Full wwPDB EM Validation Report ⓘ

Feb 29, 2024 – 10:17 PM JST

PDB ID	:	8JMI
EMDB ID	:	EMD-36422
Title	:	The cryo-EM structure of insect gustatory receptor Gr64a from Drosophila melanogaster in complex with maltose
Authors	:	Ma, D.; Guo, J.
Deposited on	:	2023-06-04
Resolution	:	2.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

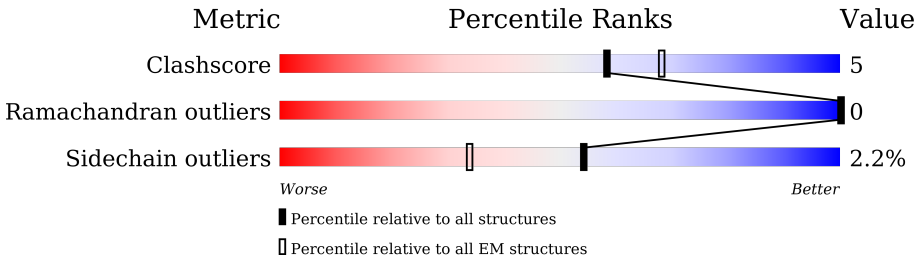
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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	A	473	72% 14% 14%
1	B	473	71% 15% 14%
1	C	473	73% 14% 14%
1	D	473	72% 14% 14%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%
2	H	2	100%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 27344 atoms, of which 13900 are hydrogens and 0 are deuteriums.

In the tables below, 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 Gustatory receptor for sugar taste 64a.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	407	Total	C	H	N	O	S	0	0
			6791	2206	3453	553	555	24		
1	B	407	Total	C	H	N	O	S	0	0
			6791	2206	3453	553	555	24		
1	C	407	Total	C	H	N	O	S	0	0
			6791	2206	3453	553	555	24		
1	D	407	Total	C	H	N	O	S	0	0
			6791	2206	3453	553	555	24		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P83293
A	-15	TRP	-	expression tag	UNP P83293
A	-14	SER	-	expression tag	UNP P83293
A	-13	HIS	-	expression tag	UNP P83293
A	-12	PRO	-	expression tag	UNP P83293
A	-11	GLN	-	expression tag	UNP P83293
A	-10	PHE	-	expression tag	UNP P83293
A	-9	GLU	-	expression tag	UNP P83293
A	-8	LYS	-	expression tag	UNP P83293
A	-7	GLY	-	expression tag	UNP P83293
A	-6	GLY	-	expression tag	UNP P83293
A	-5	SER	-	expression tag	UNP P83293
A	-4	SER	-	expression tag	UNP P83293
A	-3	GLY	-	expression tag	UNP P83293
A	-2	GLY	-	expression tag	UNP P83293
A	-1	VAL	-	expression tag	UNP P83293
A	0	ASP	-	expression tag	UNP P83293
B	-16	MET	-	initiating methionine	UNP P83293
B	-15	TRP	-	expression tag	UNP P83293
B	-14	SER	-	expression tag	UNP P83293
B	-13	HIS	-	expression tag	UNP P83293
B	-12	PRO	-	expression tag	UNP P83293

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	GLN	-	expression tag	UNP P83293
B	-10	PHE	-	expression tag	UNP P83293
B	-9	GLU	-	expression tag	UNP P83293
B	-8	LYS	-	expression tag	UNP P83293
B	-7	GLY	-	expression tag	UNP P83293
B	-6	GLY	-	expression tag	UNP P83293
B	-5	SER	-	expression tag	UNP P83293
B	-4	SER	-	expression tag	UNP P83293
B	-3	GLY	-	expression tag	UNP P83293
B	-2	GLY	-	expression tag	UNP P83293
B	-1	VAL	-	expression tag	UNP P83293
B	0	ASP	-	expression tag	UNP P83293
C	-16	MET	-	initiating methionine	UNP P83293
C	-15	TRP	-	expression tag	UNP P83293
C	-14	SER	-	expression tag	UNP P83293
C	-13	HIS	-	expression tag	UNP P83293
C	-12	PRO	-	expression tag	UNP P83293
C	-11	GLN	-	expression tag	UNP P83293
C	-10	PHE	-	expression tag	UNP P83293
C	-9	GLU	-	expression tag	UNP P83293
C	-8	LYS	-	expression tag	UNP P83293
C	-7	GLY	-	expression tag	UNP P83293
C	-6	GLY	-	expression tag	UNP P83293
C	-5	SER	-	expression tag	UNP P83293
C	-4	SER	-	expression tag	UNP P83293
C	-3	GLY	-	expression tag	UNP P83293
C	-2	GLY	-	expression tag	UNP P83293
C	-1	VAL	-	expression tag	UNP P83293
C	0	ASP	-	expression tag	UNP P83293
D	-16	MET	-	initiating methionine	UNP P83293
D	-15	TRP	-	expression tag	UNP P83293
D	-14	SER	-	expression tag	UNP P83293
D	-13	HIS	-	expression tag	UNP P83293
D	-12	PRO	-	expression tag	UNP P83293
D	-11	GLN	-	expression tag	UNP P83293
D	-10	PHE	-	expression tag	UNP P83293
D	-9	GLU	-	expression tag	UNP P83293
D	-8	LYS	-	expression tag	UNP P83293
D	-7	GLY	-	expression tag	UNP P83293
D	-6	GLY	-	expression tag	UNP P83293
D	-5	SER	-	expression tag	UNP P83293
D	-4	SER	-	expression tag	UNP P83293

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P83293
D	-2	GLY	-	expression tag	UNP P83293
D	-1	VAL	-	expression tag	UNP P83293
D	0	ASP	-	expression tag	UNP P83293

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

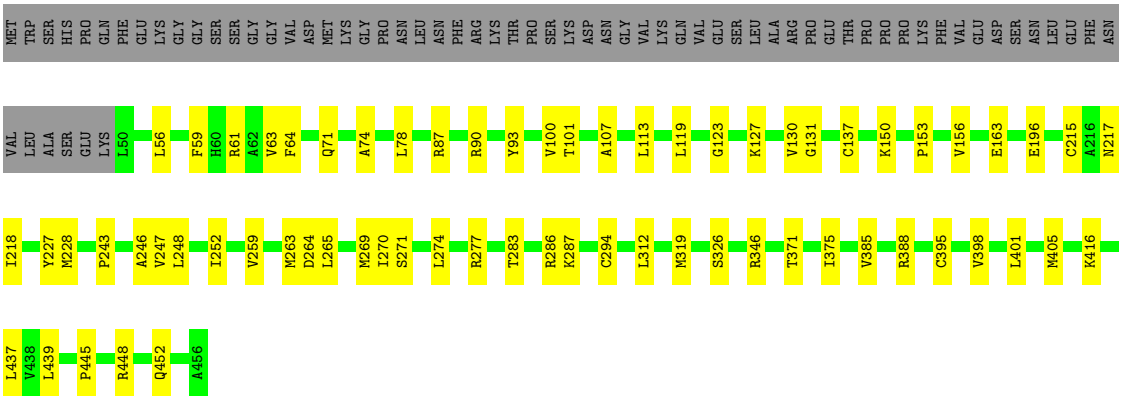
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	H	O	0	0
			45	12	22	11		
2	F	2	Total	C	H	O	0	0
			45	12	22	11		
2	G	2	Total	C	H	O	0	0
			45	12	22	11		
2	H	2	Total	C	H	O	0	0
			45	12	22	11		

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.

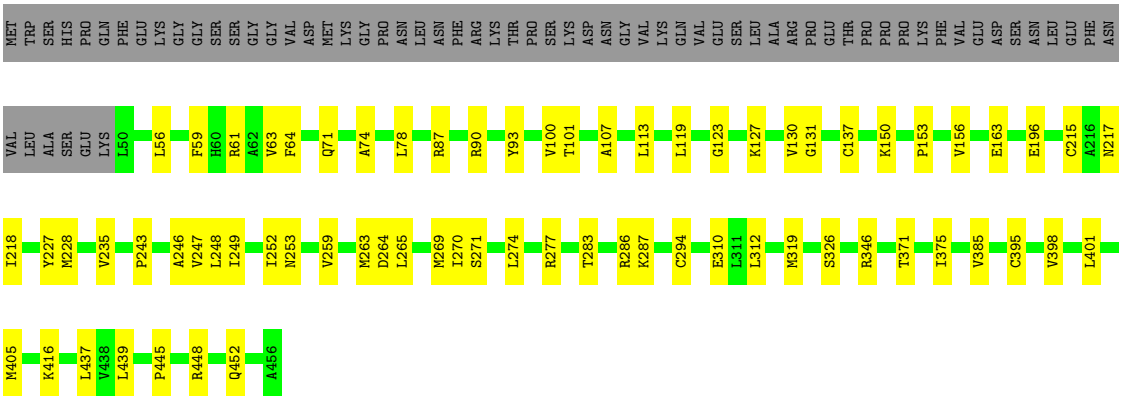
• Molecule 1: Gustatory receptor for sugar taste 64a

Chain A:



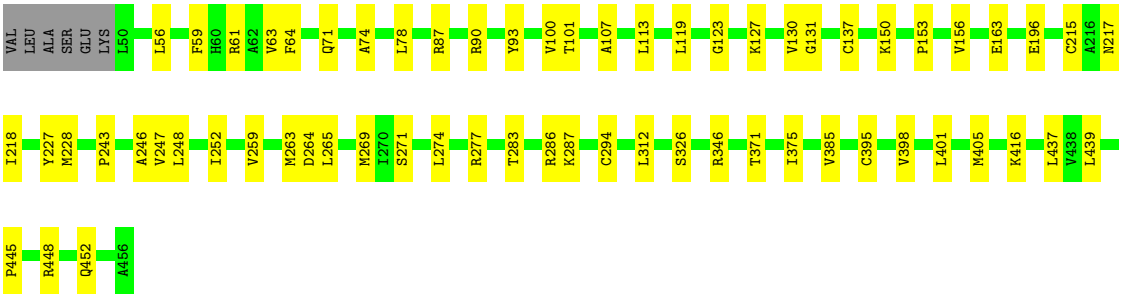
• Molecule 1: Gustatory receptor for sugar taste 64a

Chain B:



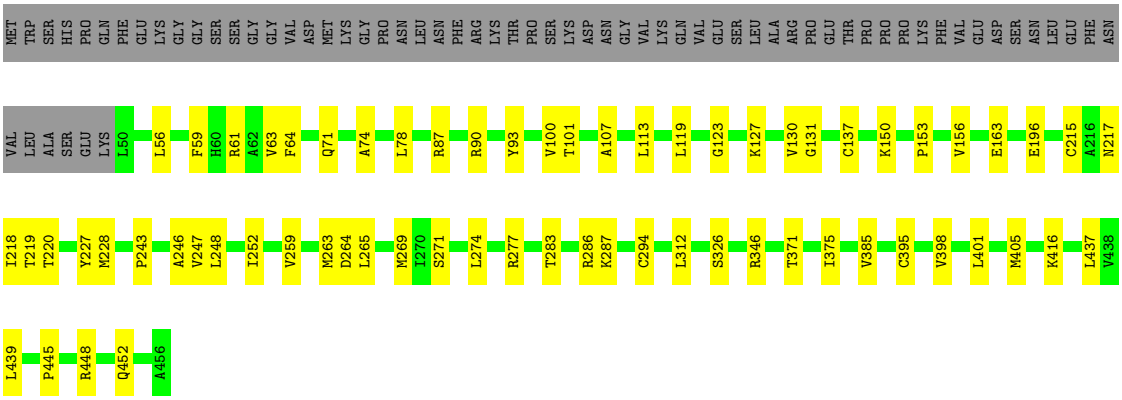
• Molecule 1: Gustatory receptor for sugar taste 64a

Chain C:



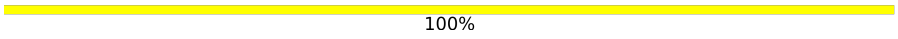
• Molecule 1: Gustatory receptor for sugar taste 64a

Chain D:



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

Chain E:

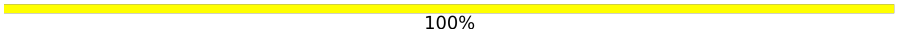


• Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:

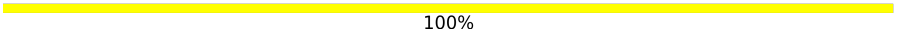
• Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G:



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

Chain H:



BGC1
C2TG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	529197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, BGC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/3422	0.48	0/4641
1	B	0.25	0/3422	0.48	0/4641
1	C	0.25	0/3422	0.48	0/4641
1	D	0.25	0/3422	0.48	0/4641
All	All	0.25	0/13688	0.48	0/18564

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	3338	3453	3453	35	0
1	B	3338	3453	3453	36	0
1	C	3338	3453	3453	33	0
1	D	3338	3453	3453	34	0
2	E	23	22	21	0	0
2	F	23	22	21	1	0
2	G	23	22	21	0	0
2	H	23	22	21	0	0
All	All	13444	13900	13896	133	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 (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ALA:HB2	1:B:100:VAL:HG12	1.67	0.77
1:A:74:ALA:HB2	1:A:100:VAL:HG12	1.66	0.77
1:D:74:ALA:HB2	1:D:100:VAL:HG12	1.67	0.76
1:C:74:ALA:HB2	1:C:100:VAL:HG12	1.67	0.74
1:B:264:ASP:OD2	1:B:326:SER:OG	2.10	0.69
1:C:264:ASP:OD2	1:C:326:SER:OG	2.10	0.69
1:A:264:ASP:OD2	1:A:326:SER:OG	2.11	0.68
1:D:264:ASP:OD2	1:D:326:SER:OG	2.10	0.68
1:B:107:ALA:HB1	1:B:252:ILE:HD13	1.78	0.64
1:C:228:MET:HG3	1:C:246:ALA:HB1	1.80	0.64
1:D:107:ALA:HB1	1:D:252:ILE:HD13	1.79	0.63
1:D:228:MET:HG3	1:D:246:ALA:HB1	1.80	0.63
1:A:107:ALA:HB1	1:A:252:ILE:HD13	1.80	0.62
1:A:228:MET:HG3	1:A:246:ALA:HB1	1.80	0.62
1:C:107:ALA:HB1	1:C:252:ILE:HD13	1.80	0.62
1:B:228:MET:HG3	1:B:246:ALA:HB1	1.81	0.61
1:C:74:ALA:HB1	1:C:101:THR:HA	1.83	0.60
1:D:59:PHE:O	1:D:63:VAL:HG22	2.01	0.60
1:B:59:PHE:O	1:B:63:VAL:HG22	2.01	0.60
1:A:74:ALA:HB1	1:A:101:THR:HA	1.83	0.60
1:B:74:ALA:HB1	1:B:101:THR:HA	1.83	0.60
1:C:59:PHE:O	1:C:63:VAL:HG22	2.01	0.60
1:A:59:PHE:O	1:A:63:VAL:HG22	2.01	0.59
1:D:74:ALA:HB1	1:D:101:THR:HA	1.83	0.59
1:C:56:LEU:O	1:C:61:ARG:NH1	2.38	0.56
1:B:56:LEU:O	1:B:61:ARG:NH1	2.38	0.56
1:D:56:LEU:O	1:D:61:ARG:NH1	2.38	0.56
1:A:56:LEU:O	1:A:61:ARG:NH1	2.38	0.55
1:D:71:GLN:NE2	1:D:78:LEU:O	2.41	0.54
1:B:71:GLN:NE2	1:B:78:LEU:O	2.41	0.53
1:A:71:GLN:NE2	1:A:78:LEU:O	2.41	0.52
1:C:71:GLN:NE2	1:C:78:LEU:O	2.42	0.52
1:B:119:LEU:O	1:B:123:GLY:N	2.43	0.52
1:D:119:LEU:O	1:D:123:GLY:N	2.43	0.51
1:A:119:LEU:O	1:A:123:GLY:N	2.44	0.51
1:C:119:LEU:O	1:C:123:GLY:N	2.44	0.51
1:B:346:ARG:NH2	1:B:452:GLN:O	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:ARG:NH2	1:C:452:GLN:O	2.38	0.50
1:C:248:LEU:O	1:C:252:ILE:HG13	2.12	0.50
1:A:248:LEU:O	1:A:252:ILE:HG13	2.12	0.50
1:A:346:ARG:NH2	1:A:452:GLN:O	2.38	0.49
1:D:286:ARG:HA	1:D:385:VAL:HG11	1.96	0.48
1:C:93:TYR:OH	1:C:150:LYS:NZ	2.29	0.48
1:A:286:ARG:HA	1:A:385:VAL:HG11	1.96	0.47
1:B:248:LEU:O	1:B:252:ILE:HG13	2.14	0.47
1:B:286:ARG:HA	1:B:385:VAL:HG11	1.96	0.47
1:A:243:PRO:O	1:A:247:VAL:HG23	2.15	0.47
1:C:243:PRO:O	1:C:247:VAL:HG23	2.15	0.47
1:D:215:CYS:SG	1:D:217:ASN:HB3	2.55	0.47
1:B:243:PRO:O	1:B:247:VAL:HG23	2.14	0.47
1:C:215:CYS:SG	1:C:217:ASN:HB3	2.55	0.47
1:D:248:LEU:O	1:D:252:ILE:HG13	2.15	0.47
1:A:388:ARG:NE	1:B:310:GLU:OE1	2.47	0.47
1:A:215:CYS:SG	1:A:217:ASN:HB3	2.55	0.46
1:D:243:PRO:O	1:D:247:VAL:HG23	2.14	0.46
1:D:163:GLU:OE1	1:D:277:ARG:NH2	2.47	0.46
1:A:93:TYR:OH	1:A:150:LYS:NZ	2.29	0.46
1:C:286:ARG:HA	1:C:385:VAL:HG11	1.98	0.46
1:B:215:CYS:SG	1:B:217:ASN:HB3	2.55	0.46
1:A:127:LYS:O	1:A:130:VAL:HG12	2.16	0.46
1:D:445:PRO:HA	1:D:448:ARG:HG2	1.98	0.46
1:A:274:LEU:HD13	1:A:312:LEU:HD12	1.98	0.46
1:D:346:ARG:NH2	1:D:452:GLN:O	2.38	0.46
1:B:127:LYS:O	1:B:130:VAL:HG12	2.17	0.45
1:B:274:LEU:HD13	1:B:312:LEU:HD12	1.99	0.45
1:A:130:VAL:HG13	1:A:131:GLY:N	2.32	0.45
1:C:271:SER:HA	1:C:375:ILE:HD11	1.98	0.45
1:B:271:SER:HA	1:B:375:ILE:HD11	1.98	0.45
1:C:274:LEU:HD13	1:C:312:LEU:HD12	1.99	0.45
1:C:283:THR:HG22	1:C:287:LYS:HE3	1.99	0.45
1:A:445:PRO:HA	1:A:448:ARG:HG2	1.98	0.45
1:B:163:GLU:OE1	1:B:277:ARG:NH2	2.47	0.45
1:C:130:VAL:HG13	1:C:131:GLY:N	2.32	0.45
1:D:274:LEU:HD13	1:D:312:LEU:HD12	1.99	0.45
1:A:271:SER:HB2	1:A:371:THR:HG22	1.99	0.45
1:B:445:PRO:HA	1:B:448:ARG:HG2	1.98	0.45
1:C:163:GLU:OE1	1:C:277:ARG:NH2	2.47	0.45
1:D:130:VAL:HG13	1:D:131:GLY:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:SER:HA	1:A:375:ILE:HD11	1.98	0.45
1:B:93:TYR:OH	1:B:150:LYS:NZ	2.28	0.45
1:B:130:VAL:HG13	1:B:131:GLY:N	2.32	0.45
1:B:265:LEU:O	1:B:269:MET:HG3	2.17	0.45
1:B:271:SER:HB2	1:B:371:THR:HG22	1.99	0.45
1:C:127:LYS:O	1:C:130:VAL:HG12	2.16	0.45
1:C:265:LEU:O	1:C:269:MET:HG3	2.17	0.45
1:C:445:PRO:HA	1:C:448:ARG:HG2	1.98	0.45
1:D:127:LYS:O	1:D:130:VAL:HG12	2.17	0.45
1:C:271:SER:HB2	1:C:371:THR:HG22	1.99	0.44
1:D:265:LEU:O	1:D:269:MET:HG3	2.17	0.44
1:A:283:THR:HG22	1:A:287:LYS:HE3	1.99	0.44
1:C:401:LEU:O	1:C:405:MET:HG3	2.18	0.44
1:D:271:SER:HA	1:D:375:ILE:HD11	1.98	0.44
1:D:283:THR:HG22	1:D:287:LYS:HE3	1.99	0.44
1:B:283:THR:HG22	1:B:287:LYS:HE3	1.99	0.44
1:A:395:CYS:SG	1:A:398:VAL:HG23	2.58	0.43
1:A:401:LEU:O	1:A:405:MET:HG3	2.18	0.43
1:B:401:LEU:O	1:B:405:MET:HG3	2.18	0.43
1:C:395:CYS:SG	1:C:398:VAL:HG23	2.58	0.43
1:D:93:TYR:OH	1:D:150:LYS:NZ	2.29	0.43
1:D:271:SER:HB2	1:D:371:THR:HG22	1.99	0.43
1:D:401:LEU:O	1:D:405:MET:HG3	2.18	0.43
1:B:395:CYS:SG	1:B:398:VAL:HG23	2.58	0.43
1:D:395:CYS:SG	1:D:398:VAL:HG23	2.58	0.43
1:A:163:GLU:OE1	1:A:277:ARG:NH2	2.47	0.43
1:C:153:PRO:O	1:C:156:VAL:HG12	2.19	0.43
1:B:437:LEU:HD22	1:D:439:LEU:HD21	2.01	0.42
1:C:439:LEU:HD21	1:D:437:LEU:HD22	2.01	0.42
1:A:153:PRO:O	1:A:156:VAL:HG12	2.19	0.42
1:B:153:PRO:O	1:B:156:VAL:HG12	2.19	0.42
1:C:74:ALA:HB1	1:C:101:THR:CA	2.49	0.42
1:A:437:LEU:HD22	1:B:439:LEU:HD21	2.01	0.42
1:A:227:TYR:CD1	1:A:227:TYR:C	2.93	0.42
1:A:439:LEU:HD21	1:C:437:LEU:HD22	2.01	0.42
1:C:227:TYR:C	1:C:227:TYR:CD1	2.93	0.42
1:B:227:TYR:CD1	1:B:227:TYR:C	2.93	0.42
1:A:259:VAL:O	1:A:263:MET:HG3	2.20	0.42
1:B:235:VAL:HG11	1:B:249:ILE:CD1	2.50	0.41
1:B:259:VAL:O	1:B:263:MET:HG3	2.20	0.41
1:D:153:PRO:O	1:D:156:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:TYR:CD1	1:D:227:TYR:C	2.93	0.41
1:D:74:ALA:HB1	1:D:101:THR:CA	2.49	0.41
1:D:259:VAL:O	1:D:263:MET:HG3	2.20	0.41
1:A:270:ILE:HG13	1:A:319:MET:SD	2.60	0.41
1:B:217:ASN:O	1:B:218:ILE:C	2.59	0.41
1:C:259:VAL:O	1:C:263:MET:HG3	2.20	0.41
1:A:265:LEU:O	1:A:269:MET:HG3	2.20	0.41
1:B:253:ASN:ND2	2:F:1:BGC:O3	2.53	0.41
1:D:217:ASN:O	1:D:218:ILE:C	2.59	0.41
1:A:74:ALA:HB1	1:A:101:THR:CA	2.49	0.41
1:A:217:ASN:O	1:A:218:ILE:C	2.59	0.41
1:B:270:ILE:HG13	1:B:319:MET:SD	2.61	0.41
1:C:217:ASN:O	1:C:218:ILE:C	2.59	0.40
1:D:219:THR:O	1:D:220:THR:OG1	2.39	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 PDB entries followed by that with respect to all EM entries.

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	405/473 (86%)	393 (97%)	12 (3%)	0	100	100
1	B	405/473 (86%)	393 (97%)	12 (3%)	0	100	100
1	C	405/473 (86%)	395 (98%)	10 (2%)	0	100	100
1	D	405/473 (86%)	394 (97%)	11 (3%)	0	100	100
All	All	1620/1892 (86%)	1575 (97%)	45 (3%)	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 PDB entries followed by that with respect to all EM entries.

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	368/426 (86%)	360 (98%)	8 (2%)	52 76
1	B	368/426 (86%)	360 (98%)	8 (2%)	52 76
1	C	368/426 (86%)	360 (98%)	8 (2%)	52 76
1	D	368/426 (86%)	360 (98%)	8 (2%)	52 76
All	All	1472/1704 (86%)	1440 (98%)	32 (2%)	54 76

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	PHE
1	A	87	ARG
1	A	90	ARG
1	A	113	LEU
1	A	137	CYS
1	A	196	GLU
1	A	294	CYS
1	A	416	LYS
1	B	64	PHE
1	B	87	ARG
1	B	90	ARG
1	B	113	LEU
1	B	137	CYS
1	B	196	GLU
1	B	294	CYS
1	B	416	LYS
1	C	64	PHE
1	C	87	ARG
1	C	90	ARG
1	C	113	LEU
1	C	137	CYS
1	C	196	GLU
1	C	294	CYS
1	C	416	LYS

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Mol	Chain	Res	Type
1	D	64	PHE
1	D	87	ARG
1	D	90	ARG
1	D	113	LEU
1	D	137	CYS
1	D	196	GLU
1	D	294	CYS
1	D	416	LYS

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

Mol	Chain	Res	Type
1	B	253	ASN
1	D	253	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)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BGC	E	1	2	12,12,12	1.34	2 (16%)	17,17,17	0.85	0
2	GLC	E	2	2	11,11,12	1.61	2 (18%)	15,15,17	0.95	1 (6%)
2	BGC	F	1	2	12,12,12	1.35	3 (25%)	17,17,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	F	2	2	11,11,12	1.60	2 (18%)	15,15,17	0.94	1 (6%)
2	BGC	G	1	2	12,12,12	1.33	2 (16%)	17,17,17	0.85	0
2	GLC	G	2	2	11,11,12	1.63	2 (18%)	15,15,17	0.95	1 (6%)
2	BGC	H	1	2	12,12,12	1.35	3 (25%)	17,17,17	0.85	0
2	GLC	H	2	2	11,11,12	1.61	2 (18%)	15,15,17	0.94	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	GLC	C2-C3	-3.46	1.47	1.52
2	H	2	GLC	C2-C3	-3.43	1.47	1.52
2	F	2	GLC	C2-C3	-3.41	1.47	1.52
2	E	2	GLC	C2-C3	-3.41	1.47	1.52
2	H	1	BGC	O3-C3	2.81	1.49	1.43
2	E	1	BGC	O3-C3	2.79	1.49	1.43
2	F	1	BGC	O3-C3	2.79	1.49	1.43
2	G	1	BGC	O3-C3	2.77	1.49	1.43
2	E	2	GLC	O5-C1	2.60	1.47	1.43
2	G	2	GLC	O5-C1	2.60	1.47	1.43
2	H	2	GLC	O5-C1	2.59	1.47	1.43
2	F	2	GLC	O5-C1	2.58	1.47	1.43
2	H	1	BGC	C4-C3	-2.13	1.46	1.52
2	F	1	BGC	C4-C3	-2.11	1.46	1.52
2	E	1	BGC	C4-C3	-2.10	1.47	1.52
2	G	1	BGC	C4-C3	-2.05	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	BGC	C3-C2	-2.02	1.47	1.52
2	H	1	BGC	C3-C2	-2.01	1.47	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	GLC	C1-C2-C3	2.42	112.64	109.67
2	G	2	GLC	C1-C2-C3	2.40	112.62	109.67
2	F	2	GLC	C1-C2-C3	2.32	112.52	109.67
2	H	2	GLC	C1-C2-C3	2.30	112.49	109.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	GLC	C4-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6

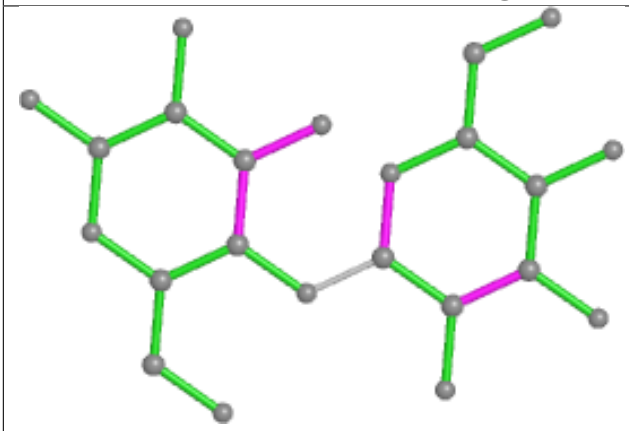
There are no ring outliers.

1 monomer is involved in 1 short contact:

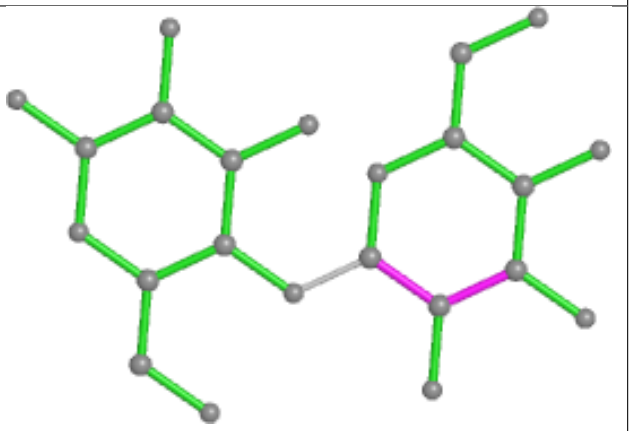
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	BGC	1	0

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

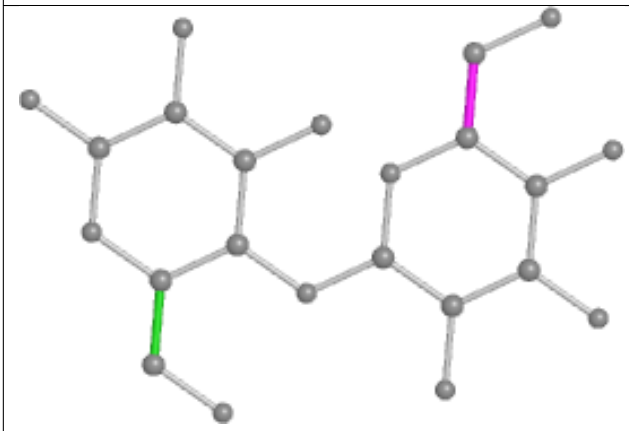
Oligosaccharide Chain E



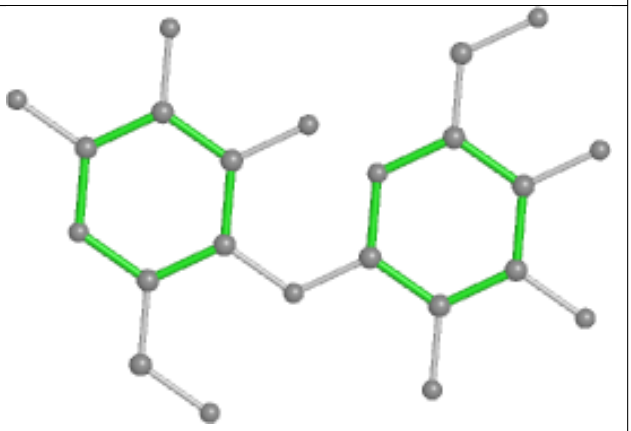
Bond lengths



Bond angles

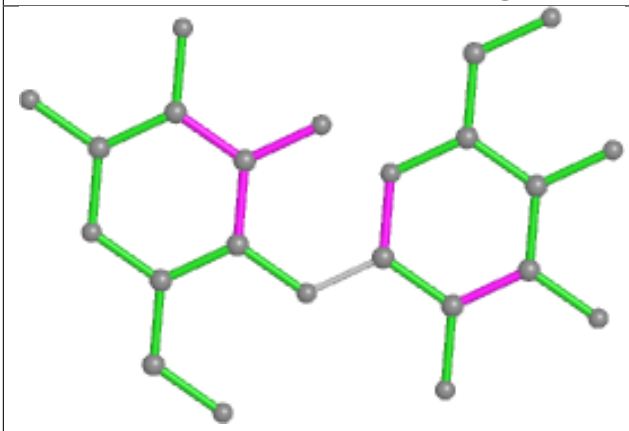


Torsions

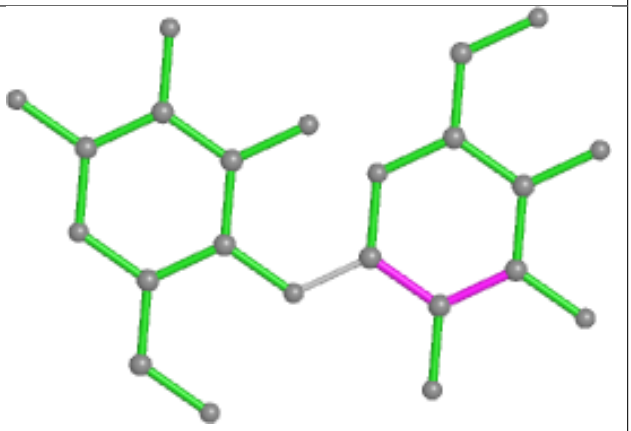


Rings

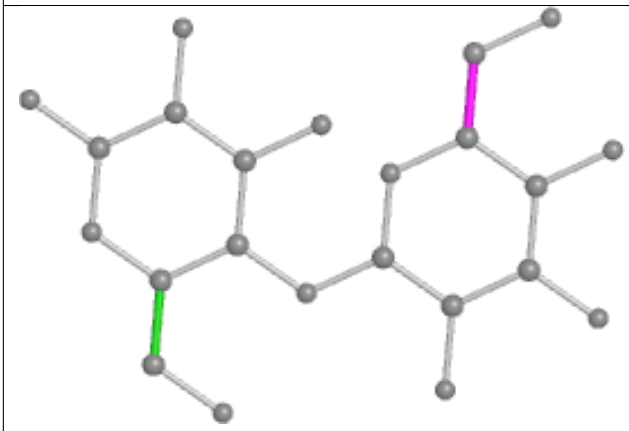
Oligosaccharide Chain F



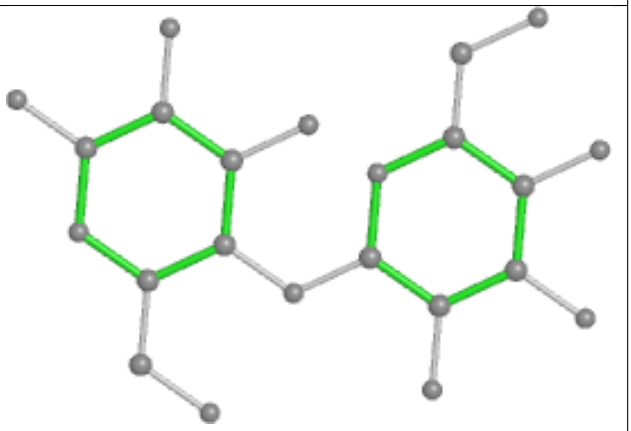
Bond lengths



Bond angles

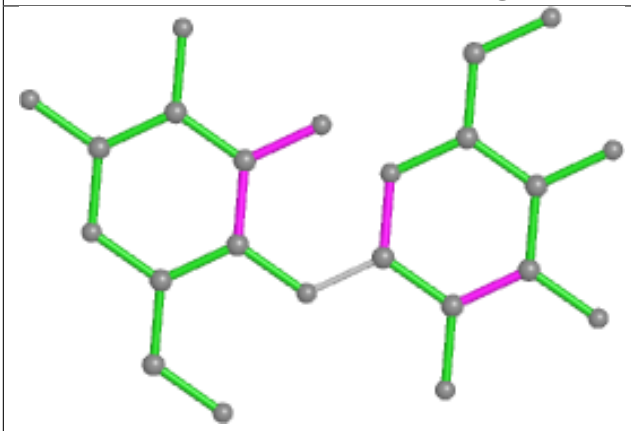


Torsions

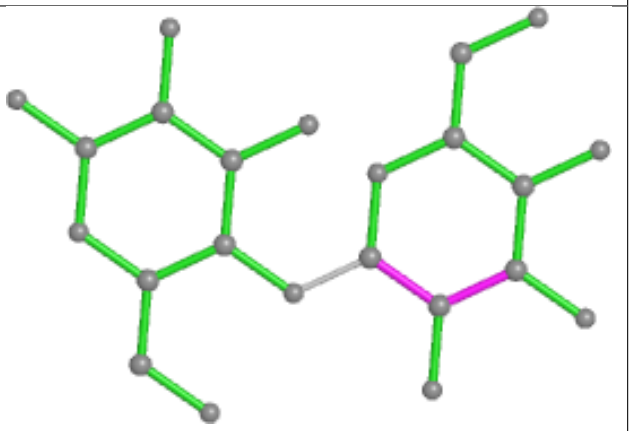


Rings

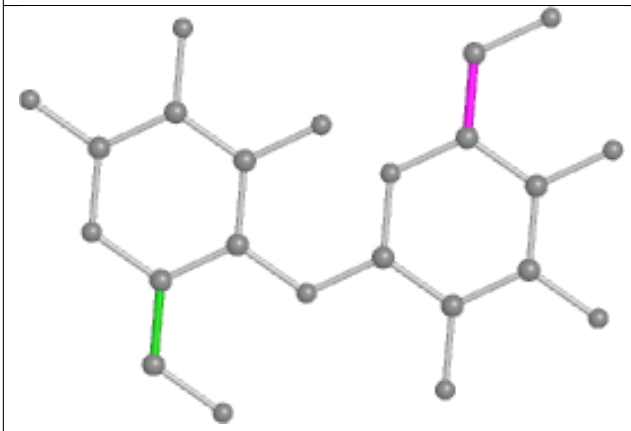
Oligosaccharide Chain G



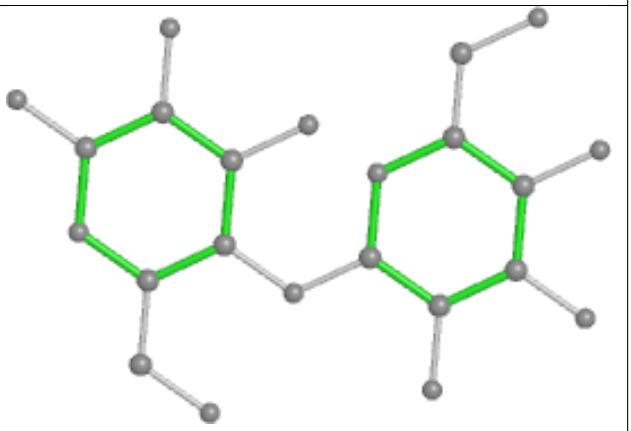
Bond lengths



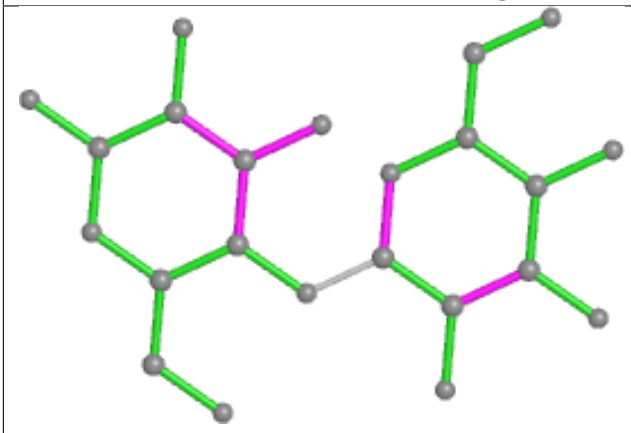
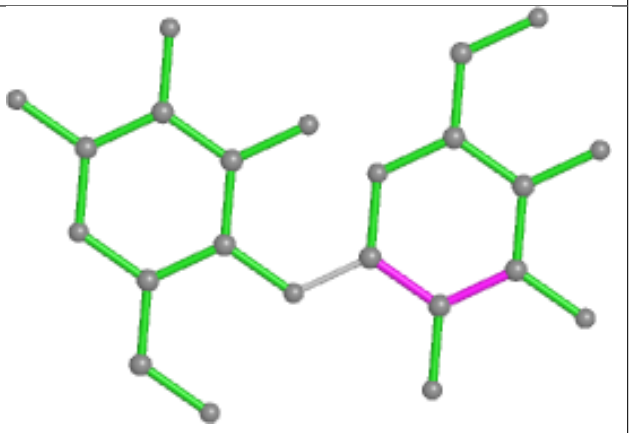
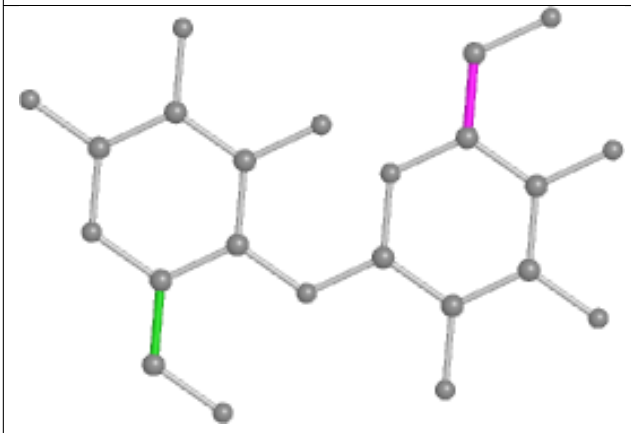
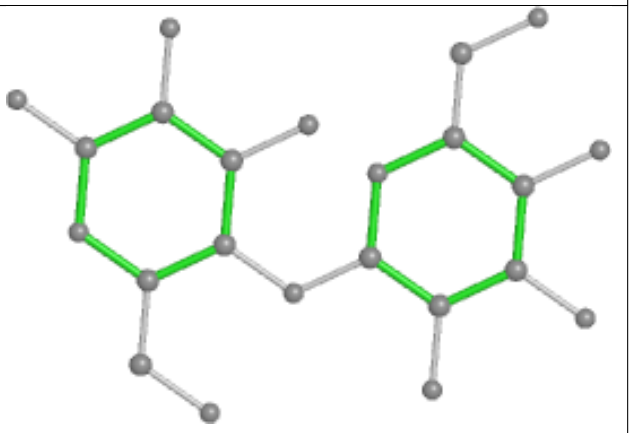
Bond angles



Torsions



Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.