wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 03:06 AM EDT

PDB ID	:	1FZD
Title	:	STRUCTURE OF RECOMBINANT ALPHAEC DOMAIN FROM HUMAN FIBRINOGEN-420
Authors	:	Spraggon, G.; Applegate, D.; Everse, S.J.; Zhang, J.-Z.; Veerapandian, L.; Redman, C.; Doolittle, R.F.; Grieninger, G.
Deposited on	:	1998-06-22
Resolution	:	2.10 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:

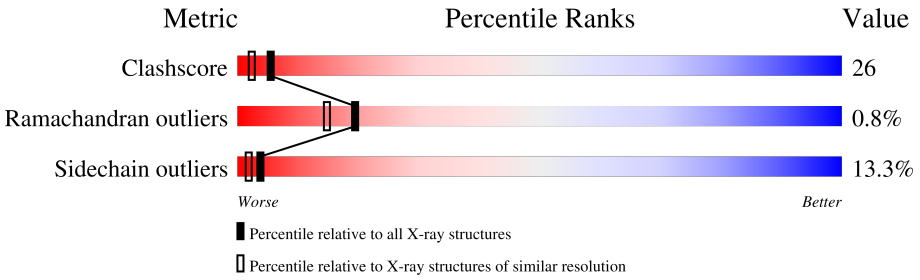
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	201	69% 19% 7%
1	B	201	73% 15% 7%
1	C	201	71% 20%
1	D	201	71% 20%
1	E	201	61% 28% 7%
1	F	201	63% 26% 8%
1	G	201	60% 30% 6%
1	H	201	55% 33% 8%

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Mol	Chain	Length	Quality of chain
2	I	6	33% 67%
2	K	6	17% 17% 67%
2	L	6	50% 50%
3	J	6	17% 83%
4	M	2	50% 50%
4	N	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	I	3	X	-	X	-
2	MAN	I	4	-	-	X	-
2	MAN	I	6	-	-	X	-
2	MAN	K	3	X	-	X	-
2	MAN	K	4	-	-	X	-
2	NAG	K	5	-	-	X	-
2	MAN	K	6	X	-	-	-
2	NAG	L	1	-	X	-	-
2	MAN	L	4	-	-	X	-
2	NAG	L	5	-	-	X	-
2	MAN	L	6	X	-	-	-
3	NAG	J	1	-	X	-	-
3	MAN	J	3	X	-	X	-
3	MAN	J	4	-	-	X	-
3	NAG	J	5	-	-	X	-
4	NAG	M	1	-	X	X	-
6	NAG	G	10	-	-	X	-
6	NAG	G	11	-	-	X	-
6	NAG	H	10	-	-	X	-
6	NAG	H	11	-	-	X	-

2 Entry composition (i)

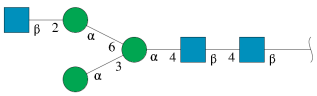
There are 7 unique types of molecules in this entry. The entry contains 13595 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FIBRINOGEN-420.

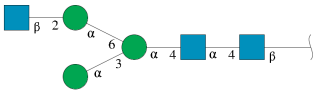
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	B	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	C	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	D	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	E	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	F	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	G	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	H	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-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
2	I	6	Total	C	N	O	0	0	0
			75	42	3	30			
2	K	6	Total	C	N	O	0	0	0
			75	42	3	30			
2	L	6	Total	C	N	O	0	0	0
			75	42	3	30			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	J	6	Total C N O 74 42 3 29	0	0	0

- 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	M	2	Total C N O 28 16 2 10	0	0	0
4	N	2	Total C N O 28 16 2 10	1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0
5	G	1	Total Ca 1 1	0	0

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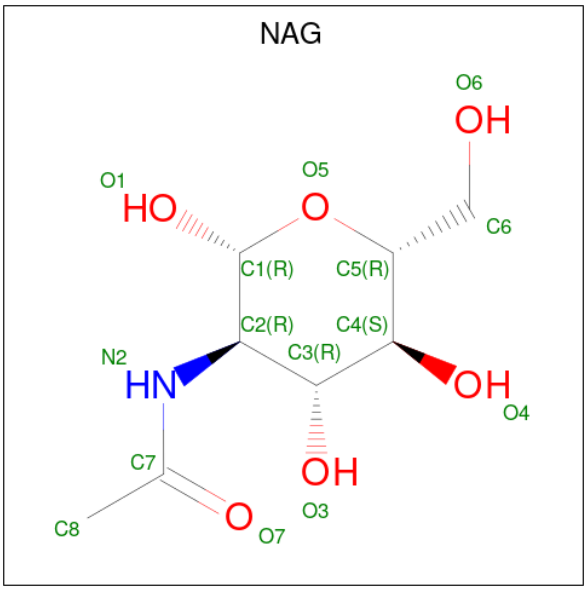
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Ca 1 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	H	1	Total C N O 14 8 1 5	0	0
6	H	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	B	76	Total O 76 76	0	0
7	C	71	Total O 71 71	0	0
7	D	74	Total O 74 74	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	52	Total O 52 52	0	0
7	F	63	Total O 63 63	0	0
7	G	56	Total O 56 56	0	0
7	H	34	Total O 34 34	0	0

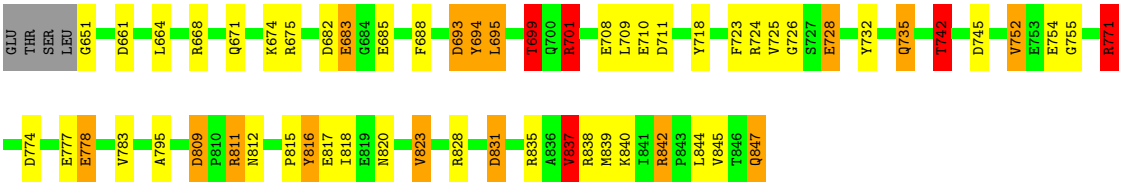
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

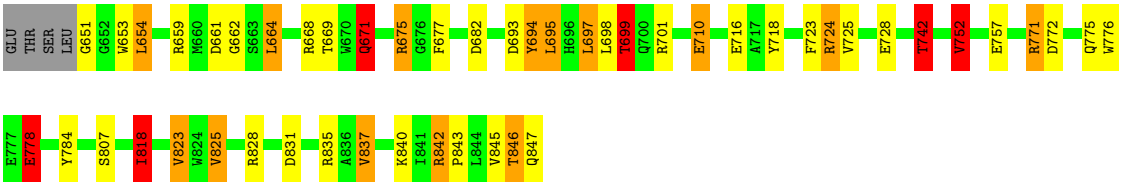
• Molecule 1: FIBRINOGEN-420

Chain A:



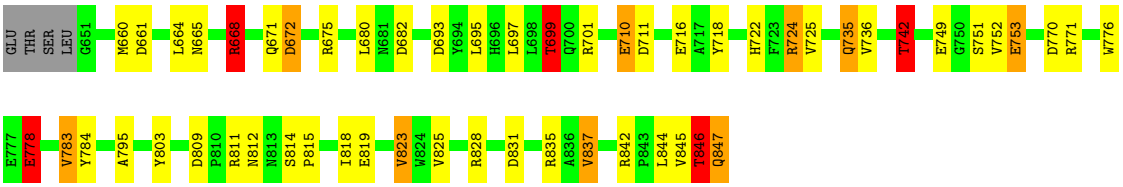
• Molecule 1: FIBRINOGEN-420

Chain B:



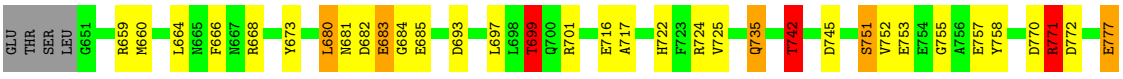
• Molecule 1: FIBRINOGEN-420

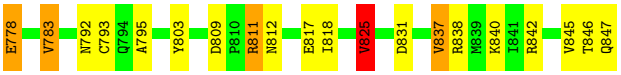
Chain C:



• Molecule 1: FIBRINOGEN-420

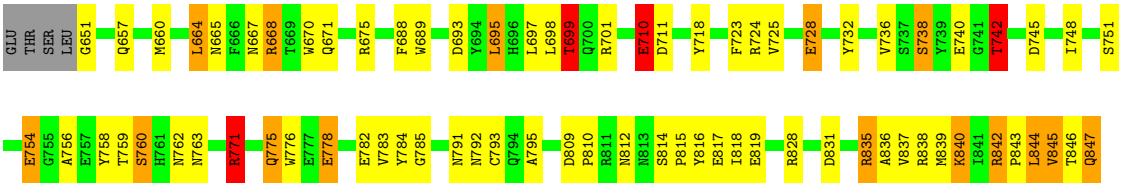
Chain D:





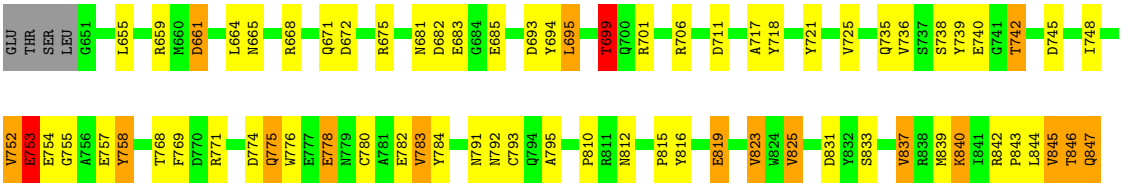
• Molecule 1: FIBRINOGEN-420

Chain E:



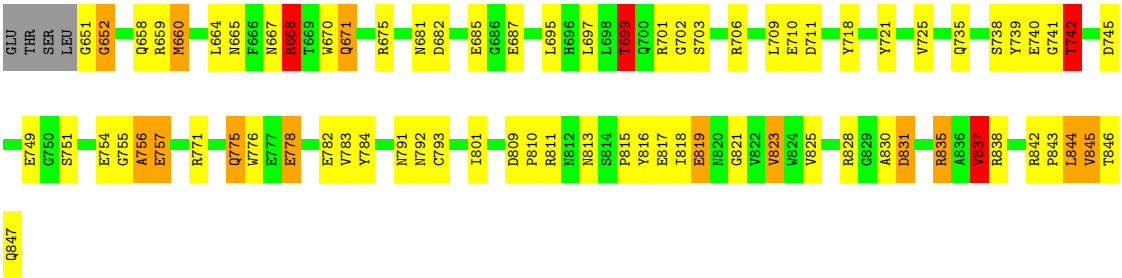
• Molecule 1: FIBRINOGEN-420

Chain F:



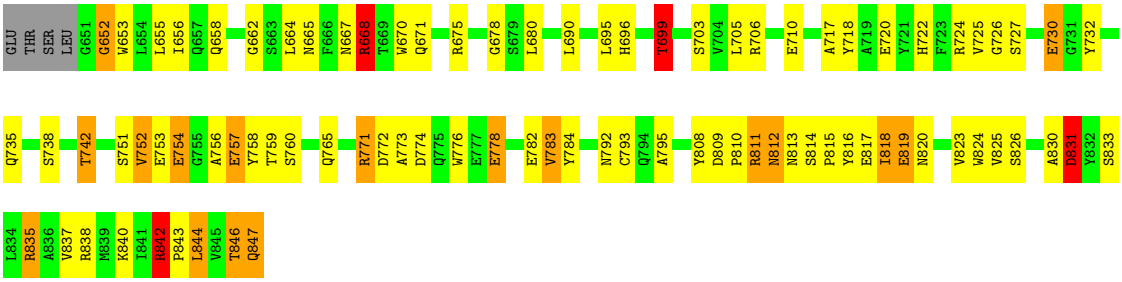
• Molecule 1: FIBRINOGEN-420

Chain G:



• Molecule 1: FIBRINOGEN-420

Chain H:



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

Chain I:

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

Chain K:

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

Chain L:

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

Chain J:

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

Chain M:

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

Chain N:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.25Å 105.18Å 71.14Å 104.60° 108.95° 71.47°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.2 (20.00-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC, X-PLOR	Depositor
R, R_{free}	0.195 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13595	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MAN, NAG, NDG

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	0.85	0/1628	1.96	46/2208 (2.1%)
1	B	0.82	0/1628	1.81	37/2208 (1.7%)
1	C	0.77	0/1628	1.66	28/2208 (1.3%)
1	D	0.79	0/1628	1.75	29/2208 (1.3%)
1	E	0.60	0/1628	1.41	26/2208 (1.2%)
1	F	0.58	0/1628	1.35	14/2208 (0.6%)
1	G	0.56	0/1628	1.34	12/2208 (0.5%)
1	H	0.52	0/1628	1.41	16/2208 (0.7%)
All	All	0.70	0/13024	1.60	208/17664 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	2
1	G	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	771	ARG	CD-NE-CZ	37.32	175.85	123.60
1	B	771	ARG	CD-NE-CZ	28.31	163.23	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	668	ARG	NE-CZ-NH2	-17.90	111.35	120.30
1	D	659	ARG	NE-CZ-NH1	16.59	128.60	120.30
1	B	840	LYS	CA-CB-CG	13.12	142.26	113.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	795	ALA	Mainchain
1	B	723	PHE	Mainchain
1	C	846	THR	Mainchain
1	D	666	PHE	Mainchain
1	D	803	TYR	Mainchain

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	1585	0	1421	29	0
1	B	1585	0	1418	42	0
1	C	1585	0	1420	31	5
1	D	1585	0	1421	33	1
1	E	1585	0	1422	58	0
1	F	1585	0	1421	108	0
1	G	1585	0	1422	107	0
1	H	1585	0	1422	114	6
2	I	75	0	64	19	0
2	K	75	0	64	27	0
2	L	75	0	64	12	0
3	J	74	0	58	30	0
4	M	28	0	26	18	0
4	N	28	0	25	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	G	28	0	26	13	0
6	H	28	0	26	17	0
7	A	70	0	0	4	0
7	B	76	0	0	8	0
7	C	71	0	0	0	0
7	D	74	0	0	7	0
7	E	52	0	0	5	0
7	F	63	0	0	3	0
7	G	56	0	0	7	0
7	H	34	0	0	6	0
All	All	13595	0	11720	642	6

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 26.

The worst 5 of 642 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:F:758:TYR:CD1	1:F:792:ASN:HB3	1.25	1.63
3:J:1:NAG:C3	3:J:1:NAG:C2	1.76	1.61
1:E:667:ASN:HD21	4:M:1:NAG:C1	0.99	1.61
1:F:842:ARG:CZ	1:F:847:GLN:HB2	1.25	1.61
1:F:842:ARG:CZ	1:F:847:GLN:CB	1.83	1.56

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:GLN:OXT	1:H:678:GLY:O[1_445]	0.94	1.26
1:D:847:GLN:O	1:H:722:HIS:ND1[1_545]	1.73	0.47
1:C:847:GLN:C	1:H:678:GLY:O[1_445]	1.88	0.32
1:C:847:GLN:NE2	1:H:680:LEU:O[1_445]	2.03	0.17
1:C:847:GLN:OXT	1:H:678:GLY:C[1_445]	2.13	0.07

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	195/201 (97%)	184 (94%)	11 (6%)	0	100 100
1	B	195/201 (97%)	188 (96%)	7 (4%)	0	100 100
1	C	195/201 (97%)	184 (94%)	10 (5%)	1 (0%)	29 26
1	D	195/201 (97%)	183 (94%)	11 (6%)	1 (0%)	29 26
1	E	195/201 (97%)	187 (96%)	7 (4%)	1 (0%)	29 26
1	F	195/201 (97%)	181 (93%)	10 (5%)	4 (2%)	7 3
1	G	195/201 (97%)	176 (90%)	16 (8%)	3 (2%)	10 5
1	H	195/201 (97%)	175 (90%)	17 (9%)	3 (2%)	10 5
All	All	1560/1608 (97%)	1458 (94%)	89 (6%)	13 (1%)	19 15

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	846	THR
1	G	756	ALA
1	C	846	THR
1	F	754	GLU
1	H	652	GLY

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	159/163 (98%)	138 (87%)	21 (13%)	4 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	159/163 (98%)	140 (88%)	19 (12%)	5 2
1	C	159/163 (98%)	143 (90%)	16 (10%)	7 4
1	D	159/163 (98%)	141 (89%)	18 (11%)	6 3
1	E	159/163 (98%)	137 (86%)	22 (14%)	3 2
1	F	159/163 (98%)	131 (82%)	28 (18%)	2 1
1	G	159/163 (98%)	137 (86%)	22 (14%)	3 2
1	H	159/163 (98%)	136 (86%)	23 (14%)	3 1
All	All	1272/1304 (98%)	1103 (87%)	169 (13%)	4 2

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	812	ASN
1	G	831	ASP
1	F	833	SER
1	G	697	LEU
1	H	735	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	792	ASN
1	H	812	ASN
1	H	765	GLN
1	F	813	ASN
1	G	775	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

28 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	I	1	2,1	14,14,15	0.85	1 (7%)	17,19,21	0.72	0
2	NAG	I	2	2	14,14,15	0.55	0	17,19,21	1.18	2 (11%)
2	MAN	I	3	2	11,11,12	0.92	1 (9%)	15,15,17	1.72	3 (20%)
2	MAN	I	4	2	11,11,12	0.80	0	15,15,17	0.71	0
2	NAG	I	5	2	14,14,15	0.61	0	17,19,21	1.31	2 (11%)
2	MAN	I	6	2	11,11,12	0.98	0	15,15,17	1.73	2 (13%)
3	NAG	J	1	3,1	14,14,15	6.98	12 (85%)	17,19,21	4.22	12 (70%)
3	NDG	J	2	3	14,14,15	0.84	0	17,19,21	0.74	0
3	MAN	J	3	3	11,11,12	0.87	0	15,15,17	2.15	3 (20%)
3	MAN	J	4	3	11,11,12	1.43	2 (18%)	15,15,17	1.67	3 (20%)
3	NAG	J	5	3	14,14,15	0.85	0	17,19,21	1.43	2 (11%)
3	MAN	J	6	3	10,10,12	0.78	0	14,14,17	1.01	1 (7%)
2	NAG	K	1	2,1	14,14,15	0.47	0	17,19,21	0.71	0
2	NAG	K	2	2	14,14,15	0.66	0	17,19,21	1.28	1 (5%)
2	MAN	K	3	2	11,11,12	0.60	0	15,15,17	1.10	1 (6%)
2	MAN	K	4	2	11,11,12	0.66	0	15,15,17	1.02	1 (6%)
2	NAG	K	5	2	14,14,15	0.92	0	17,19,21	0.74	0
2	MAN	K	6	2	11,11,12	0.98	1 (9%)	15,15,17	1.08	2 (13%)
2	NAG	L	1	2,1	14,14,15	6.18	11 (78%)	17,19,21	6.48	14 (82%)
2	NAG	L	2	2	14,14,15	0.78	1 (7%)	17,19,21	0.82	1 (5%)
2	MAN	L	3	2	11,11,12	1.00	1 (9%)	15,15,17	1.69	4 (26%)
2	MAN	L	4	2	11,11,12	0.84	0	15,15,17	1.26	2 (13%)
2	NAG	L	5	2	14,14,15	0.89	0	17,19,21	1.96	5 (29%)
2	MAN	L	6	2	11,11,12	0.73	0	15,15,17	1.32	2 (13%)
4	NAG	M	1	4,1	14,14,15	8.39	11 (78%)	17,19,21	6.54	14 (82%)
4	NAG	M	2	4	14,14,15	0.59	0	17,19,21	0.72	0
4	NAG	N	1	4,1	14,14,15	0.65	0	17,19,21	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	N	2	4	14,14,15	0.80	0	17,19,21	1.47	3 (17%)

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	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	MAN	I	3	2	1/1/4/5	1/2/19/22	1/1/1/1
2	MAN	I	4	2	-	2/2/19/22	0/1/1/1
2	NAG	I	5	2	-	0/6/23/26	0/1/1/1
2	MAN	I	6	2	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	1/6/23/26	0/1/1/1
3	NDG	J	2	3	-	2/6/23/26	0/1/1/1
3	MAN	J	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	J	4	3	-	2/2/19/22	0/1/1/1
3	NAG	J	5	3	-	2/6/23/26	0/1/1/1
3	MAN	J	6	3	-	-	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	MAN	K	3	2	1/1/4/5	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	2/2/19/22	0/1/1/1
2	NAG	K	5	2	-	2/6/23/26	0/1/1/1
2	MAN	K	6	2	1/1/4/5	2/2/19/22	1/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	MAN	L	3	2	-	2/2/19/22	0/1/1/1
2	MAN	L	4	2	-	1/2/19/22	0/1/1/1
2	NAG	L	5	2	-	2/6/23/26	0/1/1/1
2	MAN	L	6	2	1/1/4/5	1/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1	NAG	O5-C5	16.98	1.77	1.43
4	M	1	NAG	O5-C1	15.26	1.68	1.43
4	M	1	NAG	C1-C2	-14.65	1.30	1.52
3	J	1	NAG	O3-C3	-14.02	1.10	1.43
3	J	1	NAG	C3-C2	11.19	1.76	1.52

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1	NAG	O5-C5-C6	-16.10	81.97	107.20
2	L	1	NAG	O5-C1-C2	-14.71	88.07	111.29
2	L	1	NAG	O7-C7-C8	12.20	144.71	122.06
4	M	1	NAG	C2-N2-C7	-10.65	107.74	122.90
2	L	1	NAG	O7-C7-N2	-10.50	102.65	121.95

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	3	MAN	C1
2	K	3	MAN	C1
2	K	6	MAN	C1
2	L	6	MAN	C1
3	J	3	MAN	C1

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	5	NAG	C3-C2-N2-C7
3	J	2	NDG	C4-C5-C6-O6
2	I	4	MAN	O5-C5-C6-O6
2	K	4	MAN	O5-C5-C6-O6
2	L	3	MAN	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	3	MAN	C1-C2-C3-C4-C5-O5
2	K	6	MAN	C1-C2-C3-C4-C5-O5

22 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	NAG	2	0

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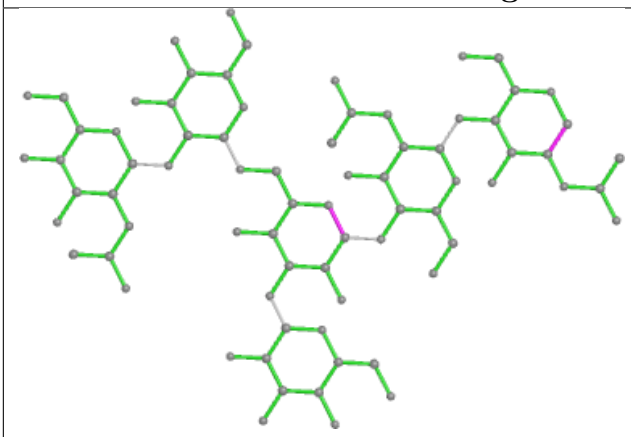
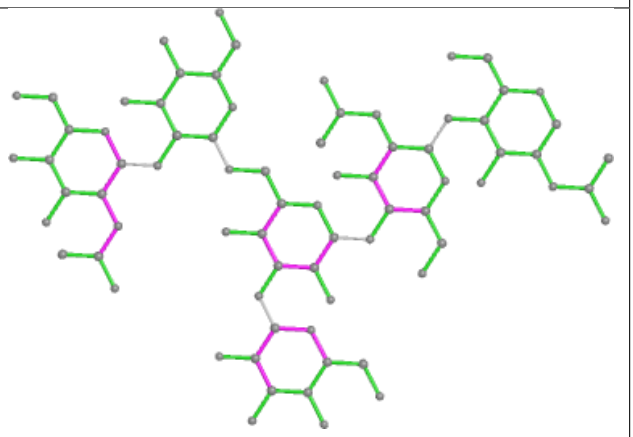
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	4	MAN	12	0
2	K	6	MAN	3	0
3	J	5	NAG	9	0
3	J	6	MAN	5	0
4	M	2	NAG	3	0
3	J	3	MAN	15	0
2	L	3	MAN	4	0
2	I	6	MAN	9	0
3	J	1	NAG	5	0
3	J	2	NDG	1	0
2	K	4	MAN	22	0
2	L	5	NAG	8	0
2	I	3	MAN	13	0
4	N	1	NAG	1	0
4	M	1	NAG	18	0
2	I	5	NAG	3	0
2	I	2	NAG	4	0
2	K	3	MAN	13	0
2	I	4	MAN	6	0
3	J	4	MAN	17	0
2	K	5	NAG	12	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.

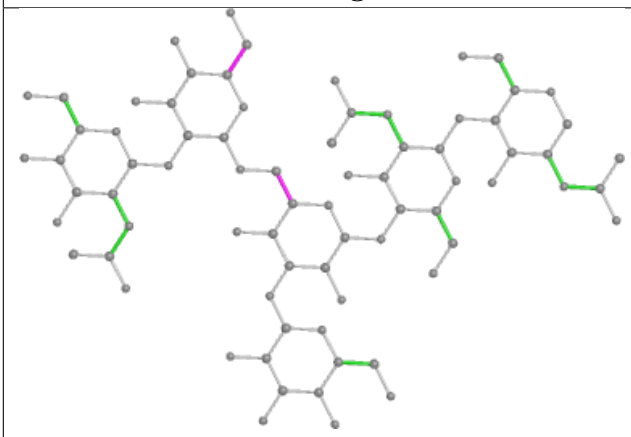
Oligosaccharide Chain I



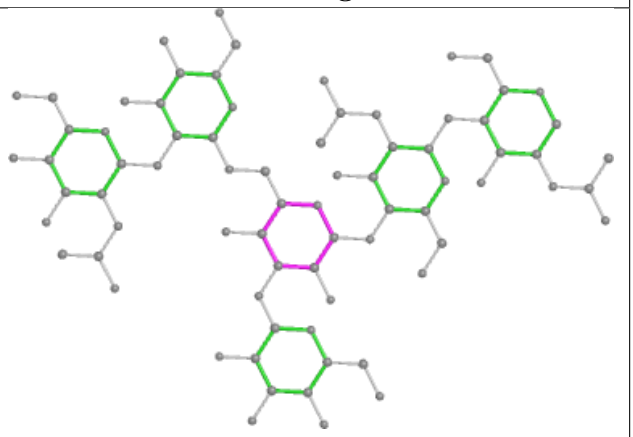
Bond lengths



Bond angles

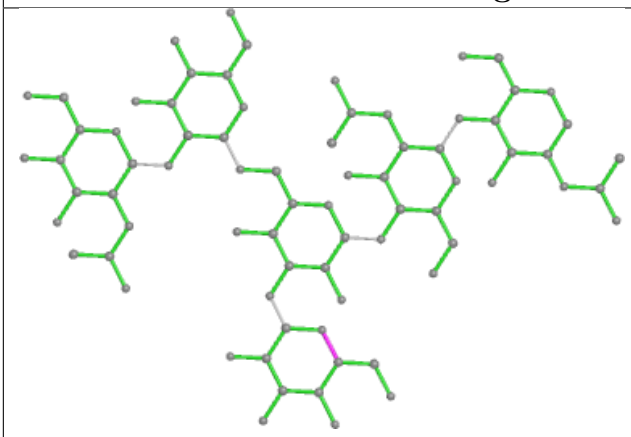


Torsions

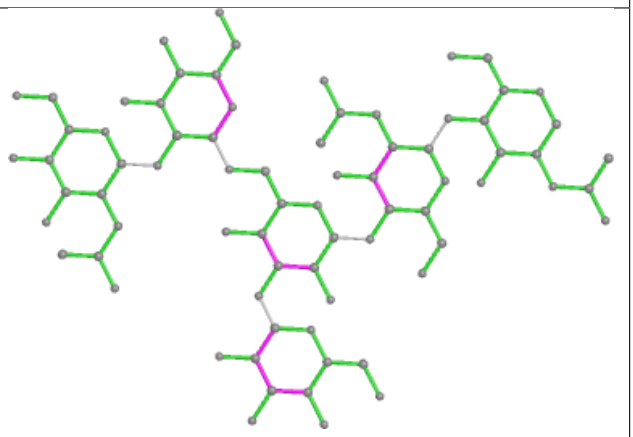


Rings

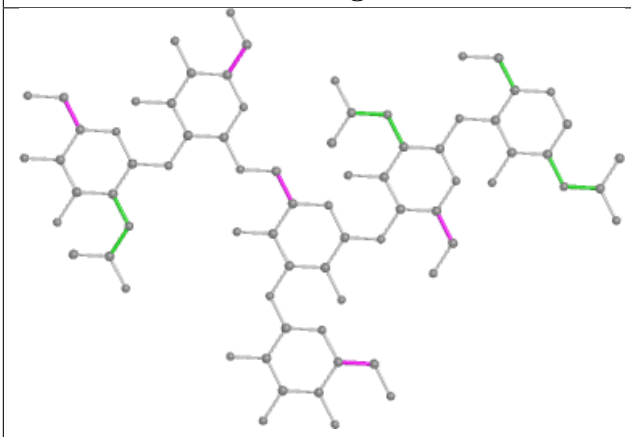
Oligosaccharide Chain K



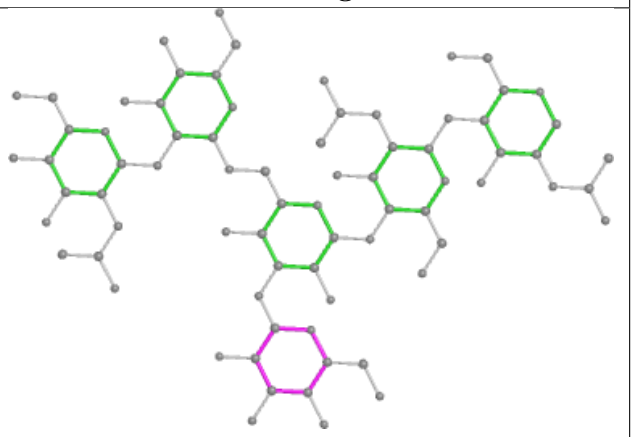
Bond lengths



Bond angles

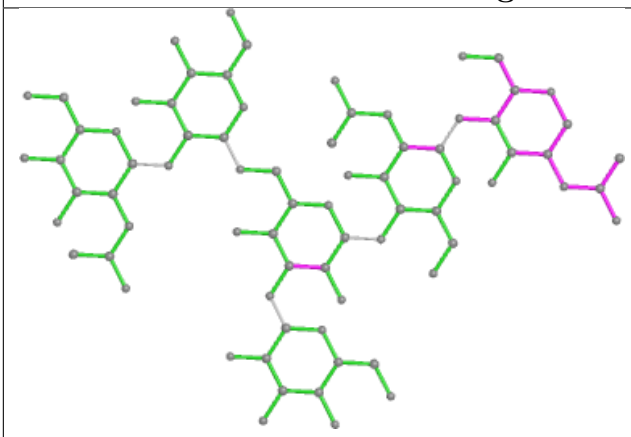


Torsions

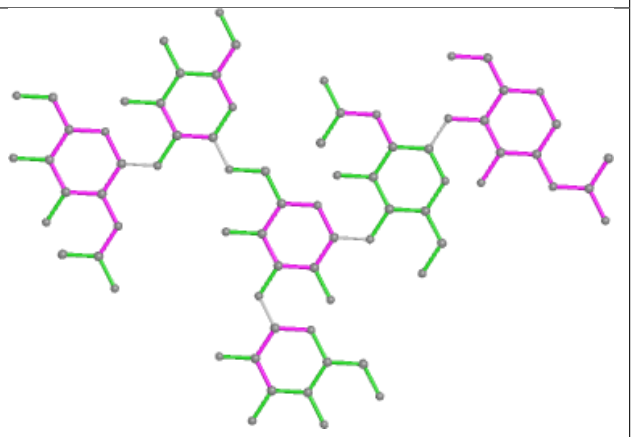


Rings

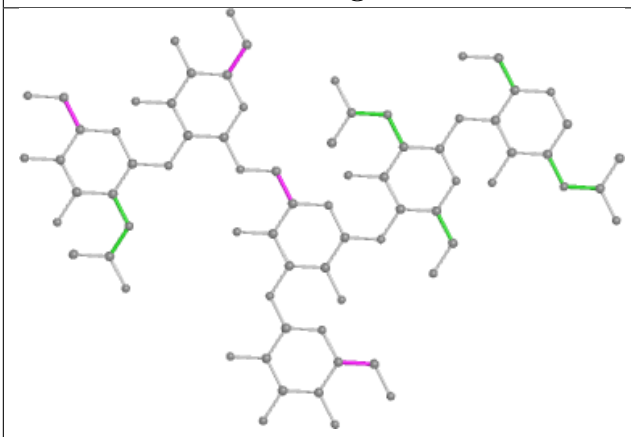
Oligosaccharide Chain L



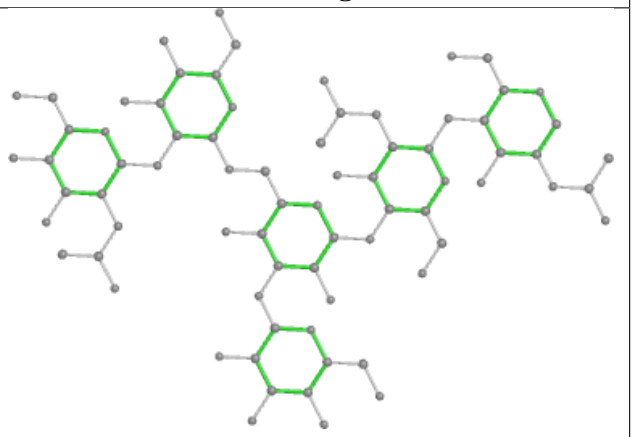
Bond lengths



Bond angles

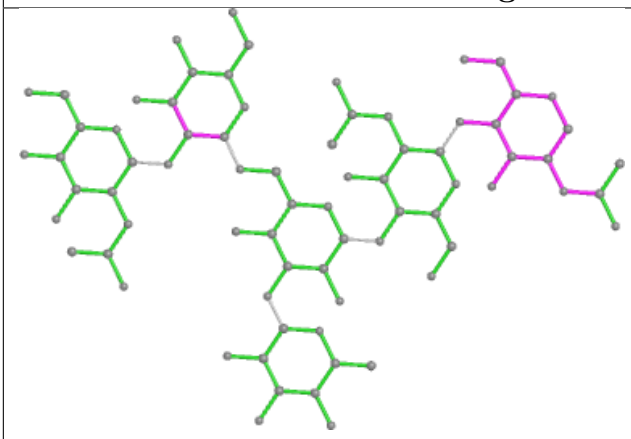


Torsions

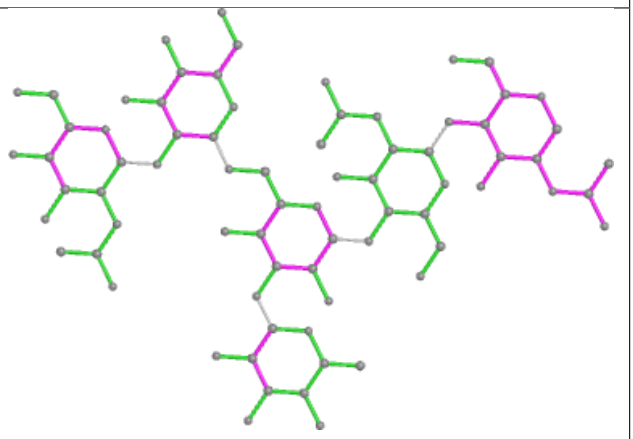


Rings

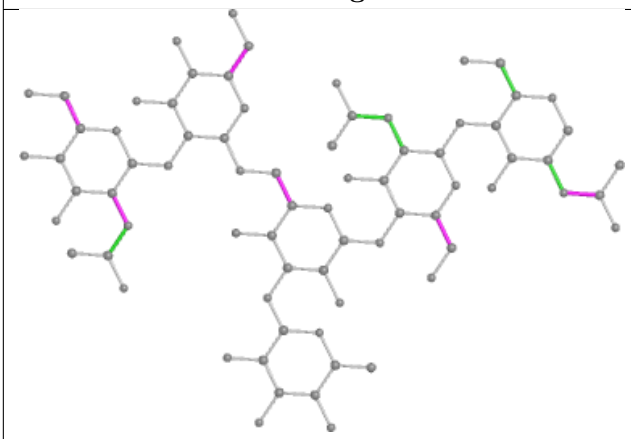
Oligosaccharide Chain J



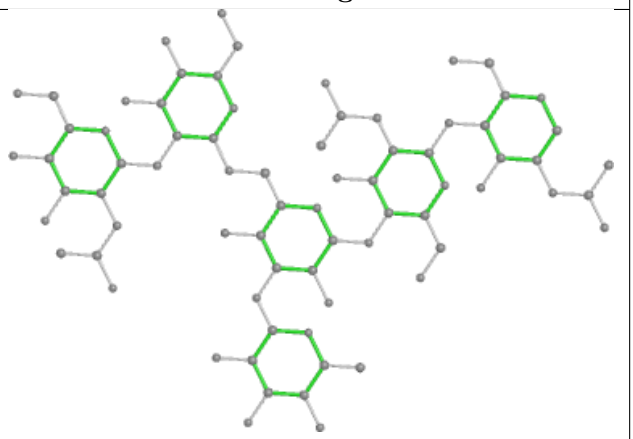
Bond lengths



Bond angles

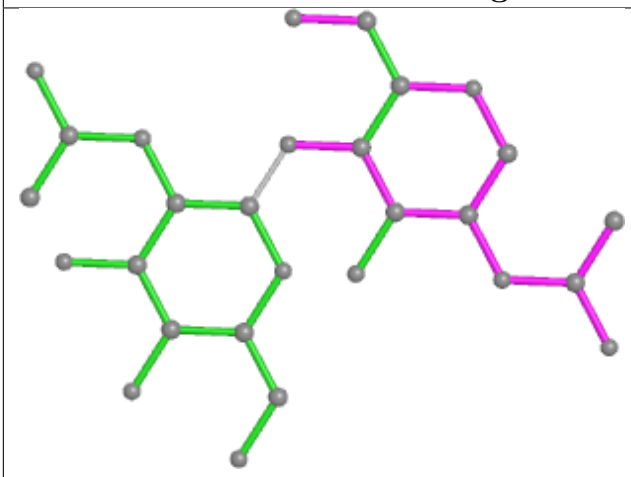


Torsions

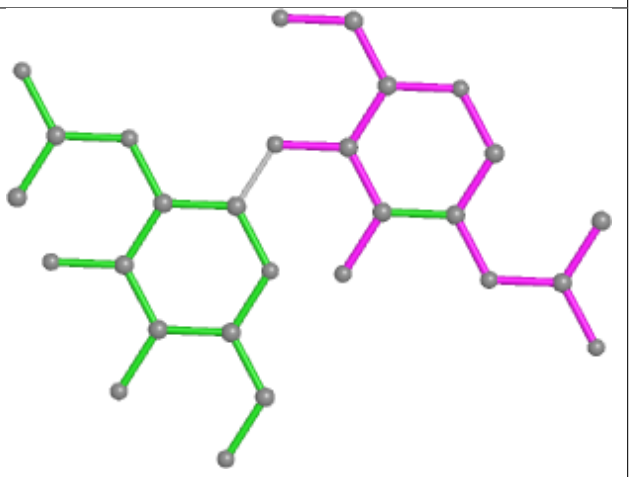


Rings

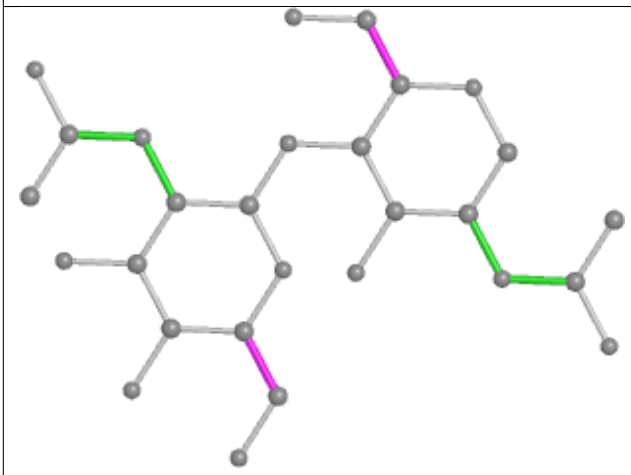
Oligosaccharide Chain M



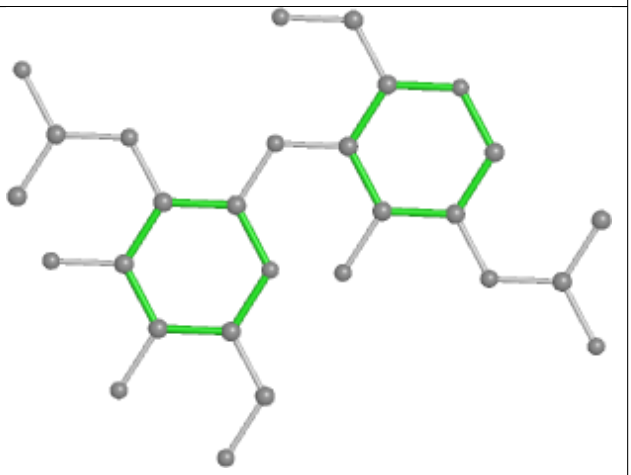
Bond lengths



Bond angles

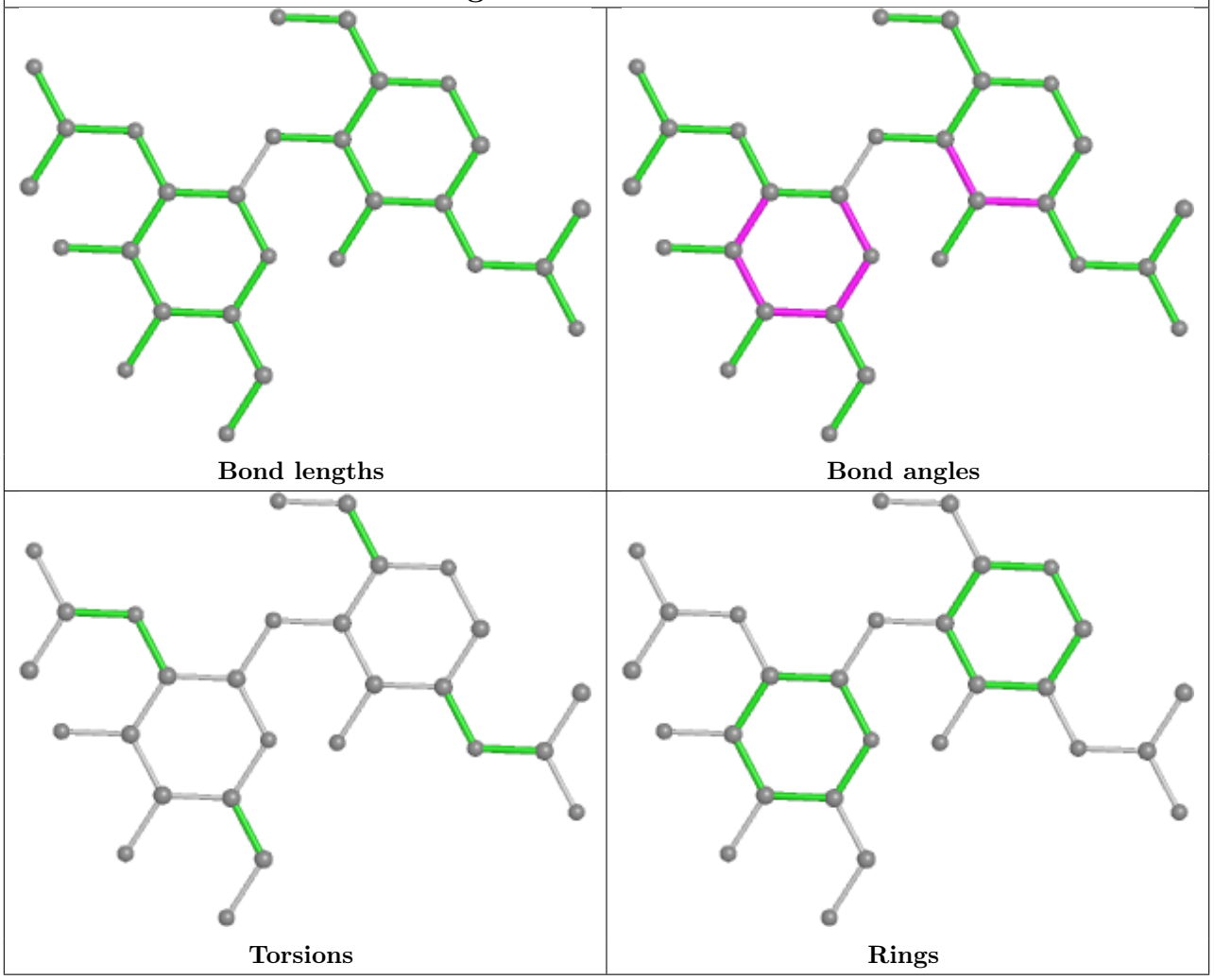


Torsions



Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	NAG	G	11	-	14,14,15	0.52	0	17,19,21	1.16	2 (11%)
6	NAG	H	11	-	14,14,15	0.71	0	17,19,21	0.79	1 (5%)
6	NAG	G	10	1	14,14,15	0.56	0	17,19,21	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	H	10	1	14,14,15	0.51	0	17,19,21	1.04	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
6	NAG	G	11	-	-	2/6/23/26	0/1/1/1
6	NAG	H	11	-	-	0/6/23/26	0/1/1/1
6	NAG	G	10	1	-	2/6/23/26	0/1/1/1
6	NAG	H	10	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	10	NAG	C3-C4-C5	3.75	116.93	110.24
6	G	11	NAG	C4-C3-C2	-3.19	106.34	111.02
6	H	10	NAG	C3-C4-C5	2.78	115.19	110.24
6	H	11	NAG	C2-N2-C7	-2.53	119.30	122.90
6	G	11	NAG	C2-N2-C7	-2.30	119.62	122.90

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	10	NAG	C4-C5-C6-O6
6	G	10	NAG	O5-C5-C6-O6
6	G	10	NAG	C4-C5-C6-O6
6	G	11	NAG	C4-C5-C6-O6
6	H	10	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	11	NAG	9	0
6	H	11	NAG	10	0
6	G	10	NAG	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	10	NAG	15	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.