wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 10:48 AM EST

PDB ID	:	6NAJ
Title	:	Integrin AlphaVBeta3 ectodomain bound to Hr10 variant of the 10th domain of Fibronectin.
Authors	:	van Agthoven, J.; Arnaout, M.A.
Deposited on	:	2018-12-05
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

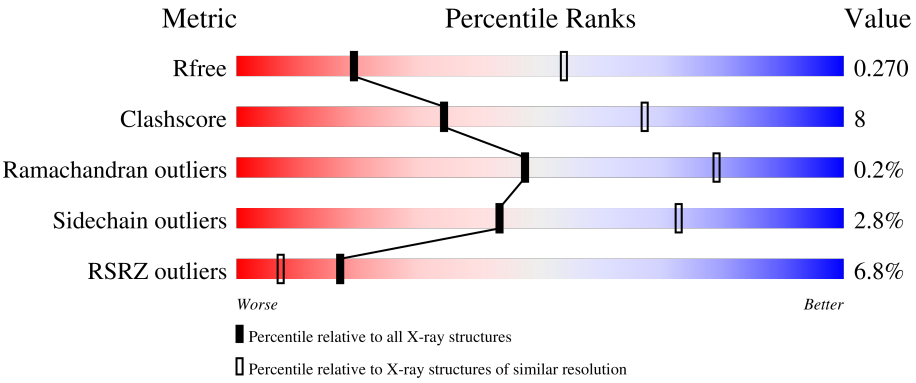
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	954	2% 77% 18%
2	B	690	10% 78% 21%
3	C	90	36% 70% 26%
4	D	2	100%
4	F	2	50% 50%

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

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
4	NAG	F	2	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13500 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	920	7163	4535	1216	1377	35	0	0	0

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	690	5294	3250	904	1070	70	0	0	0

- Molecule 3 is a protein called Fibronectin, HR10 variant.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	90	680	433	110	137	0	0	0

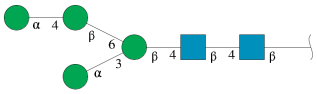
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1492	PRO	GLY	conflict	UNP P02751
C	?	-	SER	deletion	UNP P02751
C	1496	TRP	PRO	conflict	UNP P02751
C	1497	ASN	ALA	conflict	UNP P02751
C	1498	GLU	SER	conflict	UNP P02751
C	1499	GLY	SER	conflict	UNP P02751
C	1500	GLY	LYS	conflict	UNP P02751

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

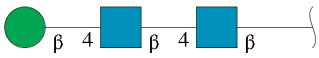
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-beta-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.



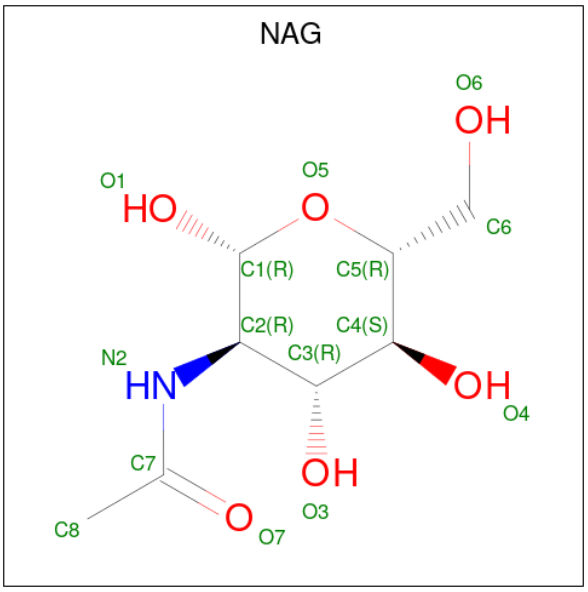
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called 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
6	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	5	Total Mn 5 5	0	0
8	B	3	Total Mn 3 3	0	0

- Molecule 9 is water.

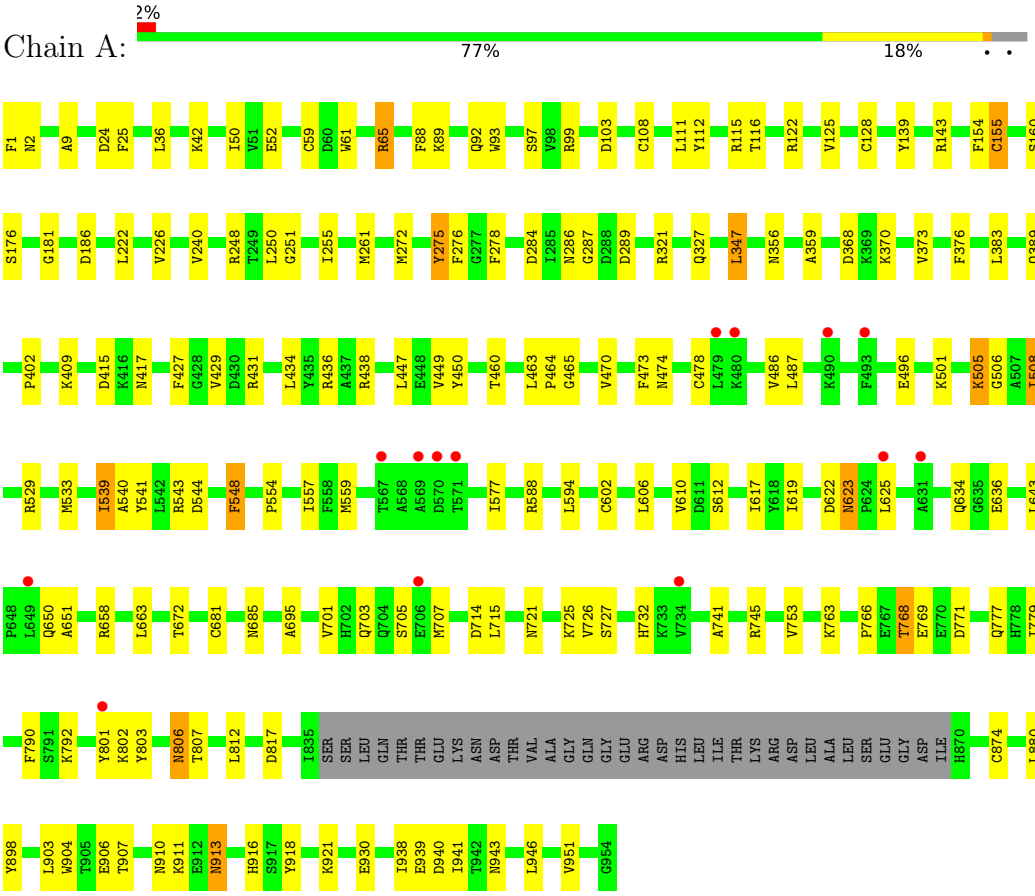
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total O 2 2	0	0
9	B	3	Total O 3 3	0	0
9	C	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

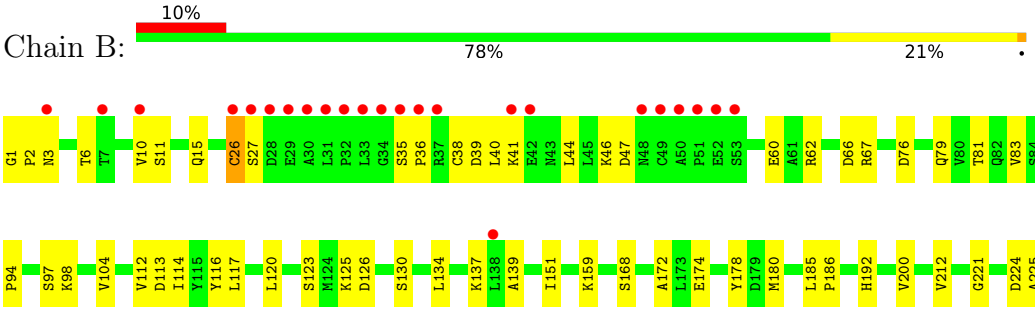
• Molecule 1: Integrin alpha-V

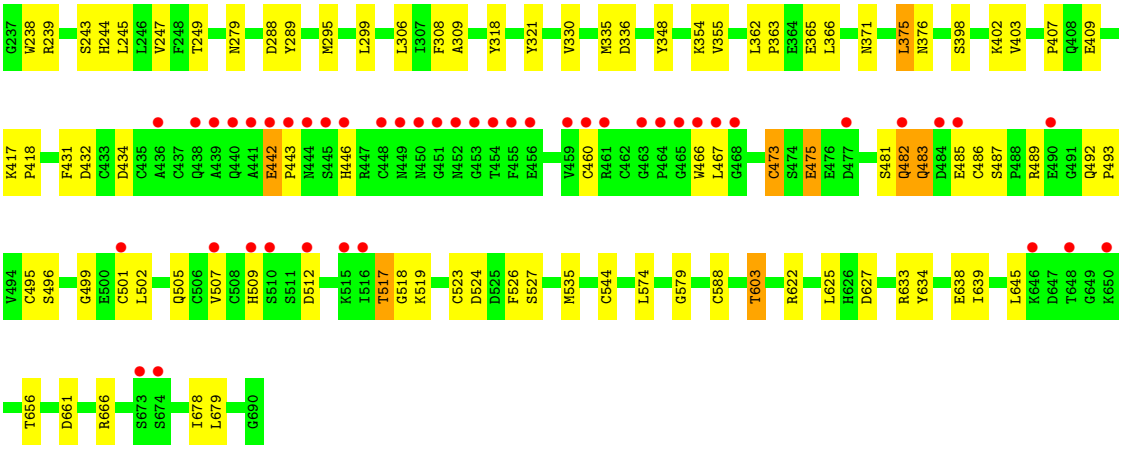
Chain A:



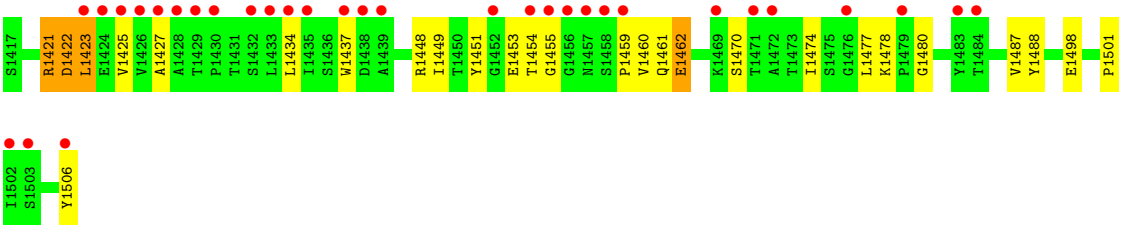
• Molecule 2: Integrin beta-3

Chain B:

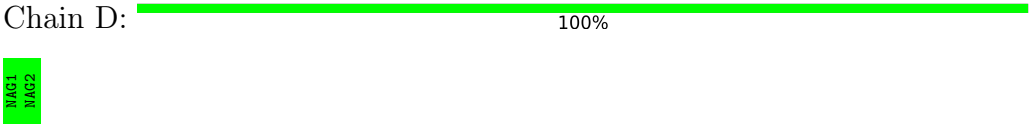




• Molecule 3: Fibronectin, HR10 variant

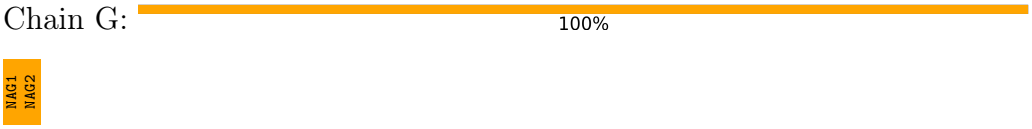


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

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

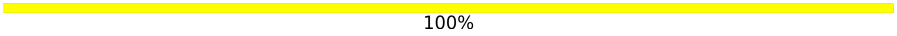


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

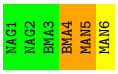
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



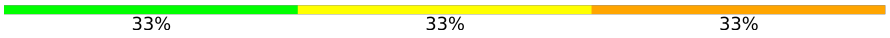
• Molecule 5: alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.71Å 129.71Å 308.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.62 – 3.10 49.62 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.9 (49.62-3.10) 90.9 (49.62-3.10)	Depositor EDS
R_{merge}	9.70	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.76 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.238 , 0.268 0.239 , 0.270	Depositor DCC
R_{free} test set	2459 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	13500	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 2.33% 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: HRG, MN, MAN, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/7319	0.50	0/9922
2	B	0.25	0/5390	0.51	0/7289
3	C	0.28	0/685	0.57	1/943 (0.1%)
All	All	0.25	0/13394	0.50	1/18154 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	5
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1423	LEU	CA-CB-CG	5.88	128.82	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	ILE	Peptide
2	B	442	GLU	Peptide
2	B	481	SER	Peptide
2	B	482	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	76	ASP	Peptide

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	7163	0	6982	109	0
2	B	5294	0	5024	94	0
3	C	680	0	659	17	0
4	D	28	0	25	0	0
4	F	28	0	25	3	0
4	G	28	0	25	1	0
4	H	28	0	25	0	0
4	J	28	0	25	0	0
5	E	72	0	61	1	0
6	I	39	0	34	1	0
7	A	70	0	65	1	0
7	B	28	0	26	1	0
8	A	5	0	0	0	0
8	B	3	0	0	0	0
9	A	2	0	0	0	0
9	B	3	0	0	0	0
9	C	1	0	0	0	0
All	All	13500	0	12976	221	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 8.

The worst 5 of 221 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)
2:B:375:LEU:HD13	2:B:633:ARG:HD2	1.66	0.78
1:A:619:ILE:HG23	1:A:703:GLN:HG3	1.67	0.77
2:B:114:ILE:HG22	2:B:245:LEU:HB2	1.69	0.74
2:B:67:ARG:HH21	2:B:86:GLN:HG2	1.52	0.74
2:B:174:GLU:HA	2:B:186:PRO:HG3	1.72	0.72

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	916/954 (96%)	857 (94%)	59 (6%)	0	100 100
2	B	688/690 (100%)	607 (88%)	77 (11%)	4 (1%)	25 59
3	C	87/90 (97%)	72 (83%)	15 (17%)	0	100 100
All	All	1691/1734 (98%)	1536 (91%)	151 (9%)	4 (0%)	47 79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	473	CYS
2	B	482	GLN
2	B	483	GLN
2	B	443	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	780/809 (96%)	757 (97%)	23 (3%)	42 72
2	B	612/612 (100%)	600 (98%)	12 (2%)	55 80
3	C	74/74 (100%)	68 (92%)	6 (8%)	11 39
All	All	1466/1495 (98%)	1425 (97%)	41 (3%)	43 73

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	376	ASN
3	C	1421	ARG
2	B	460	CYS
2	B	501	CYS
3	C	1423	LEU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HRG	C	1493	3	10,11,12	0.75	0	6,12,14	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HRG	C	1493	3	-	4/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1493	HRG	O-C-CA-CB
3	C	1493	HRG	NH1-CZ-NE-CD
3	C	1493	HRG	NH2-CZ-NE-CD
3	C	1493	HRG	CD-CG-CG'-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

19 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	$\#\|Z\|>2$
4	NAG	D	1	1,4	14,14,15	0.32	0	17,19,21	0.39	0
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	E	1	1,5	14,14,15	0.27	0	17,19,21	0.37	0
5	NAG	E	2	5	14,14,15	0.23	0	17,19,21	0.39	0
5	BMA	E	3	5	11,11,12	0.71	0	15,15,17	0.84	0
5	BMA	E	4	5	11,11,12	1.24	2 (18%)	15,15,17	1.08	1 (6%)
5	MAN	E	5	5	11,11,12	0.96	1 (9%)	15,15,17	0.87	1 (6%)
5	MAN	E	6	5	11,11,12	0.67	0	15,15,17	1.10	2 (13%)
4	NAG	F	1	1,4	14,14,15	0.44	0	17,19,21	1.34	3 (17%)
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	0.69	1 (5%)
4	NAG	G	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	H	1	2,4	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	H	2	4	14,14,15	0.89	1 (7%)	17,19,21	0.89	1 (5%)
6	NAG	I	1	2,6	14,14,15	0.20	0	17,19,21	0.46	0
6	NAG	I	2	6	14,14,15	0.61	1 (7%)	17,19,21	1.35	1 (5%)
6	BMA	I	3	6	11,11,12	0.80	0	15,15,17	1.14	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	J	1	2,4	14,14,15	0.63	1 (7%)	17,19,21	1.36	1 (5%)
4	NAG	J	2	4	14,14,15	0.23	0	17,19,21	1.28	1 (5%)

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

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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NAG	O5-C1	2.59	1.47	1.43
5	E	5	MAN	O5-C1	-2.45	1.39	1.43
5	E	4	BMA	C4-C5	2.34	1.58	1.53
4	G	2	NAG	O5-C1	2.27	1.47	1.43
4	J	1	NAG	O5-C1	2.21	1.47	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1	NAG	C1-O5-C5	4.85	118.77	112.19
4	J	2	NAG	C1-O5-C5	4.51	118.30	112.19
4	F	1	NAG	C2-N2-C7	4.34	129.09	122.90
6	I	2	NAG	C2-N2-C7	4.23	128.92	122.90
4	G	2	NAG	C1-O5-C5	3.63	117.11	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6

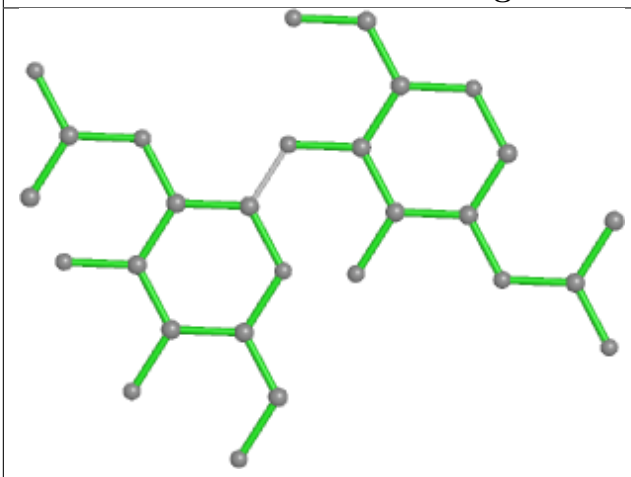
There are no ring outliers.

7 monomers are involved in 6 short contacts:

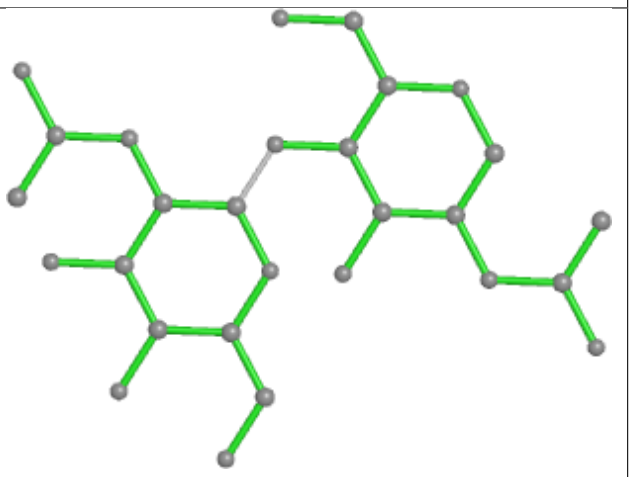
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	3	0
4	G	2	NAG	1	0
5	E	5	MAN	1	0
4	F	2	NAG	1	0
4	G	1	NAG	1	0
6	I	2	NAG	1	0
5	E	4	BMA	1	0

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

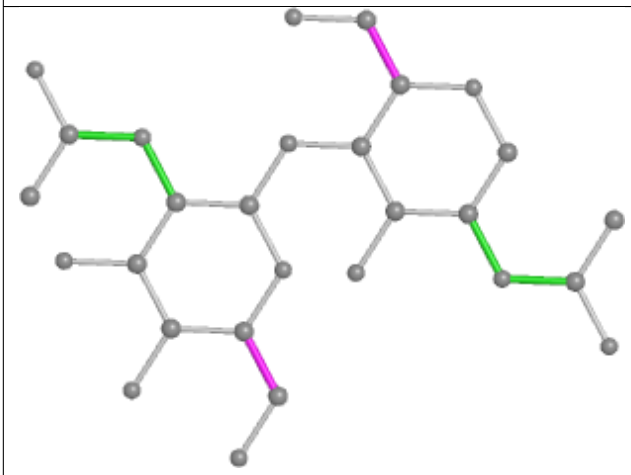
Oligosaccharide Chain D



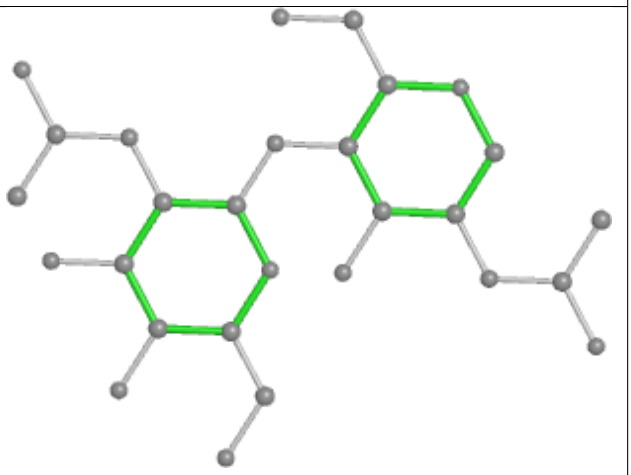
Bond lengths



Bond angles

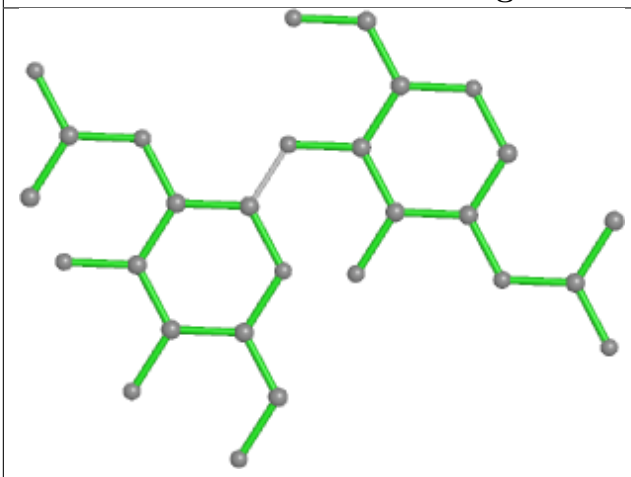


Torsions

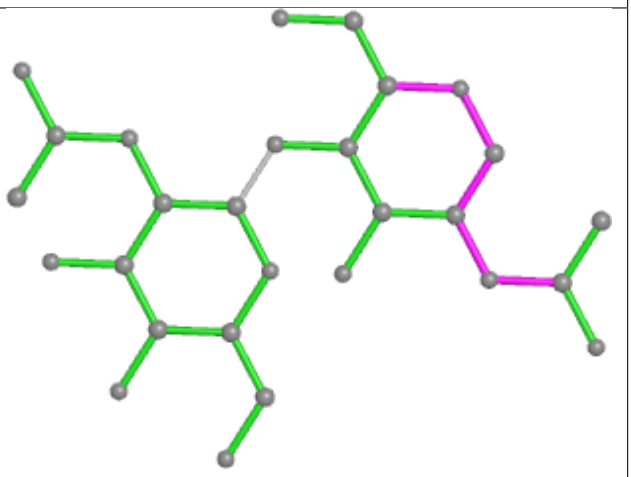


Rings

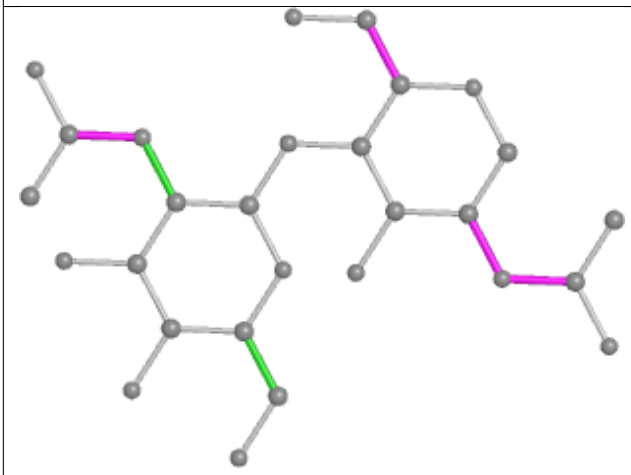
Oligosaccharide Chain F



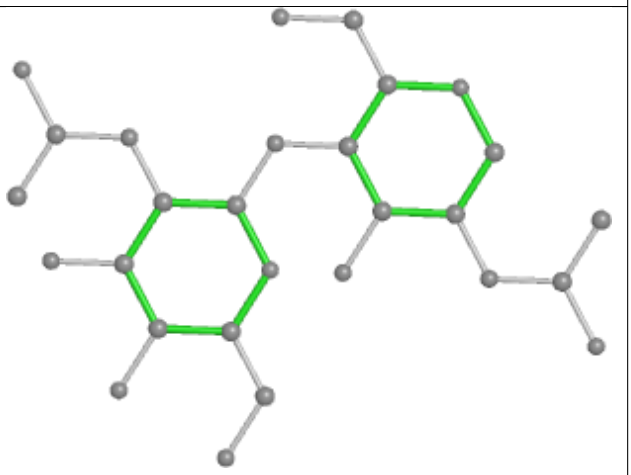
Bond lengths



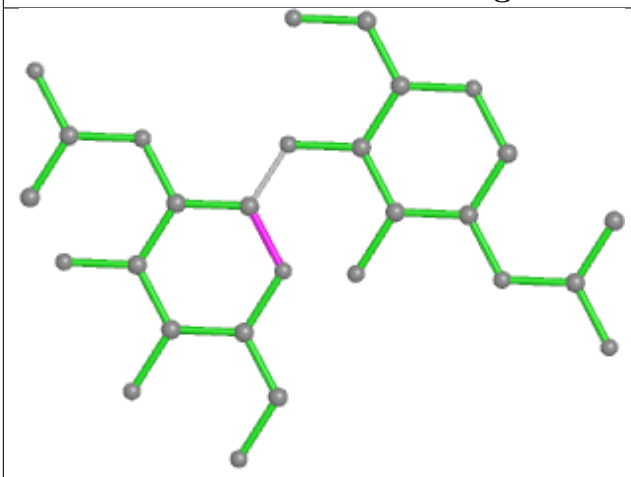
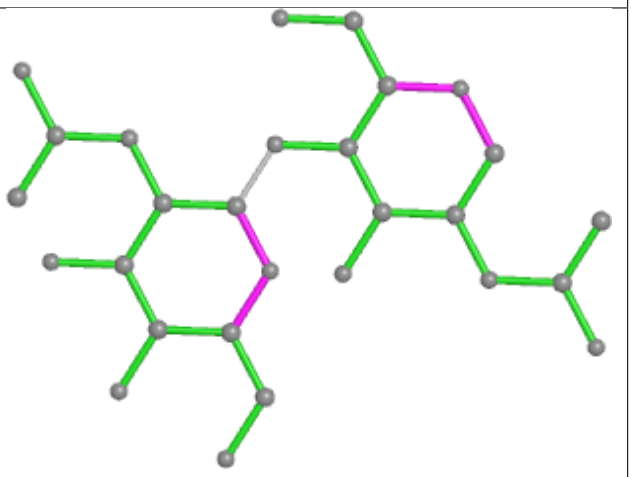
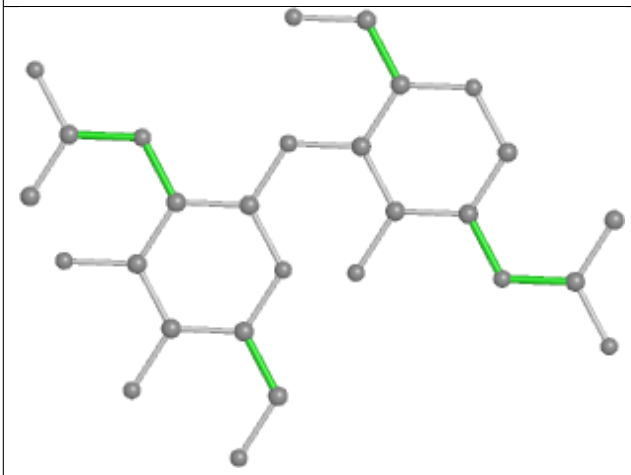
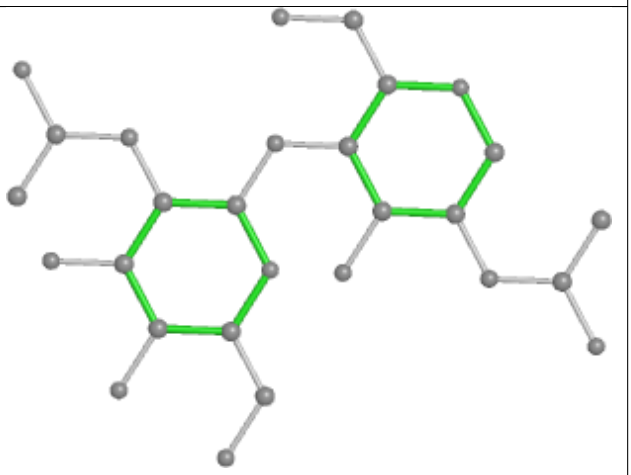
Bond angles



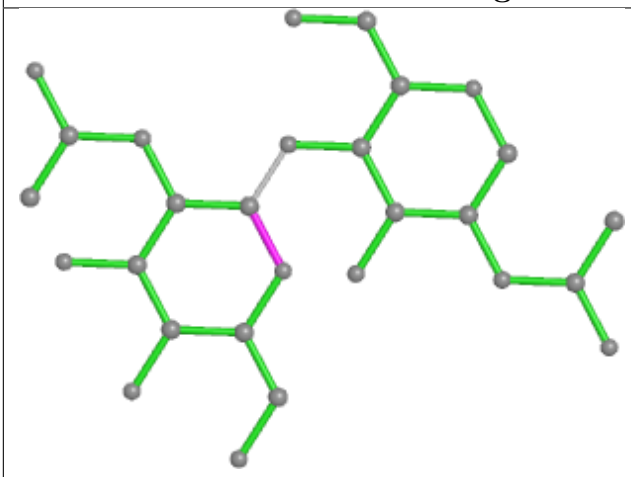
Torsions



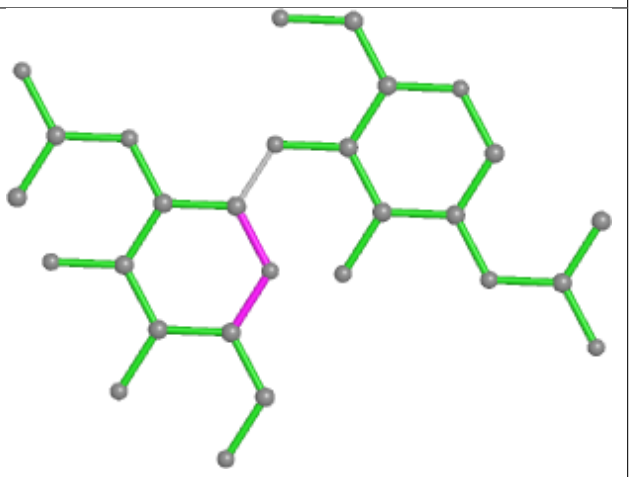
Rings

Oligosaccharide Chain G	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

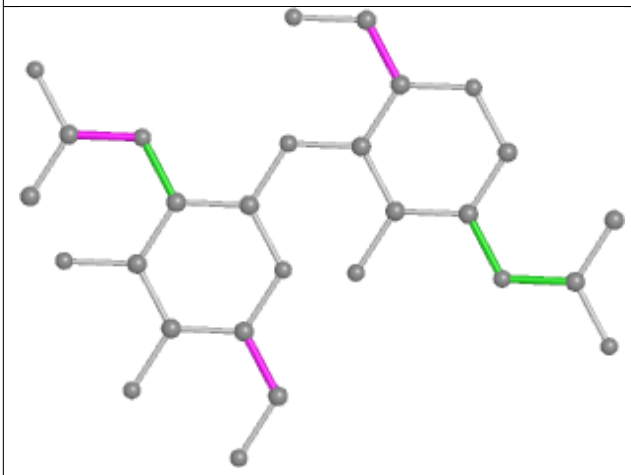
Oligosaccharide Chain H



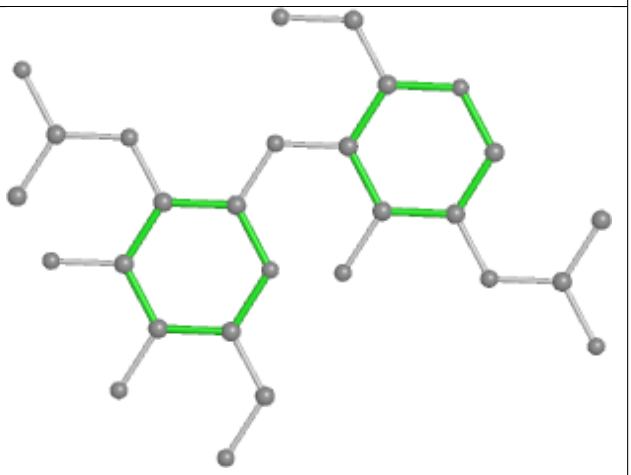
Bond lengths



Bond angles

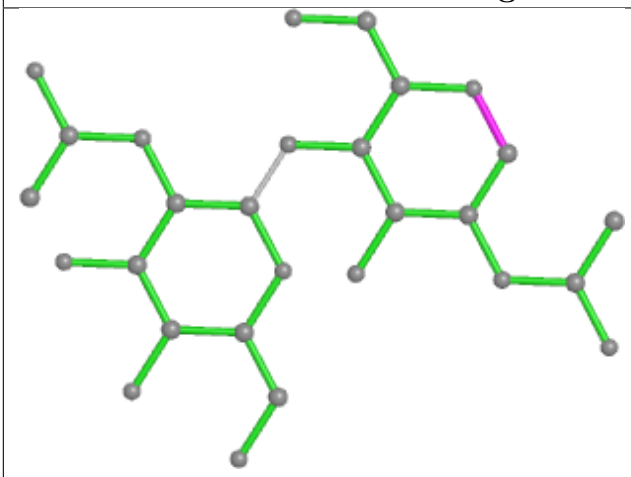


Torsions

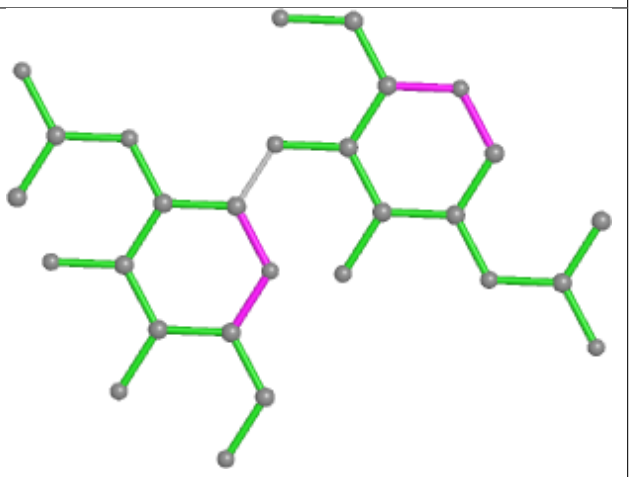


Rings

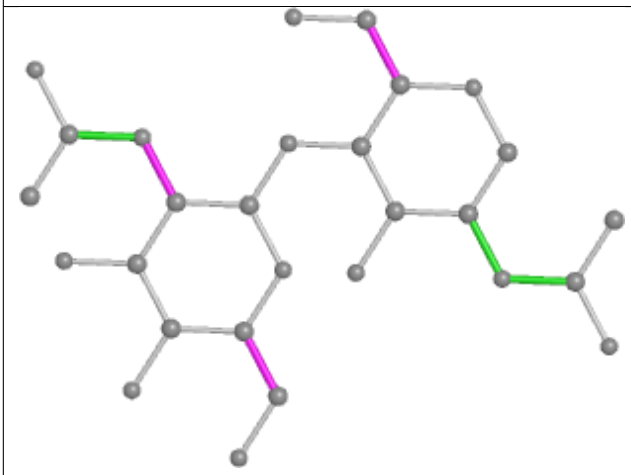
Oligosaccharide Chain J



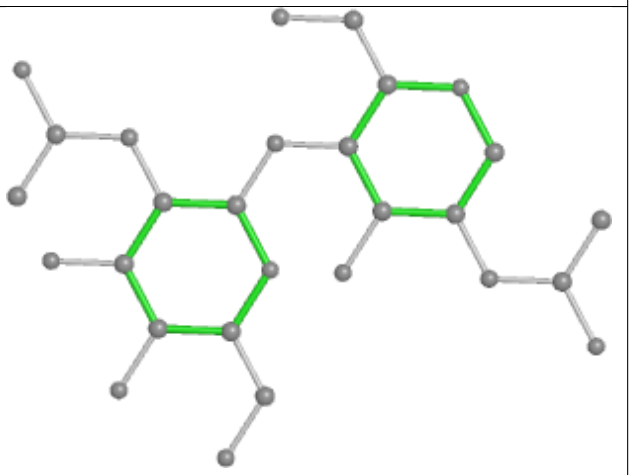
Bond lengths



Bond angles

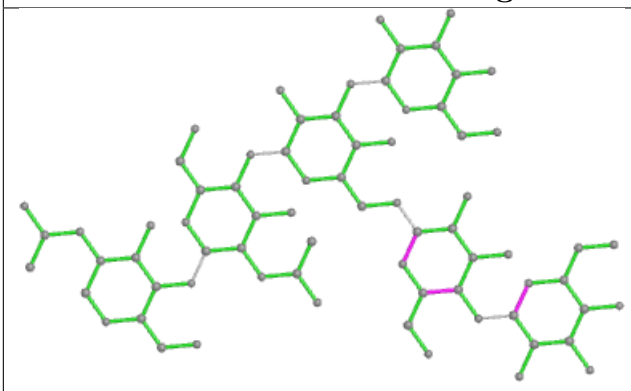


Torsions

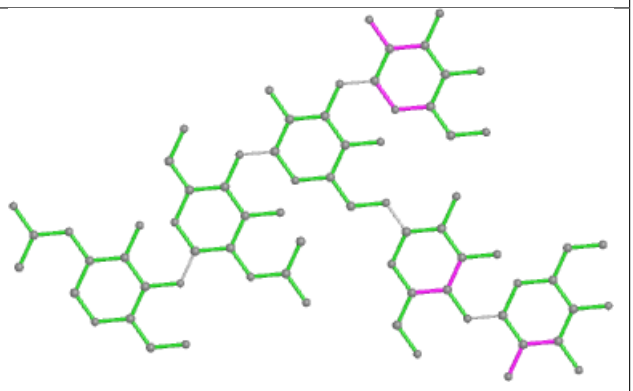


Rings

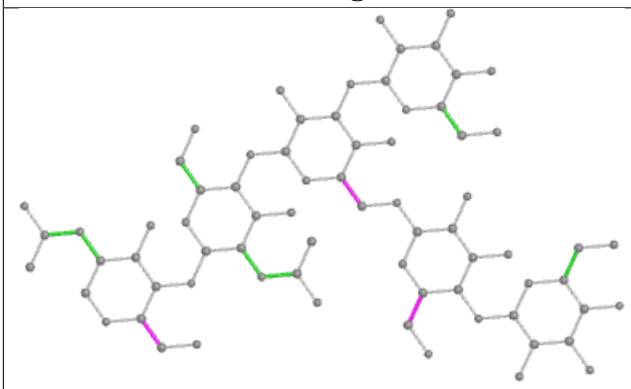
Oligosaccharide Chain E



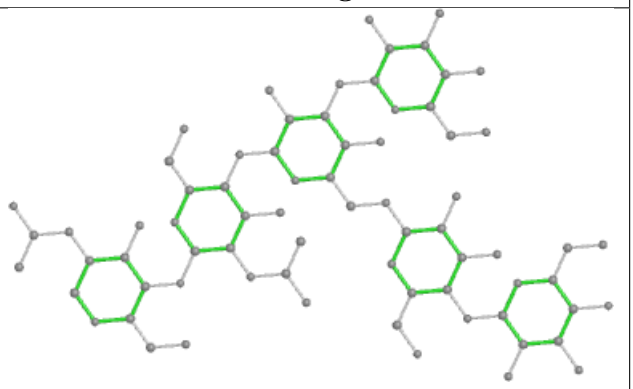
Bond lengths



Bond angles

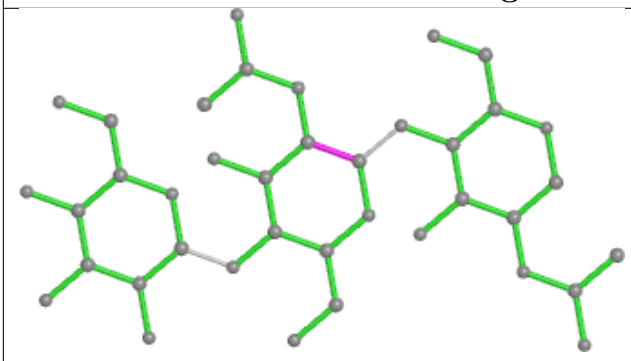


Torsions

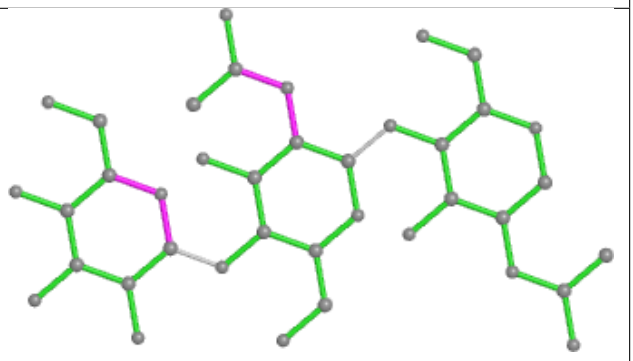


Rings

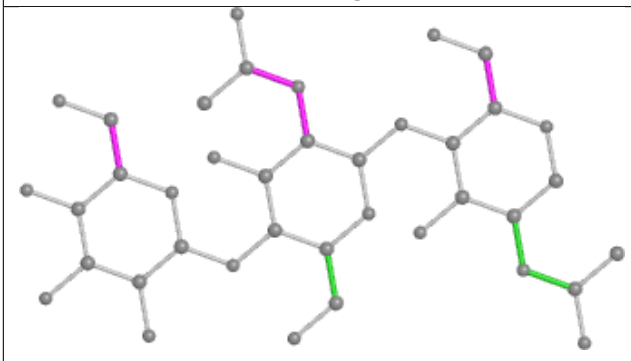
Oligosaccharide Chain I



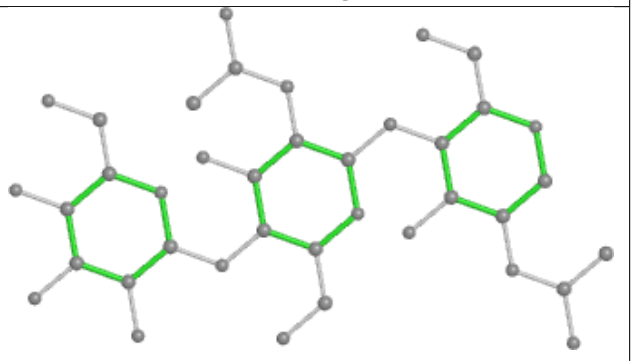
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	NAG	A	1004	1	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	A	1002	1	14,14,15	0.44	0	17,19,21	1.25	1 (5%)
7	NAG	B	702	2	14,14,15	0.20	0	17,19,21	0.47	0
7	NAG	B	701	2	14,14,15	0.64	0	17,19,21	0.84	1 (5%)
7	NAG	A	1001	1	14,14,15	0.86	1 (7%)	17,19,21	1.27	1 (5%)
7	NAG	A	1005	1	14,14,15	0.19	0	17,19,21	0.42	0
7	NAG	A	1003	1	14,14,15	0.23	0	17,19,21	0.47	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
7	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1002	1	-	3/6/23/26	0/1/1/1
7	NAG	B	702	2	-	2/6/23/26	0/1/1/1
7	NAG	B	701	2	-	2/6/23/26	0/1/1/1
7	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1005	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1003	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	NAG	O5-C1	3.08	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1001	NAG	C1-O5-C5	5.02	119.00	112.19
7	A	1002	NAG	C2-N2-C7	4.34	129.08	122.90
7	B	701	NAG	C1-O5-C5	3.26	116.61	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	702	NAG	O5-C5-C6-O6
7	A	1001	NAG	O5-C5-C6-O6
7	B	702	NAG	C4-C5-C6-O6
7	A	1001	NAG	C4-C5-C6-O6
7	A	1002	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1002	NAG	1	0
7	B	702	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	920/954 (96%)	-0.02	15 (1%) 72 51	22, 56, 111, 148	0
2	B	690/690 (100%)	0.41	69 (10%) 7 2	29, 77, 159, 204	2 (0%)
3	C	89/90 (98%)	1.67	32 (35%) 0 0	57, 110, 144, 159	0
All	All	1699/1734 (97%)	0.25	116 (6%) 17 7	22, 67, 141, 204	2 (0%)

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	36	PRO	8.1
3	C	1427	ALA	6.7
3	C	1428	ALA	6.2
2	B	35	SER	5.8
2	B	37	ARG	5.8

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

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
3	HRG	C	1493	12/13	0.91	0.23	55,57,61,62	0

6.3 Carbohydrates

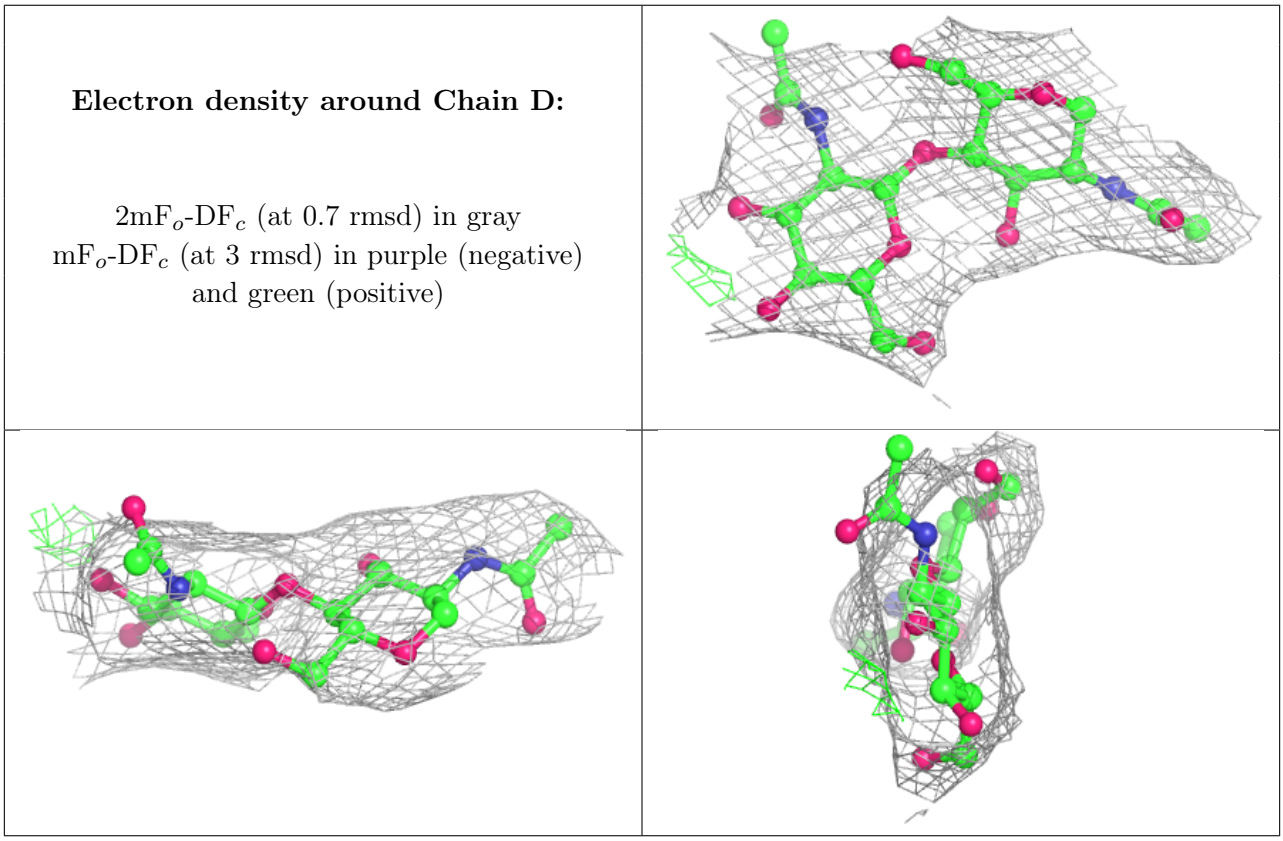
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NAG	G	2	14/15	0.60	0.35	65,94,122,126	0
6	BMA	I	3	11/12	0.69	0.21	67,95,109,113	0
4	NAG	F	2	14/15	0.75	0.43	82,111,123,127	0
4	NAG	G	1	14/15	0.75	0.26	41,78,95,115	0
4	NAG	F	1	14/15	0.77	0.29	78,95,105,111	0
4	NAG	J	2	14/15	0.79	0.31	66,117,129,133	0
4	NAG	J	1	14/15	0.80	0.30	83,90,120,126	0
4	NAG	H	2	14/15	0.81	0.27	95,104,114,116	0
5	MAN	E	6	11/12	0.83	0.24	72,81,97,97	0
5	MAN	E	5	11/12	0.85	0.24	62,81,96,105	0
5	BMA	E	4	11/12	0.87	0.14	73,77,88,94	0
6	NAG	I	2	14/15	0.88	0.30	92,104,114,130	0
4	NAG	H	1	14/15	0.89	0.22	84,92,102,105	0
4	NAG	D	2	14/15	0.90	0.20	61,70,92,107	0
5	BMA	E	3	11/12	0.92	0.13	65,73,80,88	0
5	NAG	E	2	14/15	0.92	0.18	29,45,67,83	0
6	NAG	I	1	14/15	0.93	0.14	70,86,96,102	0
4	NAG	D	1	14/15	0.95	0.15	33,46,65,79	0
5	NAG	E	1	14/15	0.96	0.17	29,34,42,58	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.

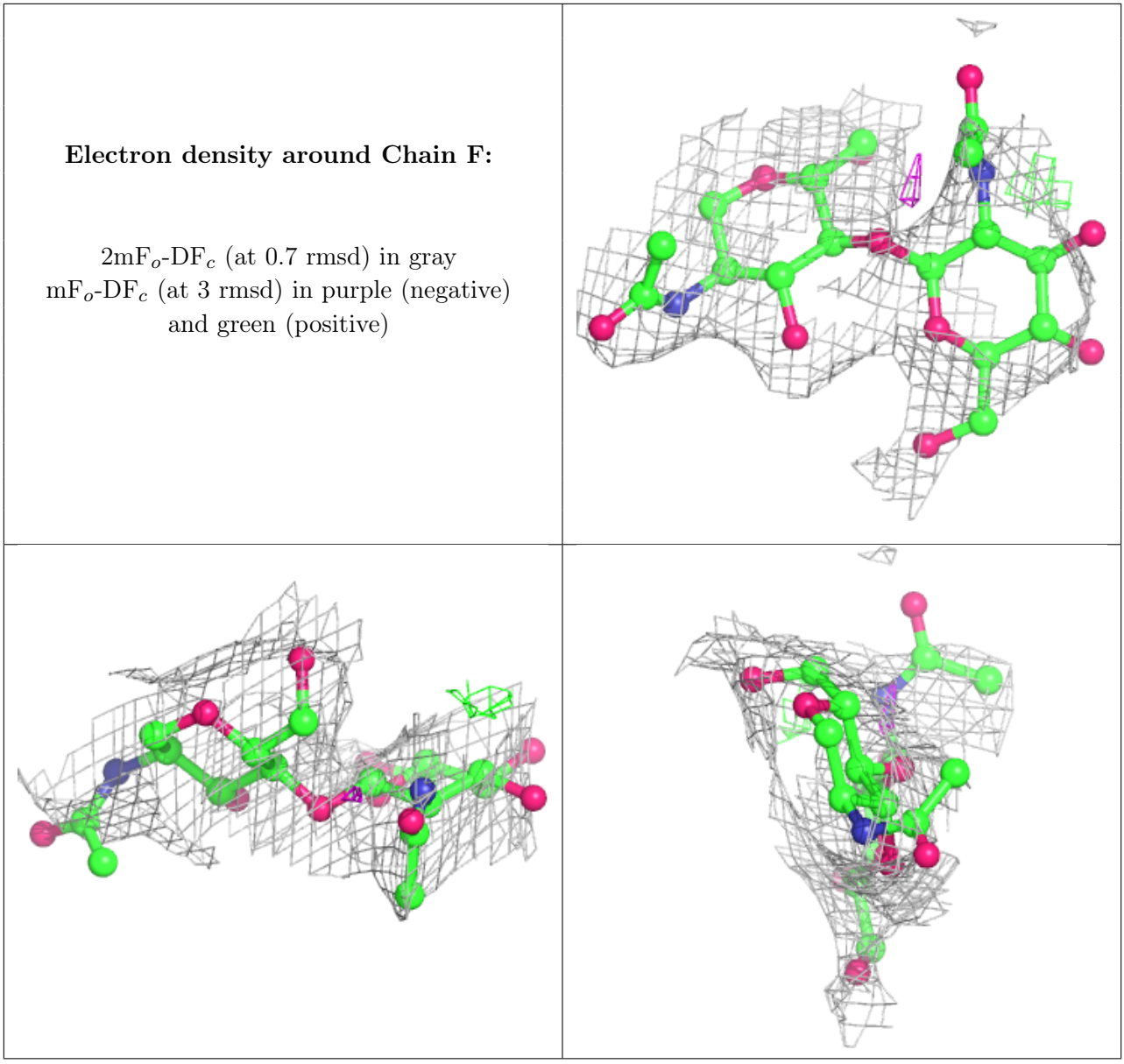
Electron density around Chain D:

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



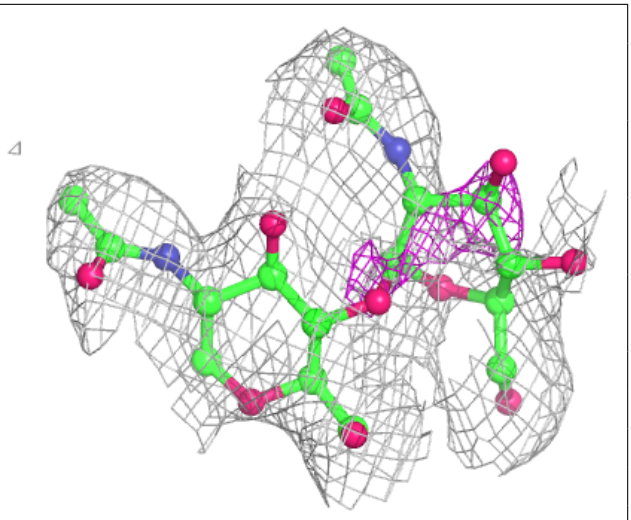
Electron density around Chain F:

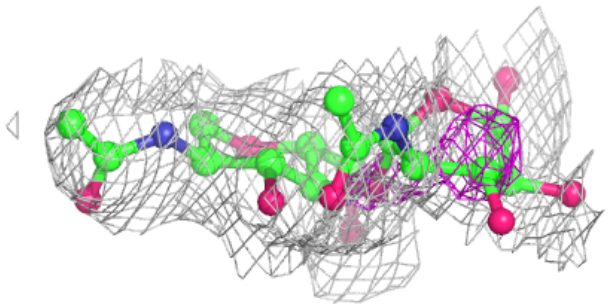
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

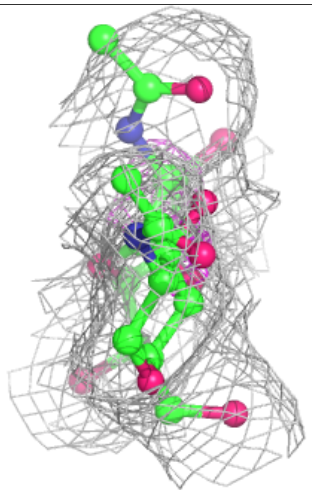


Electron density around Chain G:

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

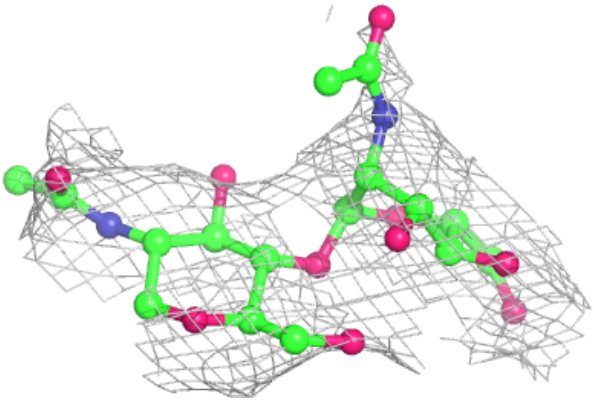


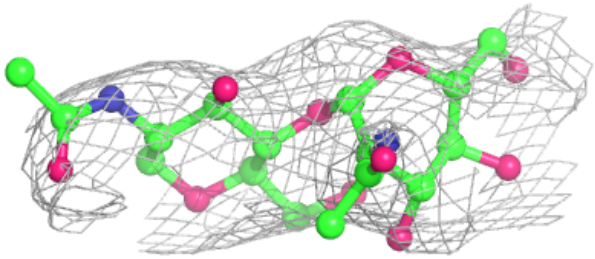


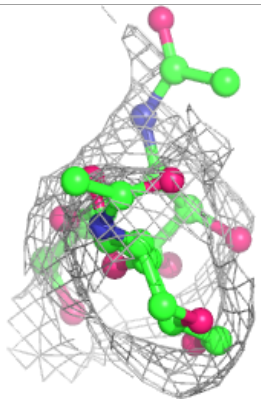


Electron density around Chain H:

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

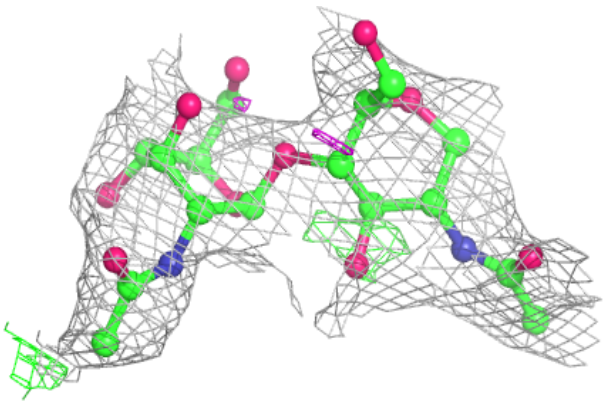


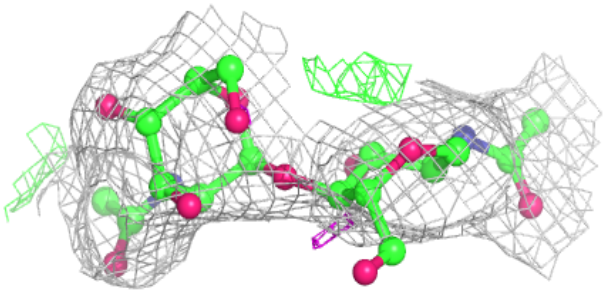




Electron density around Chain J:

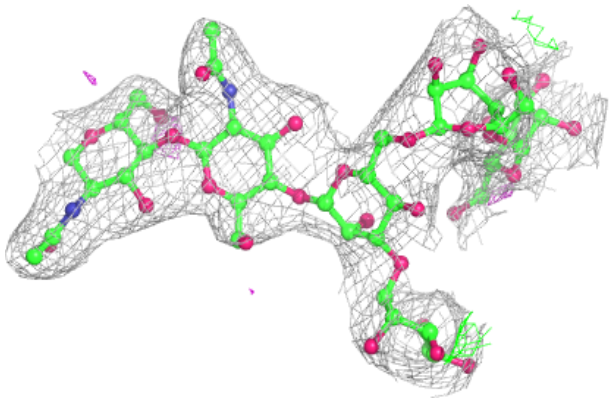
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

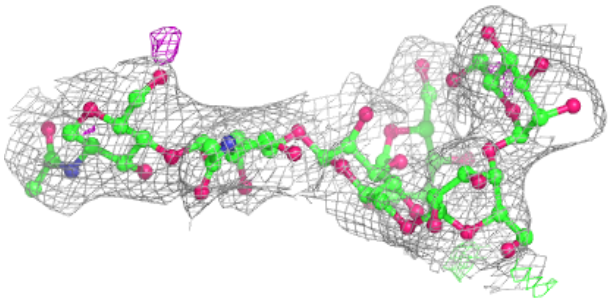


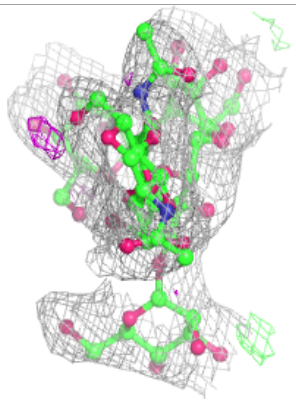


Electron density around Chain E:

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

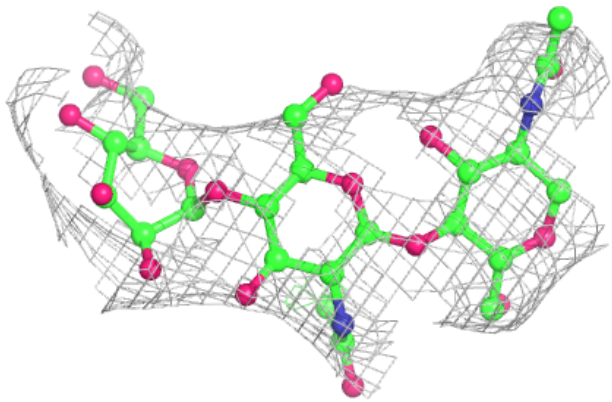


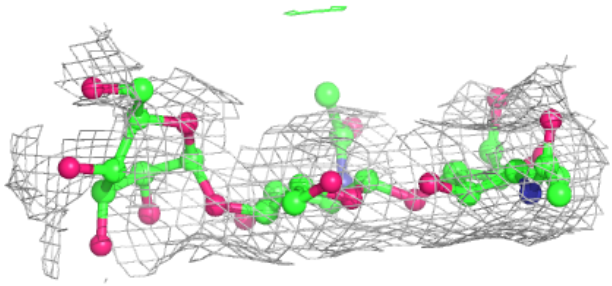


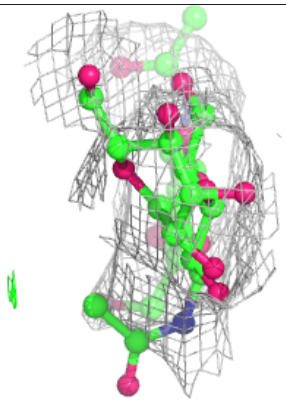


Electron density around Chain I:

$2mF_o$-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
7	NAG	A	1003	14/15	0.76	0.35	90,105,115,117	0
7	NAG	B	701	14/15	0.77	0.38	81,103,112,114	0
7	NAG	A	1001	14/15	0.79	0.26	67,80,93,97	0
7	NAG	B	702	14/15	0.81	0.22	62,85,95,100	0
7	NAG	A	1002	14/15	0.82	0.19	66,90,96,100	0
7	NAG	A	1004	14/15	0.82	0.24	60,79,92,106	0
7	NAG	A	1005	14/15	0.88	0.19	56,65,81,82	0
8	MN	A	1009	1/1	0.92	0.17	115,115,115,115	0
8	MN	B	704	1/1	0.94	0.18	70,70,70,70	0
8	MN	A	1010	1/1	0.95	0.13	70,70,70,70	0
8	MN	A	1008	1/1	0.97	0.17	72,72,72,72	0
8	MN	A	1006	1/1	0.98	0.12	68,68,68,68	0
8	MN	A	1007	1/1	0.98	0.16	69,69,69,69	0
8	MN	B	703	1/1	0.99	0.20	55,55,55,55	0
8	MN	B	705	1/1	0.99	0.21	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.