Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 06:35 am GMT

PDB ID	:	6HFY
Title	:	Influenza A virus N6 neuraminidase complex with DANA (Duck/England/56).
Authors	:	Salinger, M.T.; Hobbs, J.R.; Murray, J.W.; Laver, W.G.; Kuhn, P.; Garman, E.F.
Deposited on	:	2018-08-22
Resolution	:	1.65 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 ⓘ 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 ⓘ) were used in the production of this report:

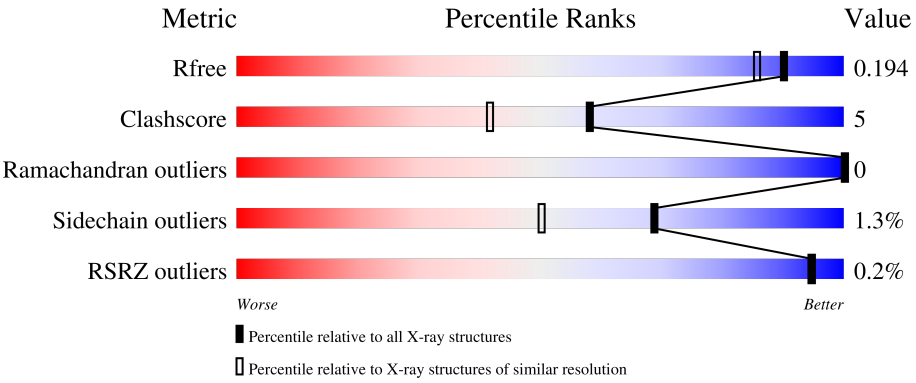
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	389	89% 10% •
1	B	389	91% 9%
1	C	389	92% 7%
1	D	389	89% 10% •
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	G	2	100%
3	F	7	100%
4	H	6	83% 17%
4	I	6	67% 33%
4	J	6	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
2	NAG	E	2	-	-	-	X
5	NAG	B	501	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14206 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.

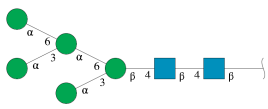
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	8	0
			3072	1912	547	585	28			
1	B	389	Total	C	N	O	S	0	12	0
			3110	1938	555	590	27			
1	C	389	Total	C	N	O	S	0	8	0
			3072	1911	545	589	27			
1	D	389	Total	C	N	O	S	0	8	0
			3082	1919	546	589	28			

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

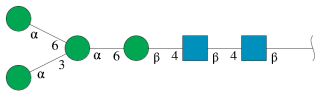
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



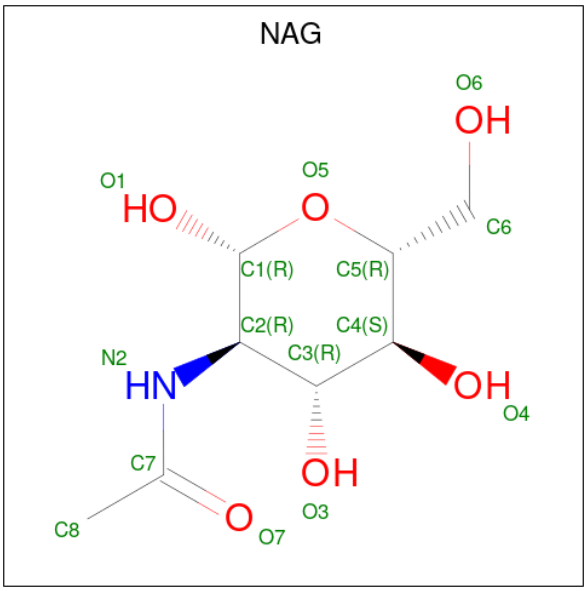
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	7	Total C N O 83 46 2 35	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	6	Total C N O 72 40 2 30	0	0	0
4	I	6	Total C N O 72 40 2 30	0	0	0
4	J	6	Total C N O 72 40 2 30	0	0	0

- 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	B	1	Total C N O 14 8 1 5	0	0

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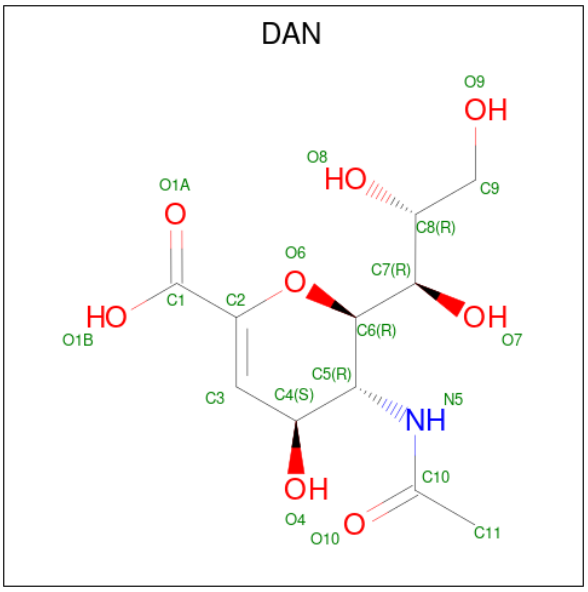
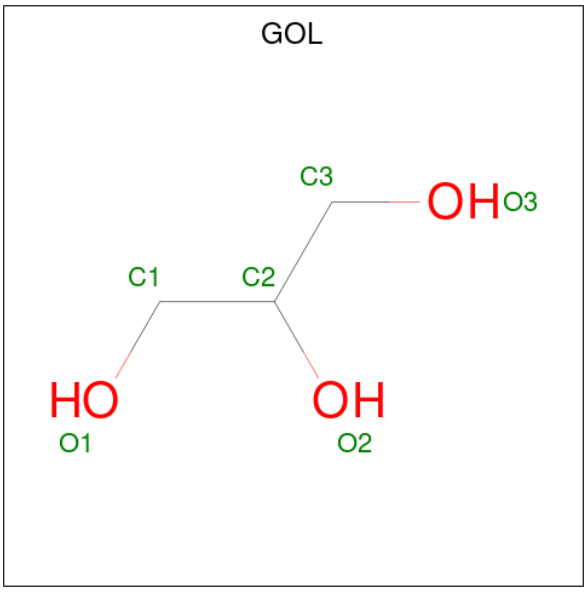
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (three-letter code: DAN) (formula: $C_{11}H_{17}NO_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	11	1	8		
6	B	1	Total	C	N	O	0	0
			20	11	1	8		
6	C	1	Total	C	N	O	0	0
			20	11	1	8		
6	D	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0
8	B	2	Total Ca 2 2	0	0
8	C	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Ca 1 1	0	0

- Molecule 9 is water.

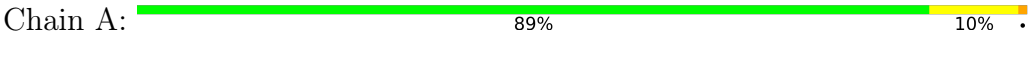
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	335	Total O 335 335	0	0
9	B	327	Total O 327 327	0	0
9	C	322	Total O 322 322	0	0
9	D	322	Total O 322 322	0	0

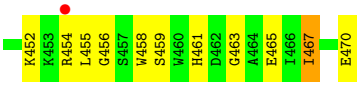
3 Residue-property plots (i)

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: Neuraminidase

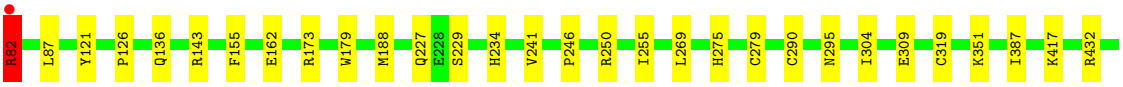
Chain A:

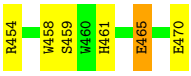




• Molecule 1: Neuraminidase

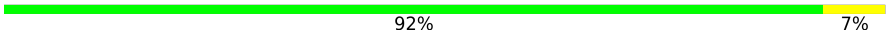
Chain B:





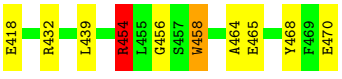
• Molecule 1: Neuraminidase

Chain C:



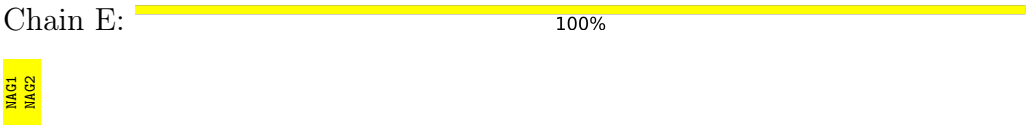
• Molecule 1: Neuraminidase

Chain D:



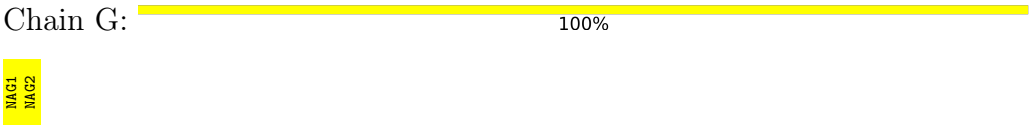
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



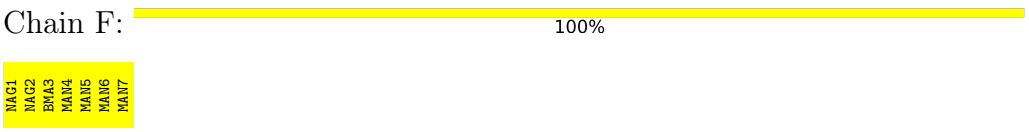
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



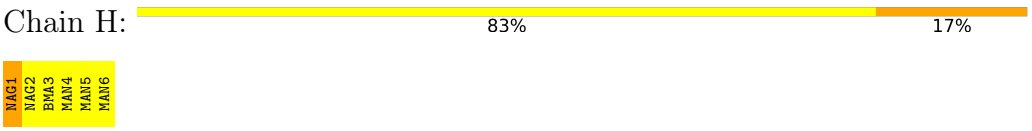
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain H:

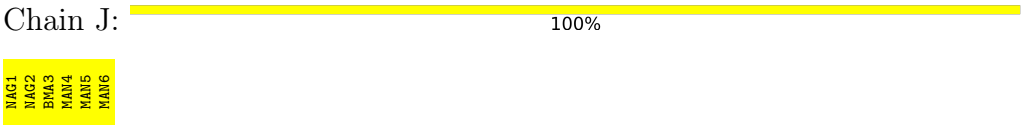


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.00Å 75.76Å 105.98Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	20.05 – 1.65 20.04 – 1.65	Depositor EDS
% Data completeness (in resolution range)	91.2 (20.05-1.65) 91.3 (20.04-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.156 , 0.185 0.167 , 0.194	Depositor DCC
R_{free} test set	9170 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	12.8	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -l,k,h 0.010 for -h,-k,l 0.010 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14206	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: BMA, NAG, GOL, CA, MAN, DAN

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	0.84	1/3147 (0.0%)	0.91	1/4267 (0.0%)
1	B	0.82	3/3186 (0.1%)	0.89	3/4318 (0.1%)
1	C	0.85	0/3147	0.89	1/4269 (0.0%)
1	D	0.88	5/3157 (0.2%)	0.94	6/4280 (0.1%)
All	All	0.85	9/12637 (0.1%)	0.91	11/17134 (0.1%)

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	2
1	B	0	3
1	C	0	3
1	D	0	2
All	All	0	10

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	465	GLU	CD-OE1	7.07	1.33	1.25
1	D	470	GLU	CD-OE2	-6.68	1.18	1.25
1	D	162	GLU	CD-OE1	6.60	1.32	1.25
1	D	418[A]	GLU	CD-OE2	6.56	1.32	1.25
1	D	418[B]	GLU	CD-OE2	6.56	1.32	1.25
1	D	230	GLU	CD-OE1	5.96	1.32	1.25
1	B	470	GLU	CD-OE2	-5.57	1.19	1.25
1	B	470	GLU	CD-OE1	-5.57	1.19	1.25
1	A	470	GLU	CD-OE1	-5.29	1.19	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	250	ARG	NE-CZ-NH1	11.73	126.16	120.30
1	D	250	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	190	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	D	432	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	D	301	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	B	250	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	B	173	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	225	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	C	143	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	211	ARG	CD-NE-CZ	5.21	130.89	123.60
1	B	143	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250[A]	ARG	Sidechain
1	A	454	ARG	Sidechain
1	B	432	ARG	Sidechain
1	B	454	ARG	Sidechain
1	B	82	ARG	Sidechain
1	C	250	ARG	Sidechain
1	C	454	ARG	Sidechain
1	C	82	ARG	Sidechain
1	D	454	ARG	Sidechain
1	D	82	ARG	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	3072	0	2944	37	0
1	B	3110	0	2987	29	0
1	C	3072	0	2937	32	0
1	D	3082	0	2953	35	0
2	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	28	0	25	0	0
3	F	83	0	70	0	0
4	H	72	0	61	2	0
4	I	72	0	61	2	0
4	J	72	0	61	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	28	0	26	0	0
5	D	14	0	13	0	0
6	A	20	0	16	0	0
6	B	20	0	16	0	0
6	C	20	0	16	0	0
6	D	20	0	16	0	0
7	A	12	0	16	1	0
7	B	18	0	24	3	0
7	C	12	0	16	1	0
7	D	12	0	16	2	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	335	0	0	6	0
9	B	327	0	0	1	0
9	C	322	0	0	3	0
9	D	322	0	0	5	0
All	All	14206	0	12325	122	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 (122) 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:C:465[A]:GLU:HG3	1:C:467:ILE:HG22	1.45	0.96
1:B:82:ARG:HH21	1:B:82:ARG:HB2	1.29	0.94
1:C:465[A]:GLU:CG	1:C:467:ILE:HG22	1.97	0.93
1:D:87:LEU:H	1:D:234:HIS:HD2	1.20	0.90
1:A:144:HIS:HE1	1:C:465[A]:GLU:H	1.21	0.88
1:C:87:LEU:H	1:C:234:HIS:HD2	1.16	0.87
1:B:465:GLU:H	1:D:144:HIS:HE1	1.23	0.86
1:C:144:HIS:HE1	1:D:465[A]:GLU:H	1.17	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:H	1:B:234:HIS:HD2	1.21	0.85
1:A:144:HIS:HE1	1:C:465[B]:GLU:H	1.22	0.84
1:B:227:GLN:HE21	1:B:241:VAL:H	1.29	0.80
1:B:82:ARG:HH21	1:B:82:ARG:CB	1.96	0.79
1:C:144:HIS:HE1	1:D:465[B]:GLU:H	1.30	0.79
1:A:87:LEU:H	1:A:234:HIS:HD2	1.30	0.77
1:D:87:LEU:H	1:D:234:HIS:CD2	2.03	0.76
1:C:227:GLN:HE21	1:C:241:VAL:H	1.33	0.76
1:D:227:GLN:HE21	1:D:241:VAL:H	1.31	0.76
1:A:227:GLN:HE21	1:A:241:VAL:H	1.33	0.75
1:D:275:HIS:HD2	1:D:295:ASN:H	1.33	0.73
1:B:87:LEU:H	1:B:234:HIS:CD2	2.07	0.73
1:C:87:LEU:H	1:C:234:HIS:CD2	2.03	0.72
1:B:234:HIS:HE1	1:B:309:GLU:OE2	1.75	0.70
1:B:188:MET:O	7:B:512:GOL:H12	1.94	0.68
1:D:336:ASN:ND2	1:D:338:ASP:H	1.92	0.67
1:C:144:HIS:CE1	1:D:465[A]:GLU:H	2.08	0.66
1:D:336:ASN:HD22	1:D:338:ASP:H	1.42	0.66
1:A:234:HIS:HE1	1:A:309:GLU:OE2	1.79	0.65
1:A:459:SER:OG	1:A:461:HIS:HD2	1.79	0.64
1:C:275:HIS:HD2	1:C:295:ASN:H	1.43	0.64
1:A:87:LEU:H	1:A:234:HIS:CD2	2.13	0.63
1:A:144:HIS:CE1	1:C:465[B]:GLU:H	2.12	0.63
1:D:234:HIS:HE1	1:D:309:GLU:OE1	1.82	0.63
7:D:510:GOL:H31	9:D:884:HOH:O	1.98	0.62
1:B:82:ARG:HH21	1:B:82:ARG:CG	2.12	0.62
1:B:275:HIS:HD2	1:B:295:ASN:H	1.47	0.62
1:A:465[A]:GLU:OE2	1:A:467[A]:ILE:HD13	1.99	0.61
1:C:459:SER:OG	1:C:461:HIS:HD2	1.83	0.61
1:B:269:LEU:HD23	7:B:513:GOL:H31	1.82	0.61
1:A:219:TRP:CD2	1:A:254:LYS:HE3	2.35	0.61
1:A:275:HIS:HD2	1:A:295:ASN:H	1.48	0.60
1:D:262:LYS:HE2	9:D:774:HOH:O	2.04	0.58
1:C:125:ASP:HB2	1:C:126:PRO:CD	2.34	0.57
1:B:459:SER:OG	1:B:461:HIS:HD2	1.87	0.57
1:A:336:ASN:HD22	1:A:338:ASP:H	1.51	0.57
1:C:254[B]:LYS:NZ	1:C:268[B]:GLU:OE2	2.38	0.56
1:B:82:ARG:HB2	1:B:82:ARG:NH2	2.12	0.56
1:A:461:HIS:H	1:A:461:HIS:CD2	2.24	0.55
1:D:310[B]:MET:HA	1:D:310[B]:MET:HE2	1.86	0.55
1:A:461:HIS:HE1	9:A:905:HOH:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ASP:HB2	1:C:126:PRO:HD2	1.89	0.54
1:A:111:ASP:O	7:A:513:GOL:H32	2.07	0.54
1:A:144:HIS:CE1	1:C:465[A]:GLU:H	2.12	0.53
1:A:165:GLN:NE2	9:A:606:HOH:O	2.41	0.53
1:B:465:GLU:H	1:D:144:HIS:CE1	2.14	0.53
1:A:275:HIS:CD2	1:A:295:ASN:H	2.28	0.52
1:A:417:LYS:HE3	9:A:914:HOH:O	2.10	0.51
1:A:310[B]:MET:HE2	9:A:680:HOH:O	2.11	0.51
1:C:234:HIS:HE1	1:C:309:GLU:OE1	1.92	0.51
1:B:82:ARG:CG	1:B:82:ARG:NH2	2.70	0.51
1:A:455:LEU:O	4:H:1:NAG:H62	2.12	0.50
1:B:417:LYS:HE3	9:B:906:HOH:O	2.12	0.50
1:C:144:HIS:HD2	9:D:729:HOH:O	1.95	0.50
1:B:82:ARG:NH2	1:B:82:ARG:HG3	2.26	0.50
1:D:275:HIS:CD2	1:D:295:ASN:H	2.21	0.50
1:A:87:LEU:N	1:A:234:HIS:HD2	2.05	0.50
1:D:336:ASN:HD22	1:D:337:CYS:N	2.10	0.50
1:C:82:ARG:HD3	1:C:187:GLY:O	2.11	0.49
1:A:456:GLY:HA2	4:H:1:NAG:O5	2.13	0.49
1:B:121:TYR:CG	1:B:229:SER:HA	2.48	0.49
1:C:273:ALA:O	7:C:511:GOL:H2	2.14	0.48
1:C:461:HIS:H	1:C:461:HIS:CD2	2.30	0.48
1:D:411:ILE:HB	1:D:413:TYR:CZ	2.48	0.48
1:B:275:HIS:CD2	1:B:295:ASN:H	2.31	0.48
1:C:275:HIS:CD2	1:C:295:ASN:H	2.28	0.48
1:A:93:GLU:HB3	1:A:452:LYS:HD3	1.96	0.48
1:A:411:ILE:HB	1:A:413:TYR:CZ	2.49	0.48
1:B:126:PRO:HD2	7:B:512:GOL:O2	2.14	0.48
1:A:279:CYS:HB3	1:A:290:CYS:HB3	1.96	0.47
1:A:250[B]:ARG:CZ	9:A:652:HOH:O	2.63	0.46
1:D:309:GLU:C	1:D:310[B]:MET:HE3	2.37	0.46
1:C:189:SER:HB2	1:C:208:TYR:CZ	2.50	0.46
1:C:144:HIS:CE1	1:D:464:ALA:HA	2.52	0.45
1:D:310[B]:MET:HA	1:D:310[B]:MET:CE	2.46	0.45
1:B:461:HIS:H	1:B:461:HIS:CD2	2.33	0.45
1:A:144:HIS:HD2	9:C:725:HOH:O	2.00	0.45
1:B:162[B]:GLU:OE2	1:D:173:ARG:HG3	2.17	0.45
1:C:121:TYR:CG	1:C:229:SER:HA	2.52	0.45
1:D:121:TYR:CG	1:D:229:SER:HA	2.52	0.45
1:D:456:GLY:HA2	4:I:1:NAG:O5	2.17	0.44
1:A:336:ASN:ND2	1:A:338:ASP:H	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465[A]:GLU:CD	1:C:467:ILE:HG22	2.37	0.44
1:A:219:TRP:CG	1:A:254:LYS:HE3	2.52	0.44
1:C:241:VAL:HG22	1:C:255:ILE:HD12	1.98	0.44
1:D:417[B]:LYS:HE3	9:D:742:HOH:O	2.17	0.44
1:C:268[B]:GLU:OE1	9:C:601:HOH:O	2.21	0.44
1:B:319:CYS:O	1:B:387:ILE:HA	2.18	0.44
1:B:279:CYS:HB3	1:B:290:CYS:HB3	1.99	0.43
1:D:125:ASP:HB2	1:D:126:PRO:CD	2.48	0.43
1:D:318:LEU:HD23	1:D:318:LEU:HA	1.89	0.43
7:D:510:GOL:C3	9:D:884:HOH:O	2.62	0.42
1:A:319:CYS:O	1:A:335:GLY:HA3	2.19	0.42
1:D:82:ARG:HD3	1:D:187:GLY:O	2.19	0.42
1:D:310[B]:MET:HE3	1:D:310[B]:MET:N	2.35	0.42
1:D:369:LYS:HB3	1:D:369:LYS:HE2	1.96	0.42
1:A:124:CYS:HA	1:A:129:CYS:HA	2.02	0.41
1:C:198:PRO:HD3	1:D:458:TRP:HB3	2.02	0.41
1:D:465[B]:GLU:HB2	1:D:468:TYR:CD2	2.54	0.41
1:B:82:ARG:HH21	1:B:82:ARG:HG3	1.84	0.41
1:B:255[B]:ILE:HD11	1:B:304:ILE:HG21	2.02	0.41
1:A:125:ASP:HB2	1:A:126:PRO:CD	2.51	0.41
1:B:229:SER:HB3	1:B:351:LYS:HE2	2.00	0.41
1:A:463:GLY:HA3	1:B:155:PHE:CE1	2.56	0.41
1:D:454:ARG:HH22	4:I:2:NAG:H81	1.86	0.41
1:A:417:LYS:CE	9:A:914:HOH:O	2.67	0.41
1:C:333[B]:THR:HG22	9:C:830:HOH:O	2.21	0.41
1:D:82:ARG:NH2	1:D:127:GLN:OE1	2.53	0.41
1:B:246:PRO:O	1:B:275:HIS:HE1	2.04	0.41
1:A:121:TYR:CG	1:A:229:SER:HA	2.56	0.40
1:C:254[B]:LYS:NZ	1:C:268[B]:GLU:CD	2.75	0.40
1:D:336:ASN:HD22	1:D:336:ASN:C	2.24	0.40
1:A:219:TRP:CE2	1:A:254:LYS:HE3	2.57	0.40
1:D:310[B]:MET:CE	1:D:310[B]:MET:CA	3.00	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	395/389 (102%)	380 (96%)	15 (4%)	0	100	100
1	B	399/389 (103%)	384 (96%)	15 (4%)	0	100	100
1	C	395/389 (102%)	384 (97%)	11 (3%)	0	100	100
1	D	396/389 (102%)	382 (96%)	14 (4%)	0	100	100
All	All	1585/1556 (102%)	1530 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	339/331 (102%)	334 (98%)	5 (2%)	65	44
1	B	343/331 (104%)	339 (99%)	4 (1%)	71	53
1	C	339/331 (102%)	338 (100%)	1 (0%)	92	88
1	D	340/331 (103%)	332 (98%)	8 (2%)	49	23
All	All	1361/1324 (103%)	1343 (99%)	18 (1%)	69	50

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	ILE
1	A	336	ASN
1	A	458	TRP
1	A	467[A]	ILE
1	A	467[B]	ILE
1	B	82	ARG
1	B	136	GLN
1	B	179	TRP

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Mol	Chain	Res	Type
1	B	458	TRP
1	C	458	TRP
1	D	179	TRP
1	D	262	LYS
1	D	302	PRO
1	D	336	ASN
1	D	369	LYS
1	D	439	LEU
1	D	454	ARG
1	D	458	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	227	GLN
1	A	234	HIS
1	A	275	HIS
1	A	336	ASN
1	A	400	ASN
1	A	402	ASN
1	A	416	ASN
1	A	421	ASN
1	A	443	ASN
1	A	461	HIS
1	B	136	GLN
1	B	227	GLN
1	B	234	HIS
1	B	275	HIS
1	B	400	ASN
1	B	402	ASN
1	B	421	ASN
1	B	443	ASN
1	B	461	HIS
1	C	144	HIS
1	C	227	GLN
1	C	234	HIS
1	C	275	HIS
1	C	334	ASN
1	C	400	ASN
1	C	402	ASN
1	C	416	ASN

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Mol	Chain	Res	Type
1	C	421	ASN
1	C	443	ASN
1	C	461	HIS
1	D	144	HIS
1	D	227	GLN
1	D	234	HIS
1	D	275	HIS
1	D	336	ASN
1	D	400	ASN
1	D	421	ASN
1	D	443	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

29 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.74	0	17,19,21	1.35	2 (11%)
2	NAG	E	2	2	14,14,15	0.93	0	17,19,21	2.05	5 (29%)
3	NAG	F	1	3,1	14,14,15	1.46	2 (14%)	17,19,21	1.91	3 (17%)
3	NAG	F	2	3	14,14,15	0.86	1 (7%)	17,19,21	1.51	3 (17%)
3	BMA	F	3	3	11,11,12	1.05	1 (9%)	15,15,17	1.30	2 (13%)
3	MAN	F	4	3	11,11,12	1.47	2 (18%)	15,15,17	1.32	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	F	5	3	11,11,12	0.93	0	15,15,17	1.31	3 (20%)
3	MAN	F	6	3	11,11,12	1.38	3 (27%)	15,15,17	1.51	4 (26%)
3	MAN	F	7	3	11,11,12	1.57	3 (27%)	15,15,17	1.36	3 (20%)
2	NAG	G	1	1,2	14,14,15	0.96	0	17,19,21	1.21	1 (5%)
2	NAG	G	2	2	14,14,15	0.61	0	17,19,21	1.39	3 (17%)
4	NAG	H	1	1,4	14,14,15	0.82	0	17,19,21	2.36	7 (41%)
4	NAG	H	2	4	14,14,15	1.06	1 (7%)	17,19,21	1.70	5 (29%)
4	BMA	H	3	4	11,11,12	1.16	1 (9%)	15,15,17	1.18	2 (13%)
4	MAN	H	4	4	11,11,12	1.01	1 (9%)	15,15,17	1.43	1 (6%)
4	MAN	H	5	4	11,11,12	1.21	1 (9%)	15,15,17	1.48	3 (20%)
4	MAN	H	6	4	11,11,12	2.08	4 (36%)	15,15,17	1.45	2 (13%)
4	NAG	I	1	1,4	14,14,15	1.08	1 (7%)	17,19,21	1.88	5 (29%)
4	NAG	I	2	4	14,14,15	0.63	0	17,19,21	1.33	1 (5%)
4	BMA	I	3	4	11,11,12	0.84	0	15,15,17	2.16	4 (26%)
4	MAN	I	4	4	11,11,12	1.09	1 (9%)	15,15,17	1.50	2 (13%)
4	MAN	I	5	4	11,11,12	1.16	0	15,15,17	1.23	1 (6%)
4	MAN	I	6	4	11,11,12	1.67	4 (36%)	15,15,17	1.56	4 (26%)
4	NAG	J	1	1,4	14,14,15	1.33	1 (7%)	17,19,21	2.25	5 (29%)
4	NAG	J	2	4	14,14,15	1.02	1 (7%)	17,19,21	1.33	2 (11%)
4	BMA	J	3	4	11,11,12	1.29	1 (9%)	15,15,17	2.71	8 (53%)
4	MAN	J	4	4	11,11,12	1.41	2 (18%)	15,15,17	1.29	2 (13%)
4	MAN	J	5	4	11,11,12	0.93	0	15,15,17	1.49	3 (20%)
4	MAN	J	6	4	11,11,12	1.61	2 (18%)	15,15,17	2.02	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
4	MAN	H	6	4	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1
4	MAN	I	6	4	-	2/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	MAN	J	6	4	-	0/2/19/22	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	6	MAN	O2-C2	4.10	1.52	1.43
4	J	1	NAG	O5-C1	3.73	1.49	1.43
4	J	6	MAN	C2-C3	3.47	1.57	1.52
3	F	7	MAN	C2-C3	3.43	1.57	1.52
3	F	4	MAN	O4-C4	3.12	1.50	1.43
4	H	6	MAN	C2-C3	3.00	1.56	1.52
4	H	2	NAG	C1-C2	2.69	1.56	1.52
4	H	6	MAN	O5-C1	2.62	1.47	1.43
3	F	4	MAN	C2-C3	2.59	1.56	1.52
4	I	1	NAG	O5-C5	2.53	1.48	1.43
3	F	1	NAG	O5-C1	2.43	1.47	1.43
4	J	4	MAN	O5-C1	-2.41	1.39	1.43
3	F	1	NAG	C2-N2	2.37	1.50	1.46
4	I	6	MAN	C2-C3	2.37	1.56	1.52
4	H	4	MAN	O5-C1	-2.32	1.40	1.43
4	J	4	MAN	O2-C2	2.31	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	7	MAN	O2-C2	2.26	1.48	1.43
3	F	3	BMA	C2-C3	2.25	1.55	1.52
4	J	6	MAN	C4-C3	2.23	1.58	1.52
3	F	7	MAN	O5-C1	2.21	1.47	1.43
4	I	6	MAN	C4-C3	2.21	1.58	1.52
4	J	3	BMA	O3-C3	2.19	1.48	1.43
4	H	5	MAN	O4-C4	2.19	1.48	1.43
4	I	6	MAN	O3-C3	2.18	1.48	1.43
4	I	6	MAN	O5-C1	2.17	1.47	1.43
4	J	2	NAG	O5-C1	2.14	1.47	1.43
3	F	2	NAG	C2-N2	2.10	1.49	1.46
4	H	6	MAN	O3-C3	2.08	1.47	1.43
4	I	4	MAN	C2-C3	2.05	1.55	1.52
4	H	3	BMA	O3-C3	2.04	1.47	1.43
3	F	6	MAN	O3-C3	2.04	1.47	1.43
3	F	6	MAN	O5-C5	2.03	1.47	1.43
3	F	6	MAN	C4-C5	2.02	1.57	1.53

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1	NAG	O5-C1-C2	-7.12	100.05	111.29
4	J	6	MAN	C1-O5-C5	5.83	120.09	112.19
3	F	1	NAG	O5-C1-C2	-5.38	102.79	111.29
4	H	1	NAG	C1-O5-C5	5.15	119.16	112.19
4	J	3	BMA	O5-C5-C6	-5.14	99.14	107.20
4	H	1	NAG	O5-C1-C2	-4.77	103.75	111.29
4	I	1	NAG	C1-O5-C5	4.28	118.00	112.19
4	J	3	BMA	O3-C3-C2	4.23	118.10	109.99
4	I	3	BMA	C1-C2-C3	4.20	114.83	109.67
4	I	3	BMA	O2-C2-C1	-4.06	100.83	109.15
4	I	3	BMA	C2-C3-C4	-4.05	103.89	110.89
4	H	6	MAN	C1-C2-C3	-4.03	104.71	109.67
4	I	6	MAN	C1-O5-C5	3.90	117.47	112.19
4	I	3	BMA	O5-C1-C2	3.81	116.65	110.77
2	E	2	NAG	O4-C4-C5	3.74	118.59	109.30
4	H	5	MAN	C3-C4-C5	-3.64	103.74	110.24
2	E	2	NAG	C1-O5-C5	3.61	117.08	112.19
2	E	2	NAG	O3-C3-C4	-3.58	102.06	110.35
3	F	2	NAG	O6-C6-C5	-3.54	99.15	111.29
2	E	2	NAG	C1-C2-N2	-3.49	104.52	110.49
4	I	4	MAN	C1-O5-C5	3.43	116.83	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	O5-C5-C6	-3.39	101.89	107.20
4	J	5	MAN	C1-O5-C5	3.38	116.77	112.19
3	F	1	NAG	C6-C5-C4	3.38	120.91	113.00
4	J	1	NAG	C3-C4-C5	3.19	115.94	110.24
3	F	6	MAN	C1-O5-C5	3.17	116.49	112.19
4	H	3	BMA	C2-C3-C4	-3.16	105.43	110.89
4	H	1	NAG	C8-C7-N2	3.16	121.44	116.10
4	J	2	NAG	O6-C6-C5	-3.12	100.58	111.29
4	J	3	BMA	O2-C2-C1	-3.11	102.78	109.15
4	I	1	NAG	O5-C1-C2	-3.10	106.39	111.29
4	J	3	BMA	C6-C5-C4	3.07	120.19	113.00
3	F	1	NAG	O4-C4-C3	-3.06	103.28	110.35
4	J	5	MAN	O5-C5-C6	3.03	111.95	107.20
4	J	6	MAN	O2-C2-C3	3.01	116.17	110.14
4	H	4	MAN	O6-C6-C5	-2.92	101.28	111.29
4	J	4	MAN	C2-C3-C4	-2.83	106.00	110.89
4	H	2	NAG	O6-C6-C5	-2.81	101.65	111.29
3	F	2	NAG	O4-C4-C5	-2.79	102.36	109.30
3	F	7	MAN	O5-C5-C6	2.79	111.58	107.20
4	I	1	NAG	C1-C2-N2	-2.79	105.73	110.49
2	E	2	NAG	O5-C5-C6	2.78	111.56	107.20
4	J	3	BMA	C2-C3-C4	-2.77	106.09	110.89
4	H	6	MAN	O5-C5-C4	-2.75	104.12	110.83
4	J	1	NAG	C6-C5-C4	2.75	119.45	113.00
4	J	3	BMA	C1-O5-C5	2.72	115.88	112.19
3	F	5	MAN	O5-C5-C6	2.72	111.46	107.20
4	H	2	NAG	C1-O5-C5	2.71	115.86	112.19
4	H	1	NAG	C6-C5-C4	-2.69	106.69	113.00
4	J	3	BMA	O3-C3-C4	-2.67	104.17	110.35
4	I	1	NAG	O3-C3-C2	-2.66	103.96	109.47
4	H	2	NAG	O5-C5-C6	2.66	111.37	107.20
2	G	2	NAG	C8-C7-N2	-2.61	111.68	116.10
3	F	6	MAN	O4-C4-C5	2.59	115.72	109.30
3	F	2	NAG	C1-O5-C5	2.56	115.66	112.19
4	J	4	MAN	O2-C2-C1	2.55	114.38	109.15
4	I	6	MAN	C3-C4-C5	2.55	114.78	110.24
4	J	3	BMA	O5-C1-C2	2.49	114.61	110.77
2	G	1	NAG	O5-C1-C2	-2.47	107.39	111.29
4	H	1	NAG	O7-C7-N2	-2.44	117.47	121.95
4	H	1	NAG	C1-C2-N2	-2.39	106.41	110.49
3	F	3	BMA	C1-O5-C5	2.36	115.39	112.19
3	F	7	MAN	O2-C2-C3	2.35	114.85	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1	NAG	O6-C6-C5	2.35	119.36	111.29
2	G	2	NAG	O7-C7-C8	2.32	126.36	122.06
4	H	5	MAN	O5-C1-C2	-2.31	107.20	110.77
3	F	6	MAN	O2-C2-C1	-2.30	104.45	109.15
4	J	1	NAG	O3-C3-C4	-2.29	105.05	110.35
4	J	5	MAN	O5-C1-C2	-2.28	107.24	110.77
4	I	6	MAN	O3-C3-C2	-2.28	105.64	109.99
3	F	5	MAN	O5-C1-C2	-2.28	107.26	110.77
4	I	5	MAN	O3-C3-C2	-2.27	105.64	109.99
3	F	7	MAN	O5-C1-C2	2.26	114.25	110.77
3	F	3	BMA	C1-C2-C3	-2.23	106.93	109.67
4	I	2	NAG	C1-O5-C5	-2.22	109.18	112.19
4	H	2	NAG	O4-C4-C5	-2.19	103.87	109.30
4	H	2	NAG	C1-C2-N2	2.16	114.18	110.49
2	E	1	NAG	O6-C6-C5	-2.15	103.92	111.29
3	F	6	MAN	O6-C6-C5	-2.15	103.92	111.29
3	F	4	MAN	O5-C5-C6	2.15	110.57	107.20
4	H	3	BMA	O3-C3-C2	2.14	114.09	109.99
3	F	5	MAN	C3-C4-C5	-2.13	106.44	110.24
4	I	6	MAN	O3-C3-C4	2.12	115.25	110.35
4	J	6	MAN	O6-C6-C5	-2.11	104.04	111.29
4	I	4	MAN	O6-C6-C5	-2.09	104.11	111.29
2	G	2	NAG	C1-O5-C5	2.08	115.01	112.19
4	J	2	NAG	O3-C3-C4	2.06	115.12	110.35
4	H	1	NAG	C3-C4-C5	2.06	113.91	110.24
4	H	5	MAN	C1-O5-C5	2.06	114.98	112.19
4	J	1	NAG	C8-C7-N2	-2.06	112.61	116.10
3	F	4	MAN	O3-C3-C4	-2.03	105.65	110.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	6	MAN	O5-C5-C6-O6
4	I	6	MAN	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6

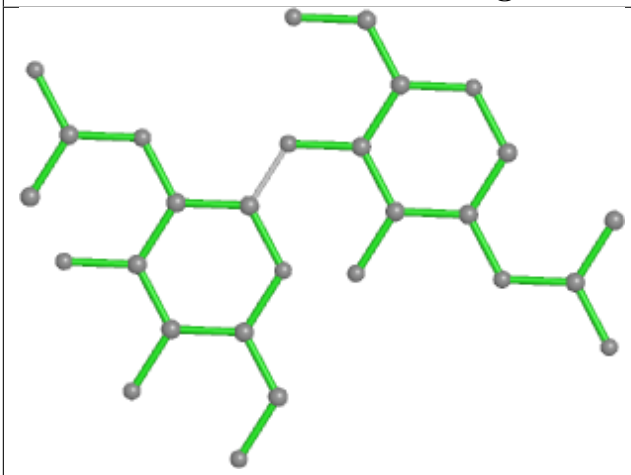
There are no ring outliers.

3 monomers are involved in 4 short contacts:

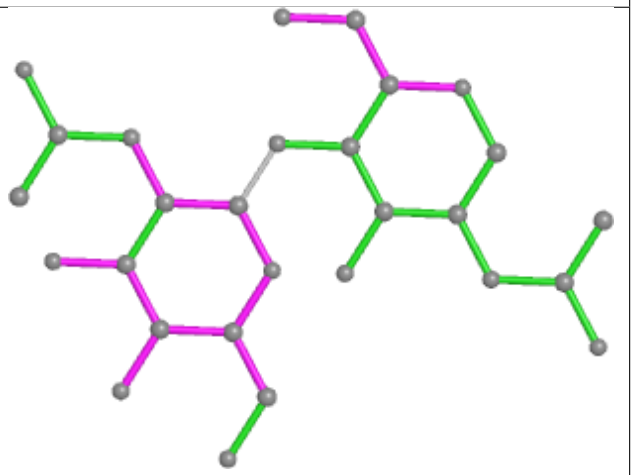
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	I	2	NAG	1	0
4	H	1	NAG	2	0

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

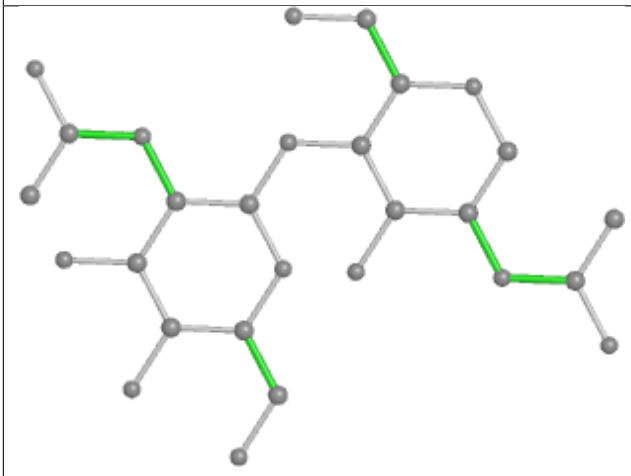
Oligosaccharide Chain E



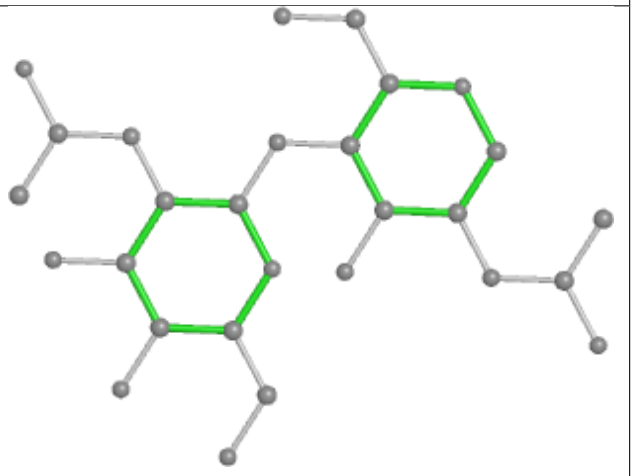
Bond lengths



Bond angles

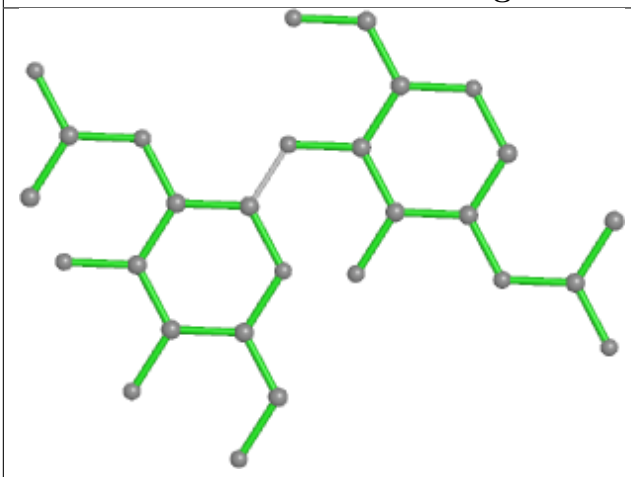


Torsions

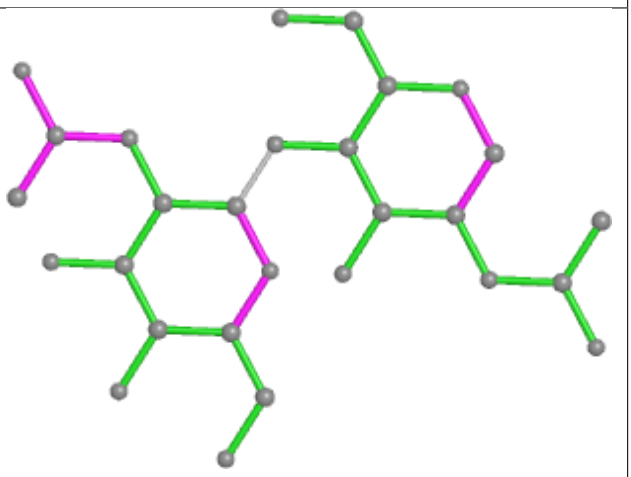


Rings

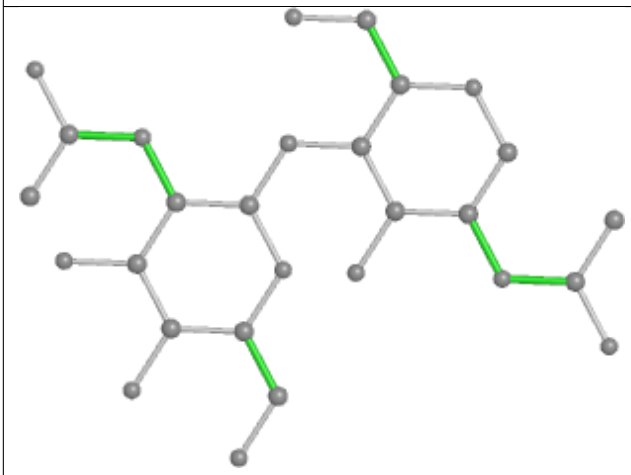
Oligosaccharide Chain G



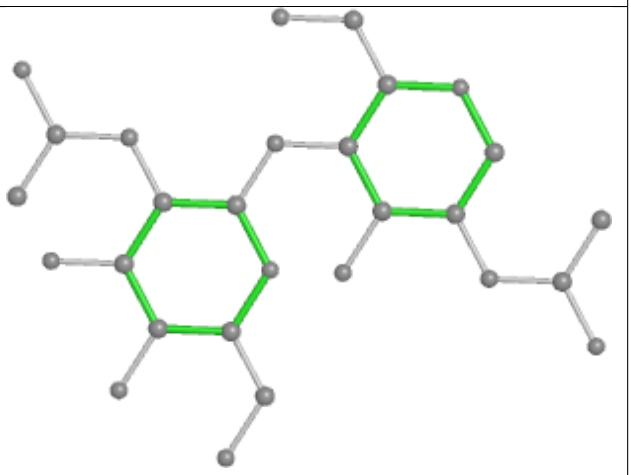
Bond lengths



Bond angles

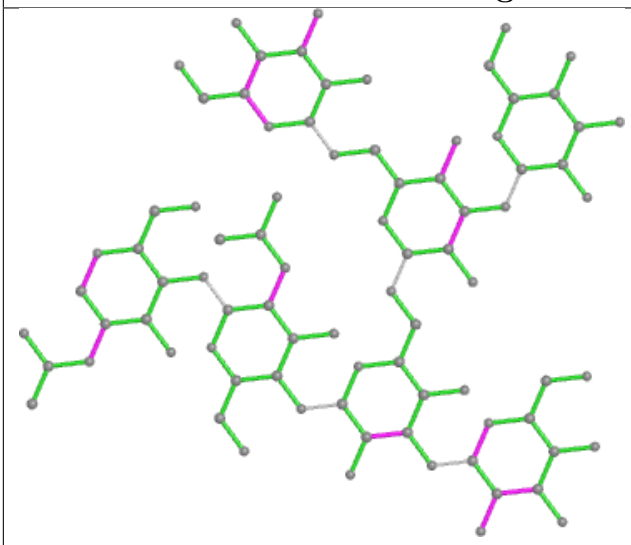


Torsions

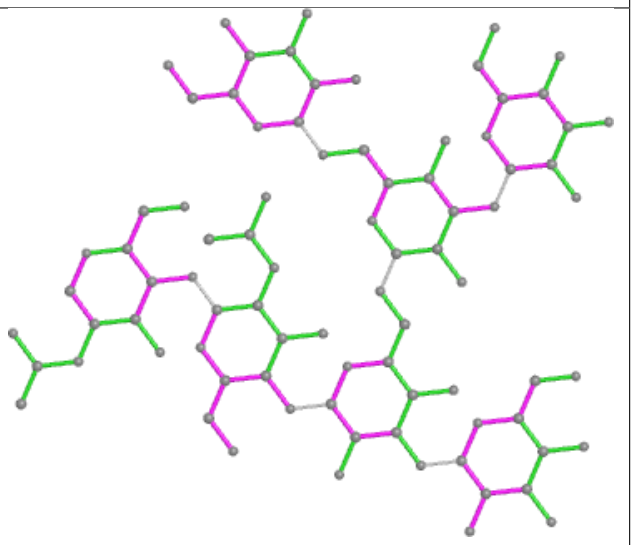


Rings

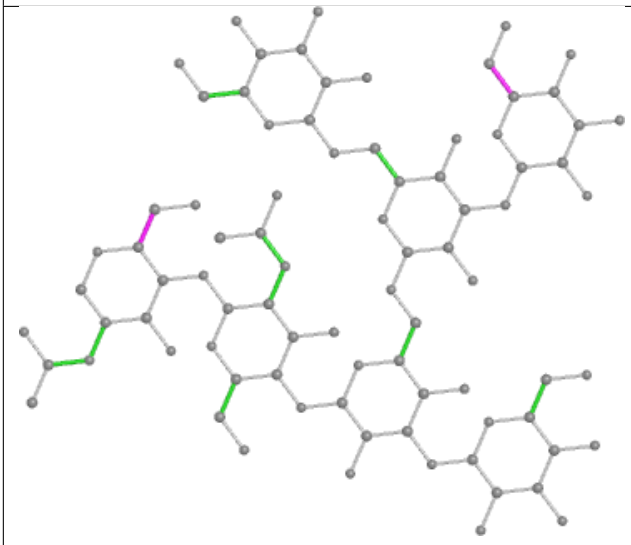
Oligosaccharide Chain F



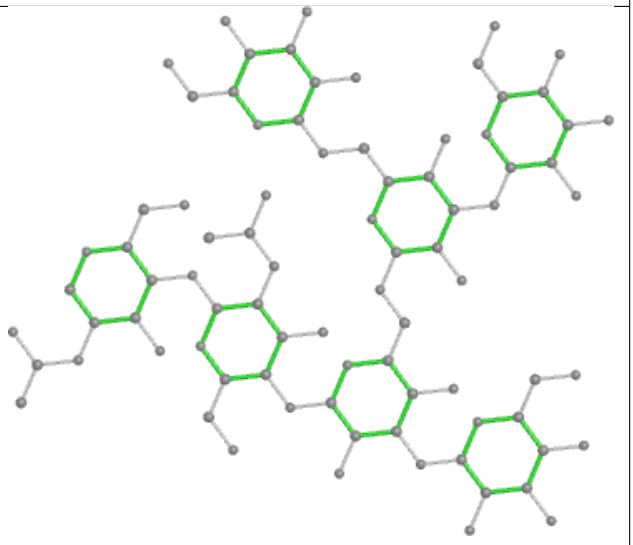
Bond lengths



Bond angles

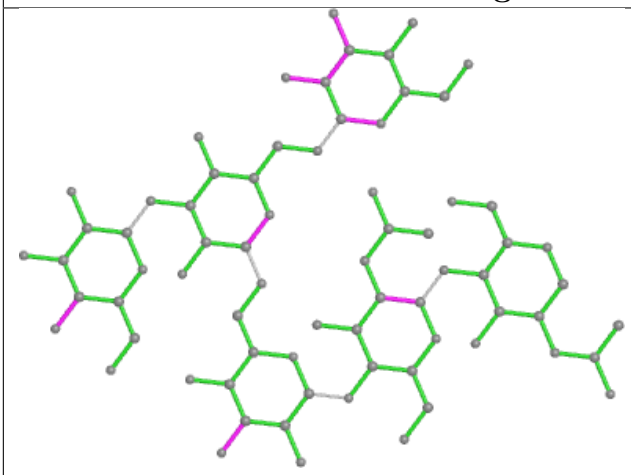


Torsions

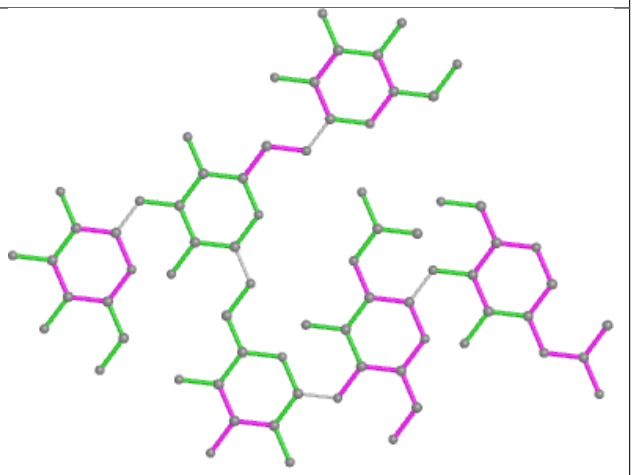


Rings

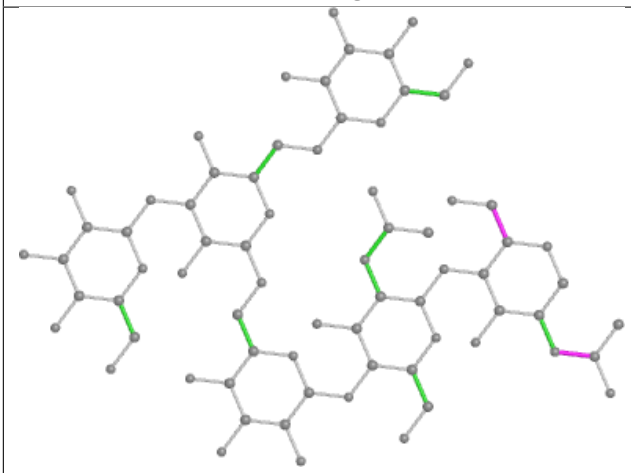
Oligosaccharide Chain H



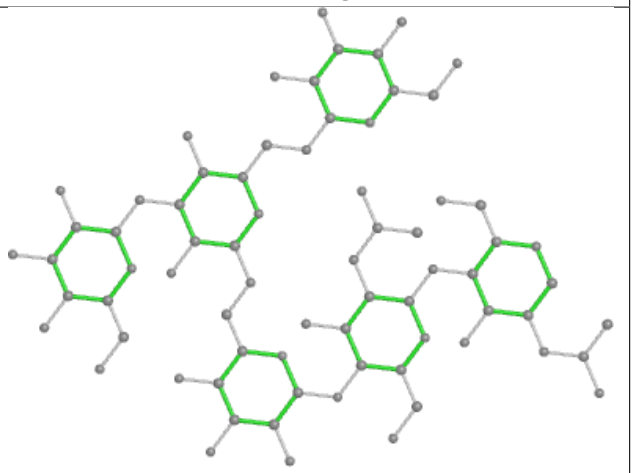
Bond lengths



Bond angles

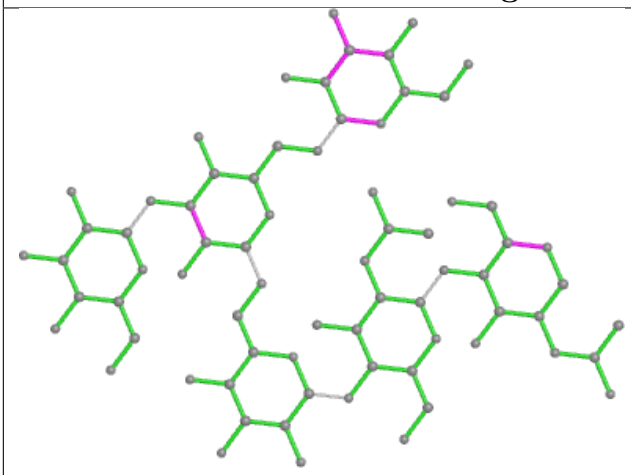


Torsions

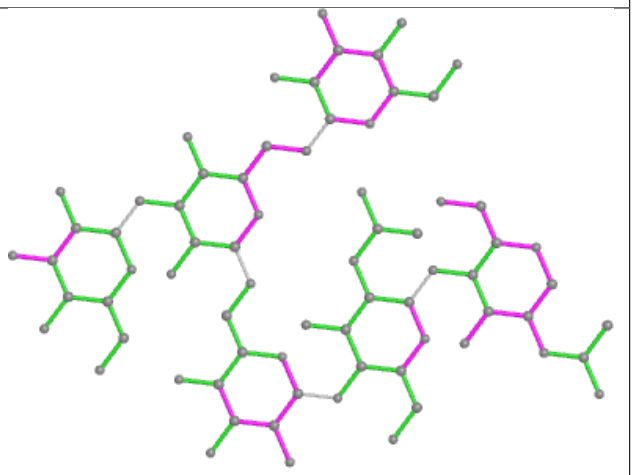


Rings

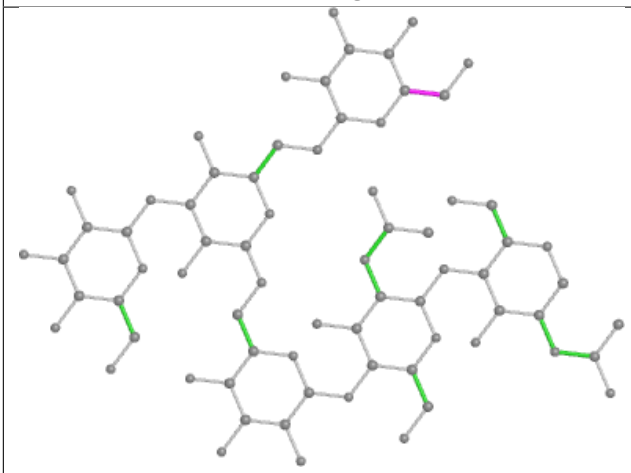
Oligosaccharide Chain I



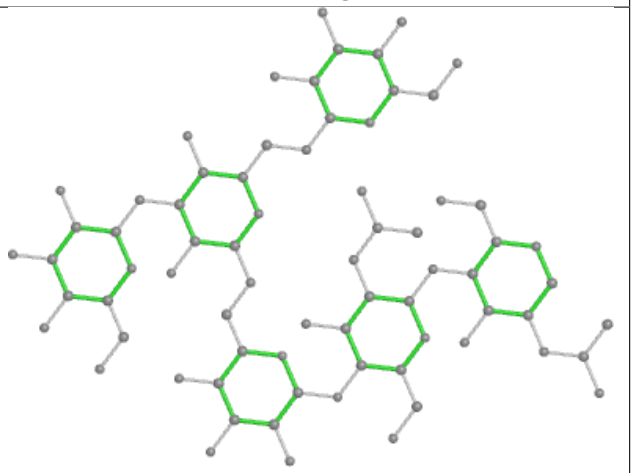
Bond lengths



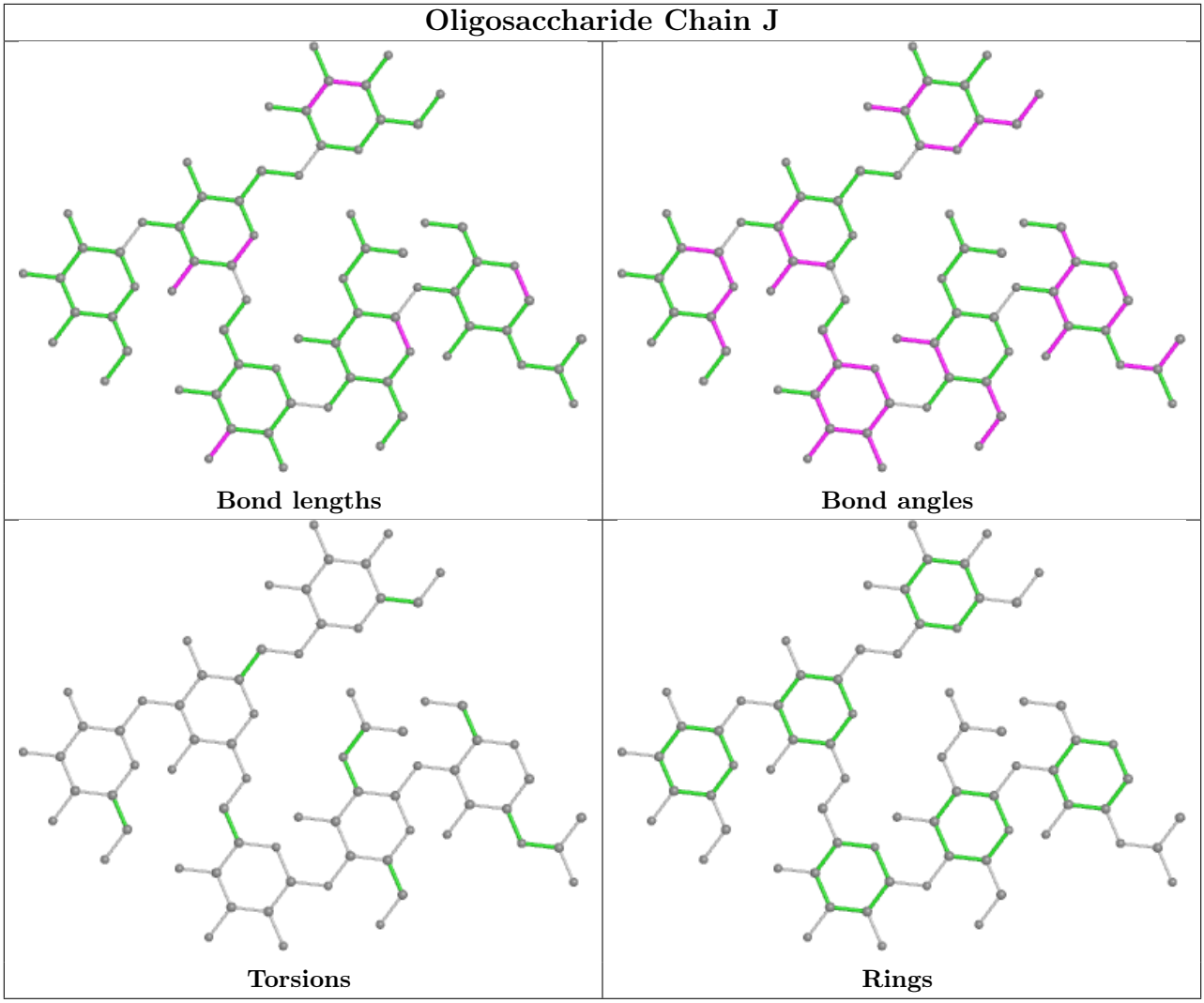
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 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	GOL	D	509	-	5,5,5	0.38	0	5,5,5	1.21	0
5	NAG	D	501	1	14,14,15	1.33	2 (14%)	17,19,21	2.04	6 (35%)
7	GOL	A	512	-	5,5,5	0.50	0	5,5,5	1.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	C	510	-	5,5,5	0.28	0	5,5,5	0.67	0
6	DAN	B	510	-	20,20,20	0.70	1 (5%)	23,28,28	0.79	1 (4%)
7	GOL	B	513	-	5,5,5	0.76	0	5,5,5	1.15	1 (20%)
5	NAG	B	501	1	14,14,15	0.96	0	17,19,21	1.80	4 (23%)
5	NAG	A	501	1	14,14,15	1.38	1 (7%)	17,19,21	1.52	3 (17%)
6	DAN	D	508	-	20,20,20	0.61	0	23,28,28	0.93	1 (4%)
7	GOL	B	512	-	5,5,5	0.85	0	5,5,5	1.18	0
5	NAG	C	501	1	14,14,15	1.15	2 (14%)	17,19,21	2.22	5 (29%)
6	DAN	A	511	-	20,20,20	0.84	1 (5%)	23,28,28	0.93	1 (4%)
7	GOL	A	513	-	5,5,5	0.60	0	5,5,5	0.65	0
7	GOL	C	511	-	5,5,5	1.27	1 (20%)	5,5,5	2.03	1 (20%)
7	GOL	D	510	-	5,5,5	0.65	0	5,5,5	1.16	0
6	DAN	C	509	-	20,20,20	0.61	0	23,28,28	0.86	0
7	GOL	B	511	-	5,5,5	0.53	0	5,5,5	1.11	0
5	NAG	C	502	1	14,14,15	1.11	1 (7%)	17,19,21	1.86	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	D	509	-	-	2/4/4/4	-
5	NAG	D	501	1	-	0/6/23/26	0/1/1/1
7	GOL	A	512	-	-	0/4/4/4	-
7	GOL	C	510	-	-	2/4/4/4	-
6	DAN	B	510	-	-	0/18/34/34	0/1/1/1
7	GOL	B	513	-	-	2/4/4/4	-
5	NAG	B	501	1	-	1/6/23/26	0/1/1/1
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
6	DAN	D	508	-	-	0/18/34/34	0/1/1/1
7	GOL	B	512	-	-	0/4/4/4	-
5	NAG	C	501	1	-	0/6/23/26	0/1/1/1
6	DAN	A	511	-	-	0/18/34/34	0/1/1/1
7	GOL	A	513	-	-	0/4/4/4	-
7	GOL	C	511	-	-	1/4/4/4	-
7	GOL	D	510	-	-	2/4/4/4	-
6	DAN	C	509	-	-	0/18/34/34	0/1/1/1
7	GOL	B	511	-	-	0/4/4/4	-
5	NAG	C	502	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	NAG	O4-C4	3.49	1.51	1.43
6	A	511	DAN	O1B-C1	-3.28	1.21	1.30
5	A	501	NAG	O5-C1	2.90	1.48	1.43
6	B	510	DAN	O1B-C1	-2.78	1.22	1.30
7	C	511	GOL	O1-C1	2.50	1.53	1.42
5	D	501	NAG	O5-C5	2.37	1.48	1.43
5	C	501	NAG	O4-C4	2.30	1.48	1.43
5	C	502	NAG	C3-C2	2.20	1.57	1.52
5	C	501	NAG	O5-C1	-2.09	1.40	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	501	NAG	O4-C4-C5	5.25	122.33	109.30
5	C	501	NAG	O4-C4-C5	4.39	120.20	109.30
5	C	502	NAG	O5-C1-C2	-4.37	104.38	111.29
5	C	501	NAG	O6-C6-C5	-4.09	97.27	111.29
5	B	501	NAG	O5-C5-C6	4.07	113.58	107.20
7	C	511	GOL	O1-C1-C2	3.91	128.94	110.20
5	C	501	NAG	O5-C5-C6	-3.62	101.53	107.20
5	A	501	NAG	C1-O5-C5	-3.59	107.33	112.19
5	C	501	NAG	C3-C4-C5	-3.52	103.96	110.24
5	D	501	NAG	C3-C4-C5	-3.41	104.16	110.24
5	C	502	NAG	O5-C5-C6	3.38	112.51	107.20
5	D	501	NAG	O5-C5-C6	-3.14	102.29	107.20
5	B	501	NAG	C8-C7-N2	-3.06	110.91	116.10
5	C	502	NAG	O3-C3-C4	-2.78	103.93	110.35
5	A	501	NAG	O5-C5-C6	2.75	111.52	107.20
5	C	501	NAG	C6-C5-C4	2.57	119.02	113.00
5	D	501	NAG	C4-C3-C2	2.42	114.57	111.02
6	A	511	DAN	O4-C4-C5	-2.34	108.37	112.61
7	B	513	GOL	O3-C3-C2	2.33	121.36	110.20
5	B	501	NAG	O7-C7-N2	2.33	126.23	121.95
5	C	502	NAG	C8-C7-N2	2.17	119.78	116.10
5	D	501	NAG	C6-C5-C4	2.13	118.00	113.00
5	D	501	NAG	O3-C3-C4	-2.12	105.45	110.35
5	A	501	NAG	C4-C3-C2	-2.09	107.96	111.02
5	B	501	NAG	O5-C5-C4	-2.09	105.75	110.83
6	B	510	DAN	O1A-C1-C2	-2.03	115.11	120.48
6	D	508	DAN	C6-C5-N5	-2.02	107.55	110.91

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	513	GOL	C1-C2-C3-O3
7	C	510	GOL	C1-C2-C3-O3
7	D	509	GOL	C1-C2-C3-O3
7	C	510	GOL	O2-C2-C3-O3
7	D	510	GOL	O2-C2-C3-O3
7	D	510	GOL	C1-C2-C3-O3
7	B	513	GOL	O2-C2-C3-O3
7	D	509	GOL	O2-C2-C3-O3
7	C	511	GOL	O2-C2-C3-O3
5	B	501	NAG	C8-C7-N2-C2

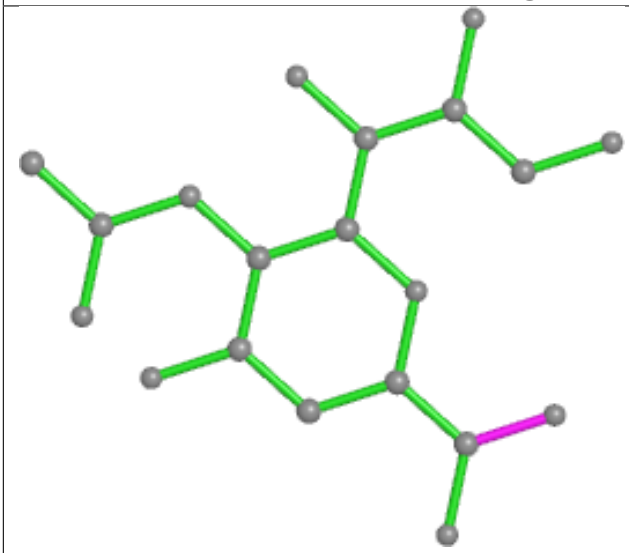
There are no ring outliers.

5 monomers are involved in 7 short contacts:

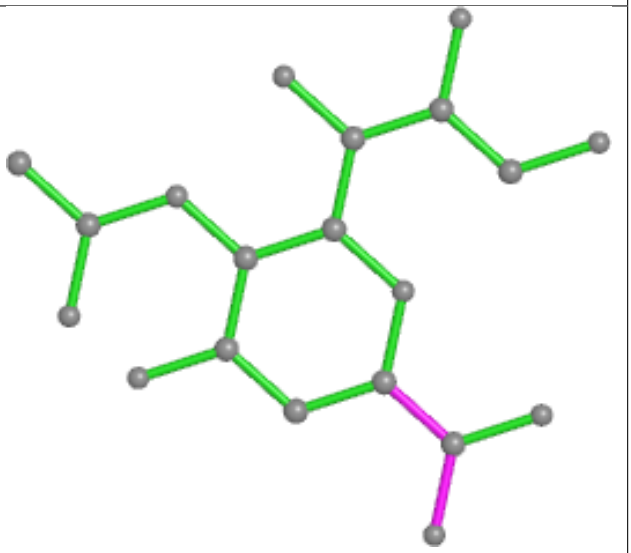
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	513	GOL	1	0
7	B	512	GOL	2	0
7	A	513	GOL	1	0
7	C	511	GOL	1	0
7	D	510	GOL	2	0

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.

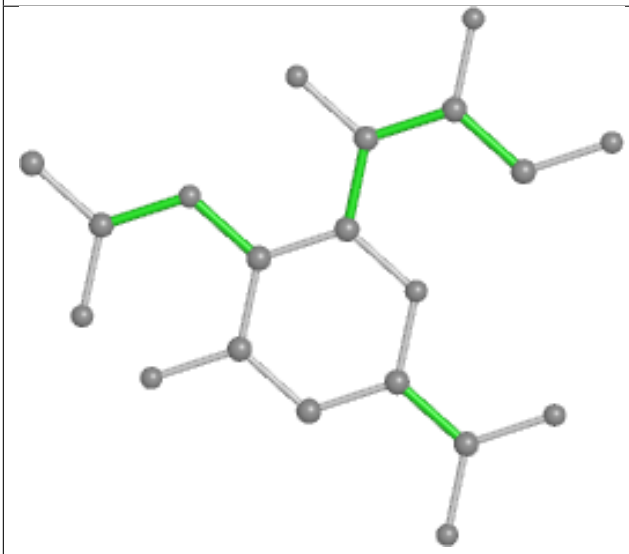
Ligand DAN B 510



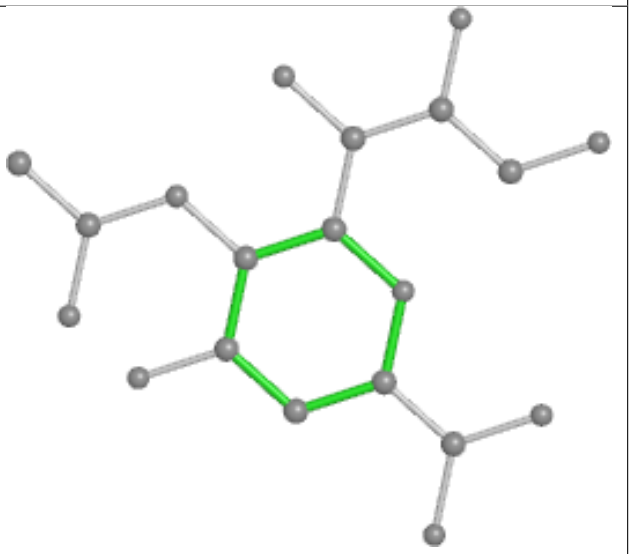
Bond lengths



Bond angles

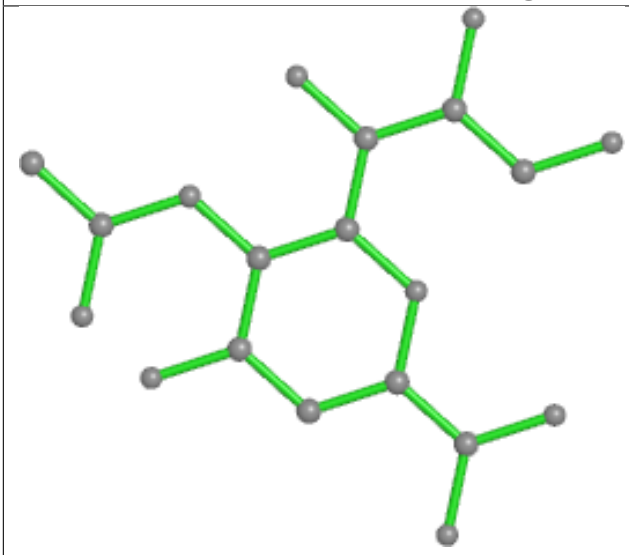


Torsions

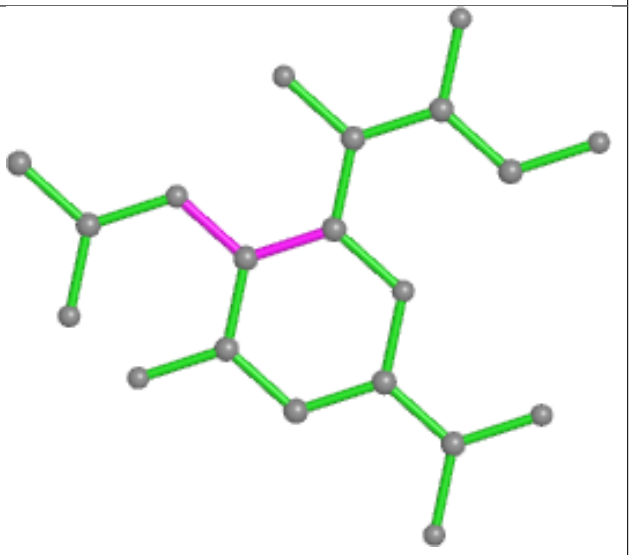


Rings

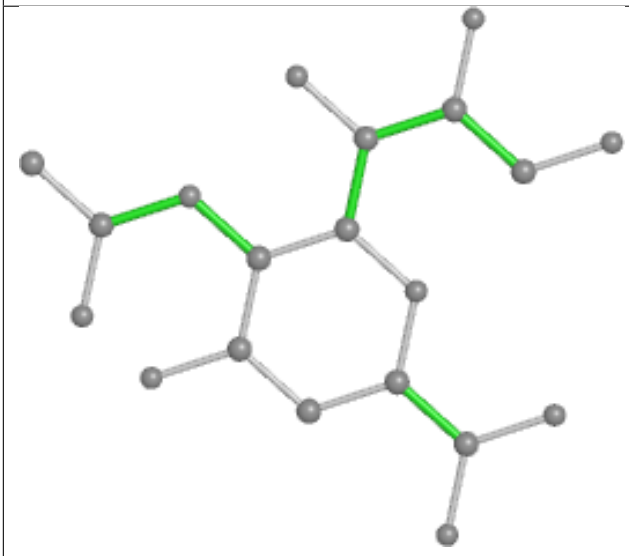
Ligand DAN D 508



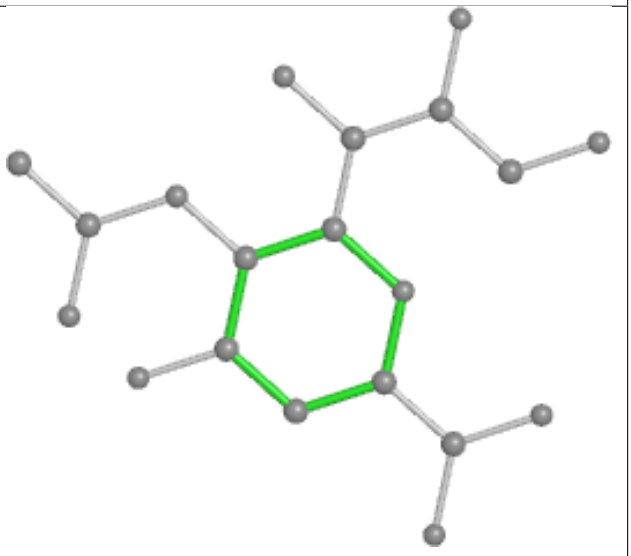
Bond lengths



Bond angles

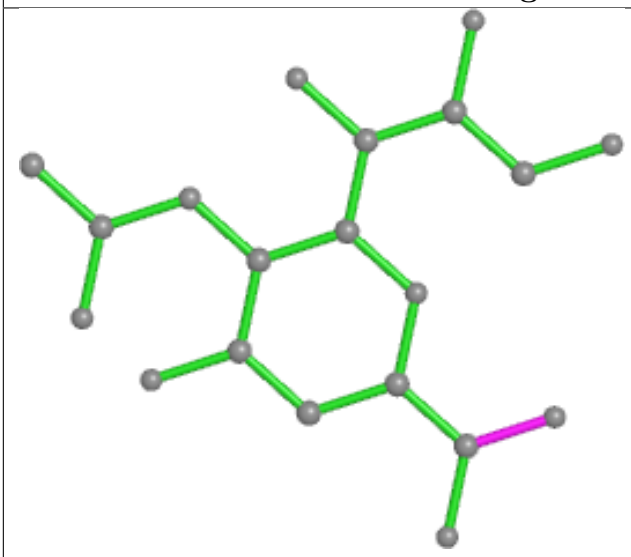


Torsions

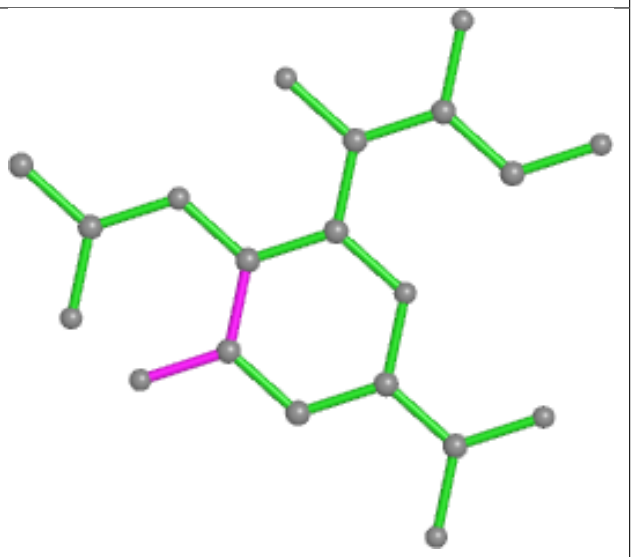


Rings

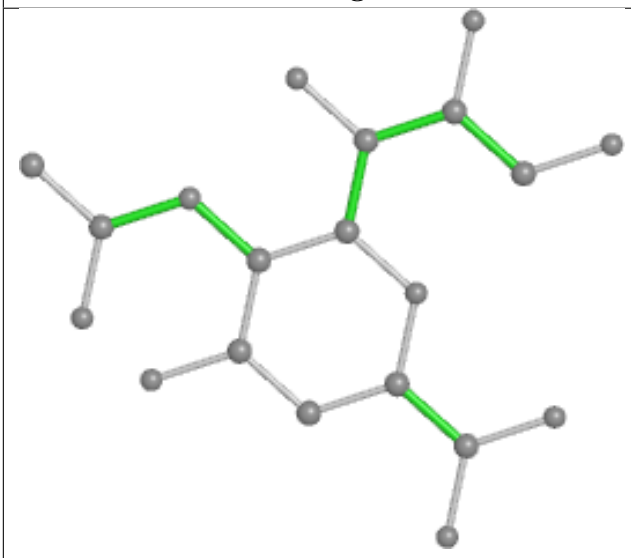
Ligand DAN A 511



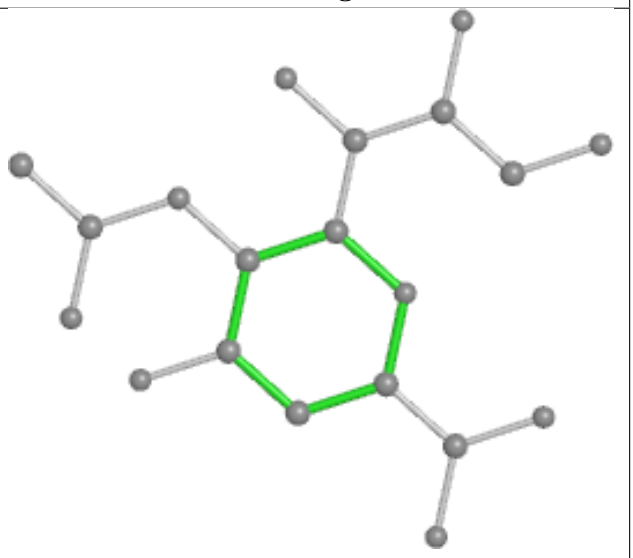
Bond lengths



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	389/389 (100%)	-0.52	1 (0%)	94	94	10, 15, 24, 33	0
1	B	389/389 (100%)	-0.56	1 (0%)	94	94	10, 14, 22, 41	0
1	C	389/389 (100%)	-0.57	1 (0%)	94	94	9, 14, 22, 37	0
1	D	389/389 (100%)	-0.53	0	100	100	10, 15, 23, 35	0
All	All	1556/1556 (100%)	-0.55	3 (0%)	95	95	9, 15, 23, 41	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	454	ARG	2.9
1	B	82	ARG	2.8
1	A	454	ARG	2.1

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	I	5	11/12	0.67	0.28	43,48,50,51	0
2	NAG	E	2	14/15	0.73	0.41	42,53,65,67	0
4	MAN	J	5	11/12	0.76	0.25	38,43,45,48	0
4	MAN	I	6	11/12	0.77	0.26	44,46,50,52	0

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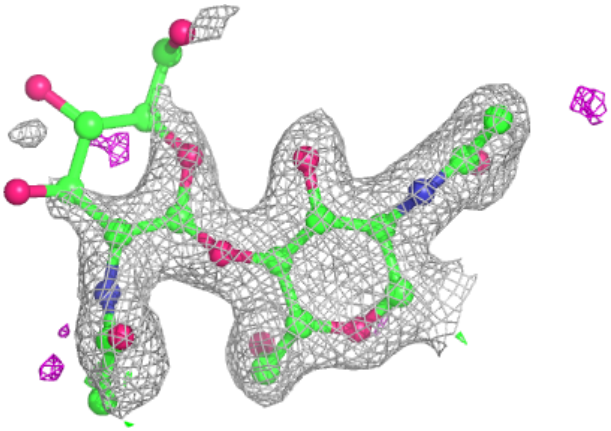
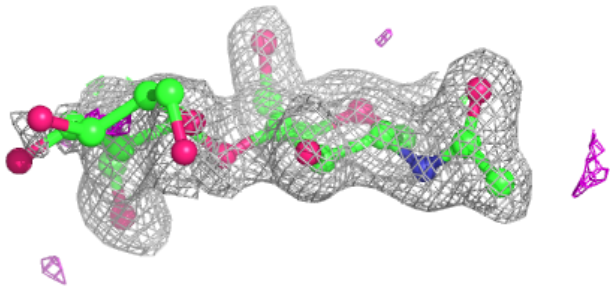
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	J	6	11/12	0.77	0.27	38,40,46,48	0
3	NAG	F	1	14/15	0.80	0.26	31,33,40,41	0
4	BMA	J	3	11/12	0.80	0.20	33,36,38,40	0
4	NAG	J	2	14/15	0.81	0.17	25,28,32,34	0
3	MAN	F	6	11/12	0.81	0.16	31,32,36,39	0
4	NAG	H	1	14/15	0.83	0.24	30,35,42,47	0
4	NAG	I	2	14/15	0.83	0.15	28,30,32,34	0
4	MAN	H	6	11/12	0.85	0.14	38,39,42,45	0
4	NAG	H	2	14/15	0.85	0.20	26,28,31,34	0
4	MAN	H	5	11/12	0.86	0.18	30,32,34,36	0
4	BMA	I	3	11/12	0.86	0.20	36,39,41,42	0
3	NAG	F	2	14/15	0.87	0.18	25,27,31,32	0
4	NAG	I	1	14/15	0.87	0.19	27,29,36,38	0
4	MAN	I	4	11/12	0.87	0.22	42,44,45,48	0
4	MAN	J	4	11/12	0.88	0.21	37,39,40,41	0
2	NAG	G	2	14/15	0.88	0.35	43,47,56,62	0
4	MAN	H	4	11/12	0.88	0.11	33,34,36,37	0
3	MAN	F	7	11/12	0.90	0.19	32,35,36,36	0
4	BMA	H	3	11/12	0.90	0.14	30,32,33,34	0
4	NAG	J	1	14/15	0.90	0.17	25,28,30,30	0
3	MAN	F	5	11/12	0.90	0.12	25,26,28,30	0
2	NAG	E	1	14/15	0.91	0.13	22,24,31,39	0
2	NAG	G	1	14/15	0.92	0.11	22,23,31,36	0
3	BMA	F	3	11/12	0.92	0.15	25,26,27,30	0
3	MAN	F	4	11/12	0.92	0.11	26,27,29,30	0

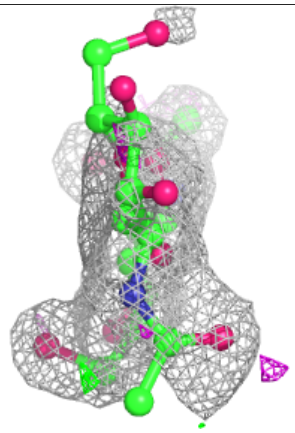
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

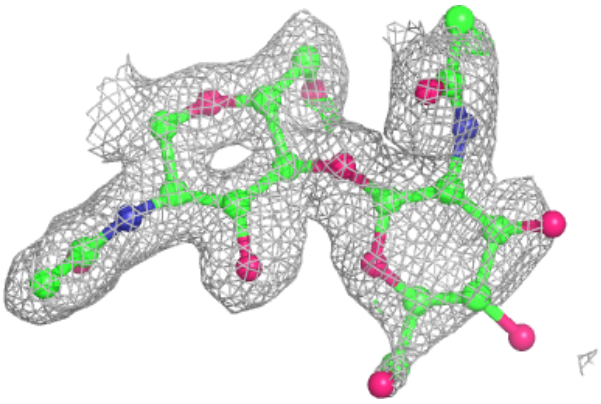


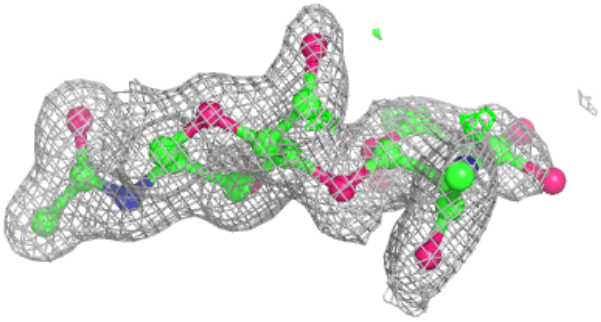


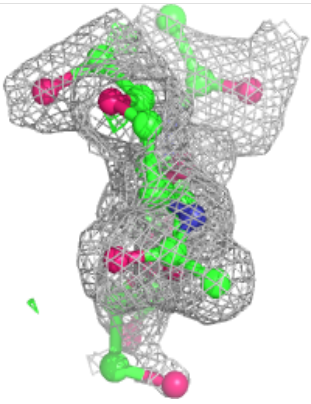


Electron density around Chain G:

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

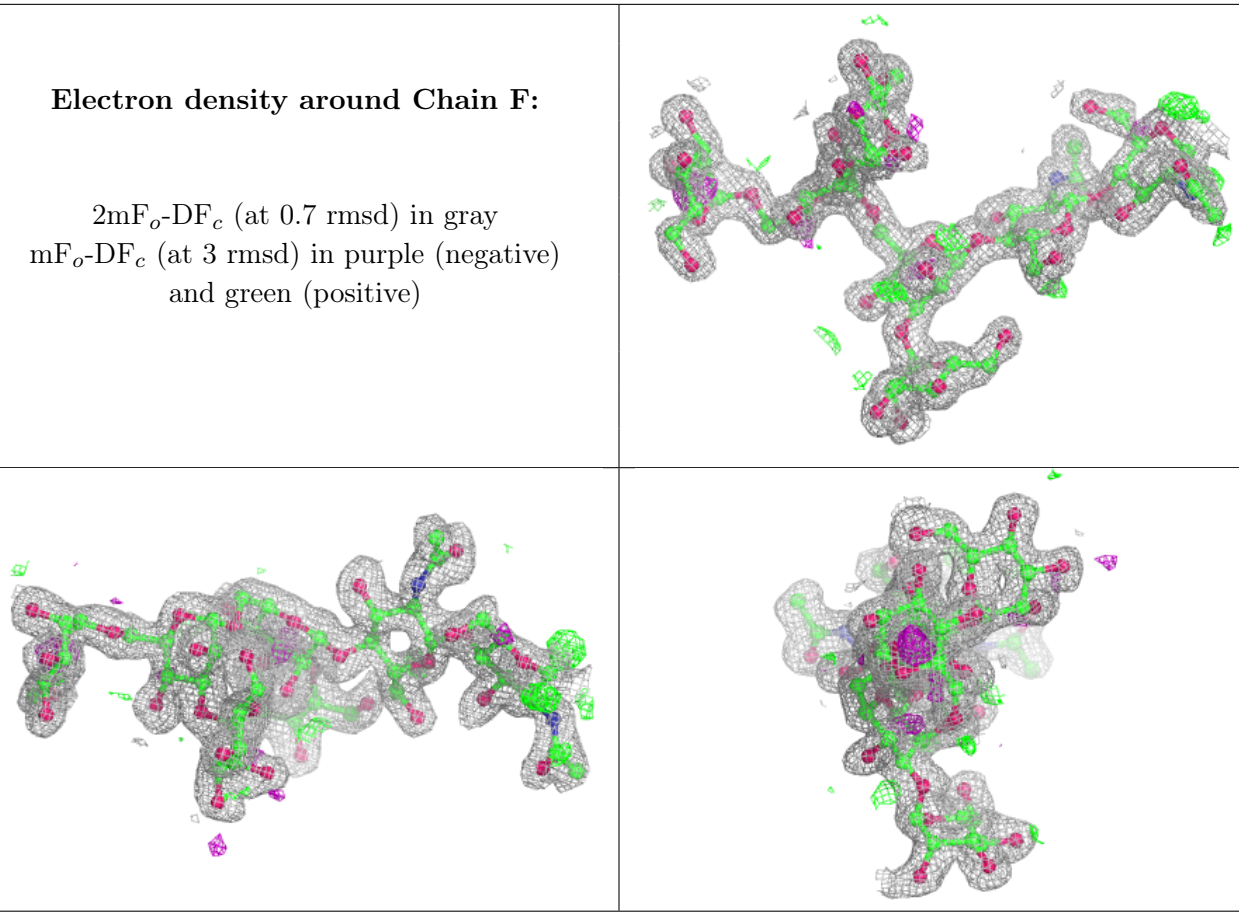






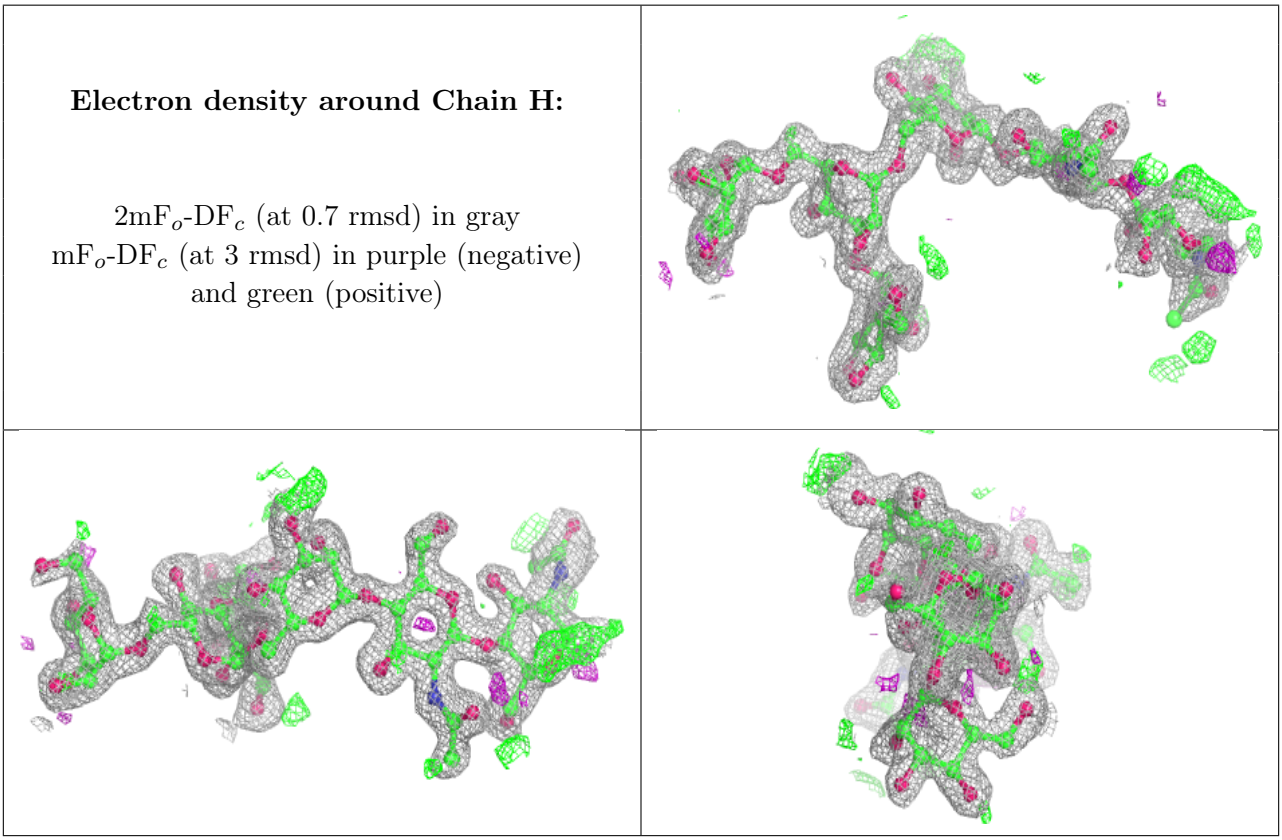
Electron density around Chain F:

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



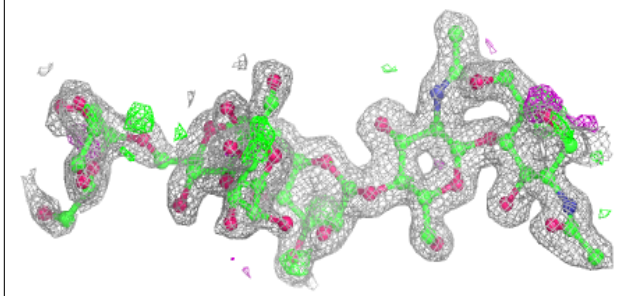
Electron density around Chain H:

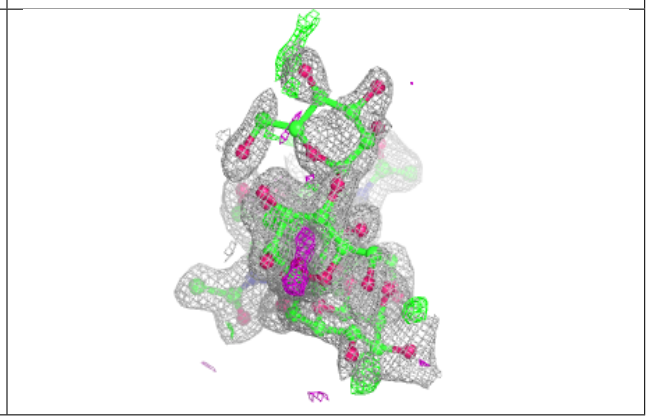
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain I:

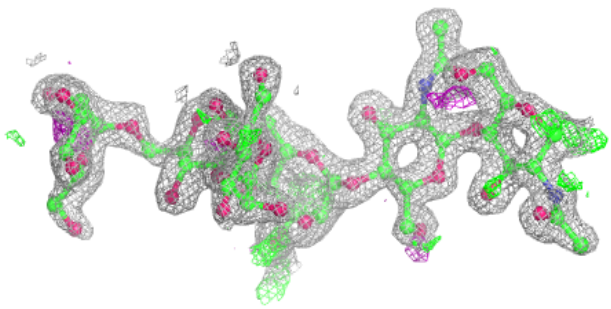
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

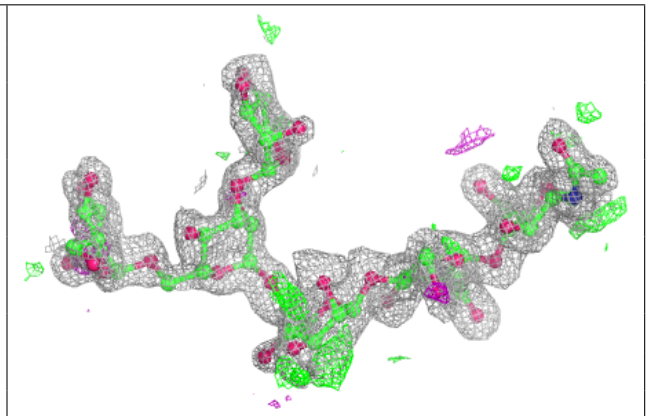




Electron density around Chain J:

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





6.4 Ligands (i)

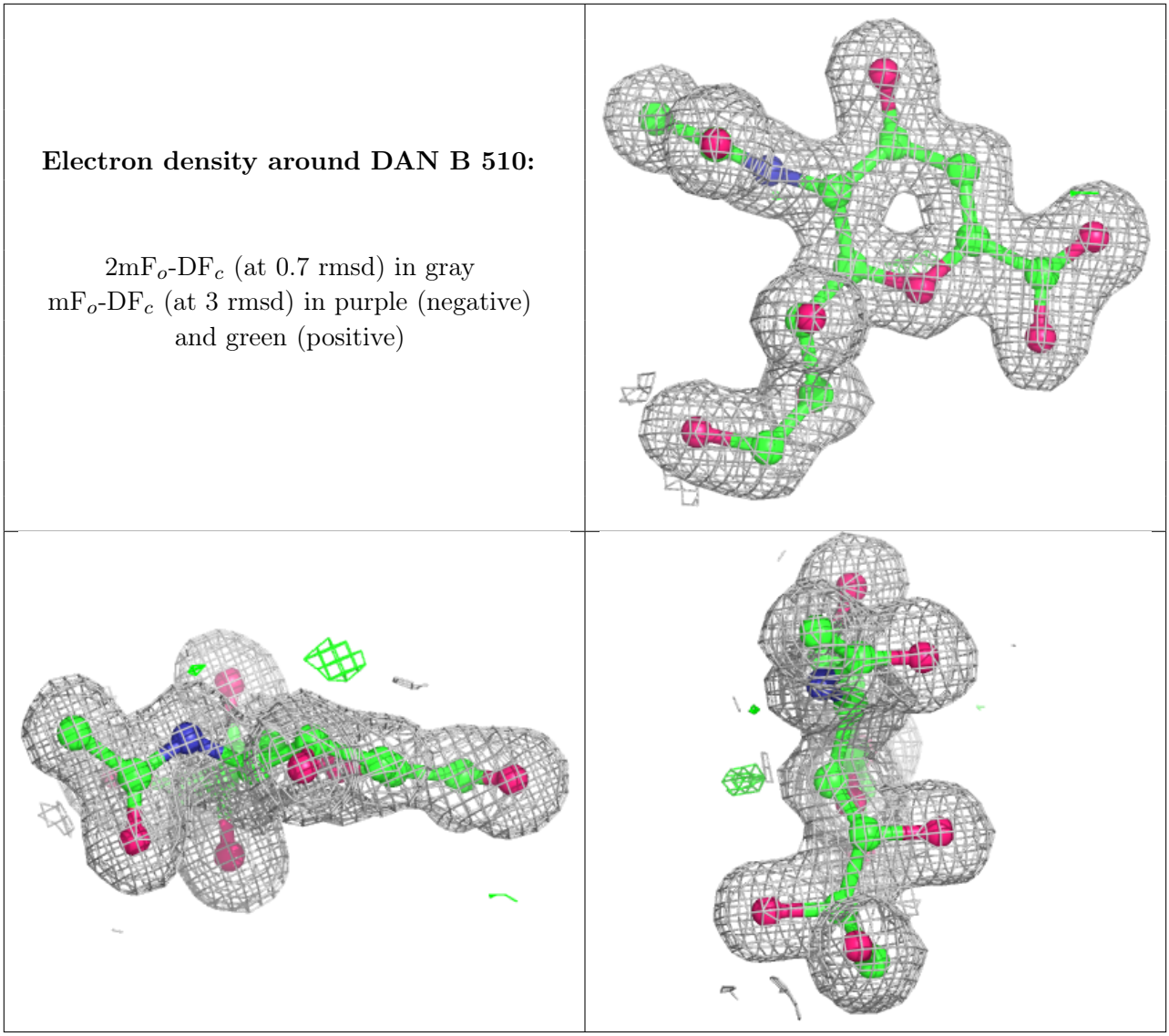
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	501	14/15	0.71	0.42	52,61,64,65	0
7	GOL	B	512	6/6	0.79	0.25	33,41,42,53	0
7	GOL	C	511	6/6	0.79	0.15	21,26,27,39	0
7	GOL	A	513	6/6	0.81	0.26	26,35,39,43	0
7	GOL	D	510	6/6	0.82	0.21	26,38,41,43	0
7	GOL	C	510	6/6	0.84	0.15	28,30,34,35	0
5	NAG	C	502	14/15	0.87	0.24	32,38,45,46	0
7	GOL	B	511	6/6	0.89	0.13	22,23,24,26	0
7	GOL	D	509	6/6	0.90	0.10	27,29,31,34	0
5	NAG	A	501	14/15	0.90	0.18	25,29,32,32	0
7	GOL	B	513	6/6	0.92	0.10	26,30,33,39	0
5	NAG	C	501	14/15	0.94	0.11	21,23,30,31	0
5	NAG	D	501	14/15	0.94	0.12	21,23,28,30	0
7	GOL	A	512	6/6	0.95	0.08	22,24,25,25	0
6	DAN	B	510	20/20	0.97	0.05	11,12,13,13	0
6	DAN	C	509	20/20	0.97	0.06	11,12,13,15	0
6	DAN	D	508	20/20	0.97	0.06	12,13,14,15	0
6	DAN	A	511	20/20	0.97	0.06	12,13,15,16	0
8	CA	A	514	1/1	0.99	0.06	22,22,22,22	0
8	CA	B	514	1/1	0.99	0.07	22,22,22,22	0
8	CA	B	515	1/1	0.99	0.20	32,32,32,32	0
8	CA	C	512	1/1	0.99	0.09	21,21,21,21	0
8	CA	D	511	1/1	0.99	0.08	23,23,23,23	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.

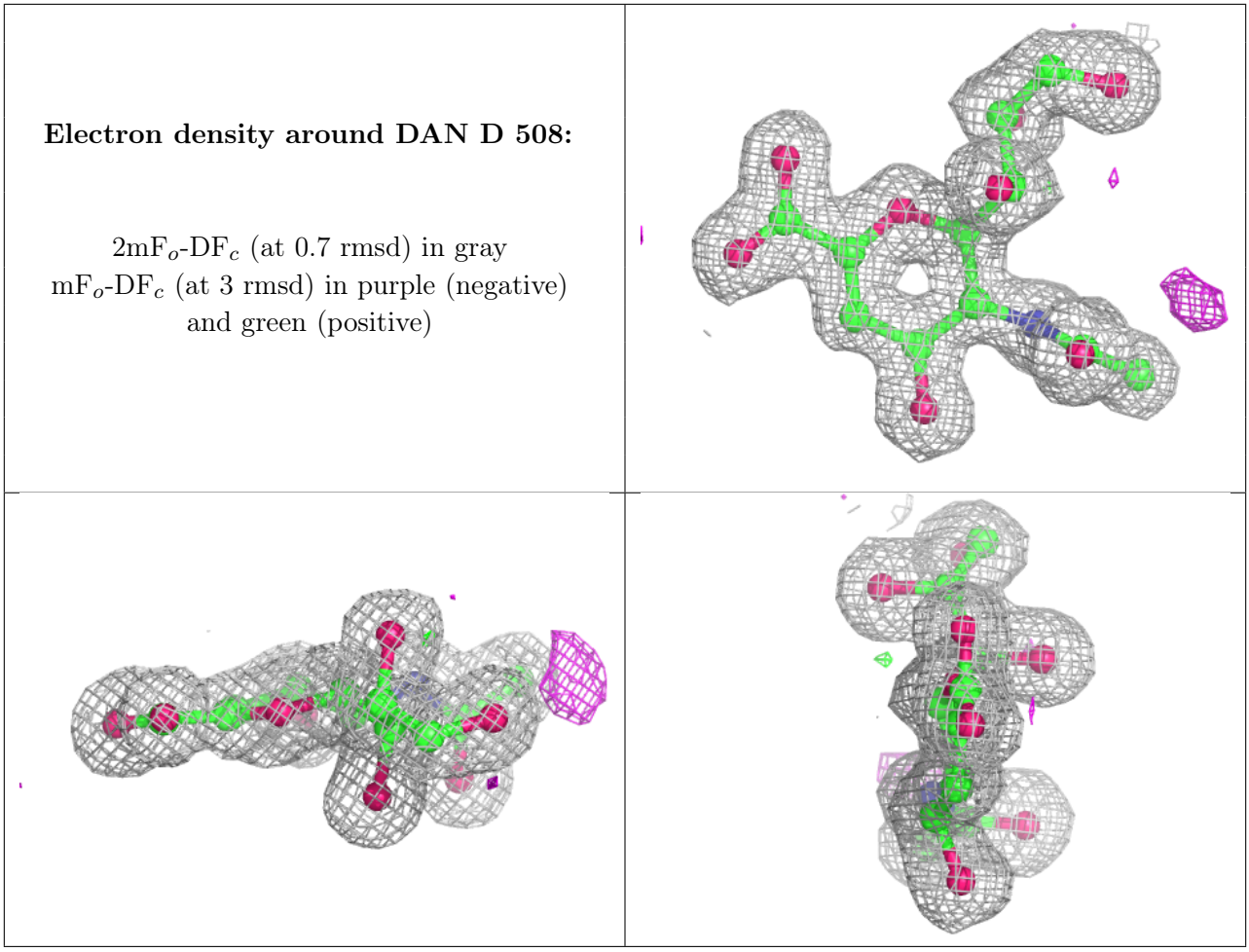
Electron density around DAN B 510:

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



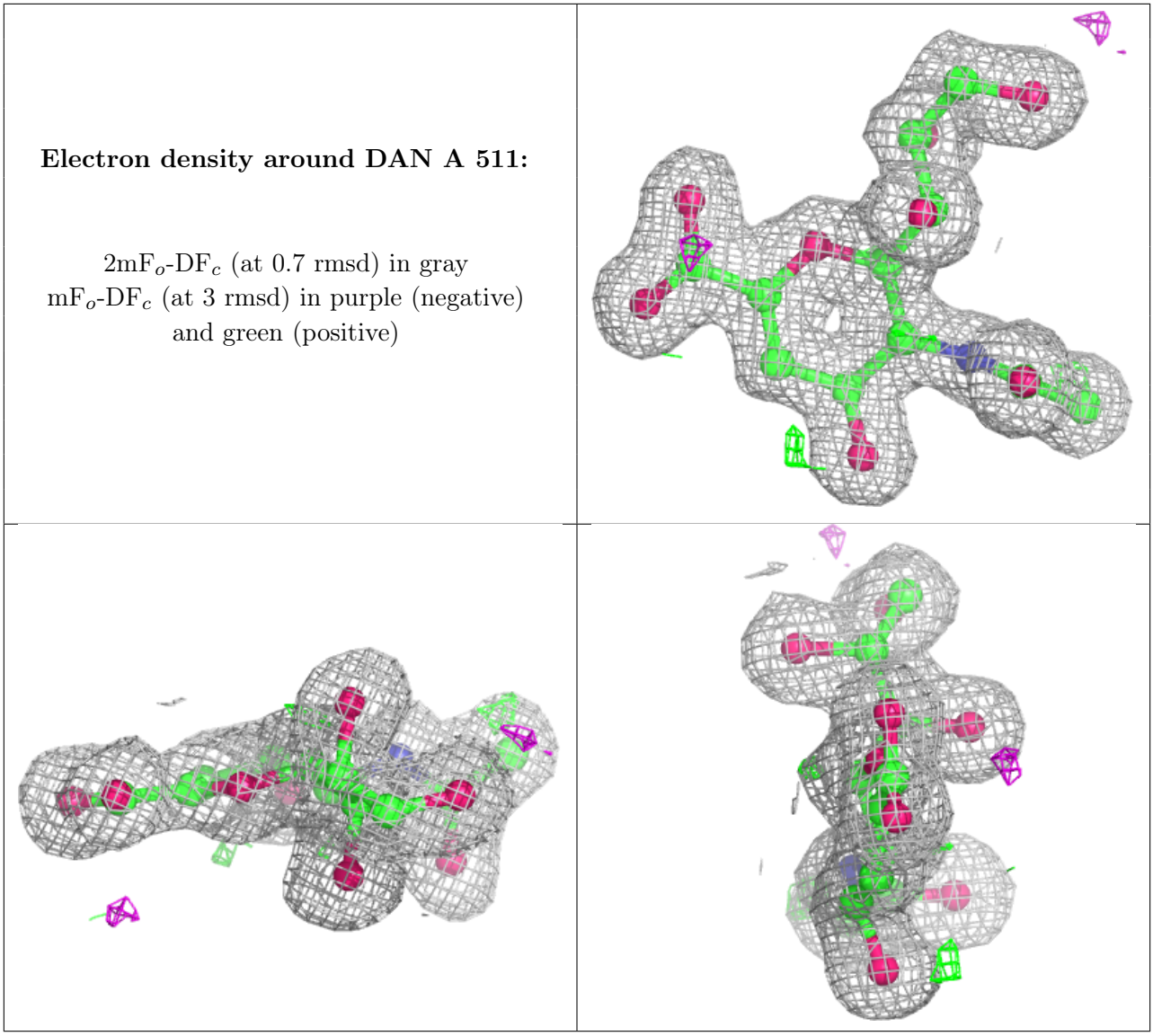
Electron density around DAN D 508:

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



Electron density around DAN A 511:

$2mF_o$-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.