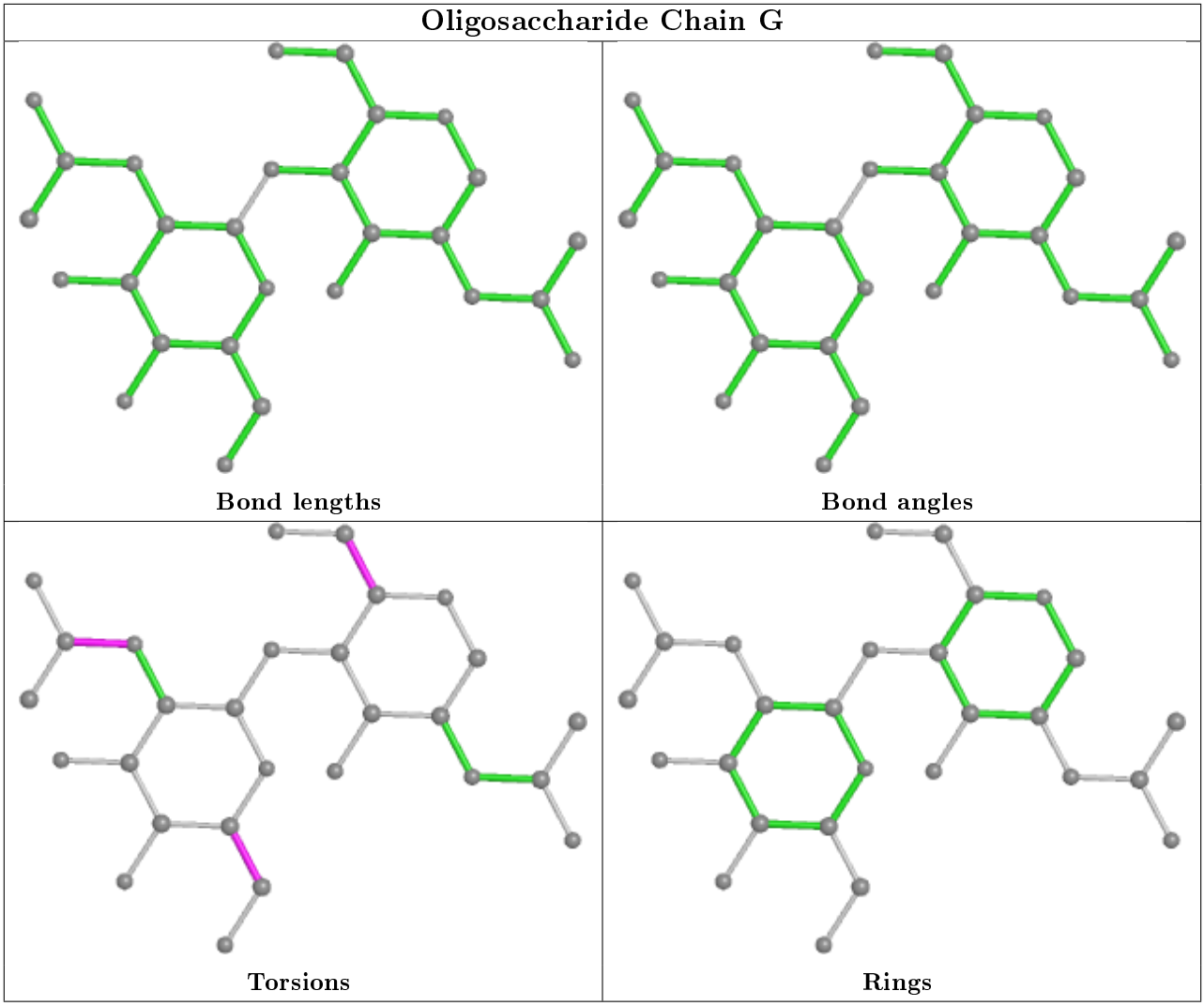
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
7	FUC	A	1012	-	10,10,11	0.50	0	14,14,16	1.25	2 (14%)
9	EDO	B	1013	-	3,3,3	0.56	0	2,2,2	0.36	0
5	NAG	B	1005	-	14,14,15	0.37	0	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	40V	A	1001	-	40,41,41	5.84	28 (70%)	49,58,58	1.94	10 (20%)
5	NAG	B	1009	1	14,14,15	0.28	0	17,19,21	0.61	0
5	NAG	B	1004	-	14,14,15	0.36	0	17,19,21	0.74	0
9	EDO	B	1012	-	3,3,3	0.48	0	2,2,2	0.35	0
6	FUL	A	1017	-	10,10,11	0.30	0	14,14,16	0.62	0
9	EDO	A	1021	-	3,3,3	0.51	0	2,2,2	0.32	0
5	NAG	B	1010	1	14,14,15	0.29	0	17,19,21	0.62	0
6	FUL	A	1010	-	10,10,11	0.30	0	14,14,16	0.63	0
5	NAG	B	1007	1	14,14,15	0.30	0	17,19,21	0.61	0
4	40V	B	1001	-	40,41,41	5.87	28 (70%)	49,58,58	1.87	10 (20%)
5	NAG	B	1003	1	14,14,15	0.29	0	17,19,21	0.62	0
6	FUL	B	1006	-	10,10,11	0.28	0	14,14,16	0.62	0
5	NAG	A	1011	1	14,14,15	0.35	0	17,19,21	0.79	0
5	NAG	B	1002	1	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	B	1008	1	14,14,15	0.36	0	17,19,21	0.74	0
9	EDO	A	1022	-	3,3,3	0.53	0	2,2,2	0.31	0
5	NAG	A	1002	1	14,14,15	0.29	0	17,19,21	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUL	B	1006	-	-	-	0/1/1/1
7	FUC	A	1012	-	-	-	0/1/1/1
9	EDO	B	1013	-	-	1/1/1/1	-
5	NAG	B	1005	-	-	2/6/23/26	0/1/1/1
4	40V	A	1001	-	-	0/22/42/42	0/5/5/5
5	NAG	B	1004	-	-	2/6/23/26	0/1/1/1
9	EDO	B	1012	-	-	0/1/1/1	-
6	FUL	A	1017	-	-	-	0/1/1/1
9	EDO	A	1021	-	-	1/1/1/1	-
5	NAG	B	1010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1011	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	1007	1	-	2/6/23/26	0/1/1/1
4	40V	B	1001	-	-	5/22/42/42	0/5/5/5
5	NAG	B	1003	1	-	1/6/23/26	0/1/1/1
9	EDO	A	1022	-	-	1/1/1/1	-
5	NAG	A	1002	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	B	1002	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1008	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
6	FUL	A	1010	-	-	-	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	40V	C07-C14	15.81	1.52	1.38
4	B	1001	40V	C07-C14	15.80	1.52	1.38
4	B	1001	40V	C10-C15	14.11	1.59	1.39
4	A	1001	40V	C10-C15	13.35	1.58	1.39
4	A	1001	40V	C13-N29	11.44	1.51	1.37
4	B	1001	40V	C13-N29	10.36	1.50	1.37
4	A	1001	40V	C24-N30	-9.66	1.22	1.48
4	B	1001	40V	C24-N30	-9.64	1.22	1.48
4	A	1001	40V	C05-C11	9.29	1.55	1.39
4	B	1001	40V	C05-C11	9.20	1.55	1.39
4	A	1001	40V	C06-C12	7.99	1.53	1.39
4	B	1001	40V	C06-C12	7.91	1.53	1.39
4	B	1001	40V	C02-C06	7.73	1.55	1.38
4	A	1001	40V	C02-C06	7.61	1.54	1.38
4	B	1001	40V	C07-C10	7.38	1.51	1.39
4	B	1001	40V	C12-C11	7.20	1.52	1.39
4	A	1001	40V	C07-C10	7.16	1.51	1.39
4	B	1001	40V	C08-N29	7.04	1.46	1.32
4	A	1001	40V	C12-C11	6.99	1.52	1.39
4	A	1001	40V	C01-C05	6.95	1.53	1.38
4	B	1001	40V	C01-C05	6.88	1.53	1.38
4	A	1001	40V	C08-N29	6.83	1.46	1.32
4	B	1001	40V	C03-C04	6.42	1.51	1.36
4	B	1001	40V	C16-N31	6.30	1.48	1.34
4	A	1001	40V	C03-C04	6.27	1.51	1.36
4	A	1001	40V	C16-N31	6.15	1.48	1.34
4	A	1001	40V	C02-C01	6.10	1.54	1.38
4	B	1001	40V	C02-C01	6.07	1.54	1.38
4	B	1001	40V	C15-C13	5.33	1.51	1.42
4	A	1001	40V	C15-C13	5.33	1.51	1.42
4	A	1001	40V	C03-C08	5.22	1.52	1.37
4	B	1001	40V	C03-C08	5.21	1.52	1.37
4	B	1001	40V	C14-C09	5.19	1.61	1.42
4	A	1001	40V	C14-C09	5.13	1.61	1.42
4	B	1001	40V	C10-C16	4.88	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	40V	C10-C16	4.70	1.57	1.50
4	A	1001	40V	C19-C20	-4.17	1.42	1.53
4	B	1001	40V	C19-C20	-3.80	1.43	1.53
4	A	1001	40V	C09-C13	3.61	1.51	1.42
4	B	1001	40V	C09-C13	3.38	1.50	1.42
4	B	1001	40V	C17-C24	3.25	1.59	1.54
4	A	1001	40V	C17-C24	3.18	1.59	1.54
4	A	1001	40V	C20-C23	-3.13	1.43	1.52
4	B	1001	40V	C20-C23	-3.06	1.43	1.52
4	B	1001	40V	C04-C09	2.99	1.48	1.42
4	B	1001	40V	C18-C24	2.83	1.58	1.54
4	A	1001	40V	C04-C09	2.66	1.47	1.42
4	B	1001	40V	C21-N30	-2.63	1.42	1.47
4	B	1001	40V	C22-N30	-2.56	1.43	1.47
4	A	1001	40V	C18-C24	2.50	1.58	1.54
4	A	1001	40V	O36-C15	2.22	1.43	1.35
4	A	1001	40V	C26-N31	-2.20	1.42	1.47
4	A	1001	40V	C22-N30	-2.20	1.43	1.47
4	B	1001	40V	O36-C15	2.14	1.42	1.35
4	B	1001	40V	C26-N31	-2.05	1.43	1.47
4	A	1001	40V	C21-N30	-2.00	1.43	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	40V	C14-C09-C13	7.03	120.18	116.70
4	B	1001	40V	C14-C09-C13	6.05	119.70	116.70
4	A	1001	40V	C27-N31-C26	5.66	123.14	116.41
4	B	1001	40V	C27-N31-C26	5.37	122.79	116.41
4	B	1001	40V	C21-N30-C22	4.35	112.48	108.19
4	A	1001	40V	C17-C11-C12	-3.34	108.26	110.56
7	A	1012	FUC	C1-C2-C3	3.29	113.71	109.67
4	A	1001	40V	C03-C08-N29	-3.21	119.01	123.94
4	B	1001	40V	C17-C11-C12	-3.11	108.42	110.56
4	A	1001	40V	C21-N30-C22	3.06	111.20	108.19
4	B	1001	40V	C20-C23-C22	3.03	112.10	108.68
4	A	1001	40V	C07-C14-C09	-3.00	118.78	122.80
4	A	1001	40V	C28-C27-N31	-2.91	106.96	113.42
4	B	1001	40V	C28-C27-N31	-2.91	106.97	113.42
4	B	1001	40V	C03-C08-N29	-2.73	119.75	123.94
4	A	1001	40V	C18-C12-C11	-2.71	108.70	110.56
4	A	1001	40V	C20-C23-C22	2.65	111.67	108.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1001	40V	C18-C12-C11	-2.63	108.75	110.56
4	B	1001	40V	C19-C21-N30	-2.56	106.97	111.28
4	B	1001	40V	C07-C14-C09	-2.48	119.47	122.80
7	A	1012	FUC	C3-C4-C5	2.25	113.28	109.77
4	A	1001	40V	C07-C10-C15	2.23	120.77	118.97

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1002	NAG	C1
5	B	1008	NAG	C1
5	A	1011	NAG	C1

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1002	NAG	C8-C7-N2-C2
5	A	1002	NAG	O7-C7-N2-C2
5	B	1005	NAG	C8-C7-N2-C2
5	B	1005	NAG	O7-C7-N2-C2
4	B	1001	40V	C18-C24-N30-C21
5	B	1002	NAG	C8-C7-N2-C2
5	B	1002	NAG	O7-C7-N2-C2
5	B	1007	NAG	O5-C5-C6-O6
5	B	1007	NAG	C4-C5-C6-O6
9	B	1013	EDO	O1-C1-C2-O2
5	B	1010	NAG	O5-C5-C6-O6
4	B	1001	40V	C27-C28-O37-C25
5	A	1002	NAG	C4-C5-C6-O6
4	B	1001	40V	C17-C24-N30-C21
5	B	1004	NAG	C1-C2-N2-C7
5	B	1002	NAG	C1-C2-N2-C7
5	B	1010	NAG	C3-C2-N2-C7
5	B	1002	NAG	C3-C2-N2-C7
5	B	1003	NAG	C3-C2-N2-C7
4	B	1001	40V	C20-C23-C26-N31
4	B	1001	40V	C22-C23-C26-N31
9	A	1022	EDO	O1-C1-C2-O2
9	A	1021	EDO	O1-C1-C2-O2
5	A	1002	NAG	O5-C5-C6-O6
5	B	1004	NAG	C3-C2-N2-C7

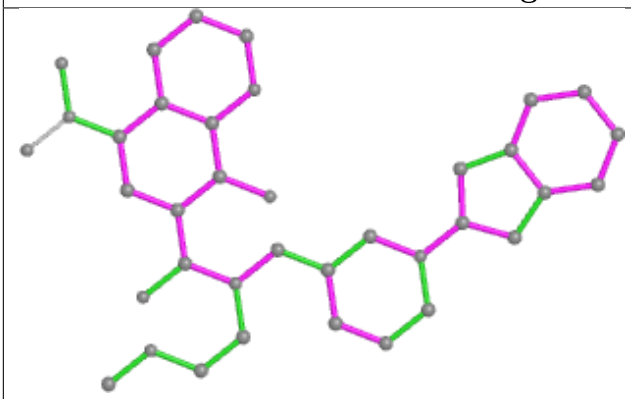
There are no ring outliers.

8 monomers are involved in 25 short contacts:

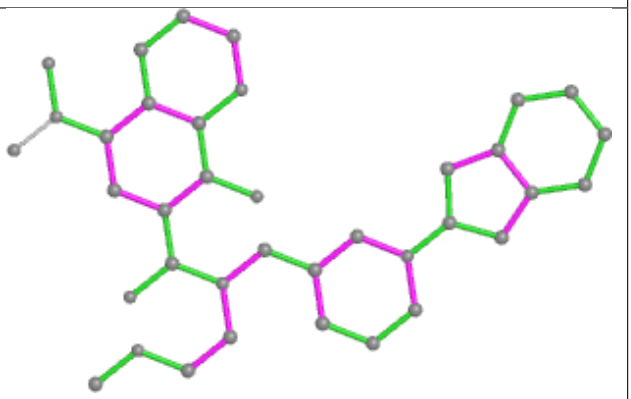
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1012	FUC	3	0
5	B	1005	NAG	4	0
4	A	1001	40V	4	0
5	B	1004	NAG	1	0
6	A	1017	FUL	2	0
6	A	1010	FUL	6	0
4	B	1001	40V	5	0
5	A	1011	NAG	3	0

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.

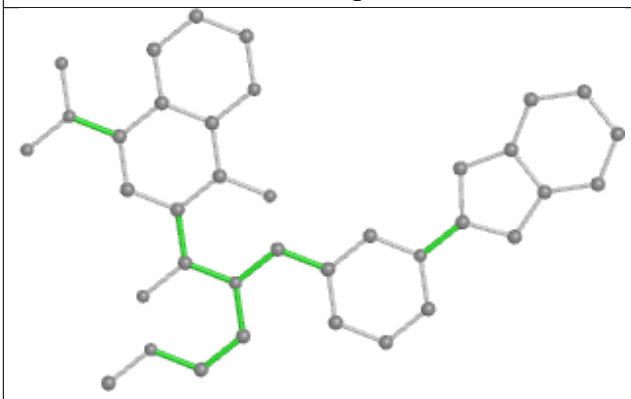
Ligand 40V A 1001



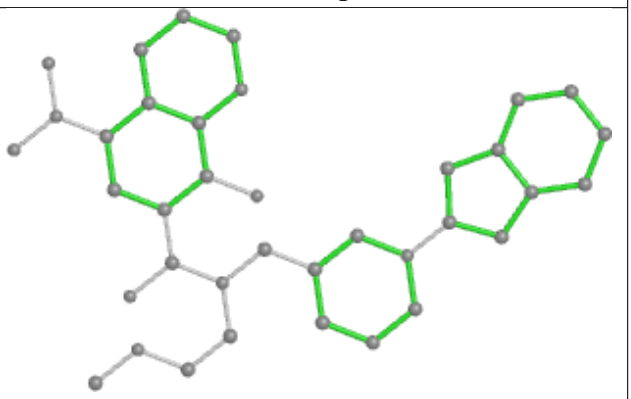
Bond lengths



Bond angles

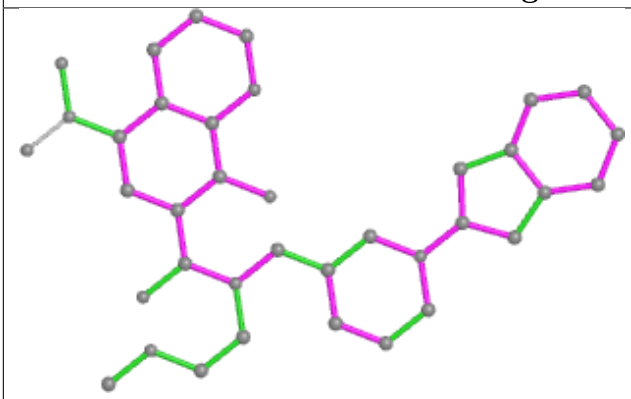


Torsions

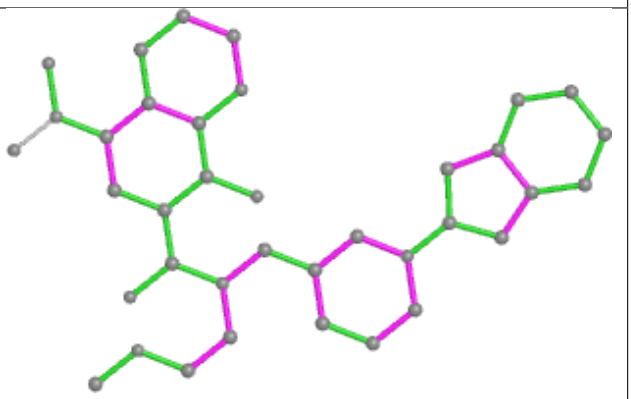


Rings

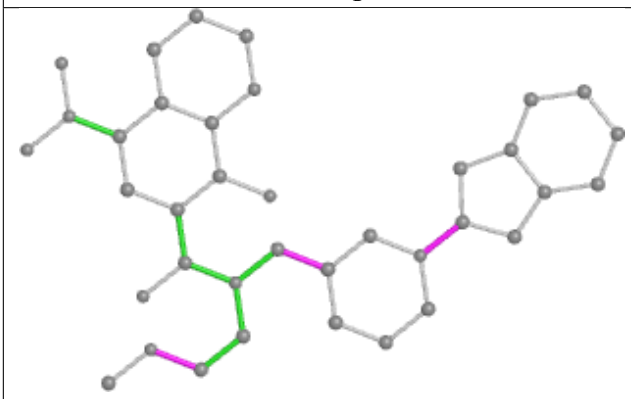
Ligand 40V B 1001



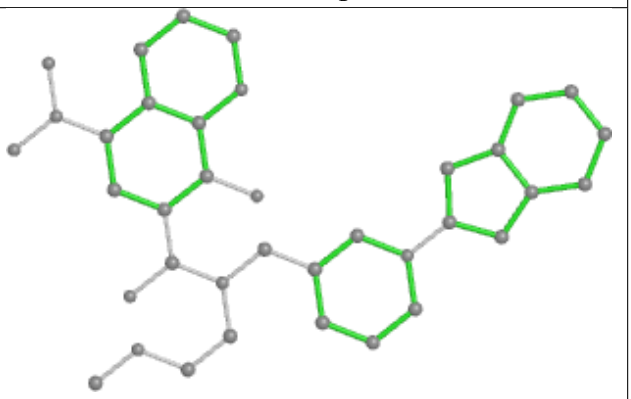
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	528/544 (97%)	-0.04	8 (1%) 73 76	41, 66, 94, 116	0
1	B	525/544 (96%)	0.18	16 (3%) 50 51	51, 73, 102, 125	0
All	All	1053/1088 (96%)	0.07	24 (2%) 60 62	41, 70, 99, 125	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	530	LEU	11.6
1	B	530	LEU	6.0
1	A	529	VAL	5.4
1	B	490	TRP	3.4
1	A	452	ARG	3.2
1	B	28	PHE	3.1
1	B	4	ILE	3.1
1	B	6	ILE	3.1
1	B	185	PHE	3.0
1	B	22	GLY	3.0
1	B	105	LYS	2.8
1	B	12	LYS	2.8
1	B	5	ILE	2.8
1	B	53	SER	2.5
1	B	50	THR	2.5
1	A	266	ASN	2.5
1	B	529	VAL	2.4
1	B	26	THR	2.4
1	B	99	ILE	2.3
1	B	364[A]	PHE	2.2
1	A	199	ALA	2.1
1	A	336	GLY	2.1
1	A	198	SER	2.0
1	A	364[A]	PHE	2.0

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

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

6.3 Carbohydrates (i)

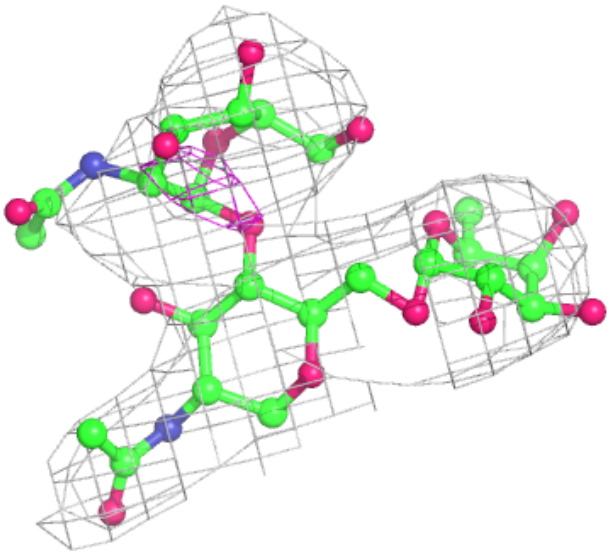
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

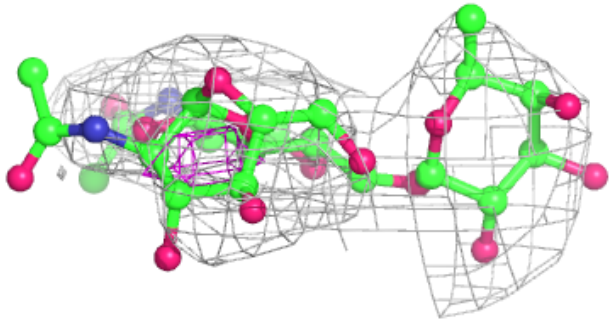
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.77	0.31	126,140,147,147	0
3	NAG	E	2	14/15	0.77	0.37	136,147,154,158	0
2	NAG	C	1	14/15	0.79	0.17	101,112,135,135	0
3	NAG	G	2	14/15	0.79	0.35	138,144,150,152	0
3	NAG	F	2	14/15	0.80	0.22	78,92,103,104	0
3	NAG	G	1	14/15	0.83	0.18	109,124,136,145	0
2	FUL	C	3	10/11	0.84	0.25	99,115,118,121	0
3	NAG	E	1	14/15	0.86	0.17	118,122,136,147	0
3	NAG	D	2	14/15	0.86	0.21	93,110,116,118	0
3	NAG	D	1	14/15	0.92	0.19	77,88,99,101	0
3	NAG	F	1	14/15	0.94	0.13	78,86,90,94	0

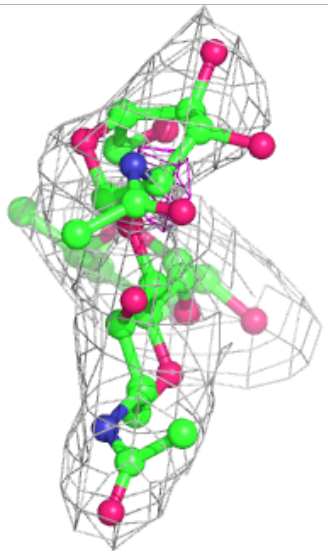
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

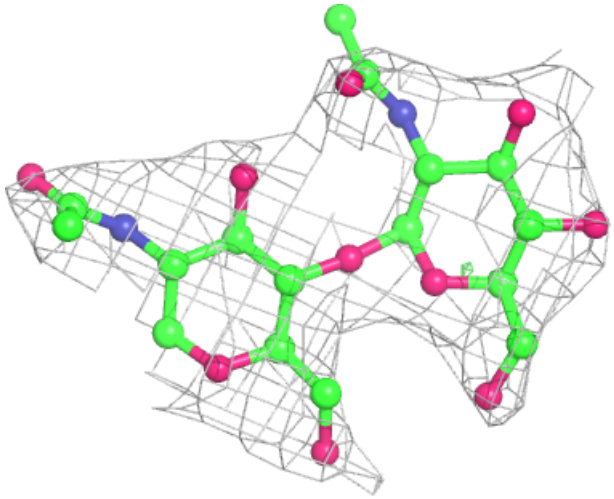


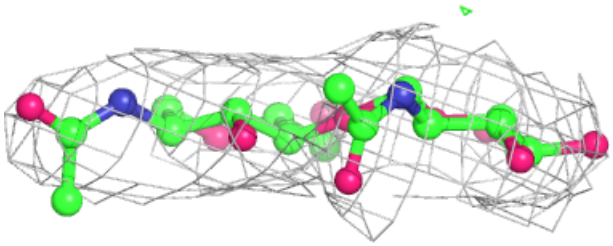


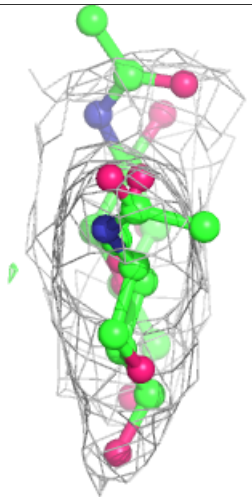


Electron density around Chain D:

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

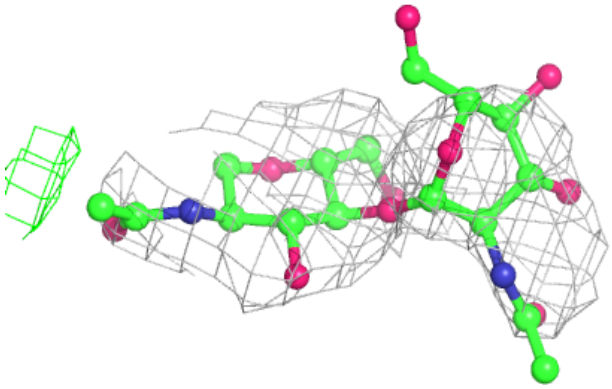


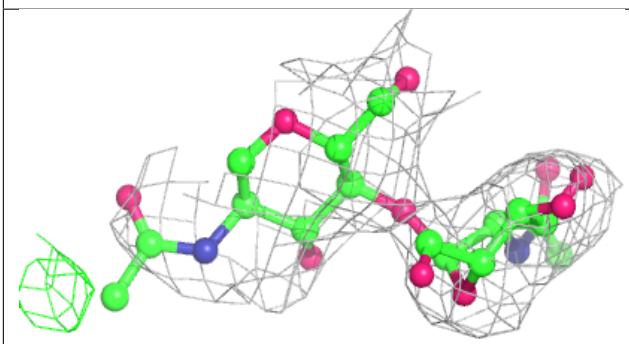


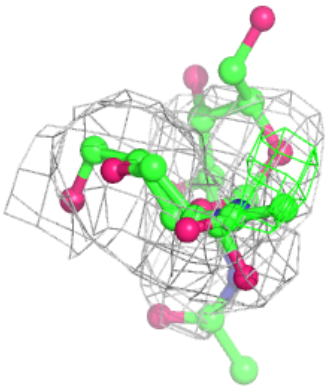


Electron density around Chain E:

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

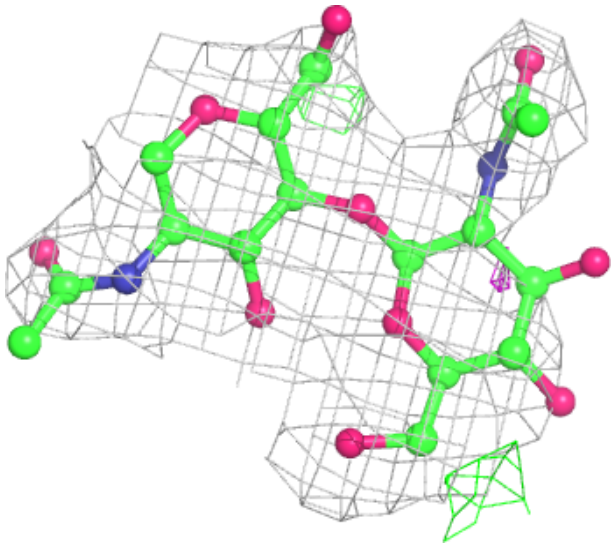


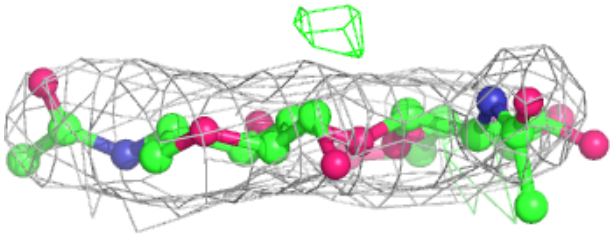


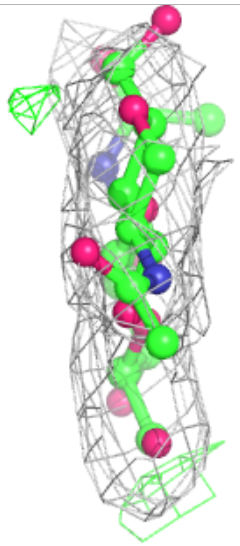


Electron density around Chain F:

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

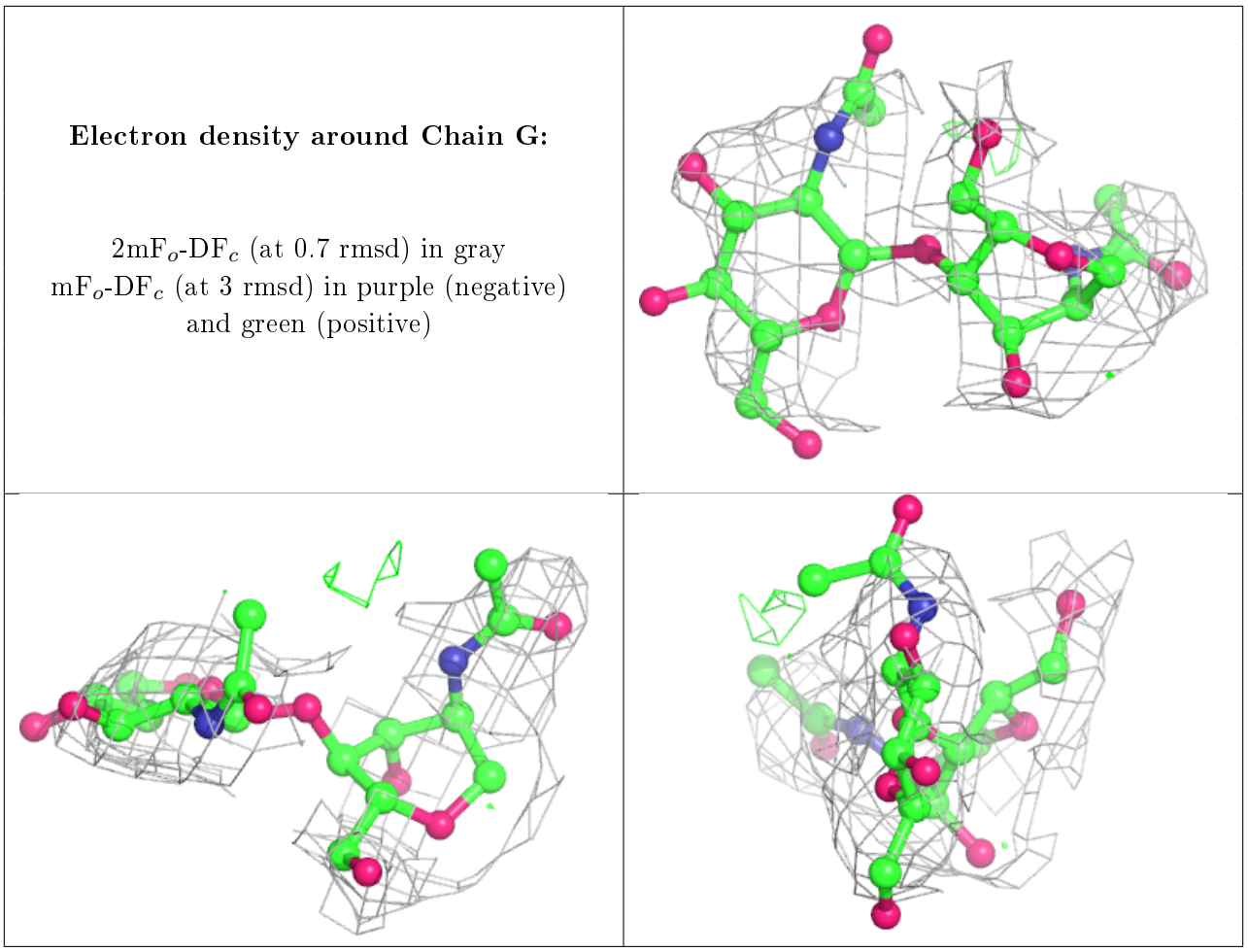






Electron density around Chain G:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	1002	14/15	0.66	0.20	118,129,138,142	0
5	NAG	B	1007	14/15	0.68	0.28	112,128,131,136	0
5	NAG	B	1003	14/15	0.70	0.25	98,112,118,129	0
8	CL	A	1020	1/1	0.73	0.30	102,102,102,102	0
7	FUC	A	1012	10/11	0.79	0.52	122,128,135,136	0
5	NAG	B	1010	14/15	0.79	0.22	108,121,128,128	0
5	NAG	A	1011	14/15	0.80	0.21	97,104,115,116	0
9	EDO	A	1021	4/4	0.81	0.20	84,85,89,91	0
5	NAG	B	1005	14/15	0.82	0.24	105,112,122,124	0
5	NAG	B	1009	14/15	0.84	0.24	109,117,122,123	0
6	FUL	A	1017	10/11	0.86	0.32	91,104,116,119	0

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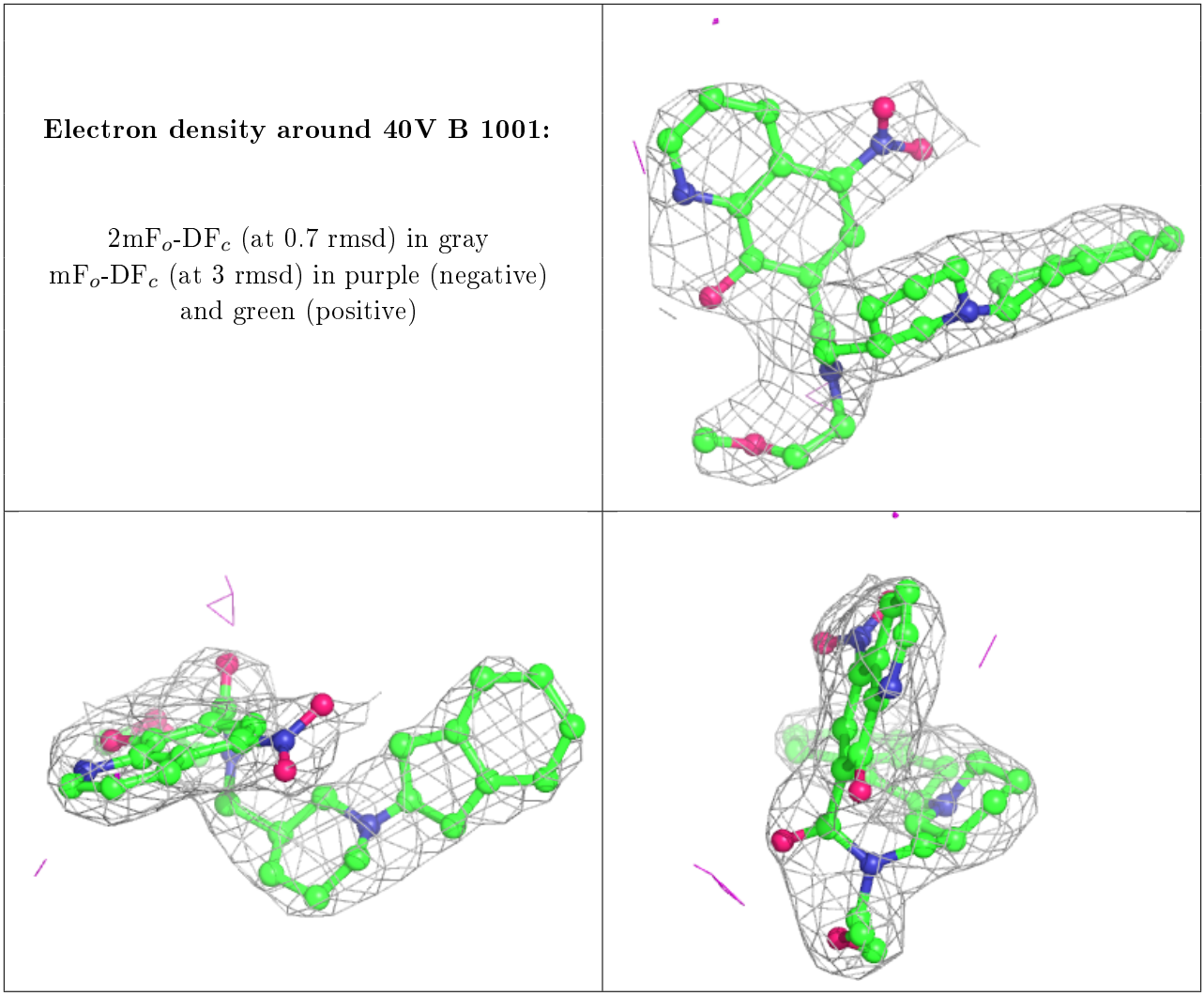
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	1004	14/15	0.87	0.31	107,113,118,121	0
6	FUL	B	1006	10/11	0.89	0.55	96,106,112,116	0
8	CL	A	1018	1/1	0.89	0.57	99,99,99,99	0
8	CL	A	1019	1/1	0.90	0.11	80,80,80,80	0
5	NAG	B	1008	14/15	0.90	0.18	89,97,103,108	0
8	CL	B	1011	1/1	0.90	0.13	76,76,76,76	0
9	EDO	A	1022	4/4	0.90	0.09	59,70,77,79	0
6	FUL	A	1010	10/11	0.91	0.24	91,111,114,114	0
5	NAG	A	1002	14/15	0.93	0.20	90,103,112,113	0
9	EDO	B	1013	4/4	0.94	0.30	51,56,66,66	0
4	40V	B	1001	37/37	0.94	0.22	53,64,74,83	0
4	40V	A	1001	37/37	0.94	0.25	51,64,79,86	0
9	EDO	B	1012	4/4	0.95	0.10	62,71,79,81	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.

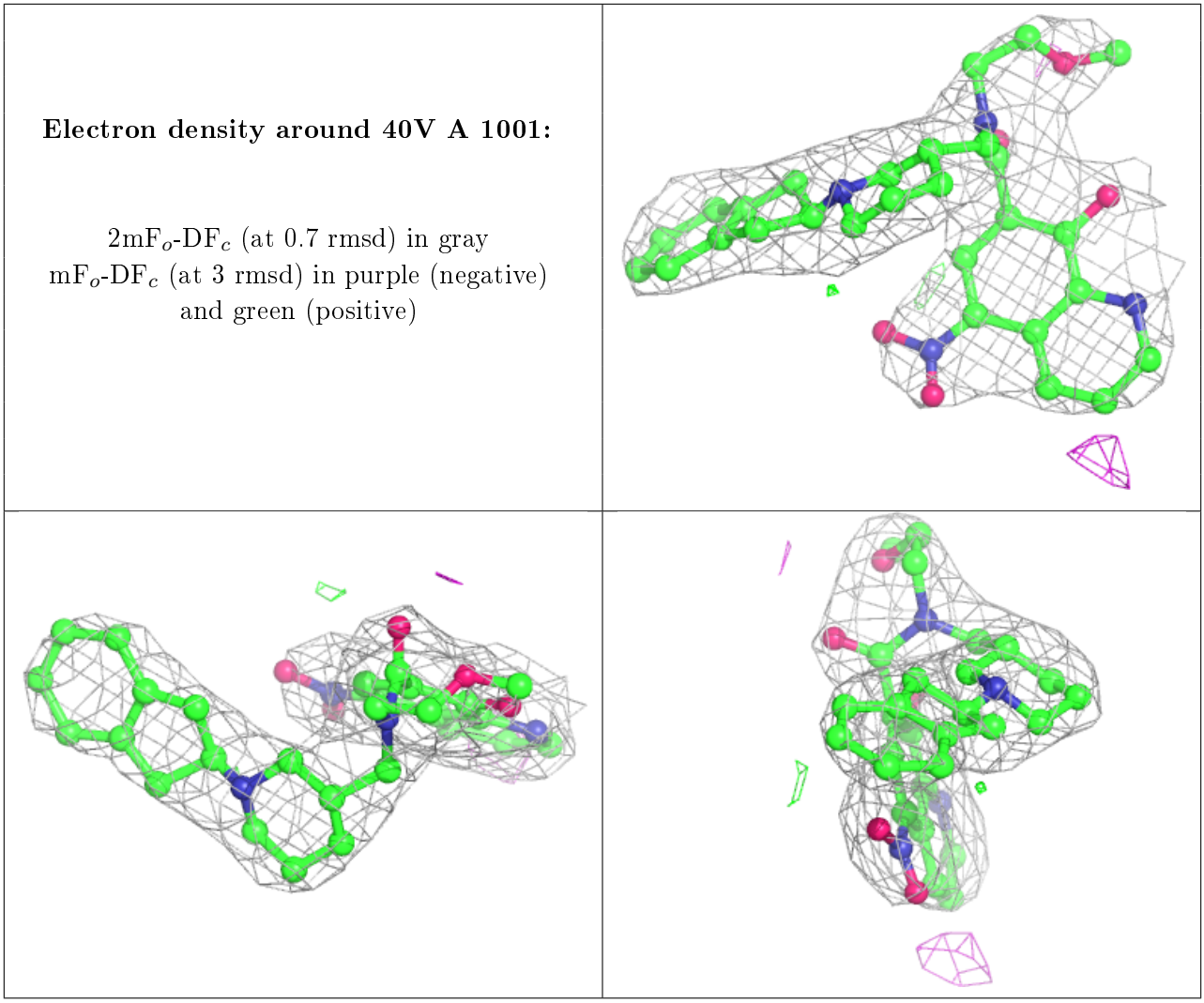
Electron density around 40V B 1001:

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



Electron density around 40V A 1001:

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



6.5 Other polymers

There are no such residues in this entry.