Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:25 PM EDT

PDB ID	:	1JU2
Title	:	Crystal structure of the hydroxynitrile lyase from almond
Authors	:	Dreveny, I.; Gruber, K.; Glieder, A.; Thompson, A.; Kratky, C.
Deposited on	:	2001-08-23
Resolution	:	1.47 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

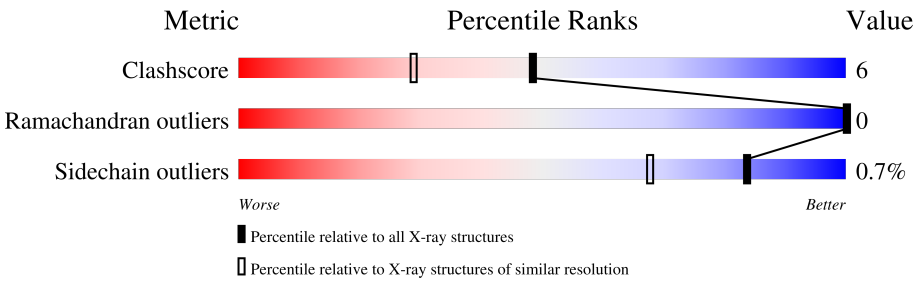
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.47 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	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	536	86% 11% .
1	B	536	84% 12% .
2	C	2	50% 50%
3	D	5	100%
3	G	5	80% 20%
4	E	5	80% 20%
5	F	2	50% 50%
6	H	4	50% 25% 25%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9995 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.

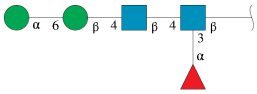
- Molecule 1 is a protein called hydroxynitrile lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	521	4033	2556	672	797	8	0	16	0
1	B	521	4019	2552	668	791	8	0	11	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

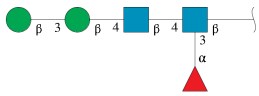
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	5	60	34	2	24	0	0	0
3	G	5	60	34	2	24	0	0	0

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

mido-2-deoxy-beta-D-glucopyranose.

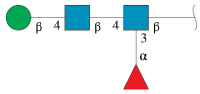


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	5	60	34	2	24	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

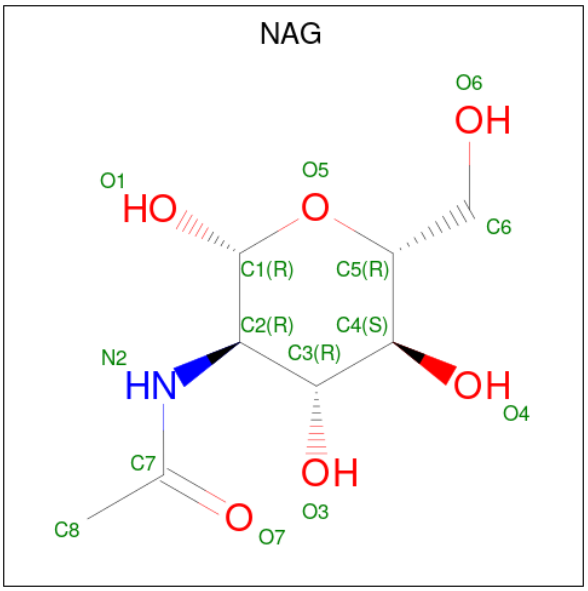
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	2	28	16	2	10	0	0	0

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



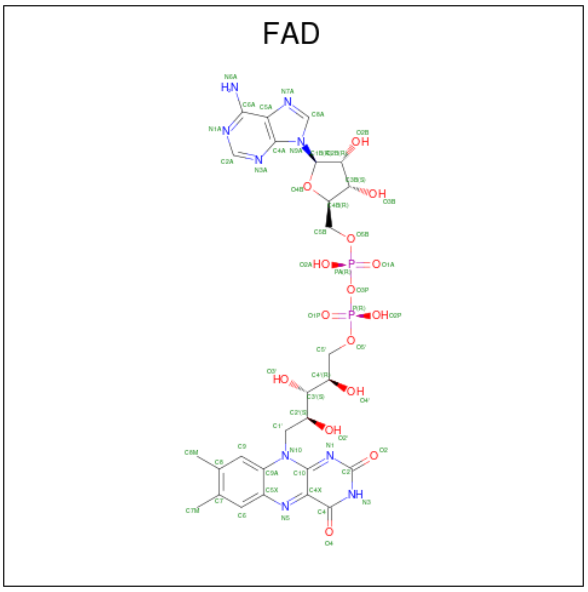
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	H	4	49	28	2	19	0	0	0

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



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

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	A	1	53	27	9	15	2	0	0

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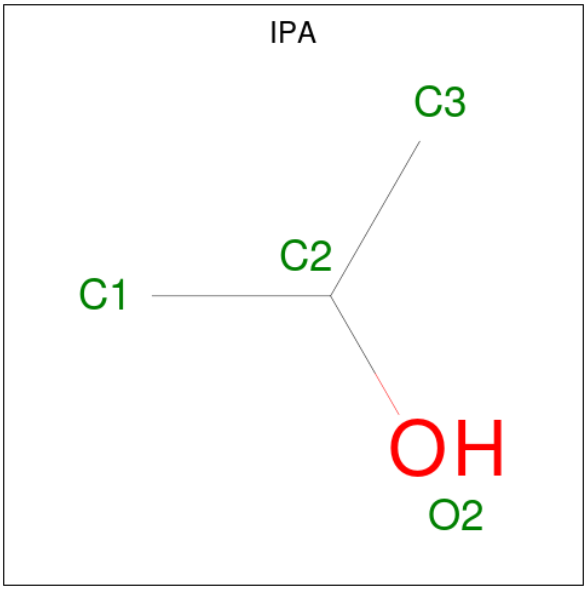
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	53	27	9	15	2	0	0

- Molecule 9 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
9	A	1	4	3	1		0	0
9	B	1	4	3	1		0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	753	753	753	0	0
10	B	763	763	763	0	0

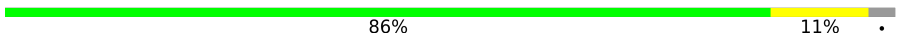
3 Residue-property plots (i)

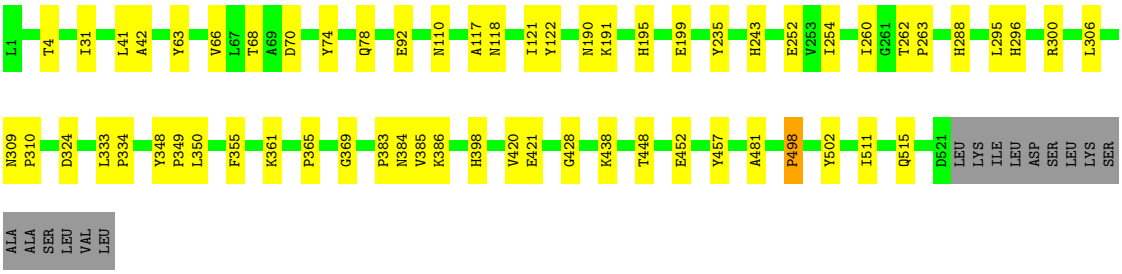
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: hydroxynitrile lyase

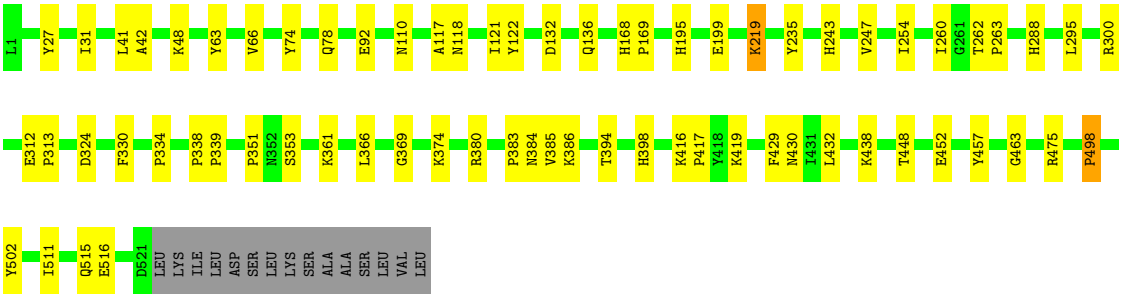
Chain A:





• Molecule 1: hydroxynitrile lyase

Chain B:



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

Chain C:

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

Chain D: 100%

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

Chain G: 80% 20%

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

Chain E: 80% 20%

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

Chain F: 50% 50%

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

Chain H: 50% 25% 25%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.18Å 67.49Å 79.80Å 79.57° 77.78° 67.19°	Depositor
Resolution (Å)	23.23 – 1.47	Depositor
% Data completeness (in resolution range)	69.2 (23.23-1.47)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.160 , 0.186	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9995	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.30	0/4223	0.63	0/5760
1	B	0.30	0/4182	0.63	0/5705
All	All	0.30	0/8405	0.63	0/11465

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4033	0	3881	43	0
1	B	4019	0	3877	52	0
2	C	28	0	24	0	0
3	D	60	0	52	0	0
3	G	60	0	52	0	0
4	E	60	0	52	0	0
5	F	28	0	25	3	0
6	H	49	0	43	1	0
7	A	14	0	13	1	0
7	B	14	0	13	1	0
8	A	53	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	53	0	31	2	0
9	A	4	0	8	1	0
9	B	4	0	8	1	0
10	A	753	0	0	3	0
10	B	763	0	0	5	0
All	All	9995	0	8110	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (100) 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:A:420:VAL:HG23	1:A:421:GLU:HG3	1.58	0.84
1:A:121[B]:ILE:HD12	9:A:4001:IPA:H2	1.60	0.83
1:B:121[B]:ILE:HD12	9:B:4002:IPA:H2	1.60	0.83
1:B:374:LYS:HE2	1:B:384[A]:ASN:HD21	1.46	0.81
1:A:118:ASN:O	1:A:121[B]:ILE:HG12	1.87	0.73
1:A:118:ASN:O	1:A:121[A]:ILE:HG13	1.90	0.72
1:B:374:LYS:HE2	1:B:384[A]:ASN:ND2	2.04	0.72
1:B:92[B]:GLU:OE2	1:B:384[B]:ASN:OD1	2.09	0.71
1:B:118:ASN:O	1:B:121[A]:ILE:HG13	1.91	0.71
1:B:118:ASN:O	1:B:121[B]:ILE:HG12	1.90	0.70
1:A:117:ALA:HB1	1:A:121[B]:ILE:HD11	1.75	0.67
1:B:448:THR:O	1:B:452[B]:GLU:HG2	1.93	0.67
5:F:1:NAG:H61	5:F:2:NAG:H82	1.79	0.65
1:A:511:ILE:O	1:A:515:GLN:HG3	2.02	0.60
6:H:2:NAG:H62	6:H:3:BMA:O2	2.01	0.60
1:B:92[B]:GLU:CG	1:B:384[B]:ASN:HD21	2.15	0.59
1:B:117:ALA:HB1	1:B:121[B]:ILE:HD11	1.85	0.58
1:A:4:THR:HG21	1:A:191:LYS:HG3	1.85	0.58
5:F:1:NAG:H61	5:F:2:NAG:C8	2.33	0.58
1:A:110:ASN:HB2	8:A:2001:FAD:C5X	2.36	0.56
1:B:438:LYS:HG3	10:B:4419:HOH:O	2.04	0.55
1:B:31:ILE:HD12	1:B:42:ALA:HB2	1.88	0.54
1:B:369:GLY:HA3	1:B:386:LYS:O	2.08	0.54
1:B:41:LEU:HD21	1:B:254:ILE:HG21	1.89	0.54
1:B:74:TYR:O	1:B:78[B]:GLN:HG2	2.08	0.53
1:B:110:ASN:HB2	8:B:2002:FAD:C5X	2.37	0.53
1:B:511:ILE:O	1:B:515:GLN:HG3	2.08	0.53
1:A:384[B]:ASN:ND2	10:A:4745:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:THR:HB	1:B:263:PRO:HD3	1.92	0.52
1:A:110:ASN:HB2	8:A:2001:FAD:N5	2.25	0.51
1:A:369:GLY:HA3	1:A:386:LYS:O	2.10	0.51
1:B:475:ARG:NH2	1:B:516:GLU:OE2	2.44	0.51
1:A:420:VAL:HG22	1:A:428:GLY:O	2.11	0.51
1:B:132:ASP:O	1:B:136:GLN:HG3	2.11	0.50
1:A:235:TYR:CZ	1:A:243:HIS:HB2	2.47	0.49
1:B:195:HIS:HA	1:B:199:GLU:OE1	2.13	0.49
1:A:68:THR:OG1	1:A:70[B]:ASP:OD1	2.29	0.48
1:B:300:ARG:HB2	1:B:457:TYR:CD1	2.49	0.47
1:A:498:PRO:HB2	1:A:502:TYR:CE1	2.49	0.47
1:B:121[A]:ILE:HD12	1:B:122:TYR:N	2.29	0.47
1:B:63:TYR:O	1:B:66:VAL:HG22	2.15	0.47
1:A:350:LEU:HD23	10:A:4570:HOH:O	2.14	0.47
1:B:110:ASN:HB2	8:B:2002:FAD:N5	2.29	0.47
1:A:41:LEU:HD21	1:A:254:ILE:HG21	1.97	0.47
1:A:306:LEU:HD23	1:A:355:PHE:HB3	1.97	0.47
1:B:351:PRO:HB3	1:B:432:LEU:HD22	1.96	0.46
1:B:380:ARG:HD3	10:B:4543:HOH:O	2.15	0.46
1:A:195:HIS:HA	1:A:199:GLU:OE1	2.15	0.46
1:A:92[B]:GLU:OE2	1:B:92[B]:GLU:OE1	2.33	0.46
1:A:121[A]:ILE:HD12	1:A:122:TYR:N	2.31	0.46
1:B:168:HIS:HB3	1:B:169:PRO:HA	1.98	0.45
1:B:295:LEU:HD22	1:B:463:GLY:HA2	1.99	0.45
1:B:498:PRO:HB2	1:B:502:TYR:CE1	2.52	0.45
1:B:330:PHE:HA	10:B:4144:HOH:O	2.15	0.45
1:A:262:THR:HB	1:A:263:PRO:HD3	1.99	0.45
1:B:300:ARG:HB2	1:B:457:TYR:HD1	1.82	0.45
1:A:296:HIS:HB3	1:A:365:PRO:HD2	1.98	0.44
1:A:4:THR:HG1	1:A:190:ASN:HD22	1.64	0.44
1:B:338:PRO:HA	1:B:339:PRO:HD3	1.87	0.44
1:A:74:TYR:O	1:A:78[A]:GLN:HG2	2.17	0.44
1:A:110:ASN:HB2	8:A:2001:FAD:C4X	2.48	0.44
1:A:438:LYS:HG3	10:A:4204:HOH:O	2.16	0.44
1:B:235:TYR:CZ	1:B:243:HIS:HB2	2.52	0.44
1:B:260:ILE:HD12	1:B:385[B]:VAL:HG21	2.00	0.44
1:B:324:ASP:HB3	1:B:398:HIS:CG	2.53	0.43
1:A:333:LEU:HB3	1:A:334:PRO:HD2	2.00	0.43
1:B:219:LYS:CB	1:B:219:LYS:NZ	2.82	0.43
1:A:300:ARG:HB2	1:A:457:TYR:CD1	2.54	0.43
5:F:1:NAG:H61	5:F:2:NAG:C7	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LYS:HB3	1:B:417:PRO:HD3	2.02	0.42
1:B:92[B]:GLU:HG2	1:B:384[B]:ASN:HD21	1.85	0.42
1:A:295:LEU:HD22	1:A:385[B]:VAL:HG13	2.01	0.42
1:A:361:LYS:HB2	1:A:457:TYR:CD1	2.55	0.42
1:B:48:LYS:HE3	10:B:4078:HOH:O	2.20	0.42
1:A:31:ILE:HD12	1:A:42:ALA:HB2	2.02	0.42
1:A:348:TYR:CG	1:A:349:PRO:HD2	2.55	0.42
1:B:374:LYS:HD3	1:B:374:LYS:HA	1.86	0.42
7:B:607:NAG:H5	10:B:4763:HOH:O	2.19	0.42
1:A:324:ASP:HB3	1:A:398:HIS:CG	2.54	0.42
1:A:448:THR:O	1:A:452[A]:GLU:HG3	2.20	0.42
1:B:361:LYS:HB2	1:B:457:TYR:CD1	2.55	0.42
1:B:419:LYS:HE2	1:B:429:PHE:CE1	2.55	0.42
1:B:219:LYS:NZ	1:B:219:LYS:HB3	2.34	0.42
1:B:366:LEU:HD12	1:B:394:THR:HB	2.02	0.41
1:A:350:LEU:O	7:A:607:NAG:O7	2.39	0.41
1:B:31:ILE:HD12	1:B:42:ALA:CB	2.50	0.41
1:A:252:GLU:HG2	1:A:481:ALA:HA	2.03	0.41
1:B:27:TYR:O	1:B:247:VAL:HA	2.19	0.41
1:A:361:LYS:HB2	1:A:457:TYR:CE1	2.56	0.41
1:A:260:ILE:HD12	1:A:385[B]:VAL:HG21	2.02	0.41
1:A:63:TYR:O	1:A:66:VAL:HG22	2.20	0.41
1:A:309:ASN:HA	1:A:310:PRO:HD3	1.92	0.40
1:B:312:GLU:HA	1:B:313:PRO:HD3	1.95	0.40
8:A:2001:FAD:H9	8:A:2001:FAD:H1'1	1.93	0.40
1:B:260:ILE:HD12	1:B:385[A]:VAL:HG11	2.04	0.40
1:B:334:PRO:HB3	1:B:353:SER:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	535/536 (100%)	522 (98%)	13 (2%)	0	100	100
1	B	530/536 (99%)	516 (97%)	14 (3%)	0	100	100
All	All	1065/1072 (99%)	1038 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	459/456 (101%)	457 (100%)	2 (0%)	91	81
1	B	454/456 (100%)	450 (99%)	4 (1%)	78	59
All	All	913/912 (100%)	907 (99%)	6 (1%)	84	68

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

Mol	Chain	Res	Type
1	A	288	HIS
1	A	498	PRO
1	B	219	LYS
1	B	288	HIS
1	B	430	ASN
1	B	498	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	224	ASN
1	A	281	ASN
1	B	65	ASN
1	B	281	ASN
1	B	323	ASN
1	B	430	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)

23 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.75	0	17,19,21	0.74	0
2	NDG	C	2	2	14,14,15	0.72	1 (7%)	17,19,21	0.73	0
3	NAG	D	1	3,1	14,14,15	0.52	0	17,19,21	0.74	0
3	NAG	D	2	3	14,14,15	0.53	0	17,19,21	0.62	0
3	BMA	D	3	3	11,11,12	0.48	0	15,15,17	0.37	0
3	MAN	D	4	3	11,11,12	0.49	0	15,15,17	0.53	0
3	FUC	D	5	3	10,10,11	0.51	0	14,14,16	0.33	0
4	NAG	E	1	4,1	14,14,15	0.52	0	17,19,21	0.64	0
4	NAG	E	2	4	14,14,15	0.48	0	17,19,21	0.64	0
4	BMA	E	3	4	11,11,12	0.44	0	15,15,17	0.28	0
4	BMA	E	4	4	11,11,12	0.58	0	15,15,17	0.73	1 (6%)
4	FUC	E	5	4	10,10,11	0.49	0	14,14,16	0.36	0
5	NAG	F	1	5,1	14,14,15	0.54	0	17,19,21	0.61	0
5	NAG	F	2	5	14,14,15	0.47	0	17,19,21	0.75	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.53	0	17,19,21	0.72	1 (5%)
3	NAG	G	2	3	14,14,15	0.51	0	17,19,21	0.69	0
3	BMA	G	3	3	11,11,12	0.45	0	15,15,17	0.41	0
3	MAN	G	4	3	11,11,12	0.48	0	15,15,17	0.51	0
3	FUC	G	5	3	10,10,11	0.49	0	14,14,16	0.37	0
6	NAG	H	1	6,1	14,14,15	0.52	0	17,19,21	0.64	0
6	NAG	H	2	6	14,14,15	0.63	0	17,19,21	1.10	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	BMA	H	3	6	11,11,12	0.48	0	15,15,17	0.43	0
6	FUC	H	4	6	10,10,11	0.48	0	14,14,16	0.34	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NDG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1
3	FUC	D	5	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	BMA	E	4	4	-	1/2/19/22	1/1/1/1
4	FUC	E	5	4	-	-	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	FUC	G	5	3	-	-	0/1/1/1
6	NAG	H	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	4/6/23/26	0/1/1/1
6	BMA	H	3	6	-	2/2/19/22	0/1/1/1
6	FUC	H	4	6	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NDG	C1-C2	2.05	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	4	BMA	C1-O5-C5	2.40	115.44	112.19
6	H	2	NAG	C4-C3-C2	2.34	114.44	111.02
5	F	2	NAG	C2-N2-C7	-2.13	119.88	122.90
3	G	1	NAG	C2-N2-C7	-2.09	119.93	122.90
6	H	2	NAG	C3-C4-C5	2.07	113.94	110.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	4	MAN	O5-C5-C6-O6
6	H	2	NAG	C8-C7-N2-C2
3	G	4	MAN	C4-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
6	H	3	BMA	C4-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
6	H	2	NAG	O7-C7-N2-C2
2	C	2	NDG	C8-C7-N2-C2
2	C	2	NDG	O7-C7-N2-C2
3	G	2	NAG	C4-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
4	E	4	BMA	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6

All (1) ring outliers are listed below:

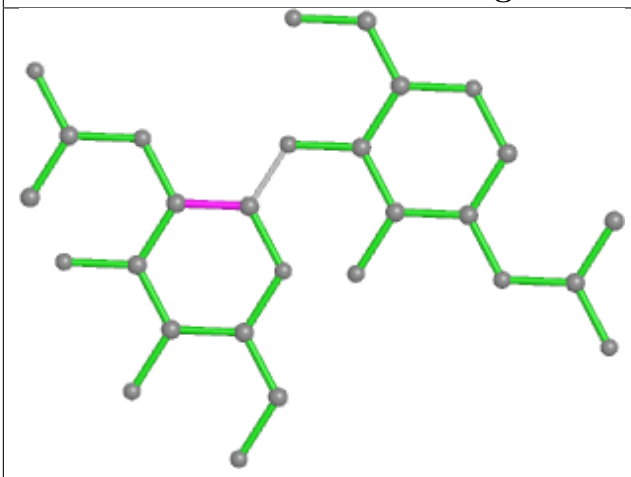
Mol	Chain	Res	Type	Atoms
4	E	4	BMA	C1-C2-C3-C4-C5-O5

4 monomers are involved in 4 short contacts:

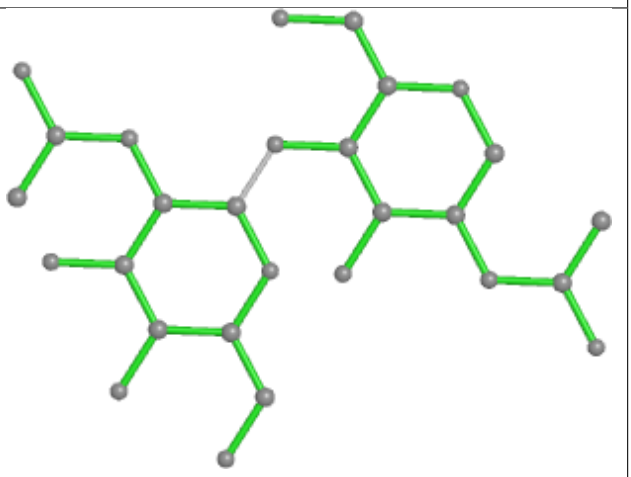
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	3	0
5	F	2	NAG	3	0
6	H	2	NAG	1	0
6	H	3	BMA	1	0

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

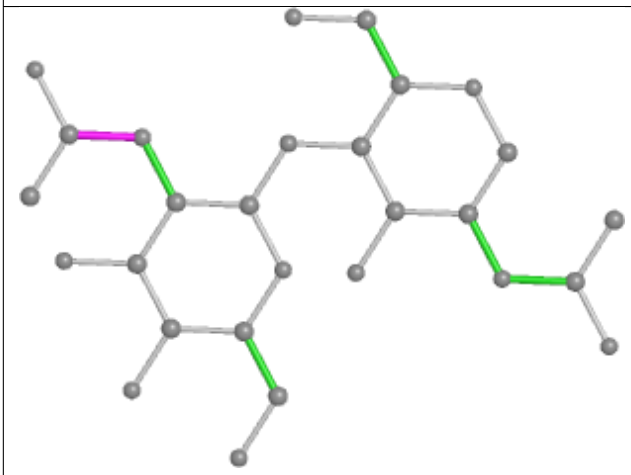
Oligosaccharide Chain C



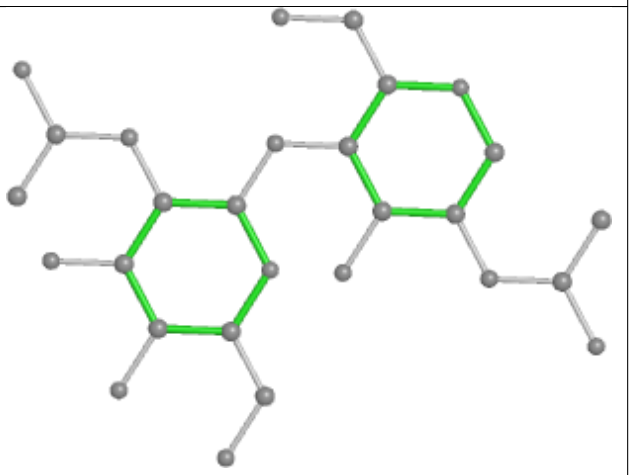
Bond lengths



Bond angles

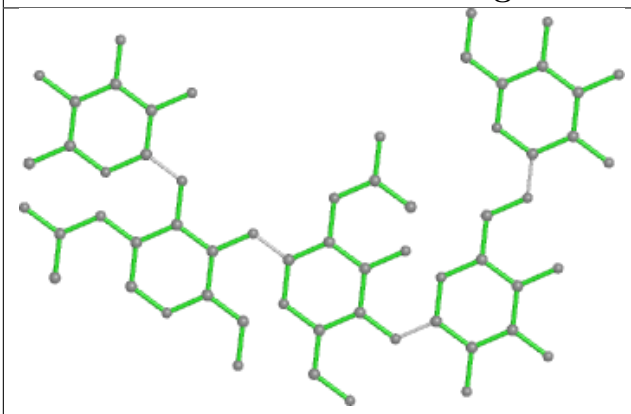


Torsions

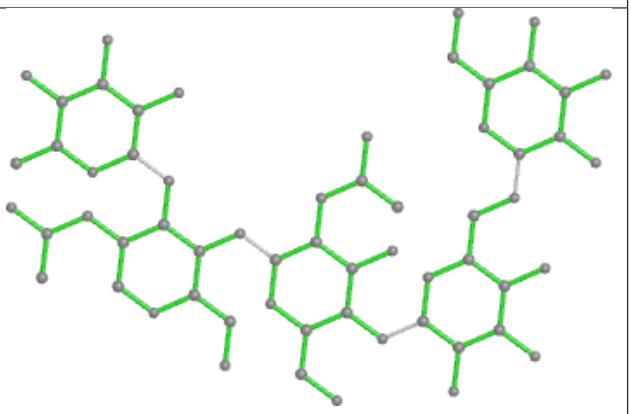


Rings

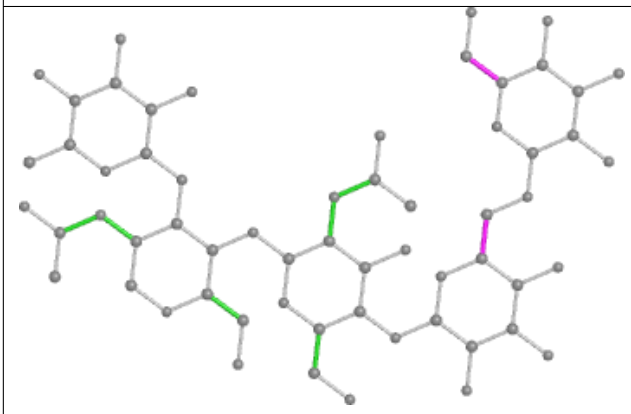
Oligosaccharide Chain D



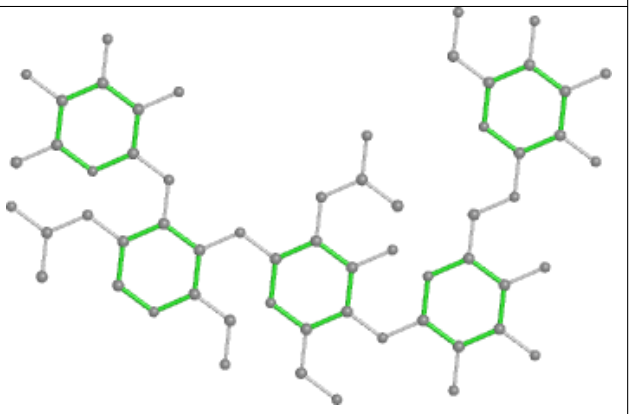
Bond lengths



Bond angles

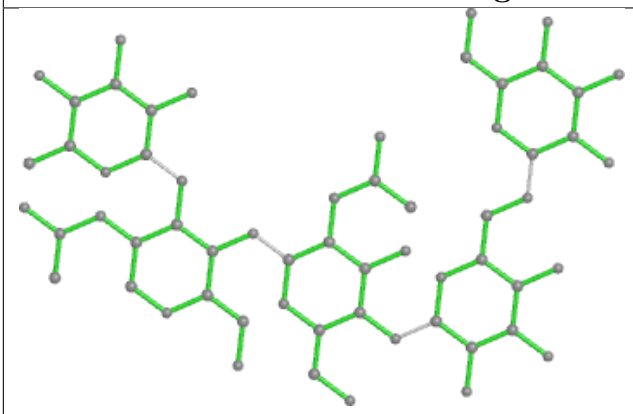


Torsions

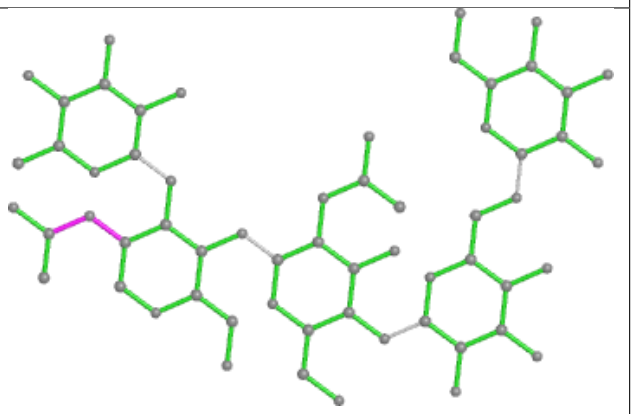


Rings

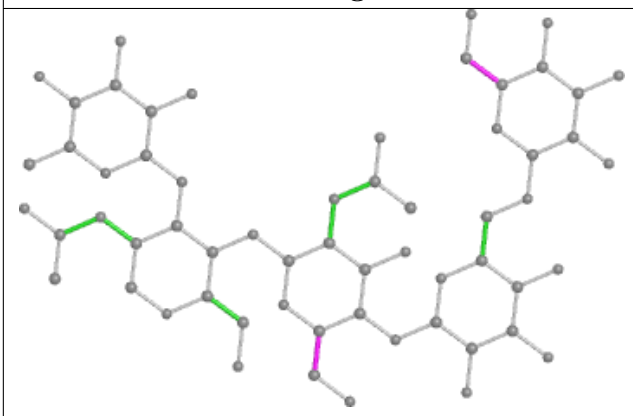
Oligosaccharide Chain G



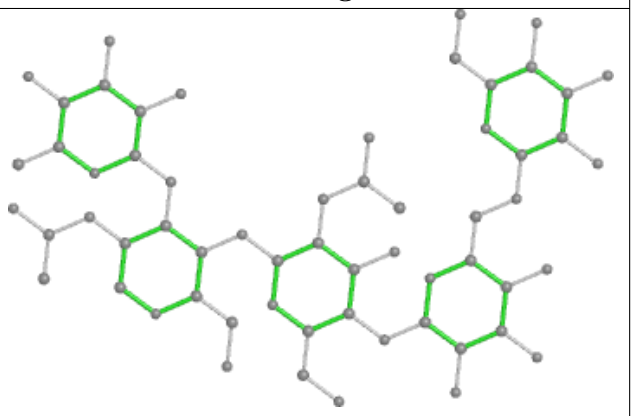
Bond lengths



Bond angles

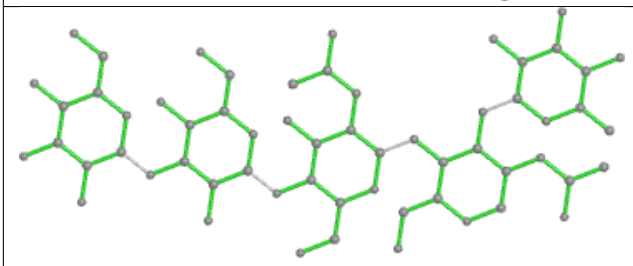


Torsions

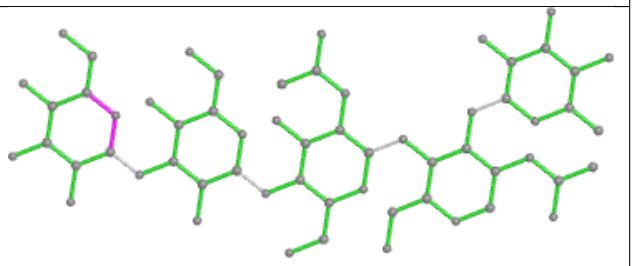


Rings

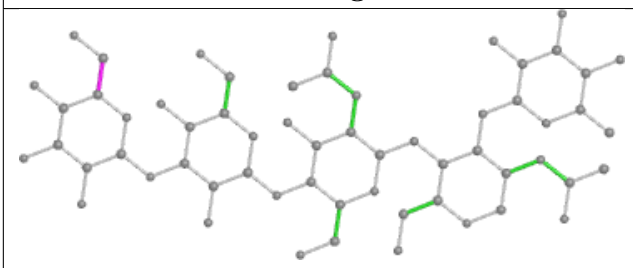
Oligosaccharide Chain E



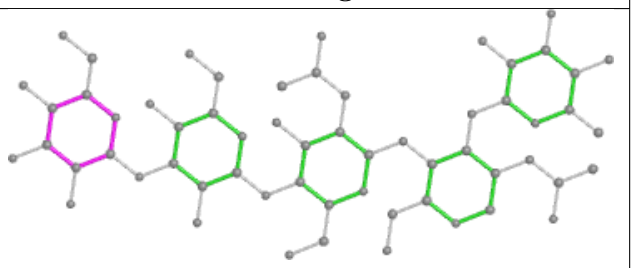
Bond lengths



Bond angles

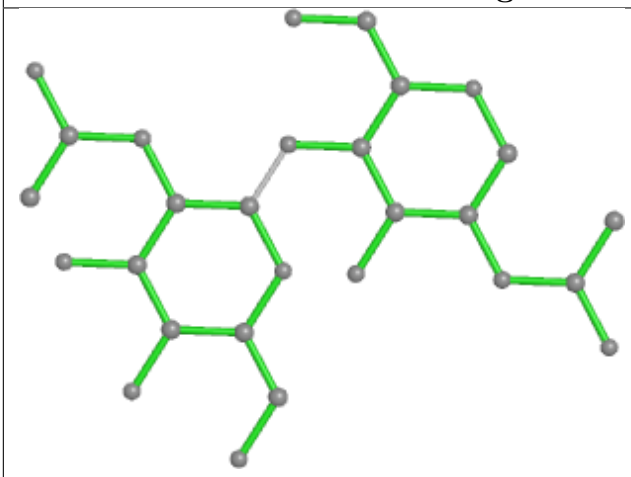


Torsions

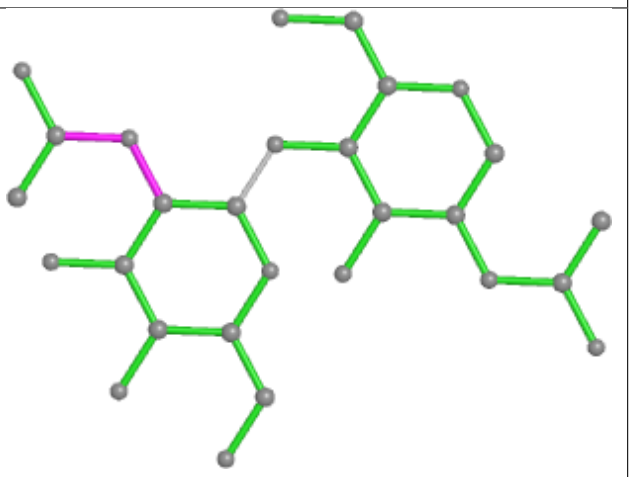


Rings

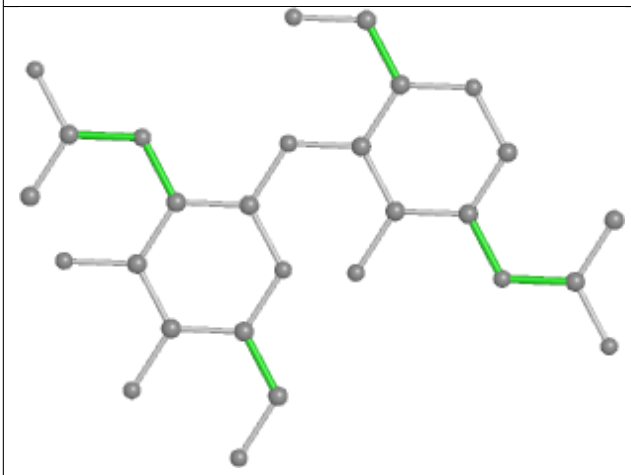
Oligosaccharide Chain F



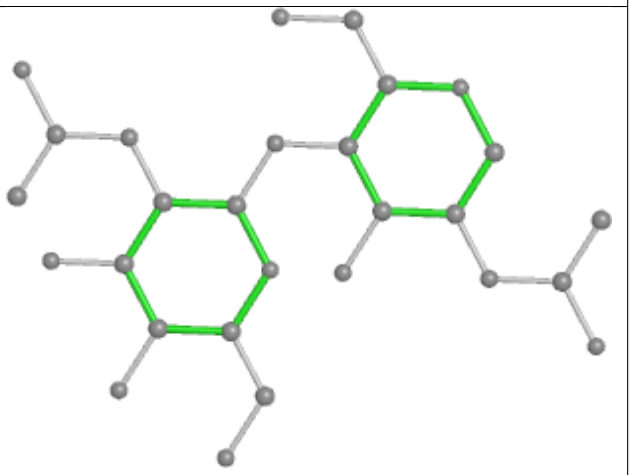
Bond lengths



Bond angles

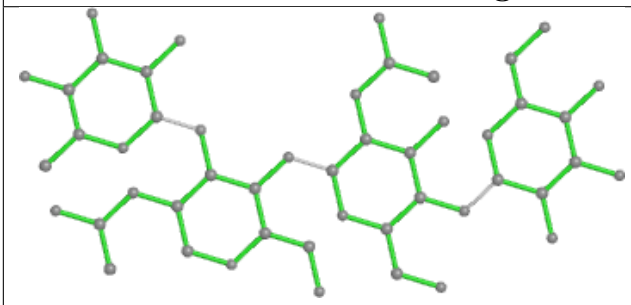


Torsions

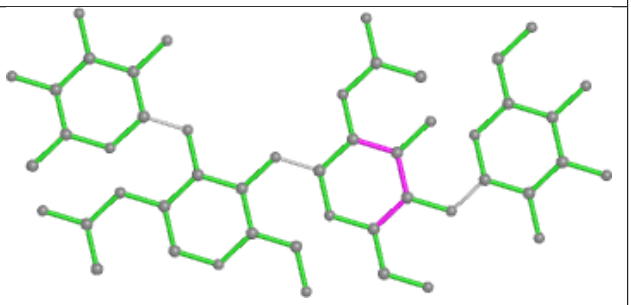


Rings

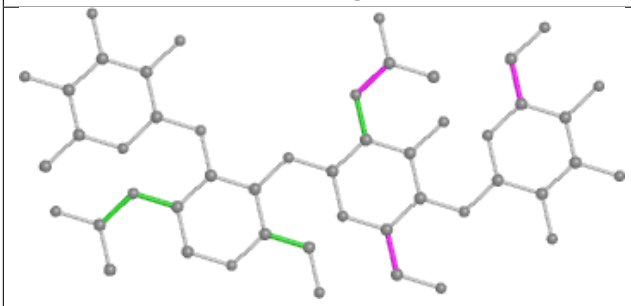
Oligosaccharide Chain H



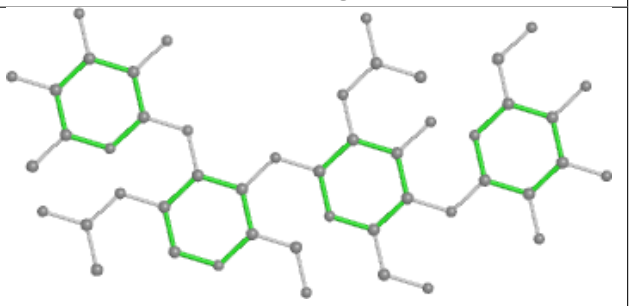
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	IPA	A	4001	-	3,3,3	0.53	0	3,3,3	0.86	0
9	IPA	B	4002	-	3,3,3	0.52	0	3,3,3	0.88	0
8	FAD	B	2002	-	53,58,58	1.79	15 (28%)	68,89,89	1.15	8 (11%)
7	NAG	A	607	1	14,14,15	0.58	0	17,19,21	0.65	0
8	FAD	A	2001	-	53,58,58	1.81	19 (35%)	68,89,89	1.15	8 (11%)
7	NAG	B	607	1	14,14,15	0.64	0	17,19,21	0.80	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FAD	B	2002	-	-	2/30/50/50	0/6/6/6
7	NAG	A	607	1	-	2/6/23/26	0/1/1/1
8	FAD	A	2001	-	-	2/30/50/50	0/6/6/6
7	NAG	B	607	1	-	0/6/23/26	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2001	FAD	O4B-C1B	4.24	1.47	1.41
8	B	2002	FAD	O4B-C1B	4.23	1.47	1.41
8	A	2001	FAD	PA-O2A	-3.83	1.37	1.55
8	B	2002	FAD	PA-O2A	-3.80	1.37	1.55
8	B	2002	FAD	C4X-N5	3.65	1.37	1.30
8	A	2001	FAD	C4X-N5	3.52	1.37	1.30
8	B	2002	FAD	P-O2P	-3.26	1.40	1.55
8	A	2001	FAD	P-O2P	-3.22	1.40	1.55
8	A	2001	FAD	C9A-N10	3.17	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	2002	FAD	C9A-N10	3.00	1.46	1.41
8	B	2002	FAD	O5'-C5'	2.90	1.55	1.44
8	B	2002	FAD	C9A-C5X	2.86	1.46	1.41
8	A	2001	FAD	O5'-C5'	2.84	1.55	1.44
8	B	2002	FAD	C8-C7	2.84	1.48	1.40
8	A	2001	FAD	C8-C7	2.72	1.47	1.40
8	A	2001	FAD	C6-C5X	2.71	1.44	1.40
8	A	2001	FAD	C9A-C5X	2.65	1.45	1.41
8	B	2002	FAD	C2A-N3A	2.62	1.36	1.32
8	B	2002	FAD	C2B-C1B	-2.57	1.49	1.53
8	B	2002	FAD	C4A-N3A	2.54	1.39	1.35
8	A	2001	FAD	C2A-N3A	2.54	1.36	1.32
8	B	2002	FAD	C6-C5X	2.47	1.43	1.40
8	A	2001	FAD	C4A-N3A	2.46	1.39	1.35
8	A	2001	FAD	C2A-N1A	2.43	1.38	1.33
8	A	2001	FAD	C2B-C1B	-2.43	1.50	1.53
8	B	2002	FAD	C2A-N1A	2.27	1.38	1.33
8	A	2001	FAD	C10-N1	2.24	1.37	1.33
8	A	2001	FAD	O4B-C4B	2.15	1.49	1.45
8	B	2002	FAD	O4B-C4B	2.11	1.49	1.45
8	A	2001	FAD	C2-N3	2.04	1.43	1.39
8	A	2001	FAD	C9-C9A	2.03	1.42	1.39
8	B	2002	FAD	C2-N3	2.03	1.43	1.39
8	A	2001	FAD	C3B-C4B	2.01	1.58	1.53
8	A	2001	FAD	C9-C8	2.00	1.42	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	2002	FAD	O5B-PA-O1A	-2.61	98.86	109.07
8	A	2001	FAD	O5B-PA-O1A	-2.59	98.96	109.07
8	B	2002	FAD	C2A-N1A-C6A	2.46	122.95	118.75
8	A	2001	FAD	C2A-N1A-C6A	2.38	122.82	118.75
8	B	2002	FAD	C5A-C6A-N1A	-2.33	115.07	120.35
8	A	2001	FAD	C5'-C4'-C3'	-2.32	107.71	112.20
8	B	2002	FAD	C5'-C4'-C3'	-2.28	107.79	112.20
8	B	2002	FAD	O4B-C1B-C2B	-2.26	103.62	106.93
8	A	2001	FAD	C5A-C6A-N1A	-2.26	115.24	120.35
8	B	2002	FAD	C5A-C6A-N6A	2.24	123.75	120.35
7	B	607	NAG	C2-N2-C7	-2.16	119.82	122.90
8	A	2001	FAD	C5A-C6A-N6A	2.13	123.58	120.35
8	A	2001	FAD	O4B-C1B-C2B	-2.10	103.85	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	2001	FAD	C4-N3-C2	-2.07	121.82	125.64
8	A	2001	FAD	C10-N1-C2	2.04	120.98	116.90
8	B	2002	FAD	C10-N1-C2	2.03	120.96	116.90
8	B	2002	FAD	C4-N3-C2	-2.01	121.92	125.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	607	NAG	O5-C5-C6-O6
7	A	607	NAG	C4-C5-C6-O6
8	A	2001	FAD	N10-C1'-C2'-O2'
8	B	2002	FAD	N10-C1'-C2'-O2'
8	A	2001	FAD	O4B-C4B-C5B-O5B
8	B	2002	FAD	O4B-C4B-C5B-O5B

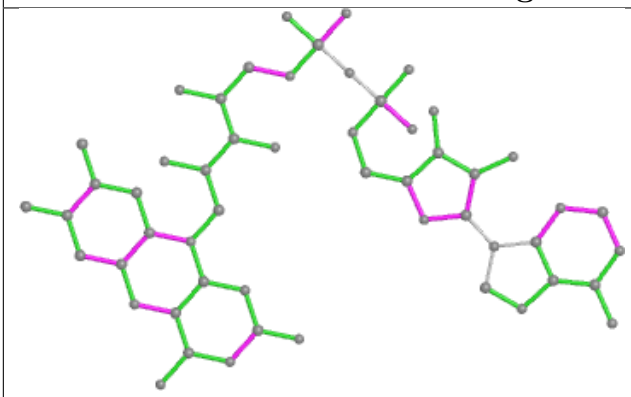
There are no ring outliers.

6 monomers are involved in 10 short contacts:

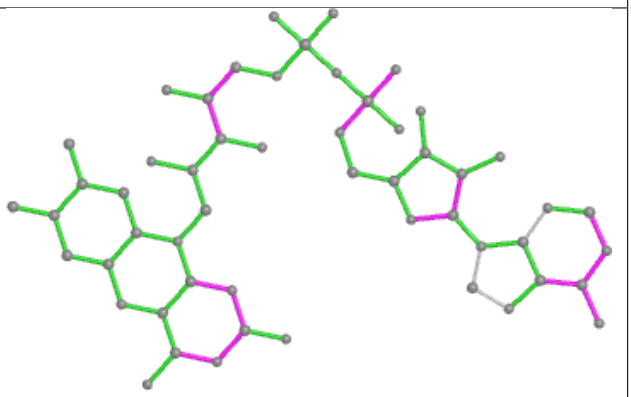
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	4001	IPA	1	0
9	B	4002	IPA	1	0
8	B	2002	FAD	2	0
7	A	607	NAG	1	0
8	A	2001	FAD	4	0
7	B	607	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

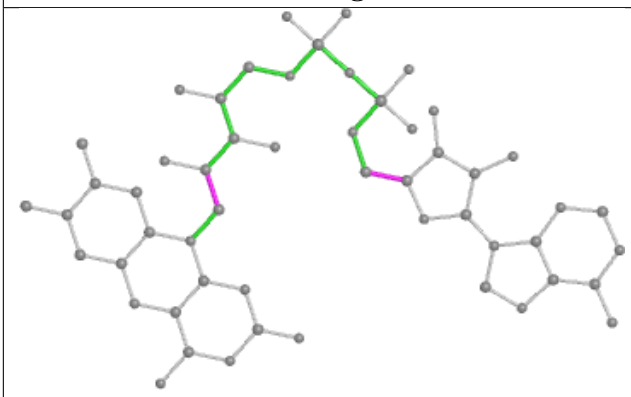
Ligand FAD B 2002



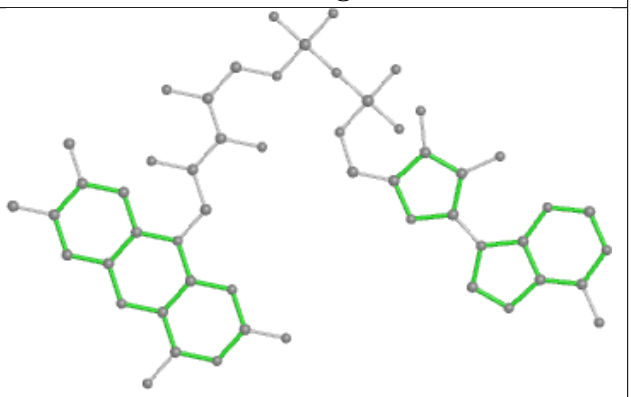
Bond lengths



Bond angles

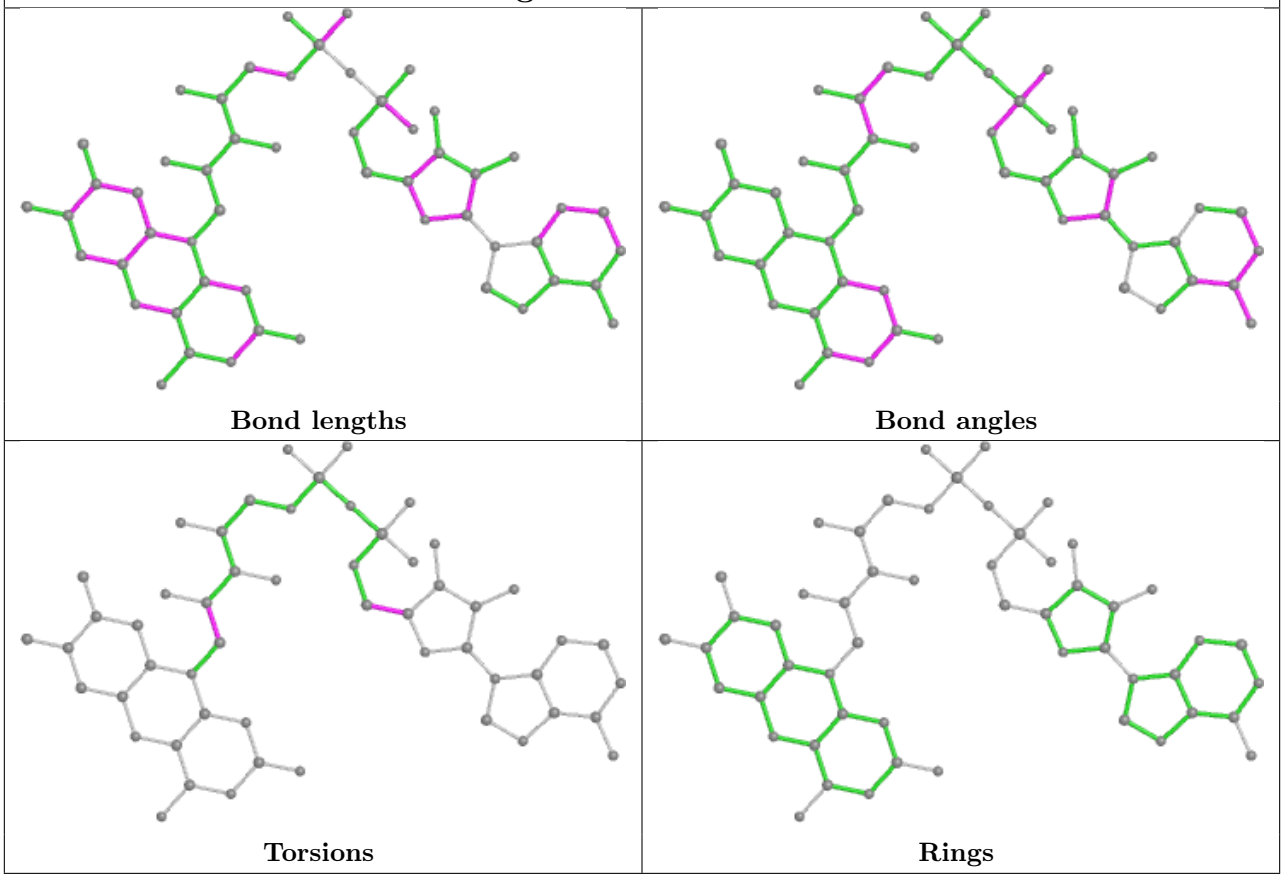


Torsions



Rings

Ligand FAD A 2001



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.