Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2025 – 06:23 PM EDT

PDB ID	:	9B7H / pdb_00009b7h
Title	:	Crystal structure of the H3 hemagglutinin COBRA TJ2
Authors	:	Dzimianski, J.V.; DuBois, R.M.
Deposited on	:	2024-03-27
Resolution	:	3.15 Å(reported)

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

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

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

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

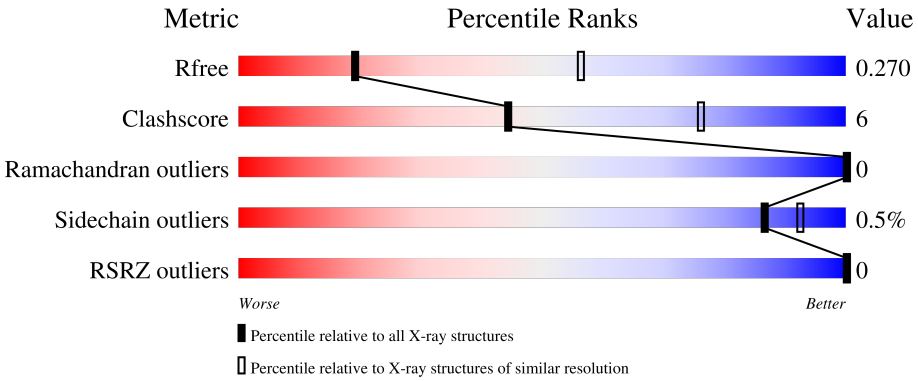
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.15 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}	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

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	323	85% 14% .
1	B	323	81% 18% .
1	C	323	85% 13% .
2	a	182	80% 15% 5%
2	b	182	79% 15% 6%

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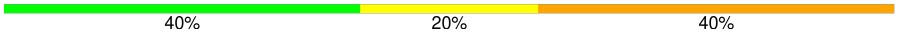
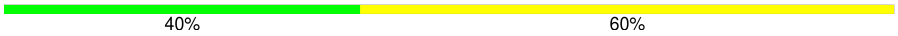
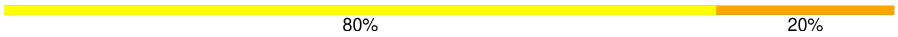
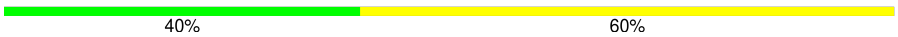
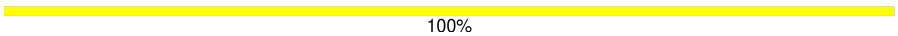
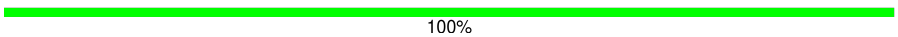
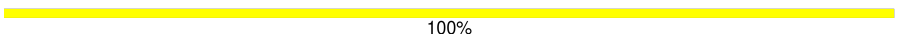
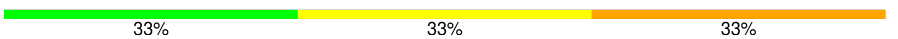
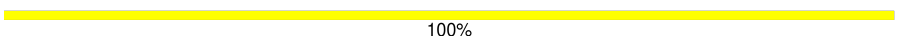
Mol	Chain	Length	Quality of chain
2	c	182	
3	D	5	
3	E	5	
3	F	5	
3	H	5	
3	J	5	
3	M	5	
3	O	5	
4	G	2	
4	K	2	
4	Q	2	
4	R	2	
5	I	3	
5	L	3	
5	P	3	
6	N	4	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12439 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2476	1547	443	474	12			
1	B	319	Total	C	N	O	S	0	0	0
			2484	1551	445	476	12			
1	C	318	Total	C	N	O	S	0	0	0
			2475	1545	443	475	12			

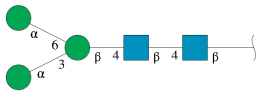
- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	172	Total	C	N	O	S	0	0	0
			1387	863	245	273	6			
2	b	171	Total	C	N	O	S	0	0	0
			1378	858	243	271	6			
2	c	172	Total	C	N	O	S	0	0	0
			1387	863	245	273	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	508	LEU	-	expression tag	UNP A0FCI1
a	509	VAL	-	expression tag	UNP A0FCI1
a	510	PRO	-	expression tag	UNP A0FCI1
a	511	ARG	-	expression tag	UNP A0FCI1
b	508	LEU	-	expression tag	UNP A0FCI1
b	509	VAL	-	expression tag	UNP A0FCI1
b	510	PRO	-	expression tag	UNP A0FCI1
b	511	ARG	-	expression tag	UNP A0FCI1
c	508	LEU	-	expression tag	UNP A0FCI1
c	509	VAL	-	expression tag	UNP A0FCI1
c	510	PRO	-	expression tag	UNP A0FCI1
c	511	ARG	-	expression tag	UNP A0FCI1

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.

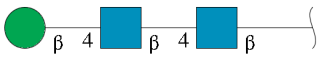


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.

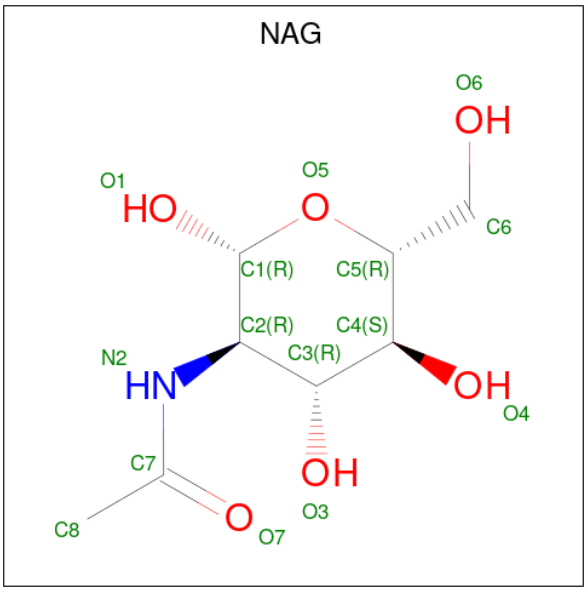


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called 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.

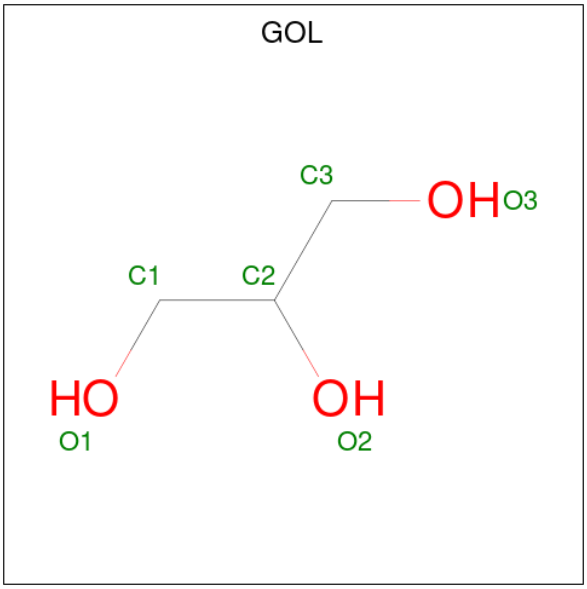
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



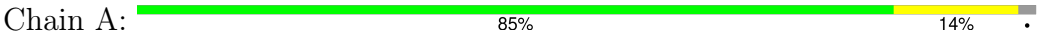
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	b	1	Total	C	O	0	0
			6	3	3		

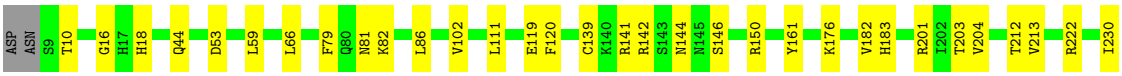
3 Residue-property plots (i)

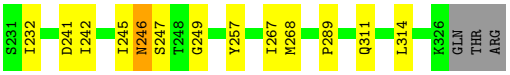
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hemagglutinin HA1

Chain A:

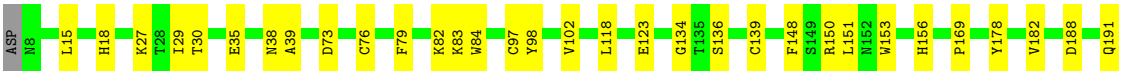






• Molecule 1: Hemagglutinin HA1

Chain B:

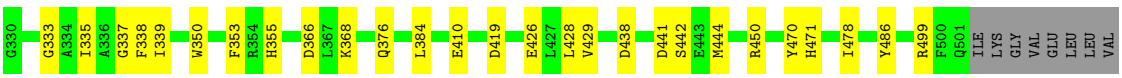


• Molecule 1: Hemagglutinin HA1

Chain C:

• Molecule 2: Hemagglutinin

Chain a:



• Molecule 2: Hemagglutinin

Chain b:

• Molecule 2: Hemagglutinin

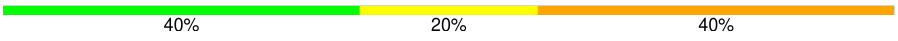
Chain c:

• Molecule 3: alpha-D-mannopyranose-(1-3)-[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 E:

• Molecule 3: alpha-D-mannopyranose-(1-3)-[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 D:



• Molecule 3: alpha-D-mannopyranose-(1-3)-[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 F:

• Molecule 3: alpha-D-mannopyranose-(1-3)-[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

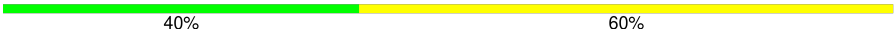
Chain H:

• Molecule 3: alpha-D-mannopyranose-(1-3)-[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:

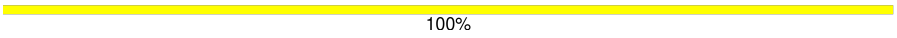
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



• Molecule 3: alpha-D-mannopyranose-(1-3)-[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 O:

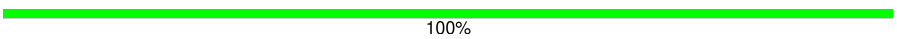


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain K:

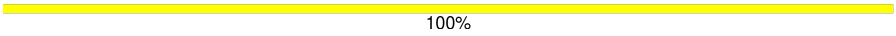


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

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

Chain R:

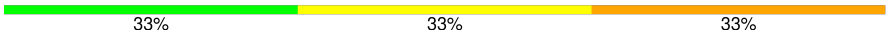


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

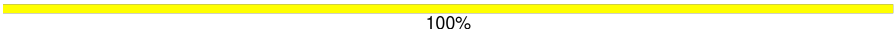


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

• Molecule 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 N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	77.25Å 117.68Å 198.62Å 90.00° 90.95° 90.00°	Depositor
Resolution (Å)	45.66 – 3.15 45.66 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.66-3.15) 88.0 (45.66-3.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.57 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.269 0.222 , 0.270	Depositor DCC
R_{free} test set	1477 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	81.0	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 71.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12439	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: GOL, NAG, MAN, 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	0.12	0/2531	0.30	0/3440
1	B	0.16	0/2539	0.35	0/3451
1	C	0.11	0/2530	0.30	0/3440
2	a	0.11	0/1411	0.25	0/1895
2	b	0.15	0/1402	0.36	0/1883
2	c	0.11	0/1411	0.28	0/1895
All	All	0.13	0/11824	0.31	0/16004

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2476	0	2430	30	0
1	B	2484	0	2435	37	0
1	C	2475	0	2422	28	0
2	a	1387	0	1313	20	0
2	b	1378	0	1306	26	0
2	c	1387	0	1313	18	0
3	D	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	61	0	52	2	0
3	F	61	0	52	0	0
3	H	61	0	52	2	0
3	J	61	0	52	0	0
3	M	61	0	52	1	0
3	O	61	0	52	2	0
4	G	28	0	25	0	0
4	K	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	2	0
5	I	39	0	34	1	0
5	L	39	0	34	2	0
5	P	39	0	34	0	0
6	N	50	0	43	2	0
7	A	28	0	26	1	0
7	B	42	0	39	2	0
7	C	42	0	39	2	0
7	a	14	0	13	0	0
7	c	14	0	13	0	0
8	b	6	0	8	0	0
All	All	12439	0	11966	144	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 6.

All (144) 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)
6:N:1:NAG:H81	4:R:2:NAG:H83	1.67	0.76
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.76	0.68
2:a:419:ASP:OD2	2:c:391:LYS:NZ	2.29	0.65
2:b:403:GLU:OE2	2:c:405:ARG:NH1	2.30	0.65
1:A:182:VAL:HG11	1:A:213:VAL:HG11	1.79	0.64
1:C:79:PHE:HA	1:C:82:LYS:HD2	1.80	0.64
1:B:123:GLU:HB2	1:B:256:GLY:HA2	1.82	0.61
2:a:499:ARG:NH2	2:c:457:GLU:OE2	2.32	0.60
2:b:355:HIS:HB2	2:b:478:ILE:HD13	1.84	0.60
2:b:357:ASN:ND2	2:b:478:ILE:HD12	2.17	0.59
2:c:335:ILE:HG12	2:c:441:ASP:HA	1.85	0.58
1:B:280:GLU:HG2	1:B:304:ALA:HB3	1.87	0.57
1:A:222:ARG:H	6:N:2:NAG:H81	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:357:ASN:HD22	2:b:478:ILE:HD12	1.69	0.57
1:A:203:THR:HG23	1:A:212:THR:HG22	1.88	0.56
1:A:10:THR:HG22	2:a:470:TYR:HA	1.86	0.55
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.89	0.55
1:B:35:GLU:HG2	1:B:322:ASN:HB3	1.89	0.54
5:L:1:NAG:H4	5:L:2:NAG:C7	2.37	0.54
2:b:457:GLU:O	2:b:499:ARG:NH1	2.40	0.53
1:B:102:VAL:HG22	1:B:232:ILE:HB	1.90	0.53
2:c:384:LEU:HD21	2:c:428:LEU:HD21	1.89	0.53
2:b:358:SER:O	2:b:359:GLU:HB2	2.09	0.53
2:b:391:LYS:NZ	2:c:419:ASP:OD2	2.42	0.53
1:B:73:ASP:HB3	1:B:76:CYS:SG	2.49	0.52
2:c:338:PHE:HD1	2:c:339:ILE:HD12	1.75	0.52
1:C:9:SER:HA	2:c:472:LYS:HG3	1.91	0.52
1:C:200:GLY:O	1:C:215:PRO:HD2	2.10	0.52
1:B:97:CYS:O	1:B:224:ARG:NH1	2.43	0.52
1:C:182:VAL:HG11	1:C:213:VAL:HG11	1.91	0.52
1:C:218:GLY:O	1:C:220:ARG:NH1	2.44	0.51
1:A:311:GLN:NE2	2:a:426:GLU:HB2	2.26	0.51
2:b:355:HIS:HB3	2:b:478:ILE:HG21	1.93	0.51
1:C:248:THR:HG23	4:R:1:NAG:O7	2.11	0.51
2:c:357:ASN:ND2	2:c:475:ASN:OD1	2.42	0.50
2:a:353:PHE:HE1	2:a:366:ASP:HB2	1.75	0.50
1:B:27:LYS:NZ	2:b:426:GLU:OE2	2.44	0.49
1:A:86:LEU:HD11	1:A:268:MET:HB2	1.94	0.49
2:b:357:ASN:HD21	2:b:474:ASP:C	2.20	0.49
1:C:30:THR:HG23	2:b:376:GLN:HA	1.93	0.49
1:C:43:VAL:HG23	1:C:314:LEU:HB2	1.94	0.49
1:C:97:CYS:SG	1:C:98:TYR:N	2.86	0.49
1:A:204:VAL:HG22	1:A:245:ILE:HG23	1.94	0.48
1:A:241:ASP:OD1	1:A:242:ILE:N	2.45	0.48
1:B:241:ASP:OD1	1:B:242:ILE:N	2.44	0.48
1:C:222:ARG:NH2	3:M:2:NAG:O6	2.47	0.48
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.49	0.48
2:b:453:LYS:HD3	2:c:463:GLY:HA2	1.96	0.48
1:A:142:ARG:O	1:A:144:ASN:ND2	2.47	0.47
1:B:38:ASN:OD1	1:B:39:ALA:N	2.47	0.47
1:A:183:HIS:HA	1:A:230:ILE:HG22	1.96	0.47
1:A:16:GLY:C	2:a:444:MET:HE1	2.39	0.47
1:B:150:ARG:HH12	7:B:402:NAG:H5	1.80	0.47
2:b:355:HIS:NE2	2:b:362:GLY:HA3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD13	2:b:402:VAL:HG11	1.97	0.47
1:B:97:CYS:SG	1:B:98:TYR:N	2.86	0.47
1:C:132:GLN:HB2	7:C:501:NAG:H82	1.97	0.47
1:B:30:THR:HG23	2:a:376:GLN:HA	1.96	0.46
2:a:338:PHE:HD1	2:a:339:ILE:HG13	1.80	0.46
1:C:141:ARG:HH12	1:C:149:SER:HB3	1.81	0.46
1:C:222:ARG:NH1	1:C:225:ASP:OD1	2.48	0.46
1:C:182:VAL:HB	1:C:202:ILE:HD11	1.98	0.46
1:A:150:ARG:HH12	7:A:401:NAG:H5	1.79	0.46
1:A:201:ARG:O	1:A:247:SER:HA	2.16	0.46
1:B:18:HIS:CD2	1:B:18:HIS:C	2.94	0.46
2:b:410:GLU:HG3	2:c:409:LEU:HD22	1.98	0.46
1:A:314:LEU:HB3	2:a:429:VAL:HG21	1.97	0.45
1:A:66:LEU:HD22	1:A:267:ILE:HD12	1.97	0.45
2:a:384:LEU:HD21	2:a:428:LEU:HD21	1.96	0.45
2:c:369:SER:O	2:c:372:ALA:HB3	2.16	0.45
1:A:81:ASN:ND2	1:A:120:PHE:H	2.14	0.45
1:B:134:GLY:HA3	1:B:153:TRP:HB3	1.98	0.45
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.84	0.45
1:B:136:SER:HB2	1:B:153:TRP:HZ3	1.81	0.45
1:A:59:LEU:HD11	1:A:82:LYS:HD3	1.97	0.45
1:C:191:GLN:NE2	1:C:199:SER:O	2.50	0.44
1:B:182:VAL:HG22	1:B:202:ILE:HG13	2.00	0.44
1:B:222:ARG:HE	3:E:2:NAG:H2	1.82	0.44
2:b:339:ILE:HG12	2:b:465:GLY:HA3	1.98	0.44
1:B:202:ILE:HD11	1:B:249:GLY:O	2.18	0.44
2:a:410:GLU:OE2	2:b:405:ARG:HD2	2.17	0.44
1:C:81:ASN:ND2	7:C:503:NAG:O3	2.51	0.44
2:c:403:GLU:HB2	2:c:407:GLN:HB2	2.00	0.44
2:b:372:ALA:O	2:b:376:GLN:HG3	2.18	0.44
1:B:222:ARG:HD3	1:B:227:PRO:HD3	1.99	0.44
1:B:222:ARG:NH2	3:E:2:NAG:O6	2.51	0.44
1:A:79:PHE:HA	1:A:82:LYS:HD2	2.00	0.44
1:C:170:ASN:ND2	1:C:237:VAL:O	2.50	0.44
1:A:246:ASN:ND2	3:H:1:NAG:O7	2.51	0.43
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.53	0.43
1:A:81:ASN:HD22	1:A:119:GLU:HA	1.83	0.43
7:B:402:NAG:H61	5:I:2:NAG:HN2	1.83	0.43
1:C:62:GLU:O	1:C:90:ARG:HB2	2.18	0.43
1:B:188:ASP:N	1:B:188:ASP:OD1	2.50	0.43
3:O:1:NAG:O3	3:O:2:NAG:O5	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLN:HE22	2:a:426:GLU:HB2	1.83	0.43
1:B:191:GLN:HG3	1:B:197:GLN:O	2.19	0.43
2:b:355:HIS:CB	2:b:478:ILE:HG21	2.48	0.43
1:B:220:ARG:HB2	1:B:227:PRO:O	2.18	0.43
2:c:353:PHE:HE1	2:c:366:ASP:HB2	1.84	0.43
1:B:83:LYS:HE3	1:B:83:LYS:HB2	1.72	0.43
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.87	0.43
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.88	0.43
2:c:452:LYS:HE3	2:c:452:LYS:HB3	1.79	0.42
1:B:148:PHE:HB2	1:B:151:LEU:HB2	2.01	0.42
1:A:18:HIS:ND1	2:a:350:TRP:HA	2.34	0.42
2:a:355:HIS:HB2	2:a:478:ILE:HD13	2.02	0.42
2:b:332:PHE:CE2	2:b:442:SER:HB2	2.54	0.42
2:b:357:ASN:ND2	2:b:474:ASP:C	2.77	0.42
1:A:176:LYS:HB3	1:A:257:TYR:HB2	2.01	0.42
1:B:270:SER:HB2	1:B:284:PRO:HA	2.01	0.42
1:A:53:ASP:OD1	1:A:53:ASP:N	2.51	0.42
2:b:338:PHE:CD2	2:b:339:ILE:HG13	2.54	0.42
2:b:391:LYS:HA	2:b:391:LYS:HD3	1.84	0.42
1:B:29:ILE:HD11	2:b:431:LEU:HG	2.02	0.42
1:B:84:TRP:HZ3	1:B:118:LEU:HG	1.84	0.42
1:C:311:GLN:NE2	2:c:426:GLU:HB2	2.33	0.42
1:B:295:GLN:NE2	1:B:298:ASN:O	2.32	0.42
2:b:335:ILE:HG12	2:b:441:ASP:HA	2.02	0.42
1:B:169:PRO:HA	1:B:242:ILE:HG13	2.01	0.41
2:a:471:HIS:NE2	2:a:486:TYR:OH	2.52	0.41
3:D:3:BMA:H62	3:D:5:MAN:H2	1.78	0.41
1:C:40:THR:HB	3:O:1:NAG:H61	2.03	0.41
1:B:301:THR:HB	1:B:305:CYS:SG	2.60	0.41
1:C:26:VAL:HG12	1:C:315:LYS:HB2	2.02	0.41
1:C:104:ASP:HB3	1:C:234:TRP:HH2	1.86	0.41
2:a:438:ASP:O	2:a:442:SER:N	2.46	0.41
1:A:141:ARG:NH1	1:A:146:SER:OG	2.53	0.41
1:A:44:GLN:NE2	1:A:289:PRO:HD2	2.36	0.41
1:B:15:LEU:HD23	2:b:447:LEU:HG	2.03	0.41
1:B:178:TYR:CZ	1:B:257:TYR:HB3	2.55	0.41
1:C:53:ASP:OD1	1:C:53:ASP:N	2.54	0.41
3:H:1:NAG:O3	3:H:2:NAG:O5	2.26	0.41
5:L:1:NAG:H4	5:L:2:NAG:N2	2.36	0.41
1:B:156:HIS:N	1:B:194:LEU:O	2.52	0.41
2:a:368:LYS:HE2	2:a:450:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ILE:O	1:B:212:THR:HA	2.20	0.40
1:C:108:LEU:HB2	1:C:234:TRP:CZ3	2.56	0.40
2:a:333:GLY:O	2:a:337:GLY:HA3	2.20	0.40
2:a:470:TYR:CG	2:a:499:ARG:HG2	2.55	0.40
1:C:8:ASN:HB3	2:c:472:LYS:HE2	2.03	0.40
2:a:335:ILE:HG12	2:a:441:ASP:HA	2.03	0.40
1:B:79:PHE:HA	1:B:82:LYS:HD2	2.04	0.40
2:c:391:LYS:HA	2:c:391:LYS:HD3	1.93	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	316/323 (98%)	310 (98%)	6 (2%)	0	100	100
1	B	317/323 (98%)	311 (98%)	6 (2%)	0	100	100
1	C	316/323 (98%)	308 (98%)	8 (2%)	0	100	100
2	a	170/182 (93%)	165 (97%)	5 (3%)	0	100	100
2	b	169/182 (93%)	165 (98%)	4 (2%)	0	100	100
2	c	170/182 (93%)	165 (97%)	5 (3%)	0	100	100
All	All	1458/1515 (96%)	1424 (98%)	34 (2%)	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	281/286 (98%)	279 (99%)	2 (1%)	81 90
1	B	282/286 (99%)	279 (99%)	3 (1%)	70 84
1	C	281/286 (98%)	280 (100%)	1 (0%)	89 94
2	a	145/154 (94%)	145 (100%)	0	100 100
2	b	144/154 (94%)	144 (100%)	0	100 100
2	c	145/154 (94%)	145 (100%)	0	100 100
All	All	1278/1320 (97%)	1272 (100%)	6 (0%)	86 92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	CYS
1	A	246	ASN
1	B	139	CYS
1	B	246	ASN
1	B	277	CYS
1	C	139	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	75	GLN
1	A	81	ASN
1	B	80	GLN
1	B	132	GLN
1	B	144	ASN
1	B	210	GLN
1	C	210	GLN
1	C	296	ASN
2	b	357	ASN
2	b	454	GLN
2	c	363	GLN
2	c	497	ASN

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)

56 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	$\#\|Z\| > 2$
3	NAG	D	1	1,3	14,14,15	0.20	0	17,19,21	0.49	0
3	NAG	D	2	3	14,14,15	0.19	0	17,19,21	0.48	0
3	BMA	D	3	3	11,11,12	0.58	0	15,15,17	0.83	1 (6%)
3	MAN	D	4	3	11,11,12	0.65	0	15,15,17	1.10	2 (13%)
3	MAN	D	5	3	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.15	0	17,19,21	0.44	0
3	NAG	E	2	3	14,14,15	0.18	0	17,19,21	0.64	0
3	BMA	E	3	3	11,11,12	0.63	0	15,15,17	1.16	1 (6%)
3	MAN	E	4	3	11,11,12	0.82	0	15,15,17	0.82	1 (6%)
3	MAN	E	5	3	11,11,12	0.74	0	15,15,17	1.31	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.17	0	17,19,21	0.63	0
3	BMA	F	3	3	11,11,12	0.90	1 (9%)	15,15,17	0.84	0
3	MAN	F	4	3	11,11,12	0.74	0	15,15,17	1.34	2 (13%)
3	MAN	F	5	3	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
4	NAG	G	1	4,1	14,14,15	0.27	0	17,19,21	0.70	0
4	NAG	G	2	4	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.48	0	17,19,21	0.51	0
3	NAG	H	2	3	14,14,15	0.26	0	17,19,21	0.75	1 (5%)
3	BMA	H	3	3	11,11,12	0.70	0	15,15,17	1.03	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	H	4	3	11,11,12	0.77	0	15,15,17	1.32	2 (13%)
3	MAN	H	5	3	11,11,12	1.29	2 (18%)	15,15,17	1.13	1 (6%)
5	NAG	I	1	1,5	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	I	2	5	14,14,15	0.30	0	17,19,21	0.64	0
5	BMA	I	3	5	11,11,12	0.56	0	15,15,17	0.85	0
3	NAG	J	1	1,3	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	J	2	3	14,14,15	0.32	0	17,19,21	0.55	0
3	BMA	J	3	3	11,11,12	0.59	0	15,15,17	0.85	0
3	MAN	J	4	3	11,11,12	0.65	0	15,15,17	1.00	2 (13%)
3	MAN	J	5	3	11,11,12	0.67	0	15,15,17	0.97	2 (13%)
4	NAG	K	1	4,1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	K	2	4	14,14,15	0.42	0	17,19,21	0.56	0
5	NAG	L	1	1,5	14,14,15	0.20	0	17,19,21	0.70	0
5	NAG	L	2	5	14,14,15	0.52	0	17,19,21	0.69	1 (5%)
5	BMA	L	3	5	11,11,12	0.50	0	15,15,17	0.70	0
3	NAG	M	1	1,3	14,14,15	0.20	0	17,19,21	0.55	0
3	NAG	M	2	3	14,14,15	0.16	0	17,19,21	0.50	0
3	BMA	M	3	3	11,11,12	0.55	0	15,15,17	0.84	0
3	MAN	M	4	3	11,11,12	0.88	0	15,15,17	1.17	2 (13%)
3	MAN	M	5	3	11,11,12	0.60	0	15,15,17	0.99	2 (13%)
6	NAG	N	1	6,1	14,14,15	0.23	0	17,19,21	0.49	0
6	NAG	N	2	6	14,14,15	0.25	0	17,19,21	0.46	0
6	BMA	N	3	6	11,11,12	0.78	0	15,15,17	0.94	1 (6%)
6	MAN	N	4	6	11,11,12	0.79	0	15,15,17	1.36	2 (13%)
3	NAG	O	1	1,3	14,14,15	0.31	0	17,19,21	0.66	0
3	NAG	O	2	3	14,14,15	0.24	0	17,19,21	0.69	0
3	BMA	O	3	3	11,11,12	0.49	0	15,15,17	0.93	1 (6%)
3	MAN	O	4	3	11,11,12	1.78	2 (18%)	15,15,17	1.25	3 (20%)
3	MAN	O	5	3	11,11,12	0.62	0	15,15,17	0.99	2 (13%)
5	NAG	P	1	1,5	14,14,15	0.60	0	17,19,21	0.89	1 (5%)
5	NAG	P	2	5	14,14,15	0.25	0	17,19,21	0.66	0
5	BMA	P	3	5	11,11,12	0.62	0	15,15,17	0.73	0
4	NAG	Q	1	4,1	14,14,15	0.17	0	17,19,21	0.53	0
4	NAG	Q	2	4	14,14,15	0.28	0	17,19,21	0.80	1 (5%)
4	NAG	R	1	4,1	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	R	2	4	14,14,15	0.51	0	17,19,21	0.71	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	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	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	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	0/1/1/1
3	MAN	H	5	3	-	0/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	1/2/19/22	0/1/1/1
3	MAN	J	4	3	-	0/2/19/22	0/1/1/1
3	MAN	J	5	3	-	0/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	1/6/23/26	0/1/1/1
5	BMA	L	3	5	-	1/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
3	MAN	M	4	3	-	1/2/19/22	0/1/1/1
3	MAN	M	5	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	N	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	4/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	1/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1
3	MAN	O	4	3	-	0/2/19/22	0/1/1/1
3	MAN	O	5	3	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	4	MAN	O5-C1	-4.21	1.36	1.43
3	O	4	MAN	C6-C5	-3.55	1.39	1.51
3	H	5	MAN	C4-C3	2.46	1.58	1.52
3	H	5	MAN	O5-C5	2.39	1.48	1.43
3	F	3	BMA	C4-C3	2.07	1.57	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	4	MAN	C1-O5-C5	4.39	118.07	112.19
3	F	4	MAN	C1-O5-C5	4.38	118.06	112.19
3	E	5	MAN	C1-O5-C5	4.25	117.88	112.19
3	H	4	MAN	C1-O5-C5	3.24	116.52	112.19
3	D	4	MAN	C1-O5-C5	3.16	116.42	112.19
3	M	4	MAN	C1-O5-C5	3.06	116.28	112.19
3	E	3	BMA	C1-O5-C5	2.96	116.15	112.19
3	H	4	MAN	O2-C2-C3	-2.89	104.16	110.15
3	O	4	MAN	O6-C6-C5	-2.85	101.63	111.33
3	H	2	NAG	C1-O5-C5	2.73	115.84	112.19
3	M	5	MAN	C1-O5-C5	2.73	115.84	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	5	MAN	C1-O5-C5	2.71	115.82	112.19
3	O	5	MAN	C1-O5-C5	2.60	115.67	112.19
3	H	3	BMA	C1-O5-C5	2.57	115.63	112.19
3	J	5	MAN	C1-O5-C5	2.54	115.59	112.19
4	Q	2	NAG	C1-O5-C5	2.52	115.56	112.19
3	H	5	MAN	O2-C2-C3	-2.46	105.06	110.15
3	J	4	MAN	C1-O5-C5	2.45	115.47	112.19
5	P	1	NAG	C1-O5-C5	2.41	115.41	112.19
3	O	4	MAN	C6-C5-C4	-2.38	107.16	113.02
6	N	4	MAN	O2-C2-C3	-2.32	105.34	110.15
3	F	5	MAN	C1-O5-C5	2.31	115.29	112.19
5	L	2	NAG	C1-O5-C5	2.27	115.23	112.19
3	O	5	MAN	O2-C2-C3	-2.26	105.47	110.15
3	O	3	BMA	C1-O5-C5	2.23	115.18	112.19
3	D	5	MAN	O2-C2-C3	-2.18	105.64	110.15
3	F	5	MAN	O2-C2-C3	-2.17	105.66	110.15
3	O	4	MAN	O2-C2-C3	-2.15	105.70	110.15
3	D	4	MAN	O2-C2-C3	-2.14	105.71	110.15
3	M	4	MAN	O2-C2-C3	-2.14	105.72	110.15
3	J	5	MAN	O2-C2-C3	-2.12	105.76	110.15
6	N	3	BMA	O2-C2-C3	-2.12	105.76	110.15
3	H	3	BMA	O2-C2-C3	-2.11	105.77	110.15
3	F	4	MAN	O2-C2-C3	-2.11	105.77	110.15
3	E	4	MAN	O2-C2-C3	-2.11	105.78	110.15
3	J	4	MAN	O2-C2-C3	-2.09	105.82	110.15
3	M	5	MAN	O2-C2-C3	-2.08	105.84	110.15
4	G	2	NAG	C1-O5-C5	2.08	114.97	112.19
3	E	5	MAN	O2-C2-C3	-2.06	105.89	110.15
3	D	3	BMA	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	M	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6
3	M	4	MAN	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C1-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
4	K	2	NAG	C1-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
5	L	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C1-C2-N2-C7
3	O	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	K	2	NAG	C3-C2-N2-C7
4	Q	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7
5	I	2	NAG	C3-C2-N2-C7
5	L	1	NAG	C3-C2-N2-C7
5	P	2	NAG	C3-C2-N2-C7
6	N	3	BMA	O5-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	O	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
4	Q	2	NAG	C1-C2-N2-C7
5	I	2	NAG	C1-C2-N2-C7
5	P	2	NAG	C1-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
3	H	3	BMA	O5-C5-C6-O6

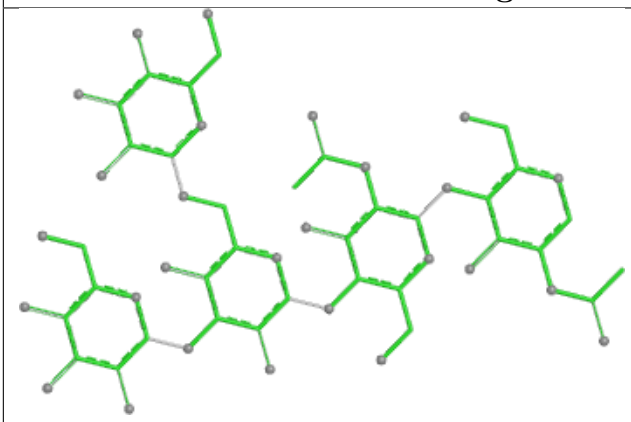
There are no ring outliers.

15 monomers are involved in 14 short contacts:

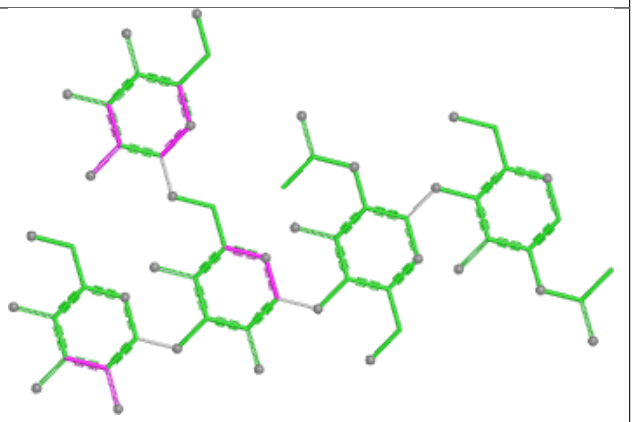
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	2	0
5	L	1	NAG	2	0
6	N	2	NAG	1	0
5	I	2	NAG	1	0
3	D	3	BMA	1	0
4	R	2	NAG	1	0
3	O	1	NAG	2	0
3	D	5	MAN	1	0
3	E	2	NAG	2	0
5	L	2	NAG	2	0
3	M	2	NAG	1	0
6	N	1	NAG	1	0
4	R	1	NAG	1	0
3	O	2	NAG	1	0
3	H	2	NAG	1	0

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

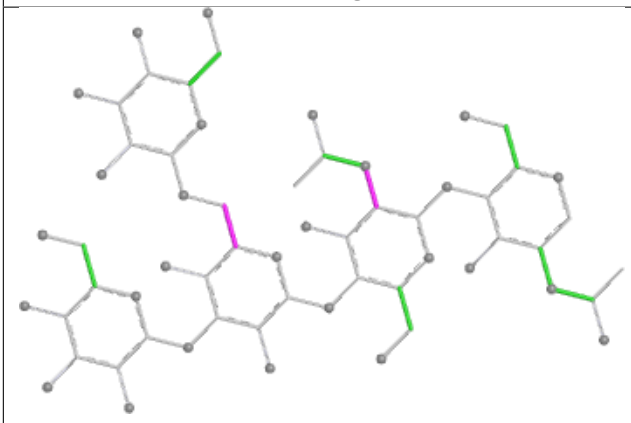
Oligosaccharide Chain E



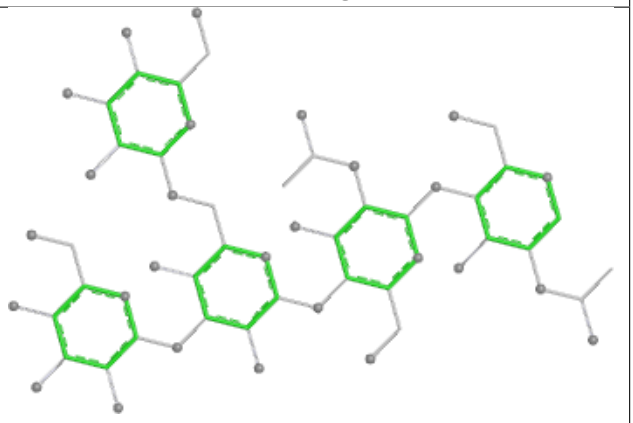
Bond lengths



Bond angles

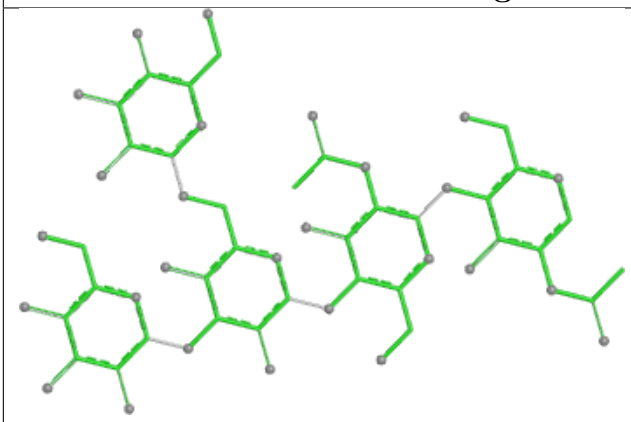


Torsions

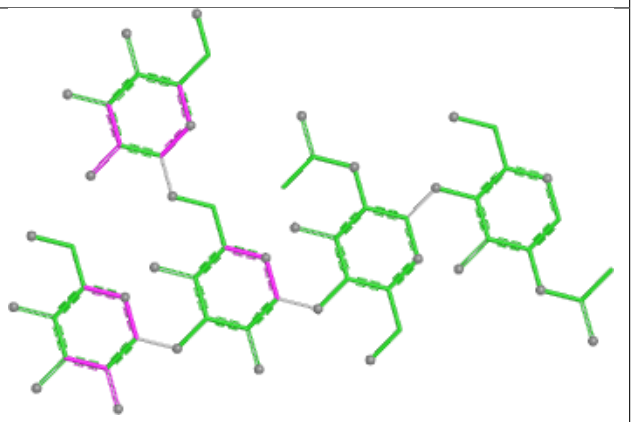


Rings

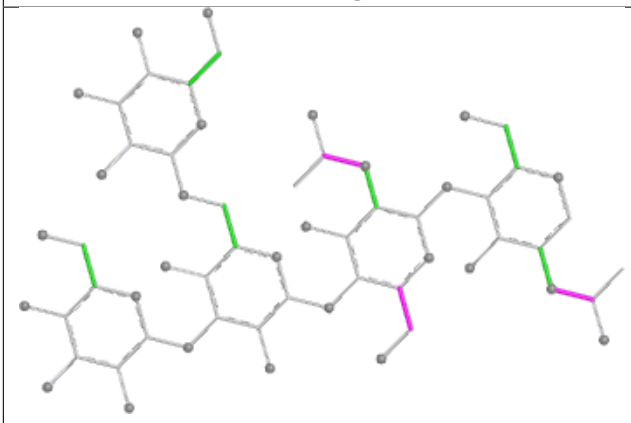
Oligosaccharide Chain D



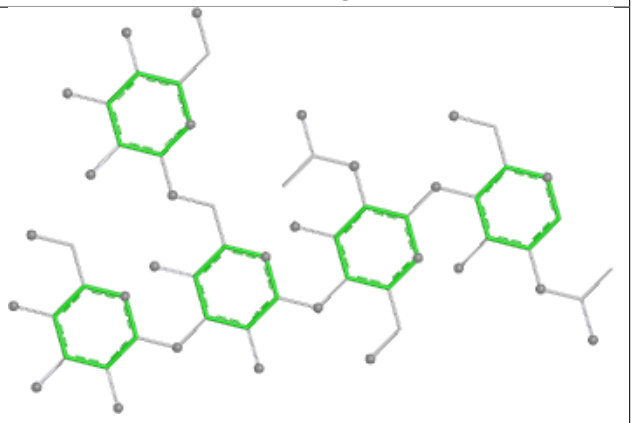
Bond lengths



Bond angles

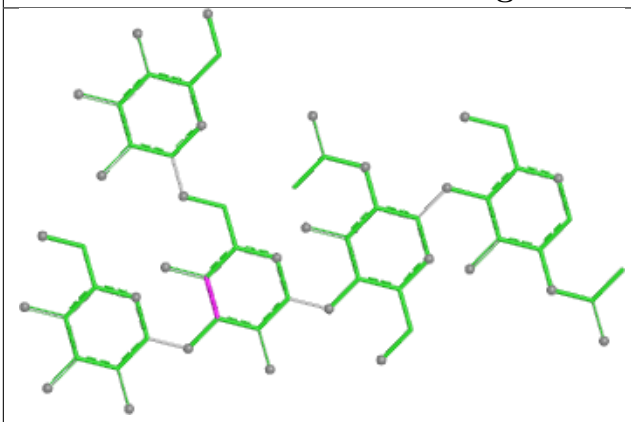


Torsions

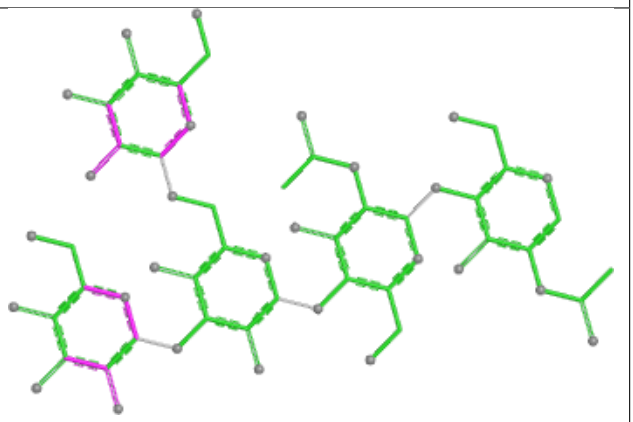


Rings

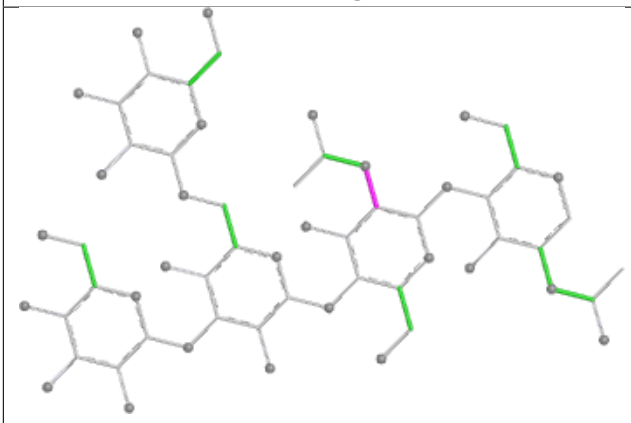
Oligosaccharide Chain F



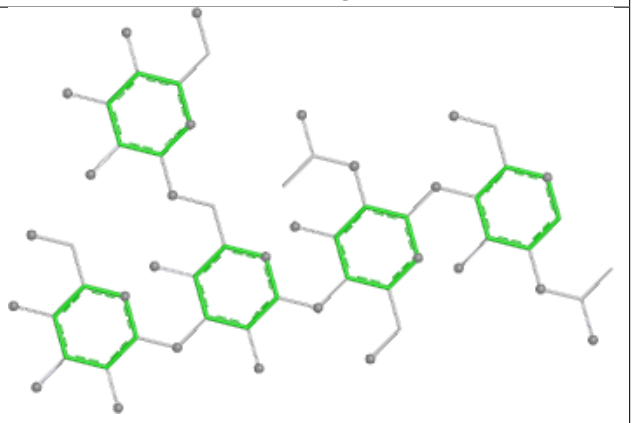
Bond lengths



Bond angles

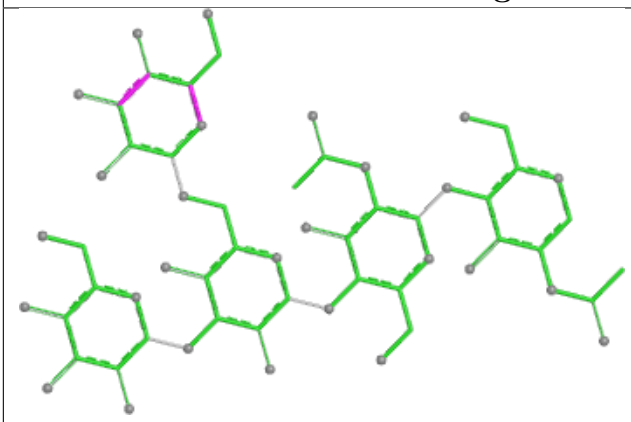


Torsions

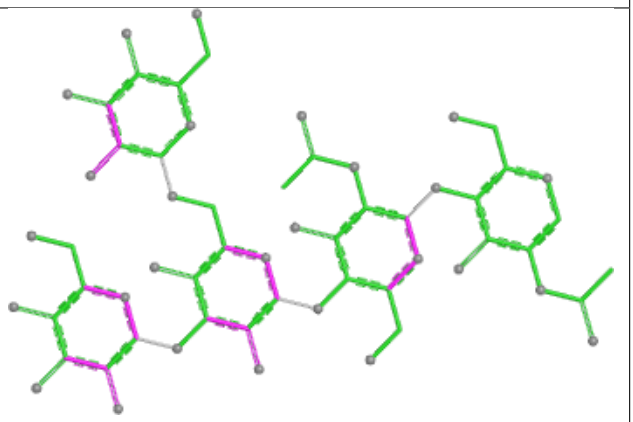


Rings

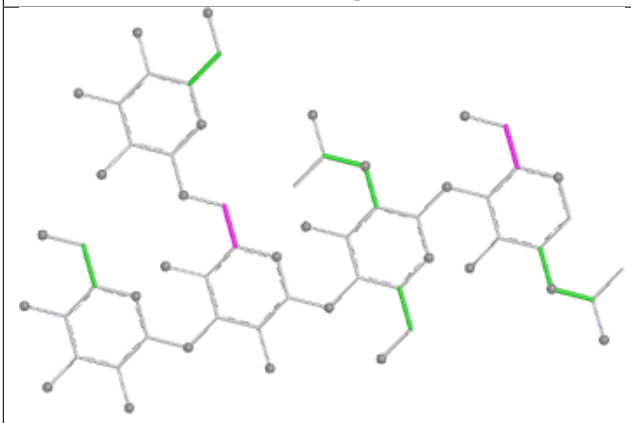
Oligosaccharide Chain H



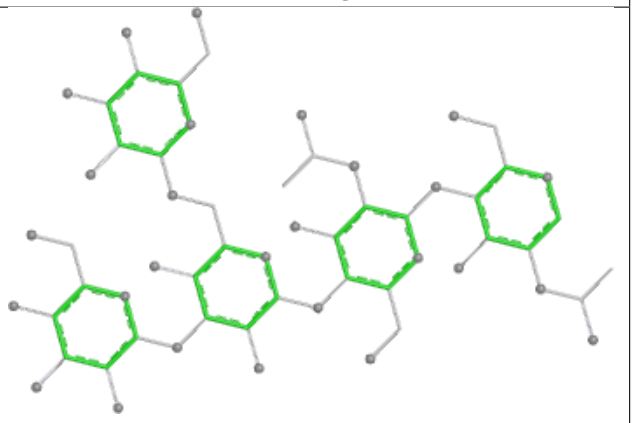
Bond lengths



Bond angles

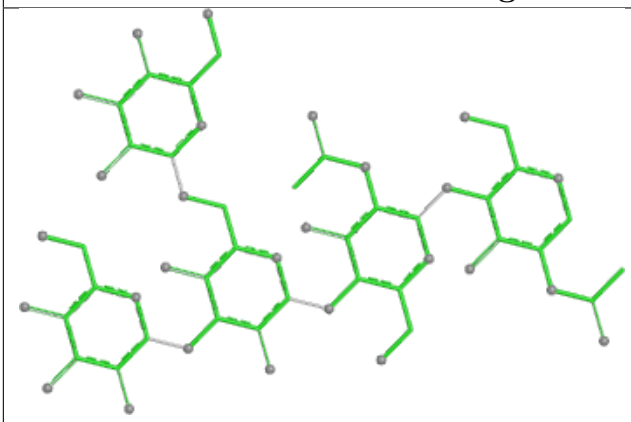


Torsions

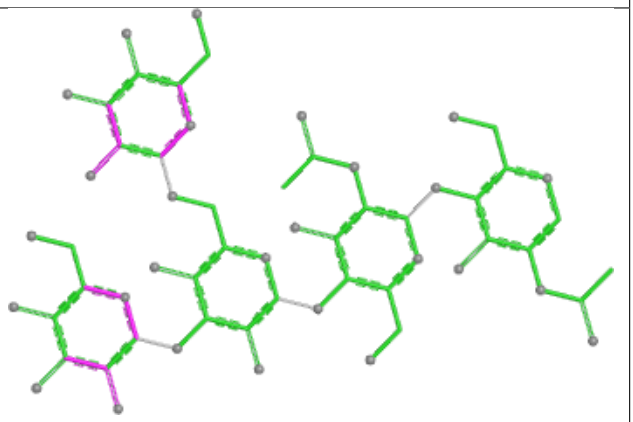


Rings

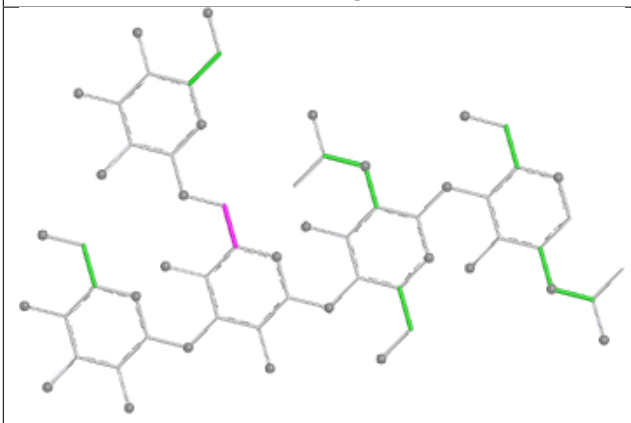
Oligosaccharide Chain J



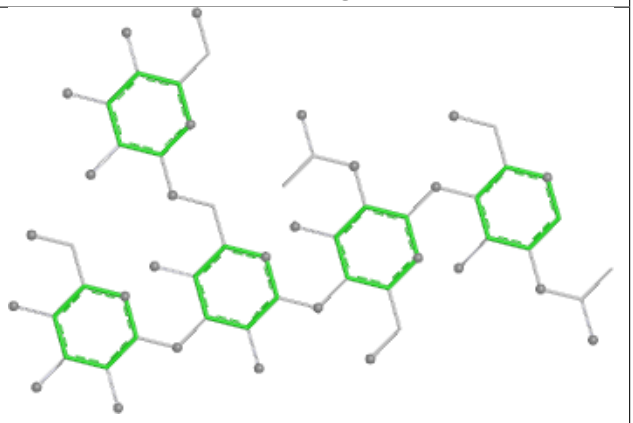
Bond lengths



Bond angles

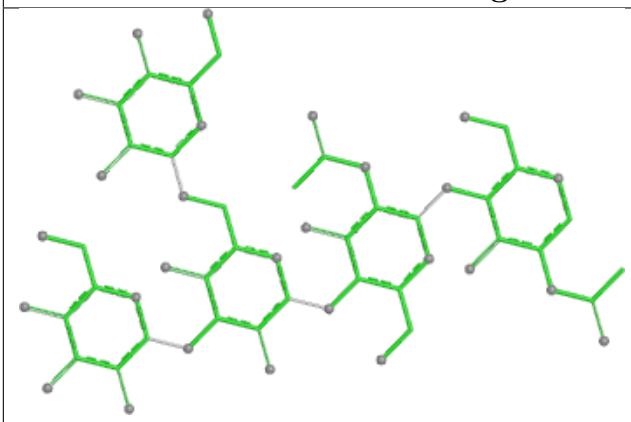


Torsions

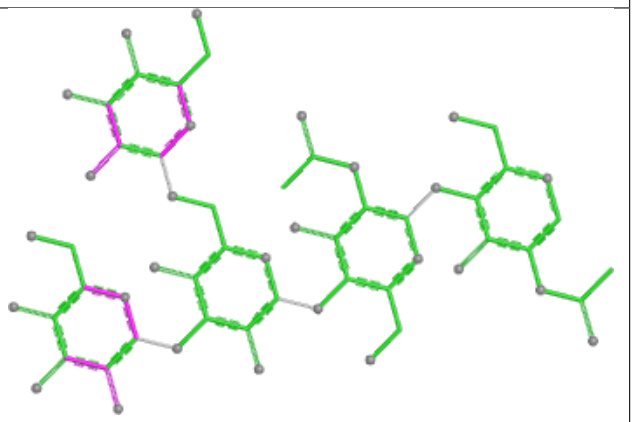


Rings

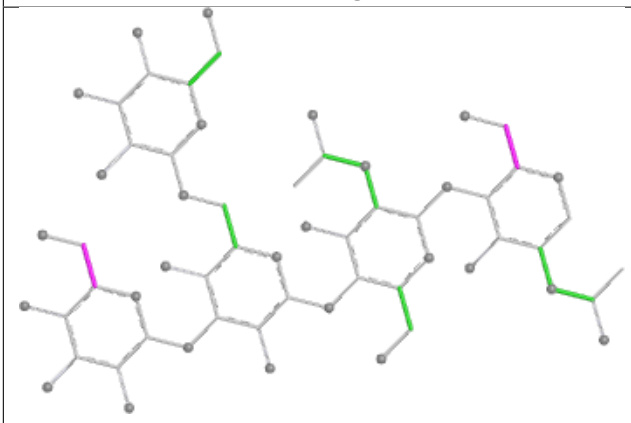
Oligosaccharide Chain M



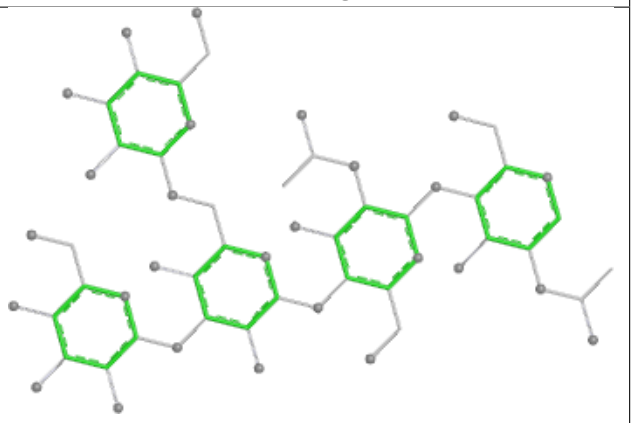
Bond lengths



Bond angles

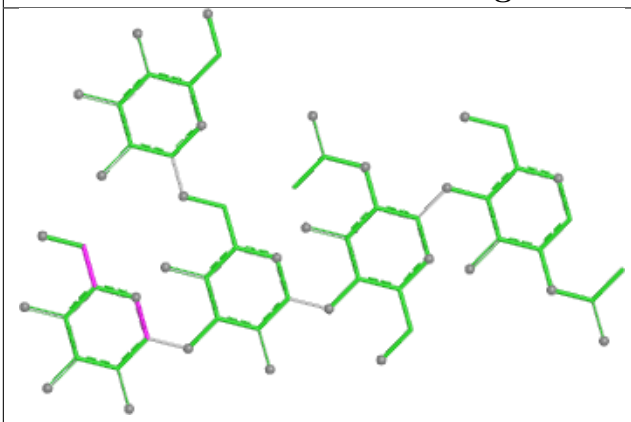


Torsions

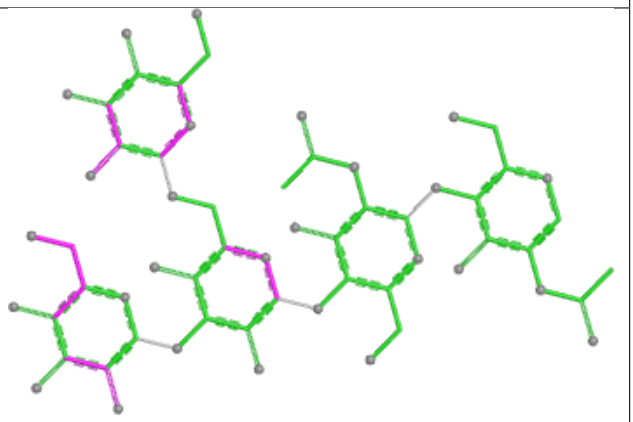


Rings

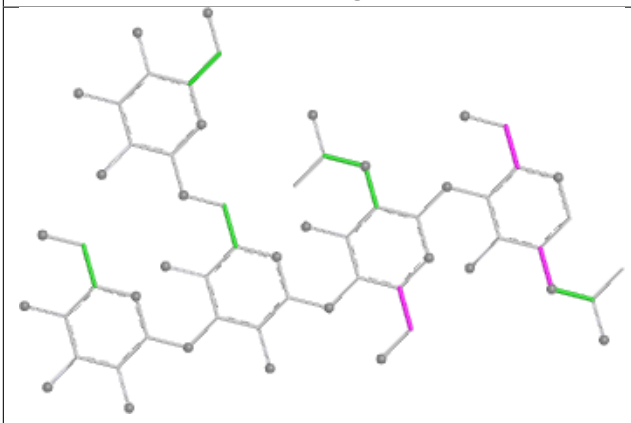
Oligosaccharide Chain O



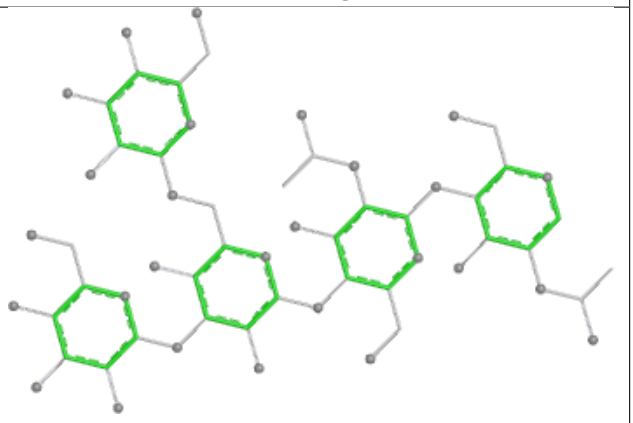
Bond lengths



Bond angles

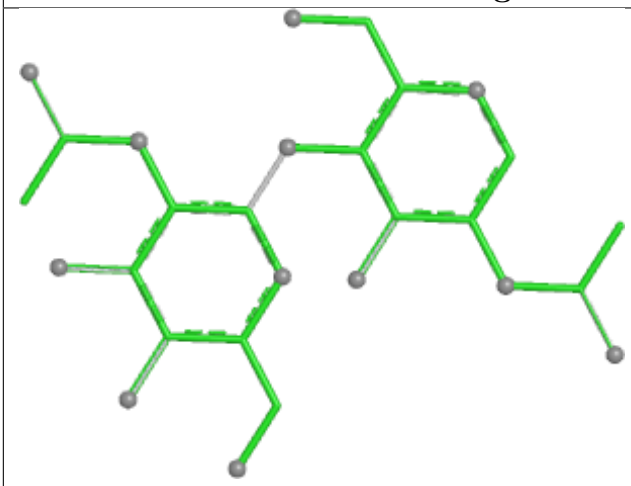


Torsions

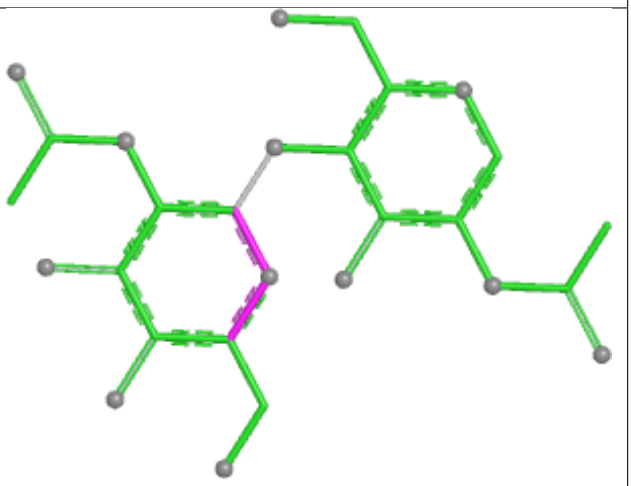


Rings

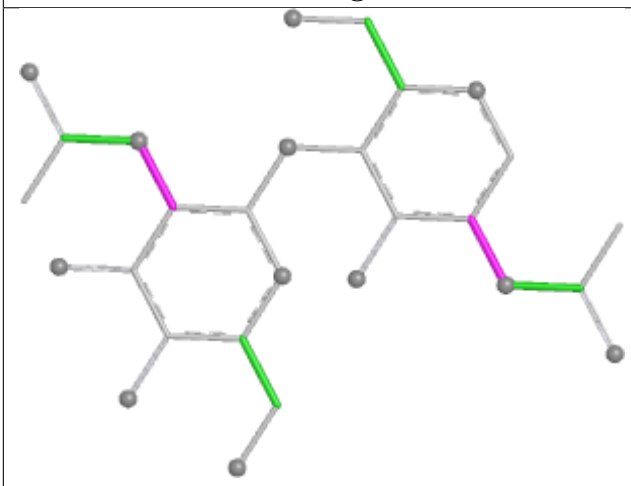
Oligosaccharide Chain G



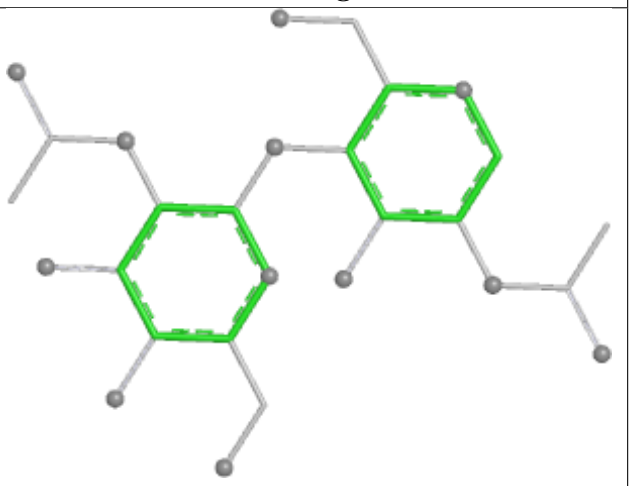
Bond lengths



Bond angles

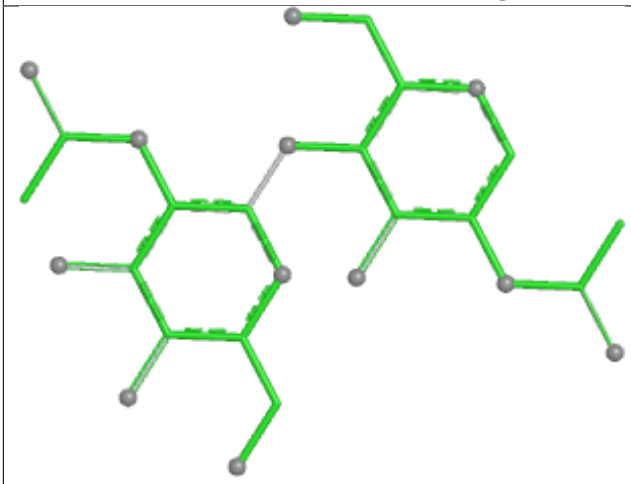


Torsions

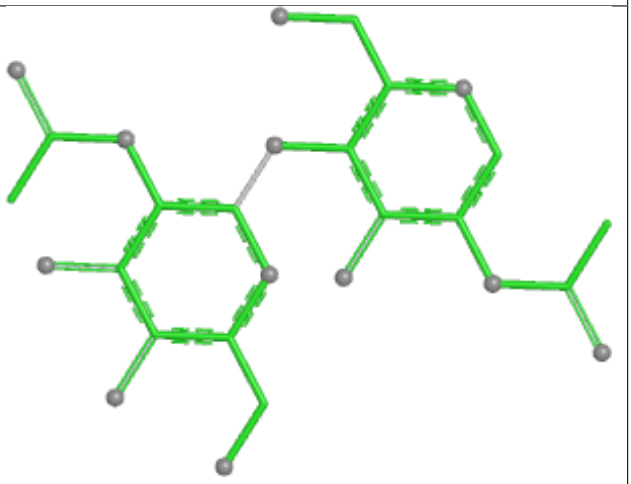


Rings

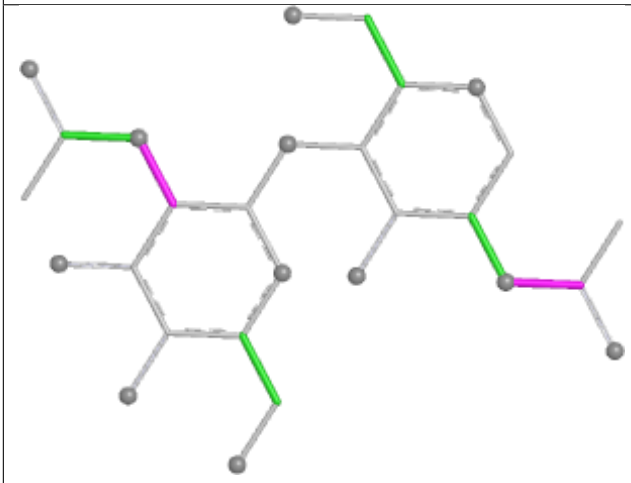
Oligosaccharide Chain K



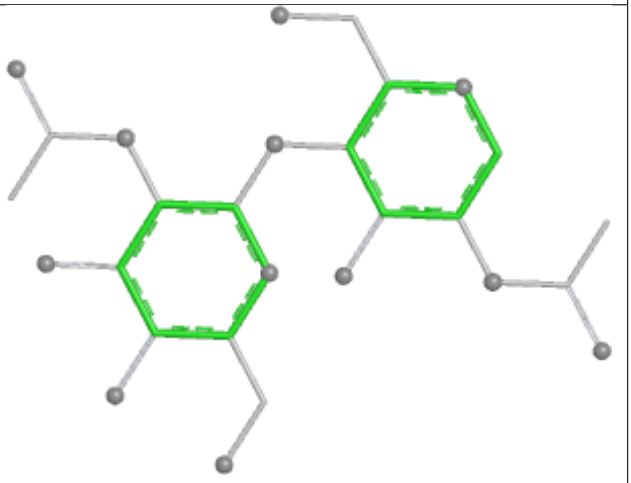
Bond lengths



Bond angles

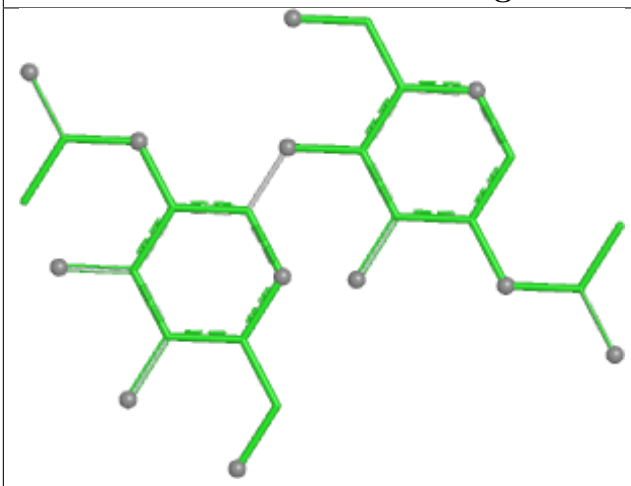


Torsions

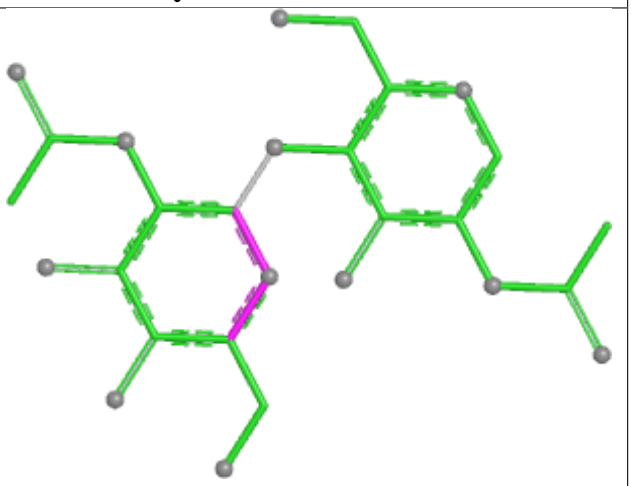


Rings

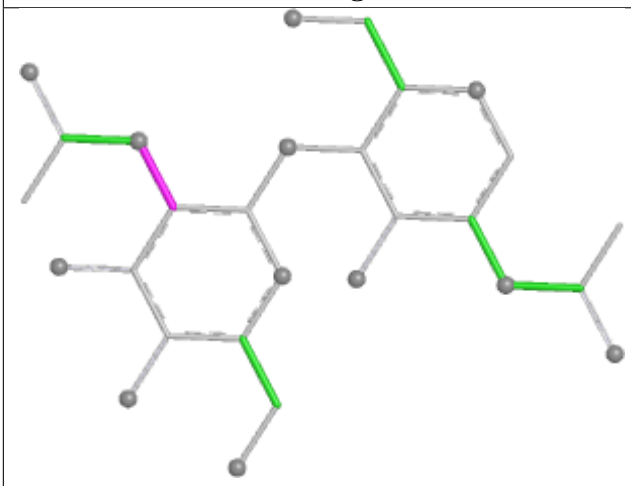
Oligosaccharide Chain Q



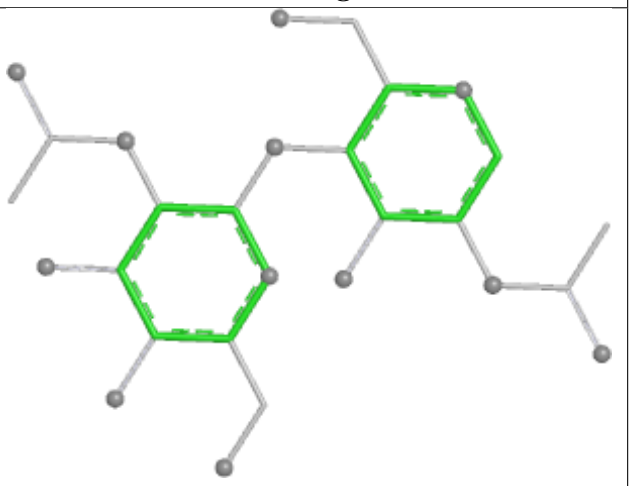
Bond lengths



Bond angles

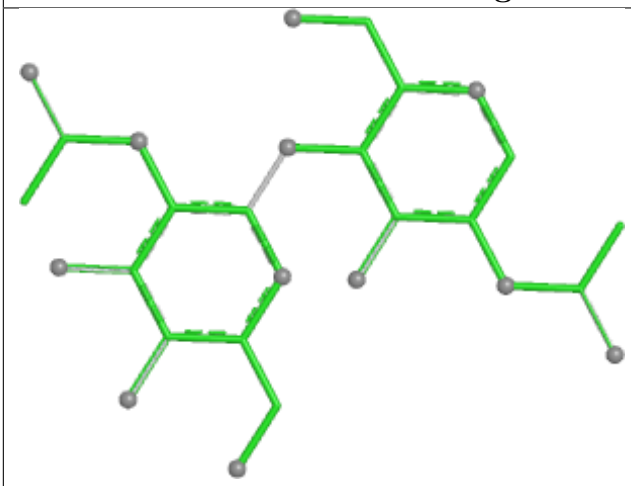


Torsions

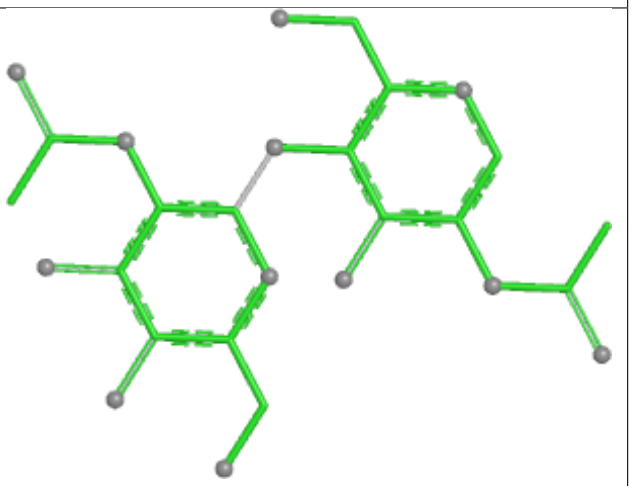


Rings

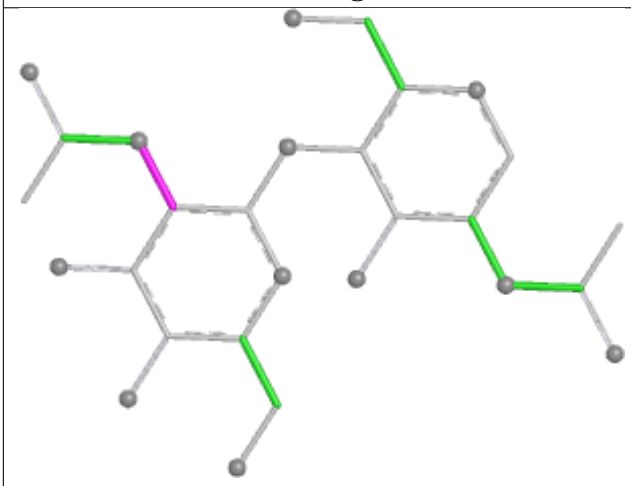
Oligosaccharide Chain R



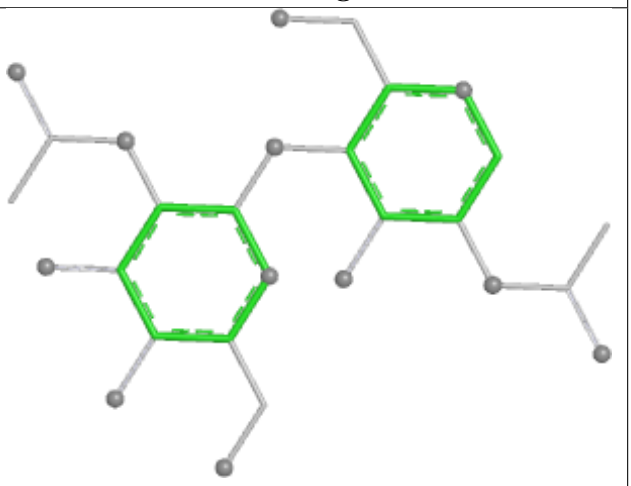
Bond lengths



Bond angles

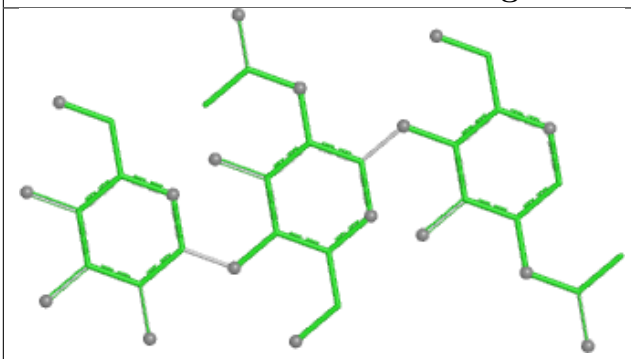


Torsions

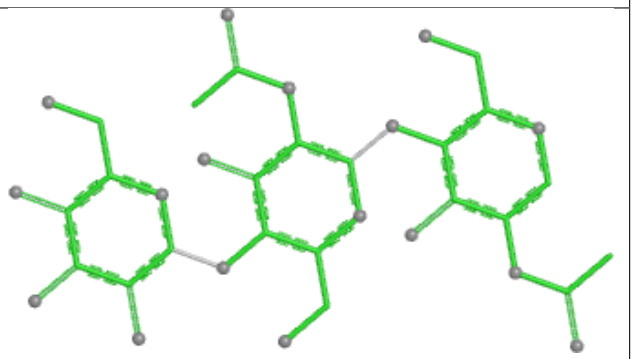


Rings

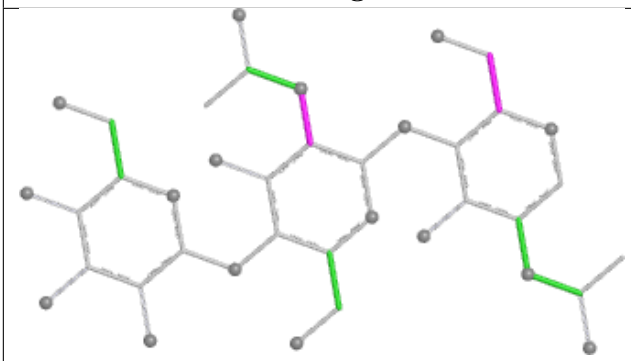
Oligosaccharide Chain I



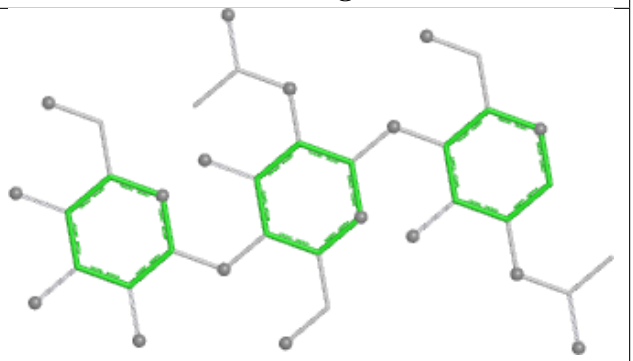
Bond lengths



Bond angles

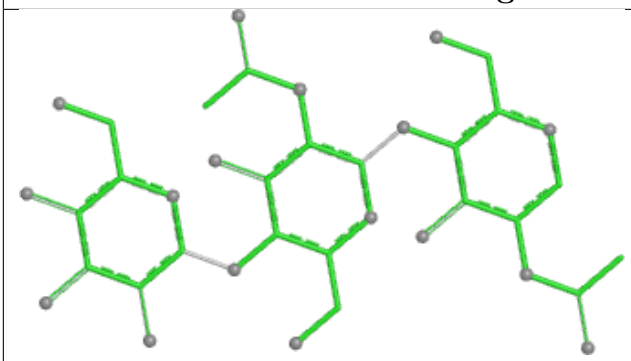


Torsions

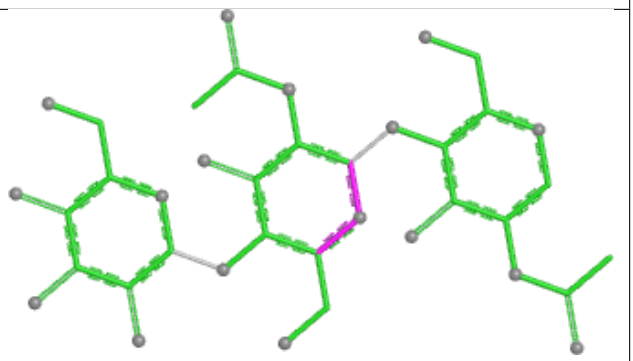


Rings

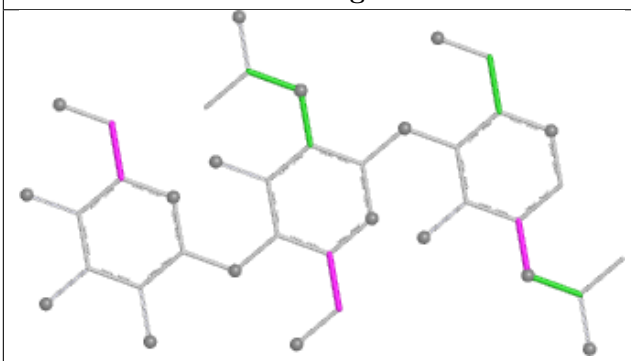
Oligosaccharide Chain L



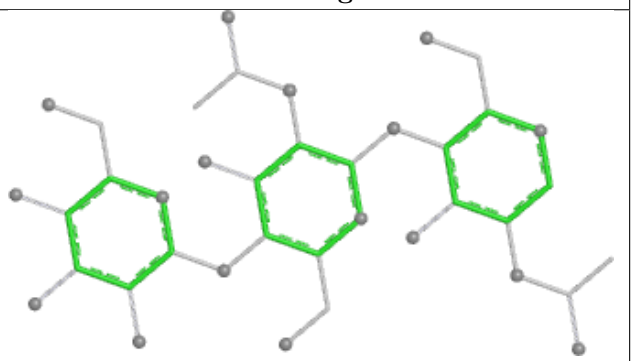
Bond lengths



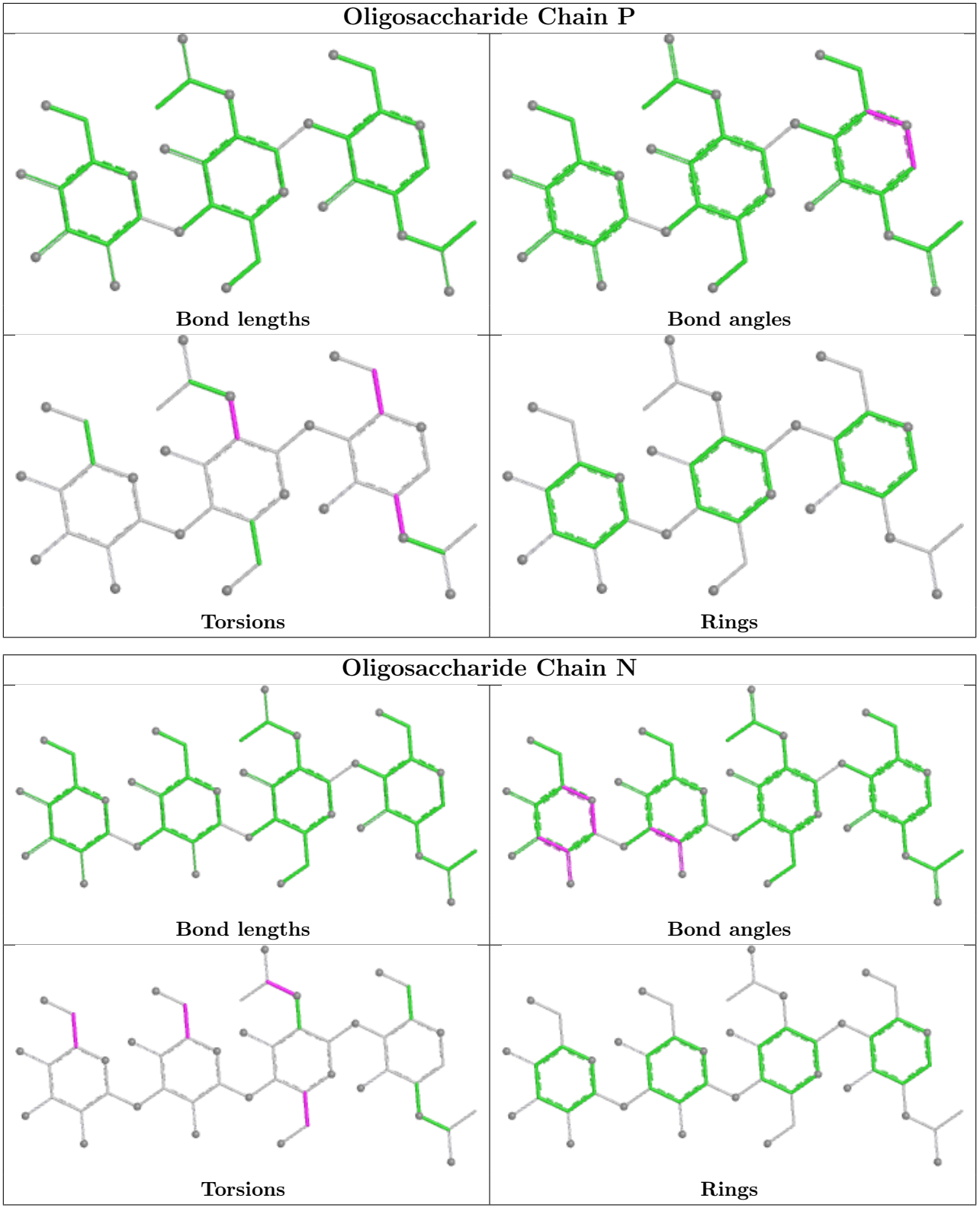
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

11 ligands 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	$\#\|Z\| > 2$
7	NAG	c	601	2	14,14,15	0.22	0	17,19,21	0.44	0
7	NAG	A	401	1	14,14,15	0.44	0	17,19,21	0.55	0
7	NAG	B	403	1	14,14,15	0.39	0	17,19,21	0.42	0
7	NAG	C	502	1	14,14,15	0.34	0	17,19,21	0.52	0
7	NAG	B	401	1	14,14,15	0.38	0	17,19,21	0.51	0
8	GOL	b	601	-	5,5,5	0.95	0	5,5,5	1.06	0
7	NAG	B	402	1	14,14,15	0.37	0	17,19,21	0.61	0
7	NAG	a	601	2	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	C	503	1	14,14,15	0.30	0	17,19,21	0.77	0
7	NAG	C	501	1	14,14,15	0.28	0	17,19,21	0.46	0
7	NAG	A	402	1	14,14,15	0.34	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	c	601	2	-	2/6/23/26	0/1/1/1
7	NAG	A	401	1	-	2/6/23/26	0/1/1/1
7	NAG	B	403	1	-	0/6/23/26	0/1/1/1
7	NAG	C	502	1	-	1/6/23/26	0/1/1/1
7	NAG	B	401	1	-	0/6/23/26	0/1/1/1
8	GOL	b	601	-	-	0/4/4/4	-
7	NAG	B	402	1	-	2/6/23/26	0/1/1/1
7	NAG	a	601	2	-	3/6/23/26	0/1/1/1
7	NAG	C	503	1	-	0/6/23/26	0/1/1/1
7	NAG	C	501	1	-	1/6/23/26	0/1/1/1
7	NAG	A	402	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	NAG	C8-C7-N2-C2
7	A	401	NAG	O7-C7-N2-C2
7	a	601	NAG	C8-C7-N2-C2
7	a	601	NAG	O7-C7-N2-C2
7	c	601	NAG	C8-C7-N2-C2
7	c	601	NAG	O7-C7-N2-C2
7	a	601	NAG	O5-C5-C6-O6
7	C	501	NAG	O5-C5-C6-O6
7	A	402	NAG	O5-C5-C6-O6
7	C	502	NAG	O5-C5-C6-O6
7	B	402	NAG	C3-C2-N2-C7
7	B	402	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	401	NAG	1	0
7	B	402	NAG	2	0
7	C	503	NAG	1	0
7	C	501	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	318/323 (98%)	-0.50	0	100	100	75, 100, 126, 148	0
1	B	319/323 (98%)	-0.49	0	100	100	72, 106, 133, 148	0
1	C	318/323 (98%)	-0.50	0	100	100	83, 111, 138, 150	0
2	a	172/182 (94%)	-0.60	0	100	100	70, 96, 113, 125	0
2	b	171/182 (93%)	-0.56	0	100	100	72, 103, 124, 156	0
2	c	172/182 (94%)	-0.55	0	100	100	74, 102, 127, 154	0
All	All	1470/1515 (97%)	-0.52	0	100	100	70, 104, 131, 156	0

There are no RSRZ outliers to report.

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

SUGAR-RSR INFOmissingINFO

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	a	601	14/15	0.39	0.10	126,146,154,155	0

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Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	c	601	14/15	0.49	0.13	123,131,148,149	0
7	NAG	C	502	14/15	0.61	0.10	121,134,145,154	0
7	NAG	A	401	14/15	0.65	0.11	102,127,151,158	0
7	NAG	C	503	14/15	0.65	0.09	124,143,149,150	0
7	NAG	B	401	14/15	0.66	0.10	92,108,131,137	0
7	NAG	B	402	14/15	0.66	0.10	127,147,154,159	0
7	NAG	C	501	14/15	0.73	0.08	99,111,124,134	0
7	NAG	B	403	14/15	0.75	0.08	111,125,138,142	0
7	NAG	A	402	14/15	0.77	0.09	122,130,142,144	0
8	GOL	b	601	6/6	0.77	0.15	77,79,101,103	0

6.5 Other polymers (i)

There are no such residues in this entry.