Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 06:56 PM EST

PDB ID	:	4RQS
Title	:	Crystal structure of fully glycosylated HIV-1 gp120 core bound to CD4 and 17b Fab
Authors	:	Kong, L.; Wilson, I.A.; Kwong, P.D.
Deposited on	:	2014-11-05
Resolution	:	4.49 Å(reported)

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

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

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

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

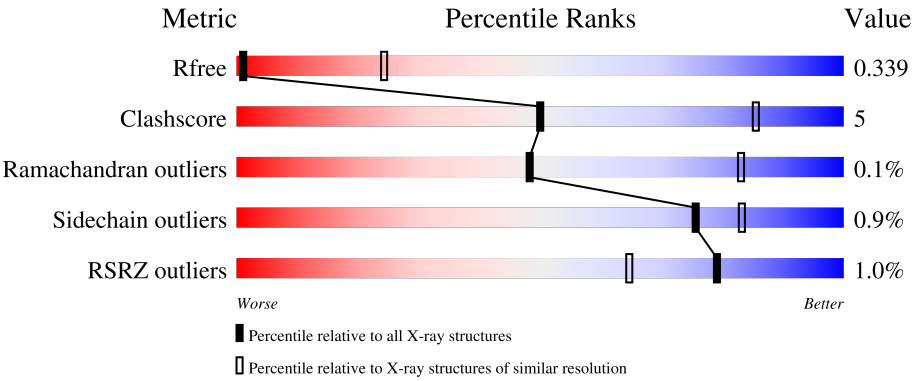
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 4.49 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	1050 (5.10-3.90)
Clashscore	180529	1106 (5.10-3.90)
Ramachandran outliers	177936	1006 (5.10-3.90)
Sidechain outliers	177891	1008 (5.12-3.88)
RSRZ outliers	164620	1046 (5.10-3.90)

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%

Mol	Chain	Length	Quality of chain
1	B	185	86% 11%
2	C	214	88% 12%
3	D	229	84% 13%
4	G	313	81% 12% 6%
5	A	9	56% 33% 11%
6	E	2	100%

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Mol	Chain	Length	Quality of chain
6	H	2	100%
6	I	2	50% 50%
6	J	2	50% 50%
7	F	3	100%
7	K	3	67% 33%
7	L	3	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7379 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 2-domain CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	181	Total	C	N	O	S	0	0	0
			1412	885	247	276	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	ASN	-	expression tag	UNP P01730
B	185	THR	-	expression tag	UNP P01730

- Molecule 2 is a protein called 17b Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1646	1028	282	331	5			

- Molecule 3 is a protein called 17b Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	223	Total	C	N	O	S	0	0	0
			1681	1064	282	330	5			

- Molecule 4 is a protein called HIV-1 YU2 gp120 core chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	295	Total	C	N	O	S	0	0	0
			2292	1441	396	435	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	79	GLY	-	expression tag	UNP P35961
G	80	ALA	-	expression tag	UNP P35961

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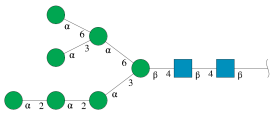
Chain	Residue	Modelled	Actual	Comment	Reference
G	81	ARG	-	expression tag	UNP P35961
G	82	SER	-	expression tag	UNP P35961
G	128	GLY	-	linker	UNP P35961
G	129	ALA	-	linker	UNP P35961
G	194	GLY	-	linker	UNP P35961
G	298	GLY	-	linker	UNP P35961
G	299	ALA	-	linker	UNP P35961
G	300	GLY	-	linker	UNP P35961

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

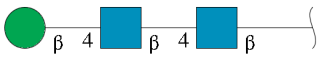


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	A	9	Total C N O 105 58 2 45	0	0	0

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

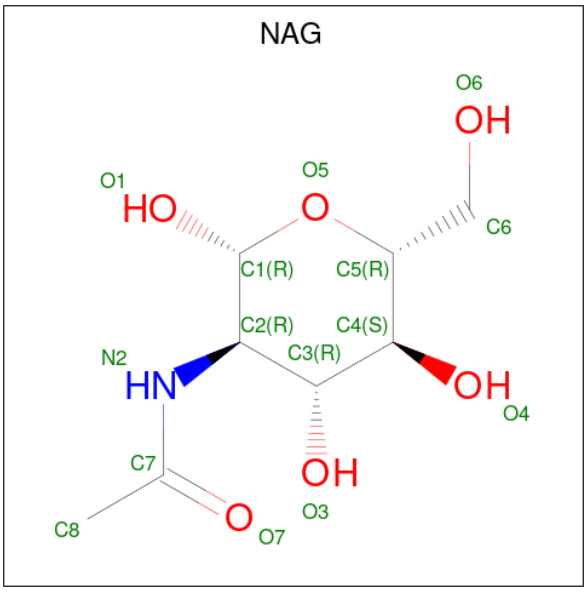
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	E	2	Total C N O 28 16 2 10	0	0	0
6	H	2	Total C N O 28 16 2 10	0	0	0
6	I	2	Total C N O 28 16 2 10	0	0	0
6	J	2	Total C N O 28 16 2 10	0	0	0

- Molecule 7 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
7	F	3	Total C N O 39 22 2 15	0	0	0
7	K	3	Total C N O 39 22 2 15	0	0	0
7	L	3	Total C N O 39 22 2 15	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



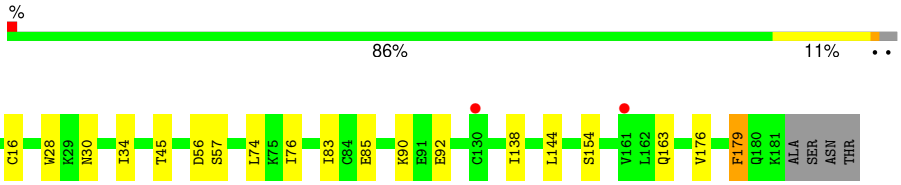
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total C N O 14 8 1 5	0	0

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.

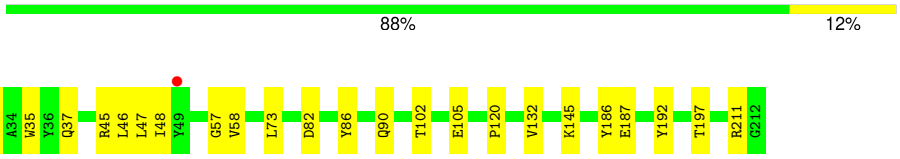
• Molecule 1: 2-domain CD4

Chain B:



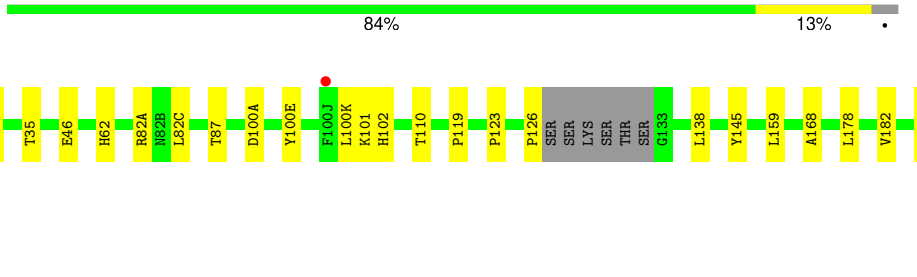
• Molecule 2: 17b Fab Light Chain

Chain C:



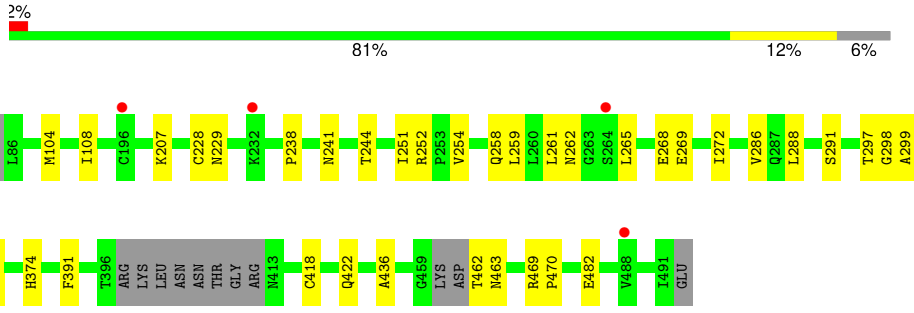
• Molecule 3: 17b Fab Heavy Chain

Chain D:



• Molecule 4: HIV-1 YU2 gp120 core chimeric protein

Chain G:



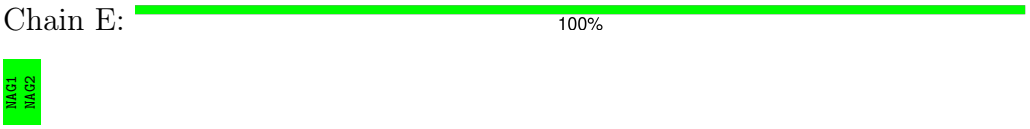
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-

(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

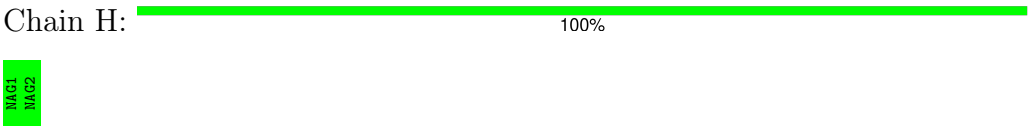
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain H:



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

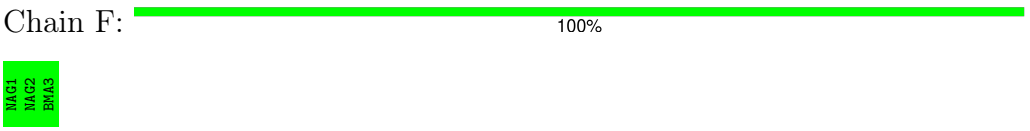
Chain I:

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

Chain J:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

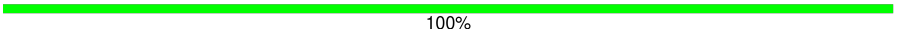
Chain F:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	171.32Å 171.32Å 151.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.50 – 4.49 47.50 – 4.49	Depositor EDS
% Data completeness (in resolution range)	95.1 (47.50-4.49) 95.0 (47.50-4.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 4.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.276 , 0.322 0.283 , 0.339	Depositor DCC
R_{free} test set	667 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	248.9	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 296.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7379	wwPDB-VP
Average B, all atoms (Å^2)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: 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	B	0.21	0/1432	0.38	0/1930
2	C	0.21	0/1683	0.38	0/2288
3	D	0.20	0/1720	0.37	0/2343
4	G	0.21	0/2337	0.40	1/3169 (0.0%)
All	All	0.21	0/7172	0.38	1/9730 (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
4	G	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	300	GLY	CA-C-N	-6.96	101.89	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	300	GLY	Peptide,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	B	1412	0	1444	13	0
2	C	1646	0	1593	13	0
3	D	1681	0	1650	17	0
4	G	2292	0	2246	29	0
5	A	105	0	88	6	0
6	E	28	0	25	0	0
6	H	28	0	25	0	0
6	I	28	0	25	1	0
6	J	28	0	25	2	0
7	F	39	0	34	0	0
7	K	39	0	34	1	0
7	L	39	0	34	0	0
8	G	14	0	13	0	0
All	All	7379	0	7236	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (75) 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)
5:A:7:MAN:C6	5:A:9:MAN:C1	2.46	0.93
4:G:297:THR:HG22	4:G:298:GLY:H	1.40	0.87
5:A:7:MAN:O6	5:A:9:MAN:C2	2.22	0.87
5:A:1:NAG:H61	5:A:2:NAG:H82	1.66	0.76
4:G:297:THR:HG22	4:G:298:GLY:N	2.03	0.72
1:B:5:LEU:HD21	1:B:163:GLN:HB3	1.74	0.69
4:G:300:GLY:CA	4:G:418:CYS:HB2	2.26	0.66
3:D:100(E):TYR:O	4:G:422:GLN:NE2	2.29	0.65
4:G:268:GLU:HG3	4:G:269:GLU:HG2	1.80	0.64
4:G:297:THR:CG2	4:G:298:GLY:H	2.15	0.59
4:G:207:LYS:HE2	4:G:436:ALA:HB3	1.85	0.58
3:D:126:PRO:HG3	3:D:138:LEU:HB3	1.85	0.58
5:A:7:MAN:O6	5:A:9:MAN:H2	2.03	0.58
3:D:197:ASN:HB3	3:D:206:LYS:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2:NAG:H82	6:J:1:NAG:H81	1.87	0.56
1:B:85:GLU:HG2	1:B:90:LYS:HG2	1.88	0.56
4:G:298:GLY:O	4:G:299:ALA:HB3	2.06	0.55
4:G:300:GLY:HA2	4:G:418:CYS:HB2	1.89	0.55
5:A:2:NAG:C8	6:J:1:NAG:H81	2.37	0.55
3:D:35:THR:HB	3:D:100(K):LEU:HD21	1.89	0.54
3:D:126:PRO:HD2	3:D:213:PRO:HA	1.89	0.54
3:D:159:LEU:HD21	3:D:182:VAL:HG21	1.90	0.53
4:G:265:LEU:HD11	4:G:291:SER:HB3	1.90	0.53
3:D:123:PRO:HD3	3:D:209:LYS:HE2	1.91	0.52
4:G:229:ASN:HB2	4:G:241:ASN:HD22	1.74	0.52
1:B:154:SER:HB2	1:B:176:VAL:HB	1.92	0.52
1:B:83:ILE:HG13	1:B:92:GLU:HG3	1.92	0.52
2:C:21:LEU:HD22	2:C:102:THR:HG21	1.92	0.51
2:C:45:ARG:NH2	2:C:57:GLY:O	2.43	0.51
4:G:363:PRO:O	4:G:469:ARG:NH1	2.39	0.50
3:D:87:THR:HG23	3:D:110:THR:HA	1.92	0.50
3:D:119:PRO:HB3	3:D:145:TYR:HB3	1.93	0.50
2:C:145:LYS:HB3	2:C:197:THR:HB	1.93	0.50
4:G:252:ARG:HD2	4:G:262:ASN:HB3	1.92	0.50
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.94	0.50
1:B:138:ILE:HG22	1:B:144:LEU:HD11	1.94	0.49
1:B:76:ILE:HD12	1:B:76:ILE:H	1.77	0.49
4:G:254:VAL:HG11	4:G:261:LEU:HB2	1.95	0.48
1:B:30:ASN:HD21	1:B:34:ILE:HB	1.78	0.48
2:C:120:PRO:HD3	2:C:132:VAL:HG22	1.97	0.47
2:C:46:LEU:HD22	3:D:101:LYS:HA	1.97	0.46
4:G:238:PRO:HD2	7:K:1:NAG:H61	1.97	0.46
1:B:56:ASP:OD1	1:B:57:SER:N	2.40	0.46
2:C:82:ASP:O	2:C:86:TYR:OH	2.26	0.46
4:G:272:ILE:HG22	4:G:286:VAL:HG22	1.97	0.46
3:D:46:GLU:OE2	3:D:62:HIS:NE2	2.48	0.46
4:G:462:THR:HA	4:G:463:ASN:HA	1.50	0.45
4:G:259:LEU:HB2	4:G:374:HIS:CE1	2.51	0.45
2:C:186:TYR:O	2:C:192:TYR:OH	2.34	0.45
2:C:12:SER:OG	2:C:105:GLU:OE1	2.27	0.45
4:G:258:GLN:NE2	4:G:371:ILE:O	2.50	0.45
4:G:288:LEU:HD21	4:G:345:ILE:HD11	1.99	0.44
3:D:27:ASP:OD2	3:D:28:THR:N	2.41	0.44
3:D:2:VAL:HG11	3:D:102:HIS:CD2	2.53	0.44
4:G:297:THR:CG2	4:G:298:GLY:N	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:VAL:HG12	1:B:74:LEU:HD11	2.00	0.43
4:G:300:GLY:HA3	4:G:418:CYS:O	2.18	0.43
4:G:229:ASN:HB2	4:G:241:ASN:ND2	2.34	0.43
2:C:21:LEU:HD12	2:C:73:LEU:HD23	2.01	0.43
2:C:35:TRP:HB2	2:C:48:ILE:HB	2.00	0.42
4:G:104:MET:O	4:G:108:ILE:HG12	2.19	0.42
3:D:168:ALA:HB2	3:D:178:LEU:HD23	2.02	0.42
1:B:179:PHE:HD1	1:B:179:PHE:HA	1.69	0.42
1:B:16:CYS:HB2	1:B:28:TRP:CZ2	2.55	0.42
1:B:16:CYS:HB2	1:B:28:TRP:HZ2	1.85	0.41
3:D:197:ASN:ND2	3:D:208:ASP:OD2	2.49	0.41
2:C:187:GLU:O	2:C:211:ARG:NH2	2.53	0.41
4:G:251:ILE:HG23	4:G:482:GLU:HG3	2.02	0.41
2:C:47:LEU:HA	2:C:58:VAL:HG21	2.03	0.41
4:G:391:PHE:CZ	4:G:470:PRO:HB3	2.55	0.41
3:D:100(A):ASP:OD1	3:D:100(A):ASP:N	2.55	0.40
1:B:45:THR:HG22	4:G:371:ILE:HD13	2.03	0.40
3:D:18:VAL:HG12	3:D:82(C):LEU:HD21	2.04	0.40
4:G:259:LEU:HD12	4:G:374:HIS:CD2	2.57	0.40
4:G:332:ASN:HD22	6:I:1:NAG:C7	2.32	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	B	179/185 (97%)	174 (97%)	5 (3%)	0	100	100
2	C	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
3	D	219/229 (96%)	216 (99%)	3 (1%)	0	100	100
4	G	289/313 (92%)	280 (97%)	8 (3%)	1 (0%)	37	72
All	All	899/941 (96%)	875 (97%)	23 (3%)	1 (0%)	48	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	300	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	B	164/167 (98%)	162 (99%)	2 (1%)	67	79
2	C	184/184 (100%)	182 (99%)	2 (1%)	70	80
3	D	187/193 (97%)	186 (100%)	1 (0%)	86	89
4	G	261/276 (95%)	259 (99%)	2 (1%)	79	84
All	All	796/820 (97%)	789 (99%)	7 (1%)	75	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	LYS
1	B	179	PHE
2	C	33	LEU
2	C	90	GLN
3	D	82(A)	ARG
4	G	228	CYS
4	G	244	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	90	GLN
3	D	171	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)

26 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	$\#\|Z\| > 2$
5	NAG	A	1	5,4	14,14,15	0.58	0	17,19,21	0.67	0
5	NAG	A	2	5	14,14,15	0.56	0	17,19,21	0.86	0
5	BMA	A	3	5	11,11,12	0.66	0	15,15,17	0.71	0
5	MAN	A	4	5	11,11,12	0.59	0	15,15,17	0.57	0
5	MAN	A	5	5	11,11,12	0.53	0	15,15,17	0.65	0
5	MAN	A	6	5	11,11,12	0.62	0	15,15,17	0.54	0
5	MAN	A	7	5	11,11,12	0.65	0	15,15,17	0.93	2 (13%)
5	MAN	A	8	5	11,11,12	0.61	0	15,15,17	0.52	0
5	MAN	A	9	5	11,11,12	0.65	0	15,15,17	0.59	0
6	NAG	E	1	6,4	14,14,15	0.51	0	17,19,21	0.73	0
6	NAG	E	2	6	14,14,15	0.53	0	17,19,21	0.55	0
7	NAG	F	1	7,4	14,14,15	0.54	0	17,19,21	0.79	0
7	NAG	F	2	7	14,14,15	0.49	0	17,19,21	0.70	0
7	BMA	F	3	7	11,11,12	0.60	0	15,15,17	0.58	0
6	NAG	H	1	6,4	14,14,15	0.52	0	17,19,21	0.77	0
6	NAG	H	2	6	14,14,15	0.49	0	17,19,21	0.66	0
6	NAG	I	1	6,4	14,14,15	0.51	0	17,19,21	0.56	0
6	NAG	I	2	6	14,14,15	0.54	0	17,19,21	0.60	0
6	NAG	J	1	6,4	14,14,15	0.53	0	17,19,21	0.66	0
6	NAG	J	2	6	14,14,15	0.52	0	17,19,21	0.61	0
7	NAG	K	1	7,4	14,14,15	0.54	0	17,19,21	0.68	0
7	NAG	K	2	7	14,14,15	0.57	0	17,19,21	0.94	0
7	BMA	K	3	7	11,11,12	0.66	0	15,15,17	0.64	0
7	NAG	L	1	7,4	14,14,15	0.52	0	17,19,21	0.70	0
7	NAG	L	2	7	14,14,15	0.53	0	17,19,21	0.63	0
7	BMA	L	3	7	11,11,12	0.62	0	15,15,17	0.57	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
5	NAG	A	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	A	2	5	-	2/6/23/26	0/1/1/1
5	BMA	A	3	5	-	0/2/19/22	0/1/1/1
5	MAN	A	4	5	-	0/2/19/22	0/1/1/1
5	MAN	A	5	5	-	1/2/19/22	0/1/1/1
5	MAN	A	6	5	-	0/2/19/22	0/1/1/1
5	MAN	A	7	5	-	2/2/19/22	0/1/1/1
5	MAN	A	8	5	-	0/2/19/22	0/1/1/1
5	MAN	A	9	5	-	0/2/19/22	0/1/1/1
6	NAG	E	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
7	NAG	F	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	F	2	7	-	2/6/23/26	0/1/1/1
7	BMA	F	3	7	-	0/2/19/22	0/1/1/1
6	NAG	H	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
6	NAG	I	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	NAG	J	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
7	NAG	K	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	NAG	L	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	7	MAN	O5-C5-C6	2.06	111.67	107.66
5	A	7	MAN	C1-O5-C5	-2.03	109.46	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
5	A	5	MAN	O5-C5-C6-O6
5	A	2	NAG	C8-C7-N2-C2
5	A	7	MAN	C4-C5-C6-O6
5	A	7	MAN	O5-C5-C6-O6
7	F	2	NAG	C4-C5-C6-O6
5	A	2	NAG	O7-C7-N2-C2
7	F	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2

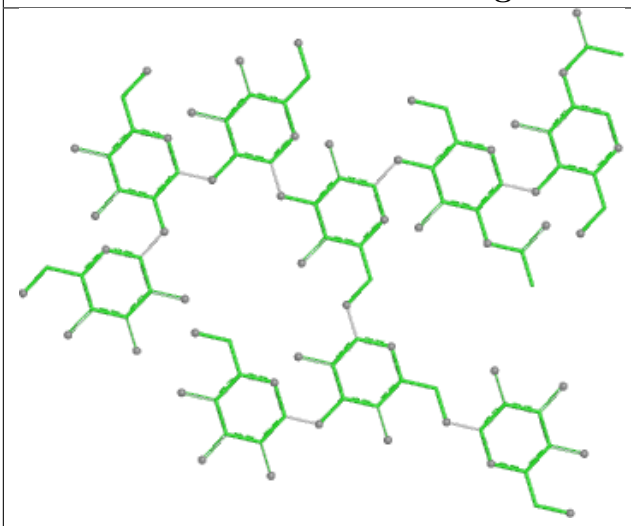
There are no ring outliers.

7 monomers are involved in 8 short contacts:

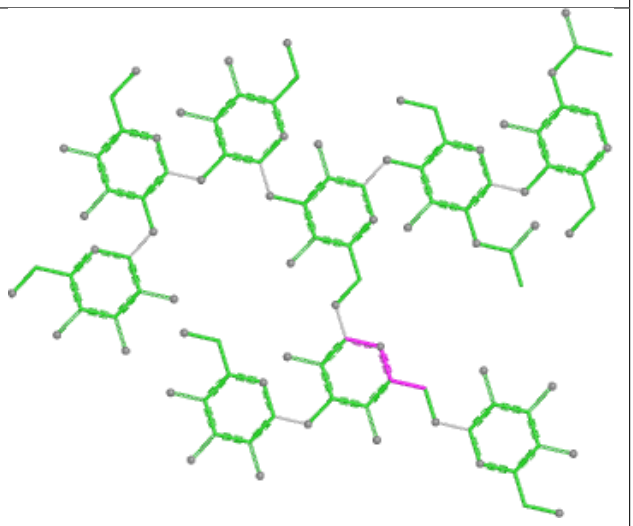
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	1	0
5	A	1	NAG	1	0
5	A	9	MAN	3	0
6	J	1	NAG	2	0
5	A	2	NAG	3	0
7	K	1	NAG	1	0
5	A	7	MAN	3	0

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

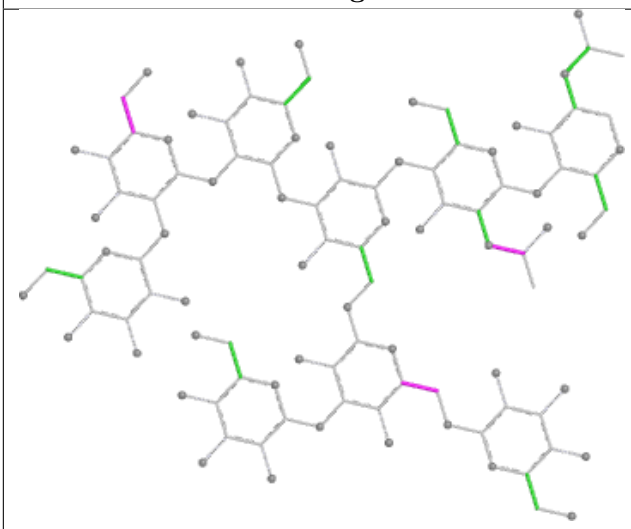
Oligosaccharide Chain A



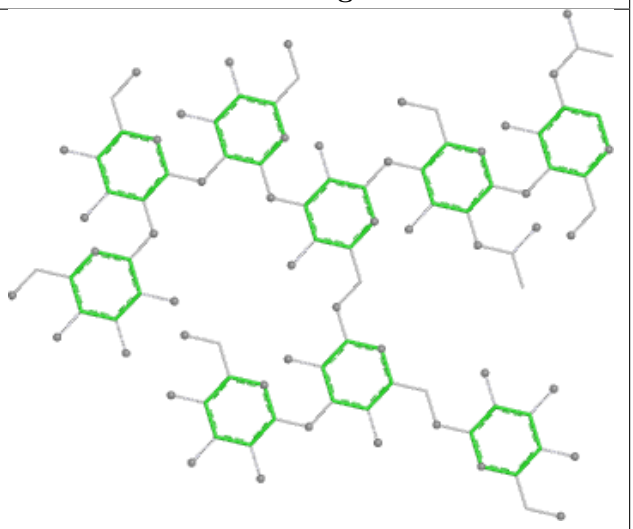
Bond lengths



Bond angles

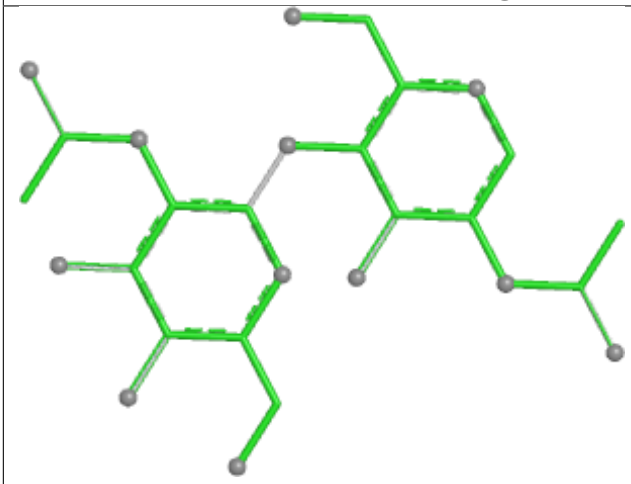


Torsions

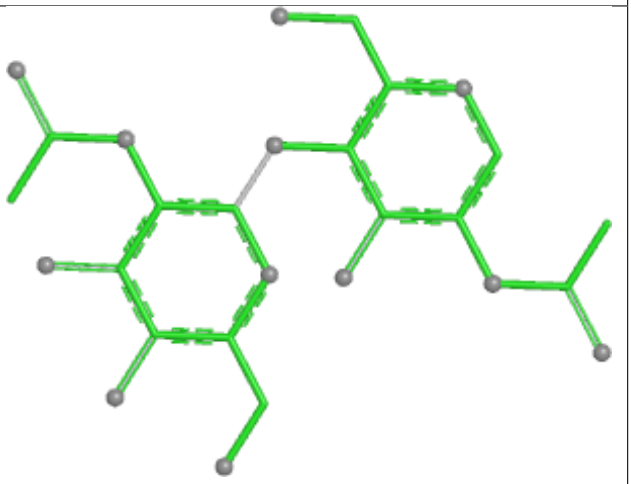


Rings

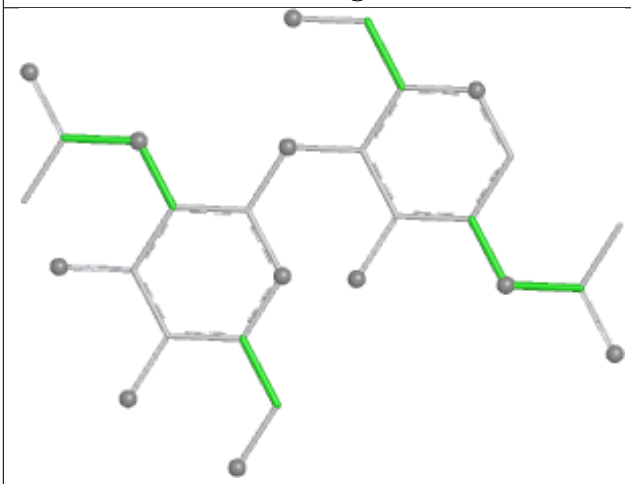
Oligosaccharide Chain E



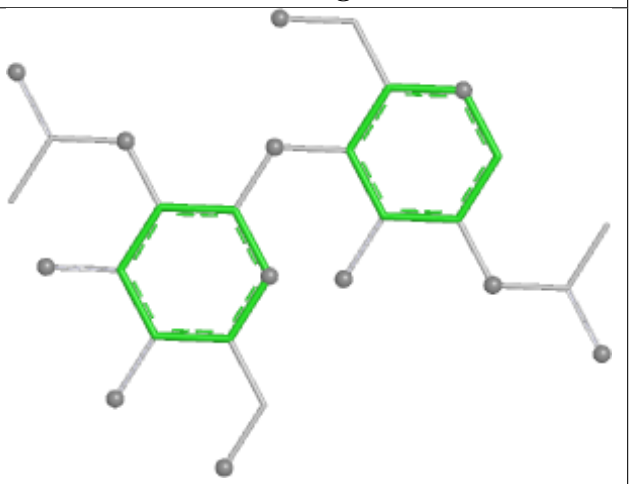
Bond lengths



Bond angles

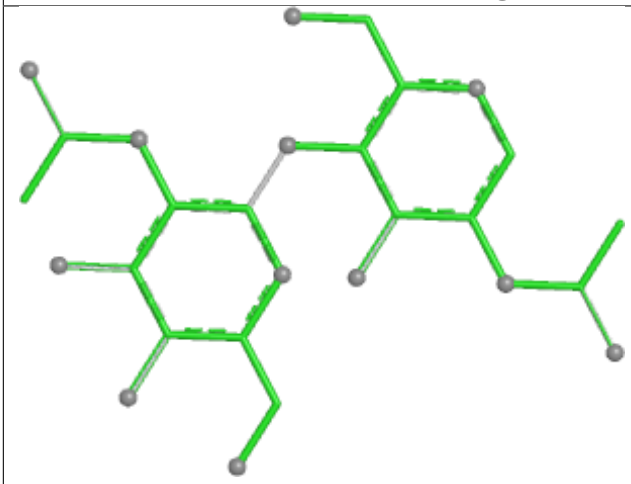


Torsions

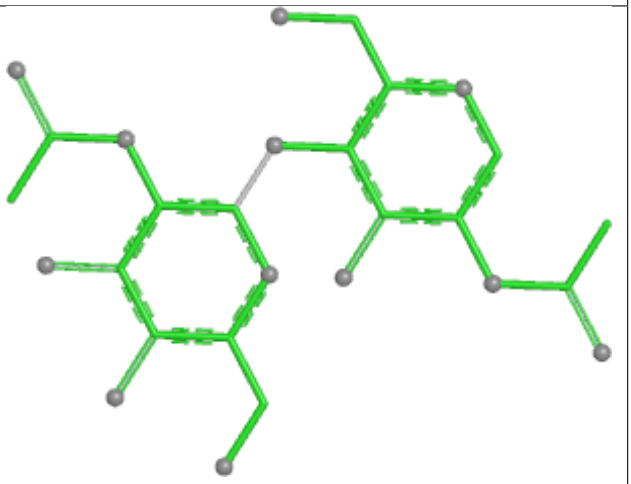


Rings

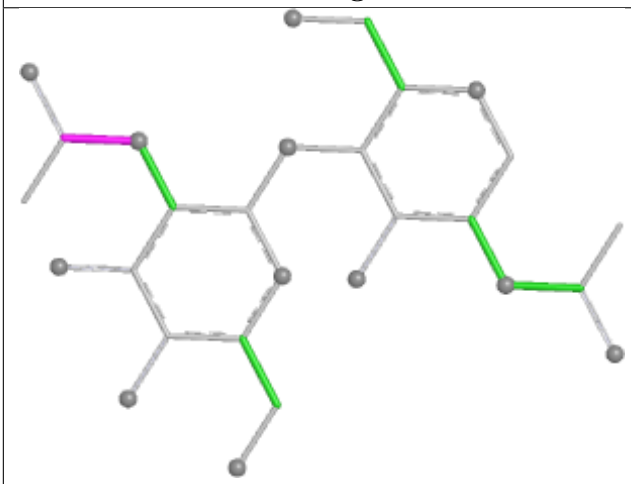
Oligosaccharide Chain H



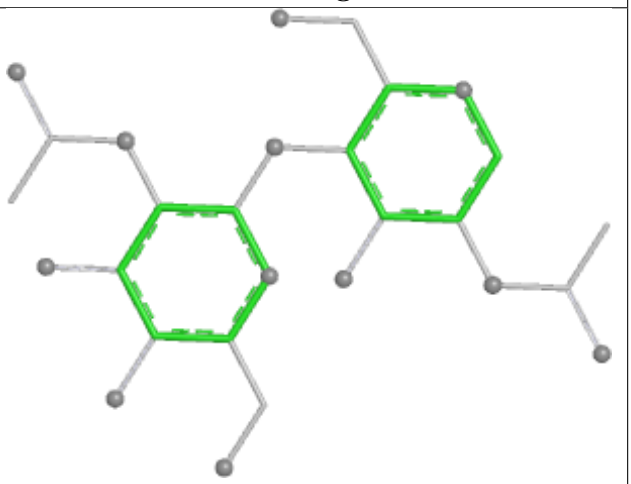
Bond lengths



Bond angles

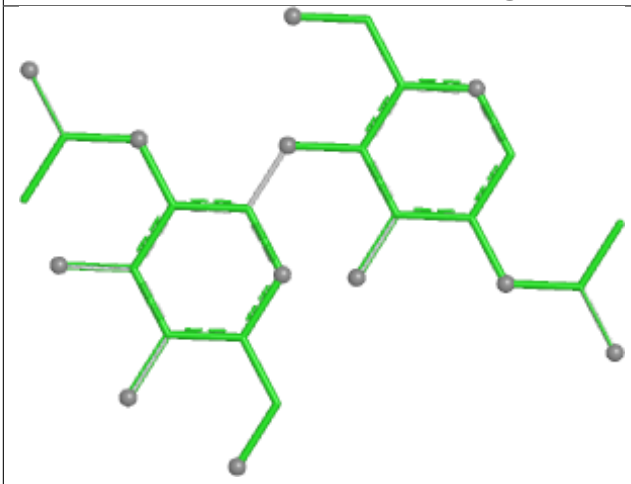


Torsions

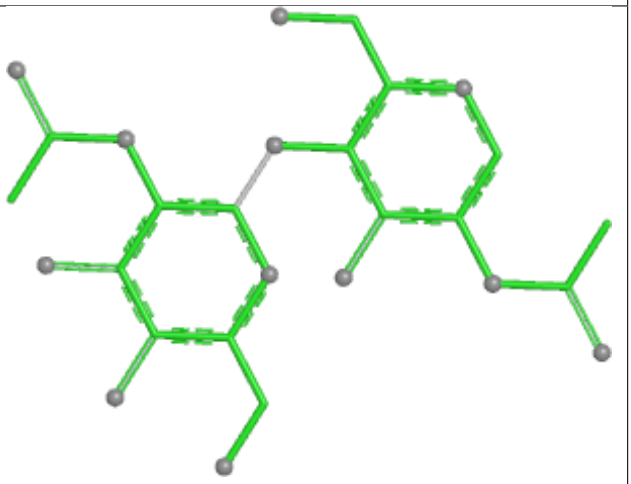


Rings

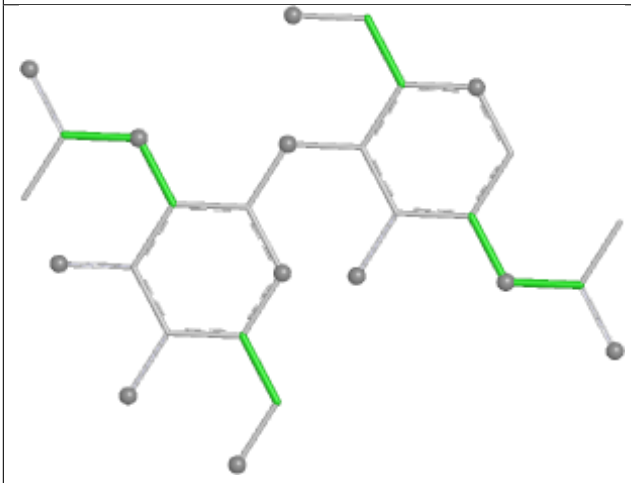
Oligosaccharide Chain I



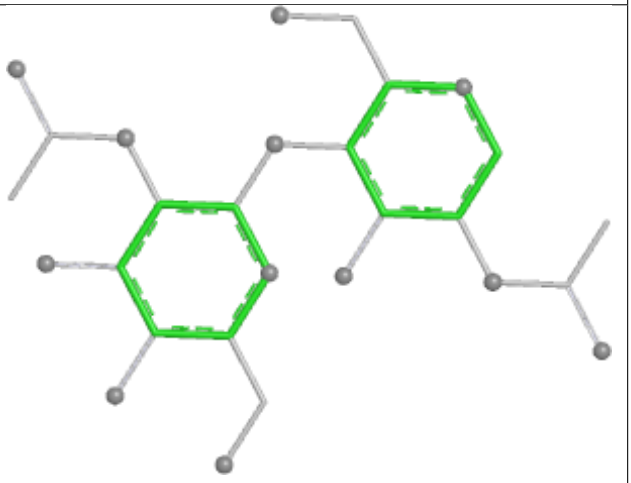
Bond lengths



Bond angles

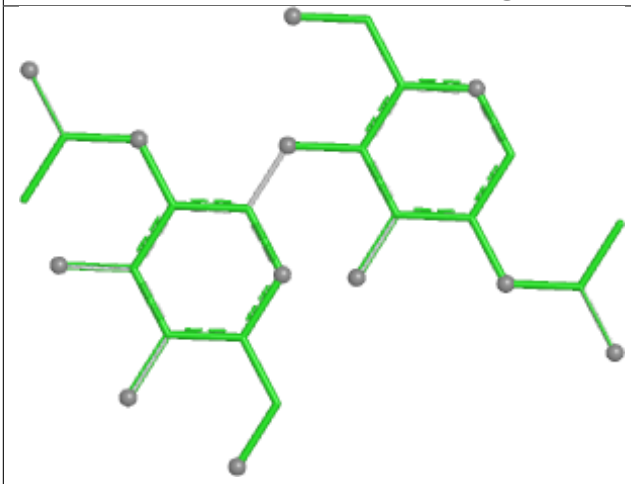


Torsions

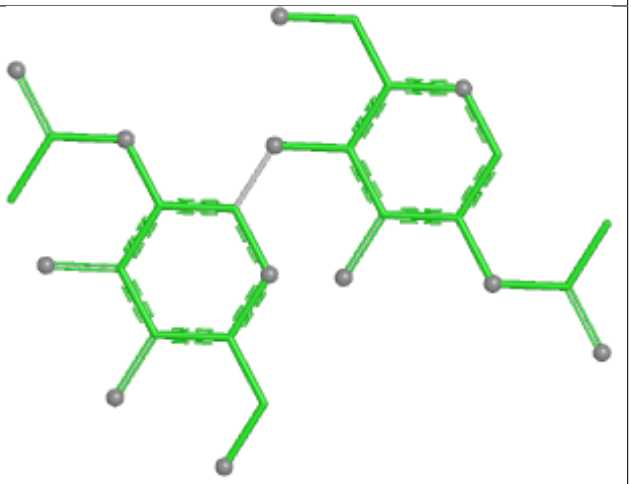


Rings

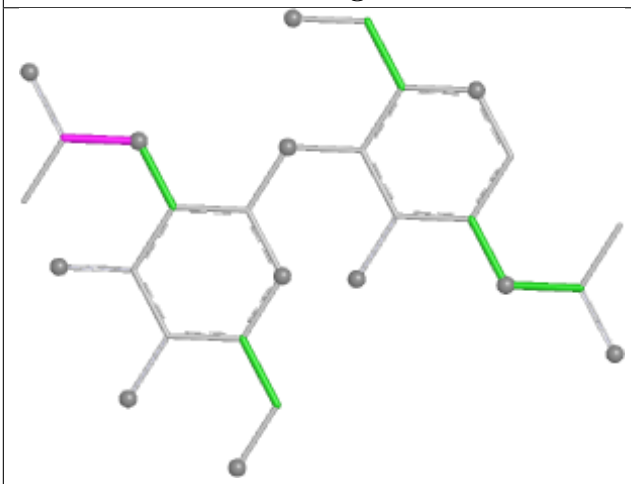
Oligosaccharide Chain J



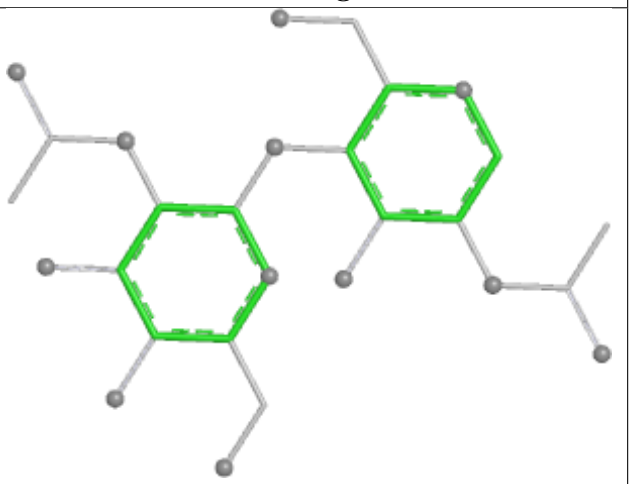
Bond lengths



Bond angles

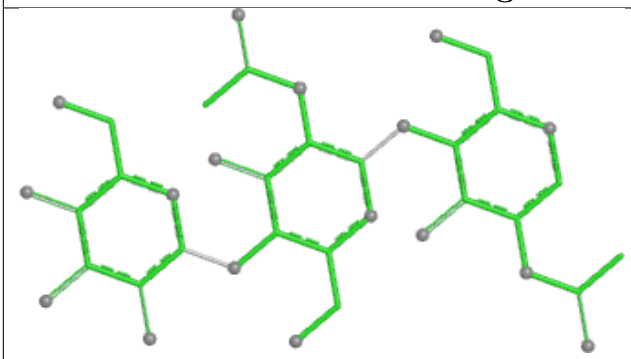


Torsions

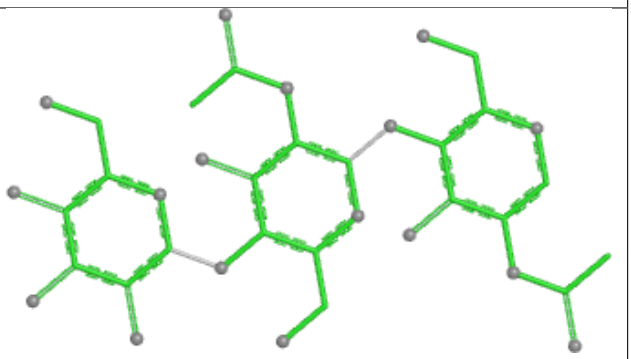


Rings

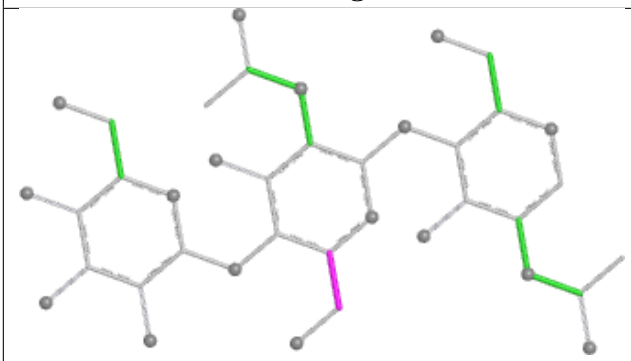
Oligosaccharide Chain F



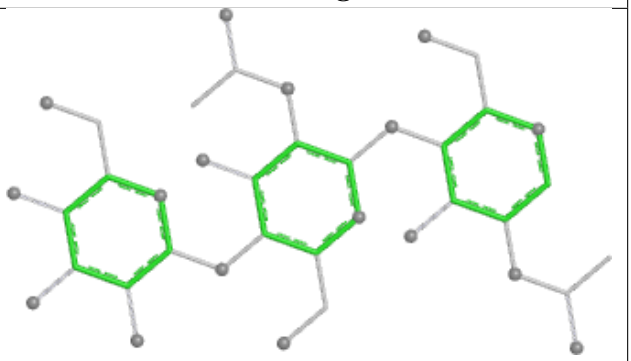
Bond lengths



Bond angles

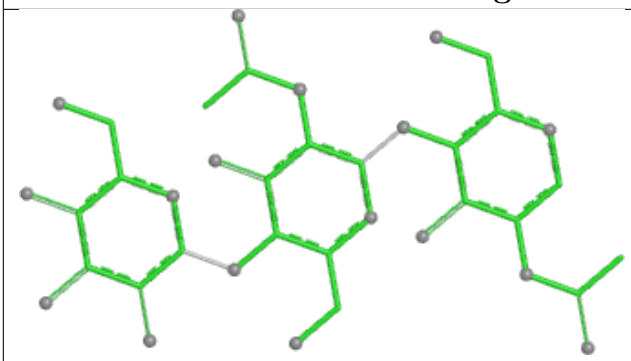


Torsions

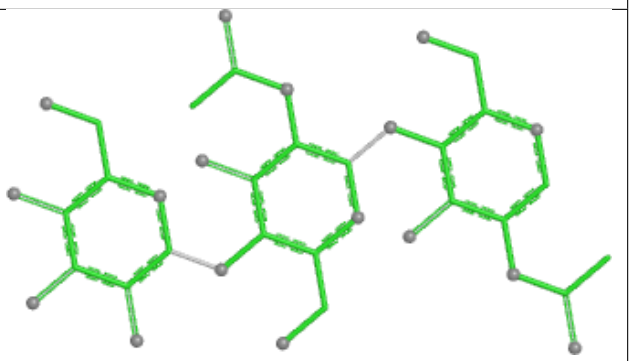


Rings

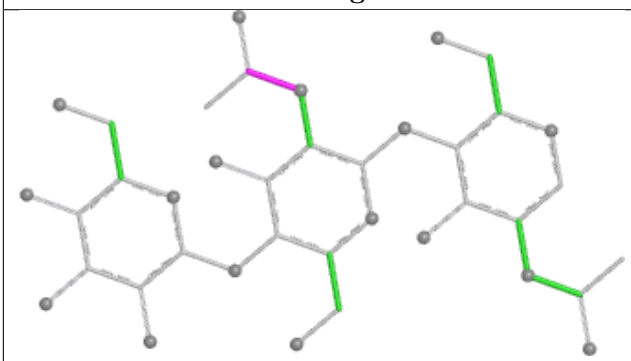
Oligosaccharide Chain K



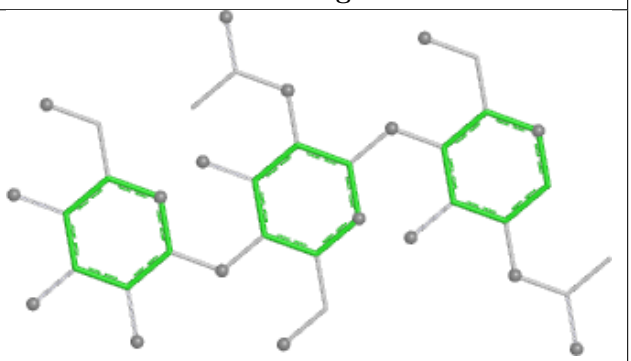
Bond lengths



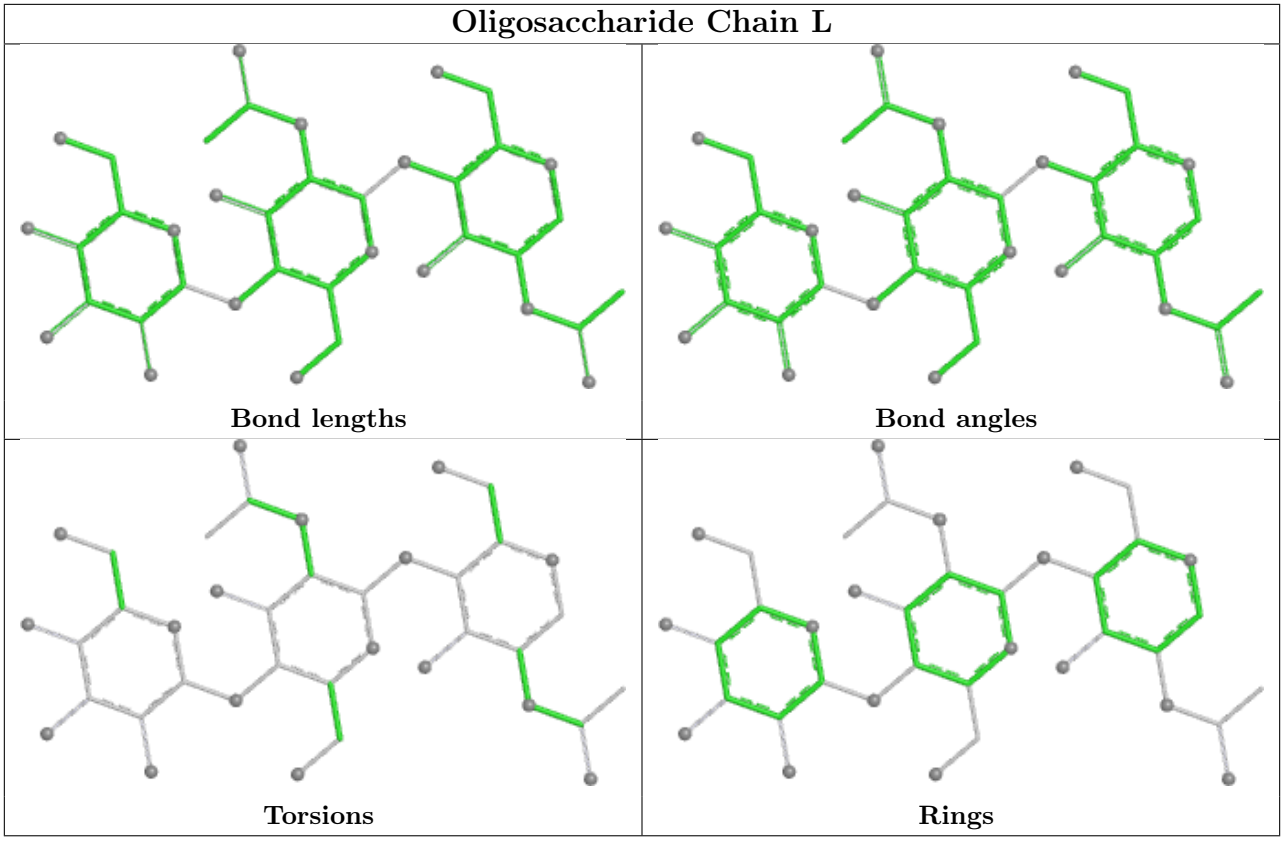
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
8	NAG	G	524	4	14,14,15	0.49	0	17,19,21	0.78	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
8	NAG	G	524	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Warning: The R factor obtained from EDS is 0.3343, which does not match the depositor's R factor of 0.2762. Please interpret the results in this section carefully.

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	B	181/185 (97%)	-0.12	2 (1%)	77	63	109, 175, 233, 284	0
2	C	214/214 (100%)	-0.27	1 (0%)	87	76	134, 237, 326, 438	0
3	D	223/229 (97%)	-0.08	1 (0%)	89	79	124, 223, 326, 448	0
4	G	295/313 (94%)	0.02	5 (1%)	69	53	103, 164, 241, 304	0
All	All	913/941 (97%)	-0.10	9 (0%)	79	65	103, 196, 311, 448	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	488	VAL	2.8
1	B	130	CYS	2.6
4	G	196	CYS	2.3
2	C	49	TYR	2.3
3	D	100(J)	PHE	2.3
4	G	232	LYS	2.3
4	G	264	SER	2.0
4	G	338	TRP	2.0
1	B	161	VAL	2.0

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
8	NAG	G	524	14/15	0.82	0.10	139,180,209,209	0

6.5 Other polymers

There are no such residues in this entry.