Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:12 PM BST

PDB ID	:	1LTT
Title	:	LACTOSE BINDING TO HEAT-LABILE ENTEROTOXIN REVEALED BY X-RAY CRYSTALLOGRAPHY
Authors	:	Sixma, T.K.; Hol, W.G.J.
Deposited on	:	1992-07-15
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

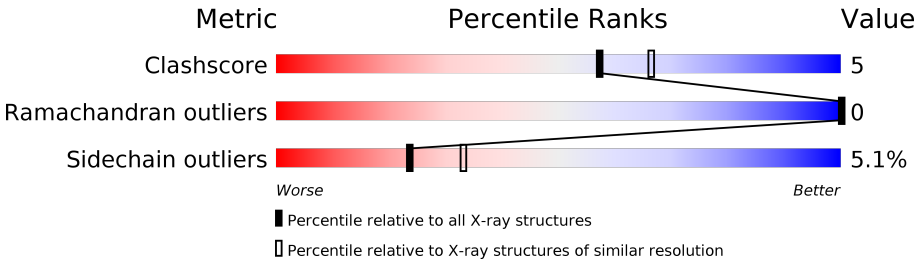
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	103	77% 21% •
1	E	103	85% 13% •
1	F	103	81% 13% 6% •
1	G	103	83% 15% •
1	H	103	81% 18% •
2	A	185	75% 21% • •
3	C	41	68% 29% •
4	B	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	I	2	100%
4	J	2	100%
4	K	2	100%
4	L	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6427 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 HEAT-LABILE ENTEROTOXIN, SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	E	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	F	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	G	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	H	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			

- Molecule 2 is a protein called HEAT-LABILE ENTEROTOXIN, SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	185	Total	C	N	O	S	0	0	0
			1511	953	276	278	4			

- Molecule 3 is a protein called HEAT-LABILE ENTEROTOXIN, SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	41	Total	C	N	O	S	0	0	0
			347	214	59	73	1			

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	B	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	2	Total C O 23 12 11	0	0	0
4	J	2	Total C O 23 12 11	0	0	0
4	K	2	Total C O 23 12 11	0	0	0
4	L	2	Total C O 23 12 11	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	65	Total O 65 65	0	0
5	E	56	Total O 56 56	0	0
5	F	37	Total O 37 37	0	0
5	G	53	Total O 53 53	0	0
5	H	51	Total O 51 51	0	0
5	A	43	Total O 43 43	0	0
5	C	29	Total O 29 29	0	0

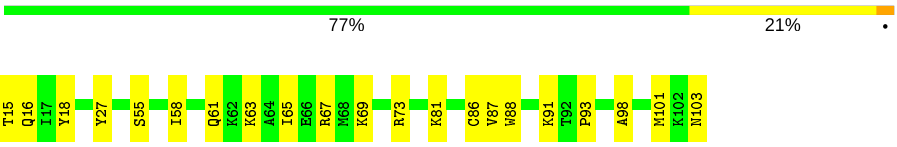
3 Residue-property plots (i)

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

Note EDS was not executed.

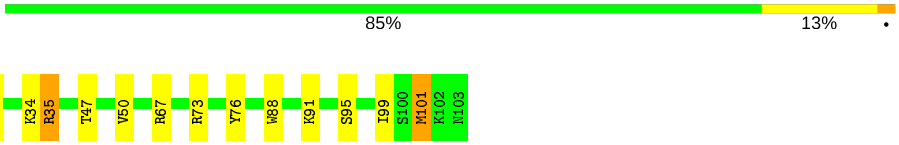
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain D:



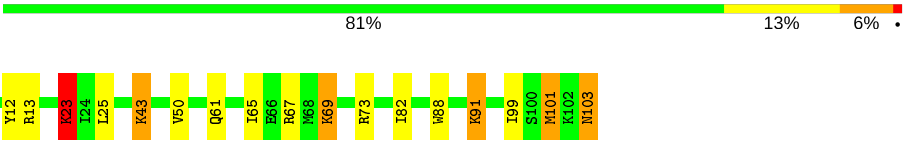
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain E:



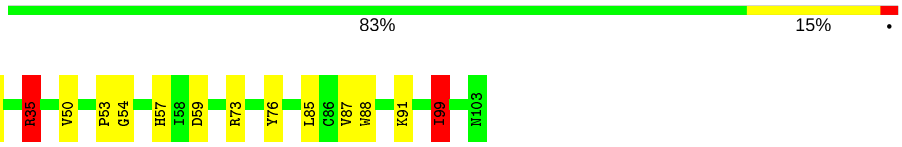
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain F:



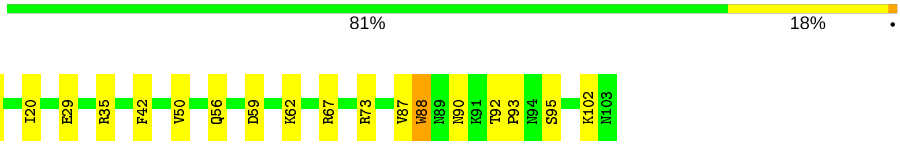
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain G:



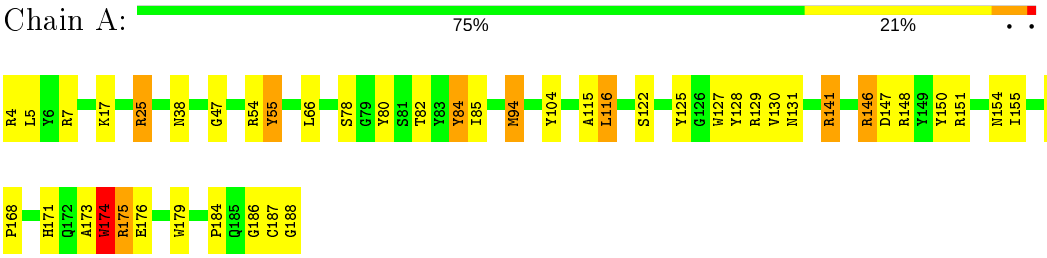
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain H:



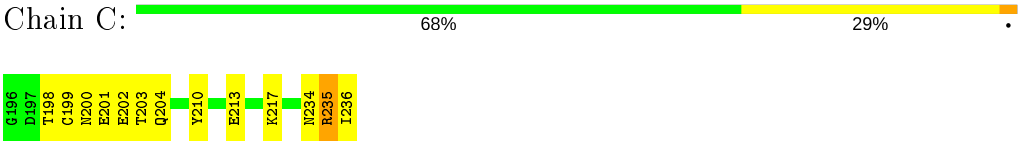
- Molecule 2: HEAT-LABILE ENTEROTOXIN, SUBUNIT A

Chain A:



• Molecule 3: HEAT-LABILE ENTEROTOXIN, SUBUNIT A

Chain C:

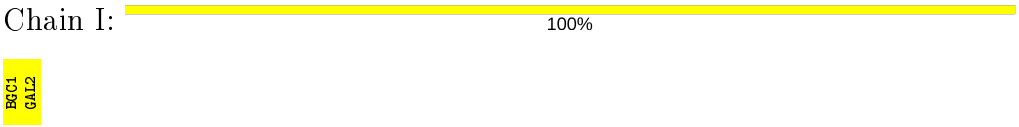


• Molecule 4: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain B:

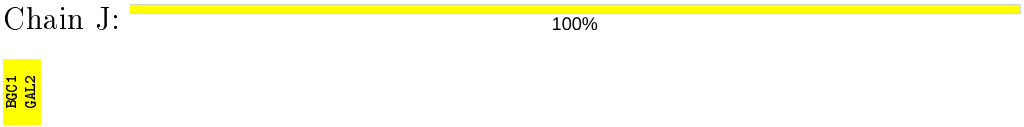
• Molecule 4: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain I:



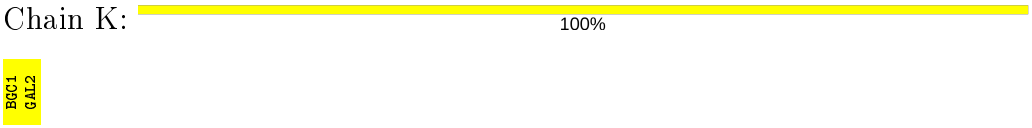
• Molecule 4: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain J:



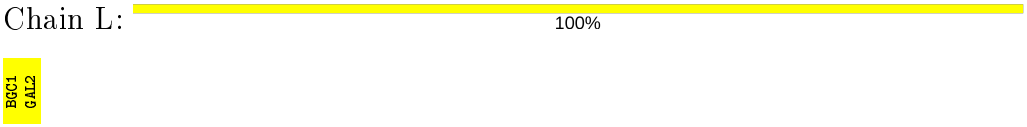
• Molecule 4: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain K:



• Molecule 4: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.80Å 101.20Å 64.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6427	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	D	0.82	0/835	1.44	9/1124 (0.8%)
1	E	0.79	0/835	1.50	13/1124 (1.2%)
1	F	0.84	0/835	1.57	15/1124 (1.3%)
1	G	0.85	0/835	1.62	10/1124 (0.9%)
1	H	0.80	0/835	1.57	13/1124 (1.2%)
2	A	0.78	0/1559	1.53	29/2120 (1.4%)
3	C	0.73	0/351	1.60	5/472 (1.1%)
All	All	0.80	0/6085	1.54	94/8212 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	235	ARG	NE-CZ-NH2	-13.72	113.44	120.30
1	H	35	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	E	67	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	G	73	ARG	NE-CZ-NH1	11.87	126.24	120.30
1	G	13	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	H	35	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	H	88	TRP	CD1-CG-CD2	9.04	113.53	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	127	TRP	CD1-CG-CD2	8.95	113.46	106.30
3	C	235	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	G	73	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	H	67	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	D	73	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	E	88	TRP	CD1-CG-CD2	8.45	113.06	106.30
2	A	25	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	D	88	TRP	CD1-CG-CD2	7.95	112.66	106.30
2	A	174	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	E	88	TRP	CE2-CD2-CG	-7.86	101.02	107.30
1	F	13	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	E	35	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	G	13	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	A	174	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	H	73	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	A	127	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	H	88	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	E	67	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	G	88	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	G	88	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	F	88	TRP	CD1-CG-CD2	7.38	112.21	106.30
1	D	12	TYR	CB-CG-CD2	-7.29	116.62	121.00
1	F	88	TRP	CE2-CD2-CG	-7.23	101.52	107.30
2	A	163	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	A	116	LEU	CA-CB-CG	7.15	131.75	115.30
2	A	179	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	E	73	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	A	128	TYR	CB-CG-CD2	-7.04	116.77	121.00
2	A	25	ARG	NE-CZ-NH2	-6.99	116.80	120.30
2	A	179	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	D	88	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	E	101	MET	CG-SD-CE	-6.64	89.58	100.20
1	D	27	TYR	CB-CG-CD2	-6.59	117.04	121.00
1	H	73	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	G	35	ARG	NE-CZ-NH1	6.55	123.57	120.30
2	A	174	TRP	CG-CD2-CE3	6.54	139.78	133.90
2	A	174	TRP	CB-CG-CD1	-6.47	118.59	127.00
2	A	127	TRP	CG-CD2-CE3	6.47	139.72	133.90
2	A	175	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	H	88	TRP	CG-CD2-CE3	6.30	139.57	133.90
2	A	55	TYR	CB-CG-CD2	-6.30	117.22	121.00
2	A	127	TRP	CG-CD1-NE1	-6.22	103.88	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	73	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	F	88	TRP	CB-CG-CD1	-6.16	119.00	127.00
2	A	150	TYR	CB-CG-CD1	-6.13	117.32	121.00
1	D	67	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	H	88	TRP	CB-CG-CD1	-6.12	119.05	127.00
1	H	88	TRP	CG-CD1-NE1	-6.10	104.00	110.10
1	G	99	ILE	CB-CA-C	-6.09	99.41	111.60
1	F	101	MET	CA-CB-CG	6.06	123.61	113.30
1	E	88	TRP	CG-CD2-CE3	6.05	139.35	133.90
1	F	67	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	F	67	ARG	NE-CZ-NH2	-6.00	117.30	120.30
3	C	213	GLU	CA-CB-CG	-5.96	100.30	113.40
1	F	23	LYS	CA-CB-CG	5.92	126.41	113.40
1	E	88	TRP	CB-CG-CD1	-5.86	119.38	127.00
1	H	12	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	F	50	VAL	N-CA-C	-5.82	95.29	111.00
3	C	210	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	G	50	VAL	N-CA-C	-5.70	95.60	111.00
2	A	7	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	13	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	H	35	ARG	CG-CD-NE	-5.68	99.86	111.80
2	A	7	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	E	18	TYR	CB-CG-CD1	-5.61	117.63	121.00
2	A	175	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	A	80	TYR	N-CA-C	-5.52	96.10	111.00
1	D	18	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	D	73	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	E	50	VAL	N-CA-C	-5.46	96.26	111.00
1	E	35	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	A	84	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	G	88	TRP	CB-CG-CD1	-5.41	119.97	127.00
2	A	127	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	F	69	LYS	CG-CD-CE	5.36	127.99	111.90
1	F	88	TRP	CG-CD2-CE3	5.36	138.72	133.90
2	A	4	ARG	NE-CZ-NH2	-5.32	117.64	120.30
3	C	236	ILE	CA-CB-CG1	-5.26	101.01	111.00
2	A	148	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	H	50	VAL	N-CA-C	-5.21	96.93	111.00
1	F	3	GLN	CA-CB-CG	-5.20	101.96	113.40
1	F	91	LYS	CA-CB-CG	-5.20	101.97	113.40
2	A	146	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	A	94	MET	CA-CB-CG	5.19	122.12	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	174	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	F	13	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	E	88	TRP	CG-CD1-NE1	-5.08	105.03	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	76	TYR	Sidechain
1	G	76	TYR	Sidechain

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	D	824	0	841	8	0
1	E	824	0	841	5	0
1	F	824	0	841	8	0
1	G	824	0	841	11	0
1	H	824	0	841	9	0
2	A	1511	0	1407	26	0
3	C	347	0	327	6	0
4	B	23	0	21	0	0
4	I	23	0	21	0	0
4	J	23	0	21	0	0
4	K	23	0	21	0	0
4	L	23	0	21	0	0
5	A	43	0	0	1	0
5	C	29	0	0	0	0
5	D	65	0	0	0	0
5	E	56	0	0	0	0
5	F	37	0	0	1	0
5	G	53	0	0	0	0
5	H	51	0	0	0	0
All	All	6427	0	6044	59	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 (59) 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:G:54:GLY:H	1:G:57:HIS:HD2	1.32	0.77
2:A:174:TRP:HB3	2:A:188:GLY:HA2	1.66	0.76
1:D:93:PRO:HG3	1:H:3:GLN:HG2	1.70	0.73
1:H:59:ASP:HA	1:H:62:LYS:HD3	1.75	0.69
3:C:198:THR:HA	3:C:201:GLU:HG2	1.75	0.68
1:G:3:GLN:HG2	1:H:93:PRO:HG3	1.76	0.68
1:G:1:ALA:HA	1:H:92:THR:O	1.93	0.68
1:F:82:ILE:HD12	1:F:99:ILE:HD11	1.78	0.66
1:F:61:GLN:O	1:F:65:ILE:HG13	1.98	0.64
2:A:84:TYR:CE2	2:A:129:ARG:HG2	2.33	0.63
1:G:53:PRO:HA	1:G:57:HIS:CD2	2.35	0.61
2:A:125:TYR:O	2:A:141:ARG:HD2	2.04	0.57
1:F:25:LEU:HB2	1:F:43:LYS:HD2	1.89	0.55
2:A:84:TYR:HE2	2:A:129:ARG:HG2	1.72	0.55
1:G:15:THR:HA	1:G:87:VAL:O	2.07	0.54
2:A:147:ASP:O	2:A:151:ARG:HB2	2.08	0.53
2:A:54:ARG:HG2	5:A:217:HOH:O	2.08	0.53
2:A:82:THR:HA	2:A:130:VAL:O	2.10	0.51
2:A:122:SER:HB2	2:A:146:ARG:HG2	1.92	0.51
2:A:168:PRO:HG2	2:A:171:HIS:HB2	1.93	0.51
1:G:54:GLY:N	1:G:57:HIS:HD2	2.05	0.51
1:D:12:TYR:OH	1:E:35:ARG:HG3	2.12	0.50
2:A:94:MET:SD	2:A:115:ALA:HB2	2.53	0.49
1:G:99:ILE:HD12	1:H:29:GLU:HB3	1.94	0.49
2:A:125:TYR:CE1	2:A:141:ARG:HD3	2.48	0.49
2:A:129:ARG:NH2	2:A:131:ASN:HD21	2.12	0.48
1:H:15:THR:HA	1:H:87:VAL:O	2.14	0.48
2:A:104:TYR:CD1	2:A:171:HIS:HE1	2.32	0.47
1:F:103:ASN:HB2	2:A:151:ARG:HH12	1.78	0.47
1:D:3:GLN:HG3	1:E:47:THR:HG21	1.98	0.46
1:F:65:ILE:HG22	1:F:69:LYS:HE2	1.97	0.46
1:H:88:TRP:HB3	1:H:90:ASN:OD1	2.15	0.46
2:A:184:PRO:HB3	3:C:202:GLU:HB3	1.99	0.45
1:D:86:CYS:HB3	1:D:98:ALA:HB3	1.98	0.45
1:G:85:LEU:HD23	1:G:99:ILE:HG23	1.98	0.45
1:G:54:GLY:H	1:G:57:HIS:CD2	2.23	0.45
2:A:25:ARG:HH11	2:A:25:ARG:HG2	1.82	0.45
3:C:217:LYS:HA	3:C:217:LYS:HD3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:ILE:HG21	1:H:42:PHE:CE1	2.53	0.43
1:H:88:TRP:HE3	1:H:95:SER:HB2	1.83	0.43
2:A:25:ARG:NH1	2:A:25:ARG:HG2	2.33	0.43
2:A:38:ASN:HA	3:C:204:GLN:OE1	2.19	0.43
1:F:12:TYR:OH	1:G:35:ARG:HB2	2.19	0.43
2:A:174:TRP:HB3	2:A:188:GLY:CA	2.43	0.42
2:A:174:TRP:CD1	2:A:187:CYS:HB3	2.54	0.42
1:D:61:GLN:HG2	1:E:31:MET:O	2.19	0.42
1:F:23:LYS:HD3	5:F:113:HOH:O	2.20	0.42
1:D:15:THR:HA	1:D:87:VAL:O	2.20	0.42
2:A:186:GLY:O	3:C:199:CYS:HB2	2.20	0.41
2:A:47:GLY:O	2:A:54:ARG:NH1	2.49	0.41
1:G:85:LEU:CD2	1:G:99:ILE:HG23	2.50	0.41
2:A:173:ALA:HA	2:A:176:GLU:HG2	2.02	0.41
1:E:99:ILE:HD13	1:E:101:MET:HE2	2.02	0.41
1:D:65:ILE:HG22	1:D:69:LYS:HE2	2.03	0.41
2:A:66:LEU:HD12	2:A:85:ILE:HG21	2.02	0.41
1:D:58:ILE:HD12	1:E:34:LYS:HE2	2.03	0.40
2:A:5:LEU:HD11	2:A:155:ILE:HD11	2.01	0.40
2:A:166:GLY:HA2	3:C:203:THR:HG21	2.04	0.40
1:F:4:THR:HB	1:F:7:GLU:HG3	2.02	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	D	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	E	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	F	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
1	G	101/103 (98%)	96 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
2	A	183/185 (99%)	175 (96%)	8 (4%)	0	100	100
3	C	39/41 (95%)	39 (100%)	0	0	100	100
All	All	727/741 (98%)	701 (96%)	26 (4%)	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	D	95/95 (100%)	87 (92%)	8 (8%)	11	13
1	E	95/95 (100%)	92 (97%)	3 (3%)	39	54
1	F	95/95 (100%)	89 (94%)	6 (6%)	18	24
1	G	95/95 (100%)	91 (96%)	4 (4%)	30	42
1	H	95/95 (100%)	93 (98%)	2 (2%)	53	70
2	A	155/155 (100%)	147 (95%)	8 (5%)	23	32
3	C	40/40 (100%)	37 (92%)	3 (8%)	13	17
All	All	670/670 (100%)	636 (95%)	34 (5%)	24	33

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	GLN
1	D	16	GLN
1	D	55	SER
1	D	63	LYS
1	D	81	LYS
1	D	91	LYS
1	D	101	MET
1	D	103	ASN
1	E	23	LYS

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Mol	Chain	Res	Type
1	E	91	LYS
1	E	95	SER
1	F	4	THR
1	F	23	LYS
1	F	43	LYS
1	F	91	LYS
1	F	101	MET
1	F	103	ASN
1	G	35	ARG
1	G	59	ASP
1	G	91	LYS
1	G	99	ILE
1	H	56	GLN
1	H	102	LYS
2	A	17	LYS
2	A	55	TYR
2	A	78	SER
2	A	116	LEU
2	A	141	ARG
2	A	154	ASN
2	A	174	TRP
2	A	175	ARG
3	C	200	ASN
3	C	234	ASN
3	C	235	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3	GLN
1	D	16	GLN
1	D	21	ASN
1	E	3	GLN
1	F	103	ASN
1	G	16	GLN
1	G	57	HIS
1	G	103	ASN
1	H	3	GLN
2	A	131	ASN
2	A	171	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BGC	B	1	4	12,12,12	0.47	0	17,17,17	0.84	1 (5%)
4	GAL	B	2	4	11,11,12	0.84	0	15,15,17	0.81	0
4	BGC	I	1	4	12,12,12	0.73	0	17,17,17	1.33	2 (11%)
4	GAL	I	2	4	11,11,12	0.93	1 (9%)	15,15,17	1.53	2 (13%)
4	BGC	J	1	4	12,12,12	1.13	1 (8%)	17,17,17	1.47	3 (17%)
4	GAL	J	2	4	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
4	BGC	K	1	4	12,12,12	1.01	1 (8%)	17,17,17	0.85	0
4	GAL	K	2	4	11,11,12	1.06	1 (9%)	15,15,17	0.86	0
4	BGC	L	1	4	12,12,12	0.91	1 (8%)	17,17,17	0.97	0
4	GAL	L	2	4	11,11,12	0.90	0	15,15,17	1.05	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
4	BGC	B	1	4	-	0/2/22/22	0/1/1/1
4	GAL	B	2	4	-	0/2/19/22	0/1/1/1
4	BGC	I	1	4	-	1/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	I	2	4	-	0/2/19/22	0/1/1/1
4	BGC	J	1	4	-	2/2/22/22	0/1/1/1
4	GAL	J	2	4	-	0/2/19/22	0/1/1/1
4	BGC	K	1	4	-	0/2/22/22	0/1/1/1
4	GAL	K	2	4	-	0/2/19/22	0/1/1/1
4	BGC	L	1	4	-	2/2/22/22	0/1/1/1
4	GAL	L	2	4	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2	GAL	C4-C5	2.60	1.58	1.53
4	I	2	GAL	C2-C3	2.56	1.56	1.52
4	K	1	BGC	C4-C5	2.26	1.57	1.53
4	J	1	BGC	C6-C5	2.08	1.58	1.51
4	L	1	BGC	C6-C5	2.06	1.58	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	2	GAL	C1-C2-C3	-4.07	104.67	109.67
4	J	1	BGC	C4-C3-C2	-3.96	103.91	110.82
4	I	1	BGC	C3-C4-C5	3.88	117.16	110.24
4	J	2	GAL	C1-O5-C5	3.53	116.98	112.19
4	J	2	GAL	O3-C3-C2	-2.44	105.32	109.99
4	J	1	BGC	O4-C4-C3	2.43	115.96	110.35
4	B	1	BGC	C3-C4-C5	2.42	114.56	110.24
4	I	1	BGC	O4-C4-C5	-2.30	103.58	109.30
4	I	2	GAL	O2-C2-C3	2.13	114.41	110.14
4	J	1	BGC	O3-C3-C4	2.13	115.27	110.35
4	L	2	GAL	C2-C3-C4	-2.00	107.43	110.89

There are no chirality outliers.

All (5) torsion outliers are listed below:

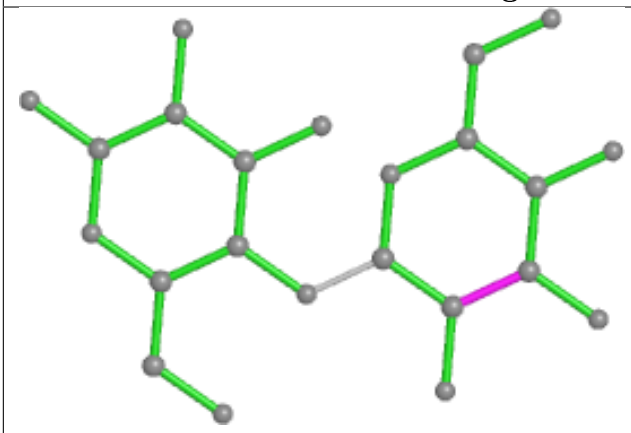
Mol	Chain	Res	Type	Atoms
4	J	1	BGC	O5-C5-C6-O6
4	I	1	BGC	O5-C5-C6-O6
4	J	1	BGC	C4-C5-C6-O6
4	L	1	BGC	C4-C5-C6-O6
4	L	1	BGC	O5-C5-C6-O6

There are no ring outliers.

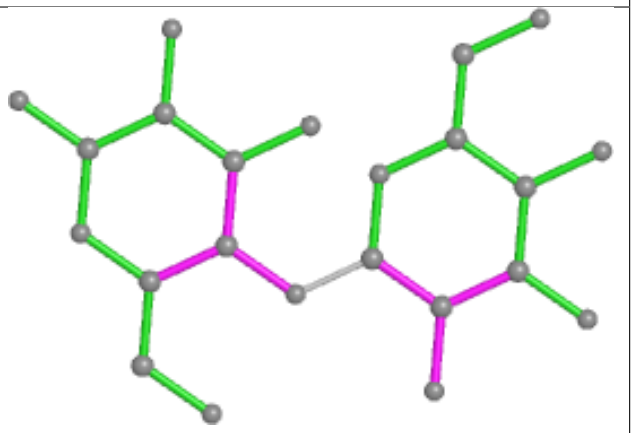
No monomer is involved in short contacts.

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

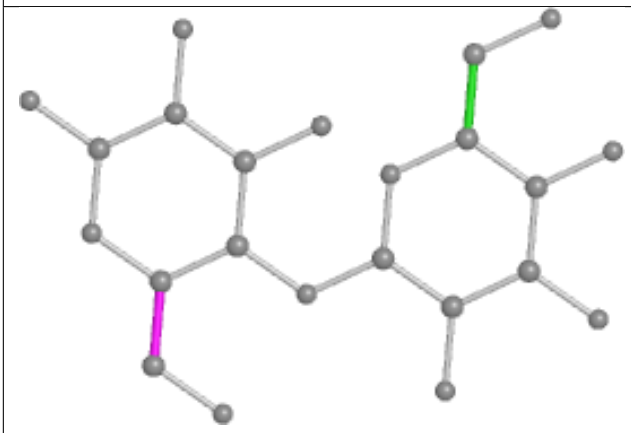
Oligosaccharide Chain I



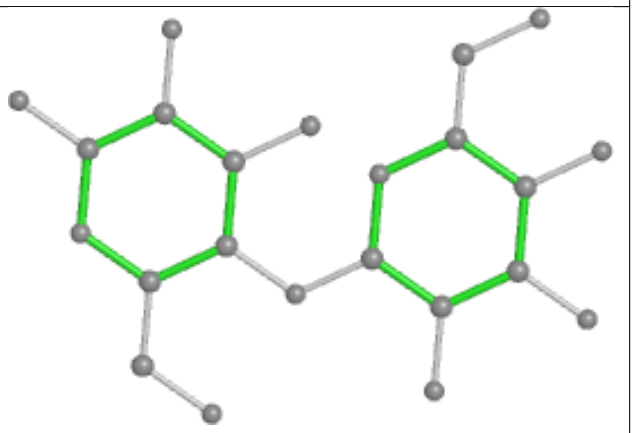
Bond lengths



Bond angles

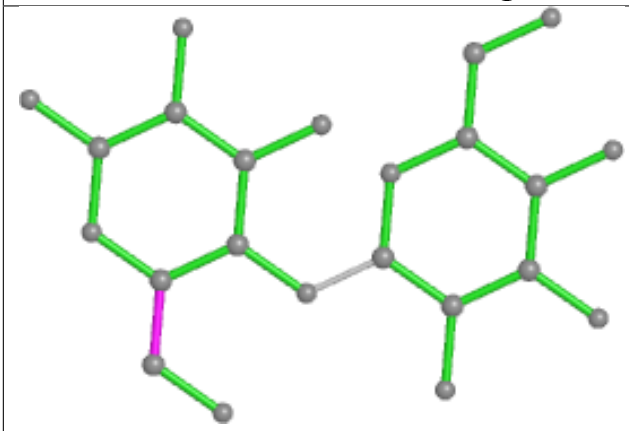


Torsions

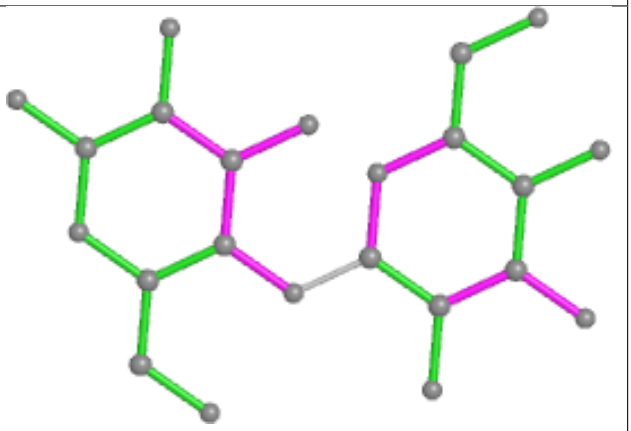


Rings

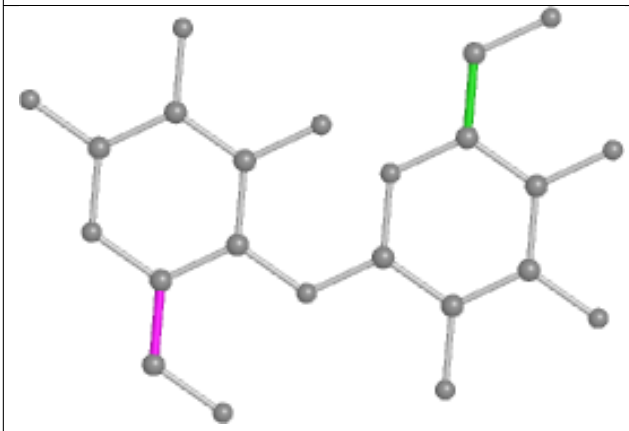
Oligosaccharide Chain J



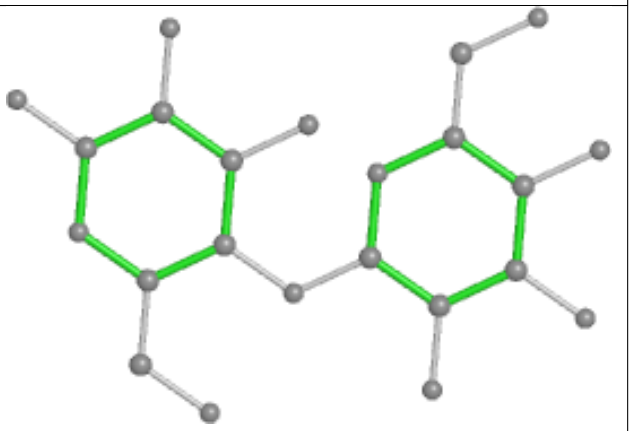
Bond lengths



Bond angles

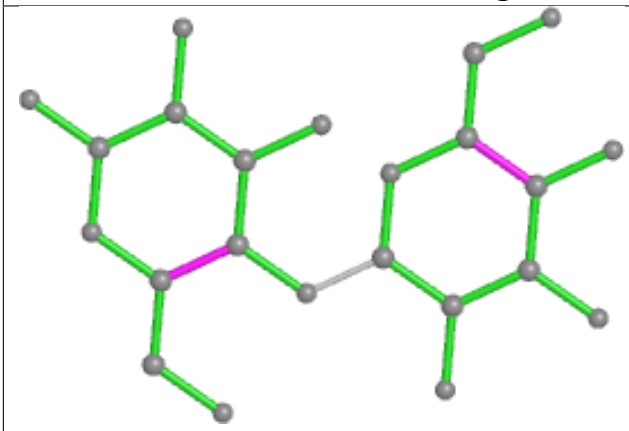


Torsions

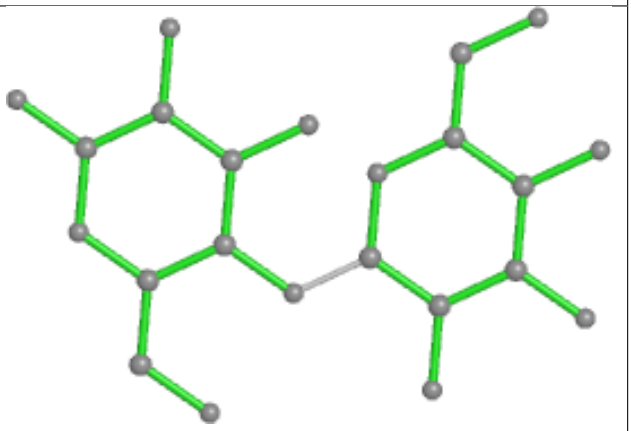


Rings

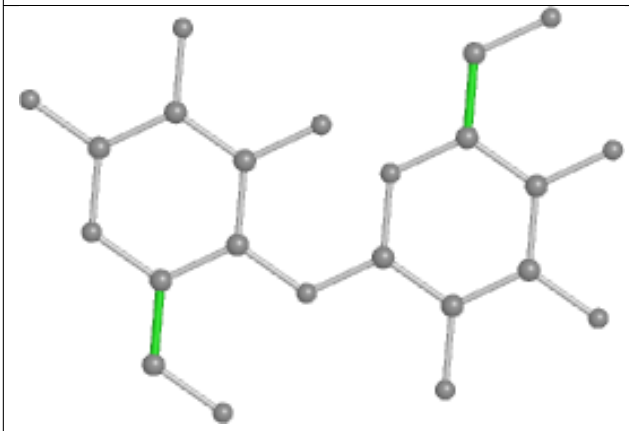
Oligosaccharide Chain K



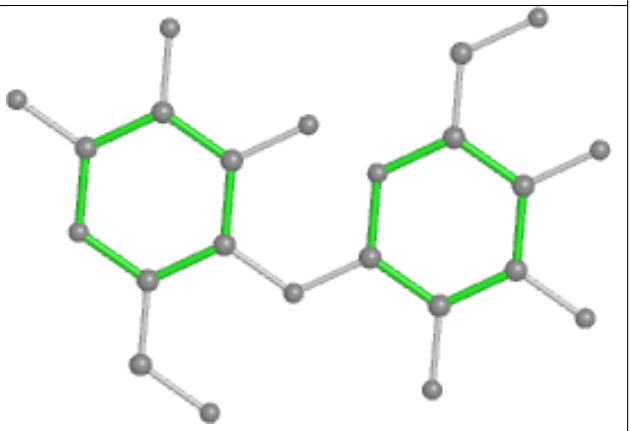
Bond lengths



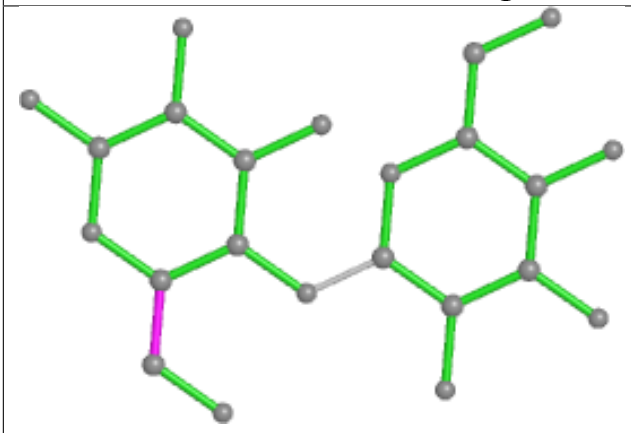
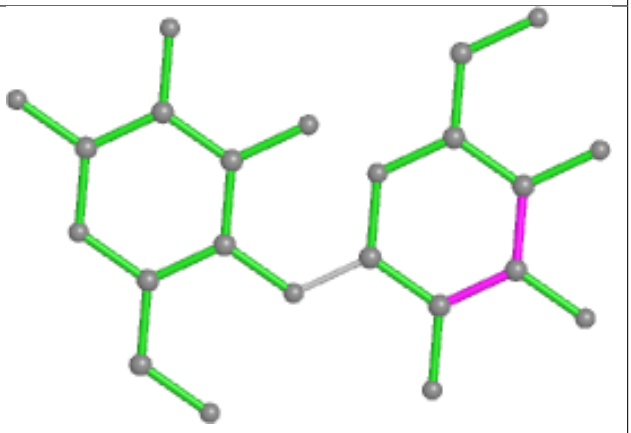
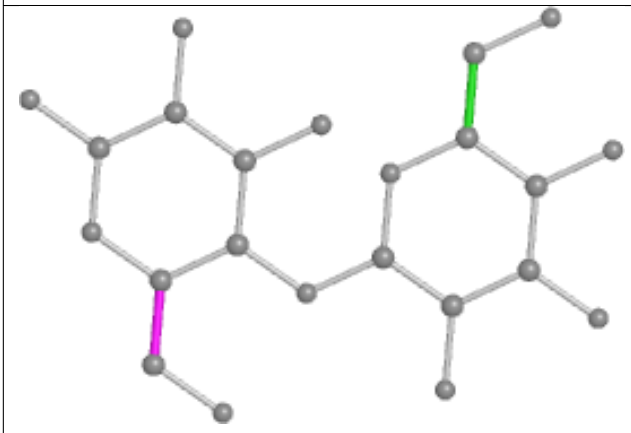
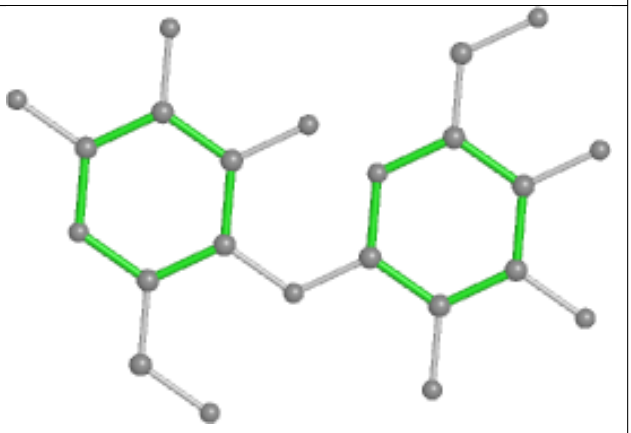
Bond angles



Torsions



Rings

Oligosaccharide Chain L	
 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.