Full wwPDB X-ray Structure Validation Report (i)

Mar 16, 2022 – 02:15 PM EDT

PDB ID	:	6CK9
Title	:	Crystal Structure of HIV-1 ConC_Base0 Prefusion Env Trimer in Complex with Human Antibody Fragment 3H109L and 35O22 variants at 3.5 Angstrom
Authors	:	Lai, Y.-T.; Kwong, P.D.
Deposited on	:	2018-02-27
Resolution	:	2.71 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 following versions of software and data (see references (i)) were used in the production of this report:

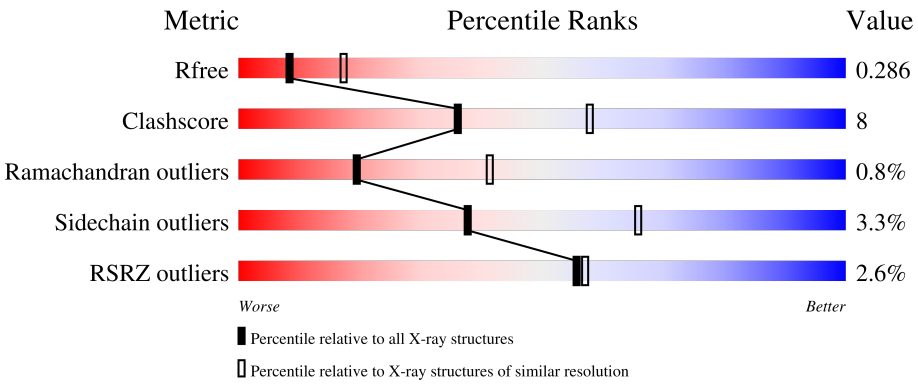
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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

Mol	Chain	Length	Quality of chain
1	B	153	.% 65% 19% 16%
2	D	134	6% 76% 17% • •
3	E	114	6% 70% 16% • 12%
4	G	463	.% 64% 27% • 7%
5	H	244	4% 74% 15% 10%

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Mol	Chain	Length	Quality of chain
6	L	217	80% 16%
7	A	5	20% 80%
8	C	6	17% 67% 17%
9	F	4	50% 50%
10	I	2	100%
10	K	2	100%
10	M	2	100%
10	O	2	100%
10	P	2	100%
11	J	2	100%
12	N	10	20% 70% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	K	2	-	-	-	X
10	NAG	O	2	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 10056 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 gp41 ectodomain of Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	129	1030	655	173	196	6	0	0	0

- Molecule 2 is a protein called 35O22 scFv heavy chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	128	994	630	168	191	5	0	0	0

- Molecule 3 is a protein called 35O22 scFv light chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	100	762	480	125	151	6	0	0	0

- Molecule 4 is a protein called gp120 of Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	430	3403	2140	597	639	27	0	0	0

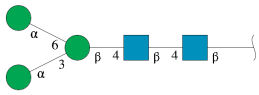
- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	H	219	1670	1065	271	328	6	0	0	0

- Molecule 6 is a protein called 3H109L Fab light chain.

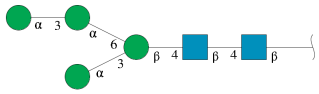
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	L	211	1604	1009	276	312	7	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	A	5	61	34	2	25	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	C	6	72	40	2	30	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

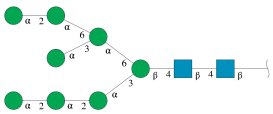
- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

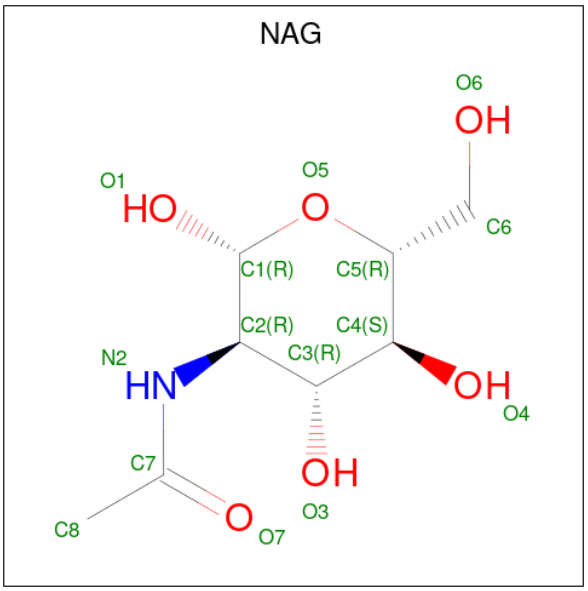
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	J	2	28	16	2	10	0	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	N	10	116	64	2	50	0	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



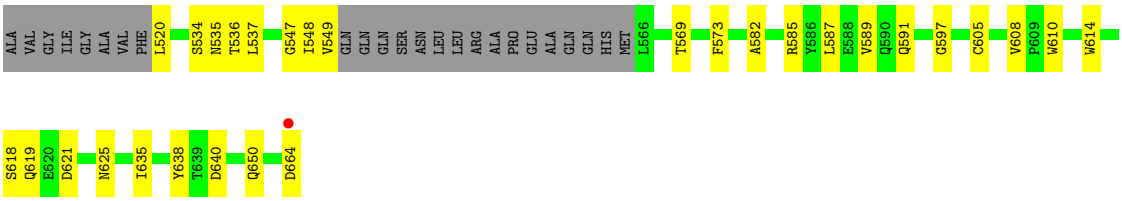
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	B	1	14	8	1	5	0	0
			Total	C	N	O		
13	B	1	14	8	1	5	0	0
			Total	C	N	O		
13	G	1	14	8	1	5	0	0
			Total	C	N	O		
13	G	1	14	8	1	5	0	0
			Total	C	N	O		
13	G	1	14	8	1	5	0	0
			Total	C	N	O		
13	G	1	14	8	1	5	0	0
			Total	C	N	O		
13	G	1	14	8	1	5	0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

3 Residue-property plots (i)

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

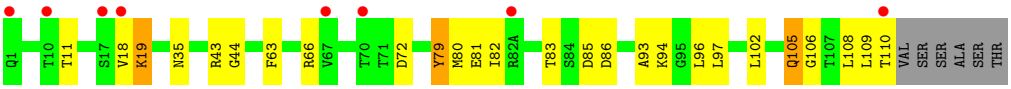
• Molecule 1: gp41 ectodomain of Envelope glycoprotein gp160

Chain B:



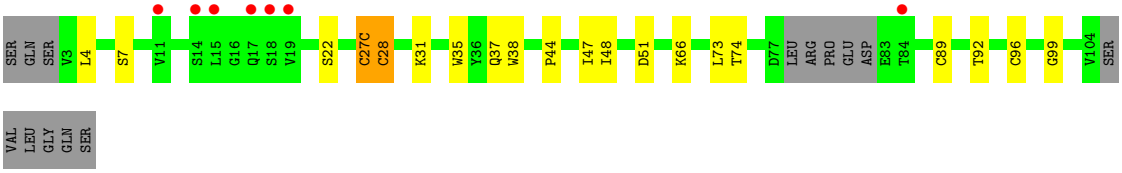
• Molecule 2: 35O22 scFv heavy chain portion

Chain D:



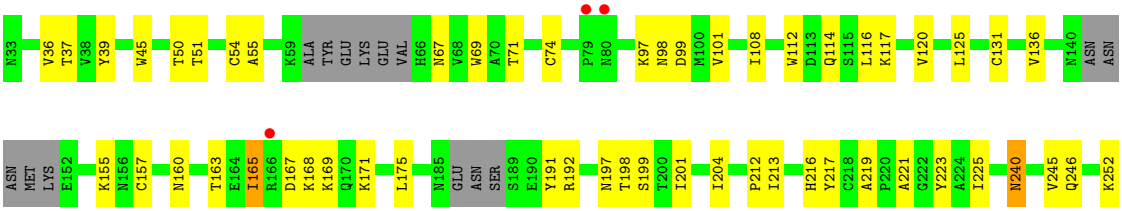
• Molecule 3: 35O22 scFv light chain portion

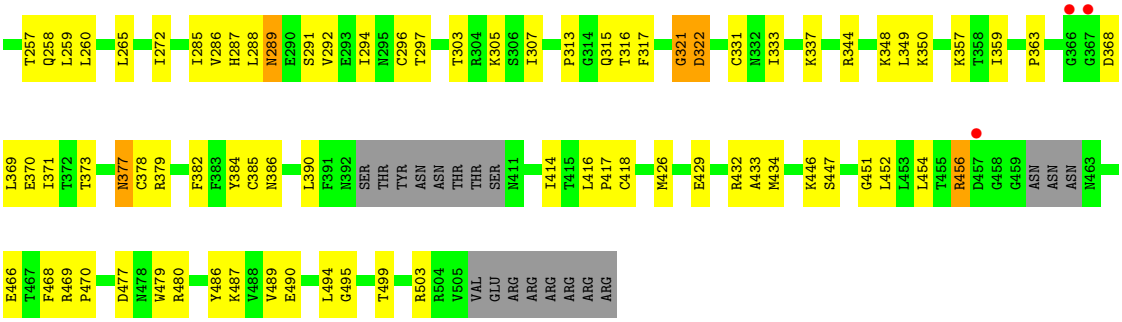
Chain E:



• Molecule 4: gp120 of Envelope glycoprotein gp160

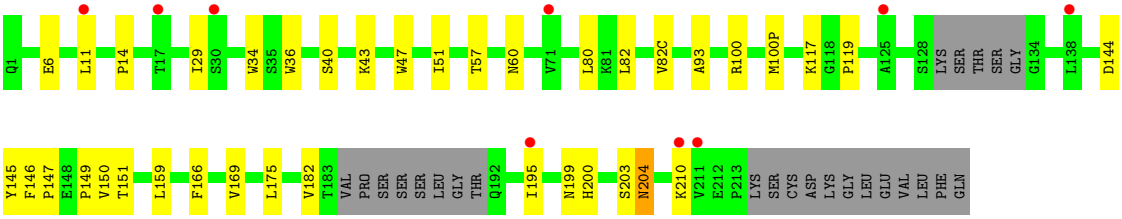
Chain G:





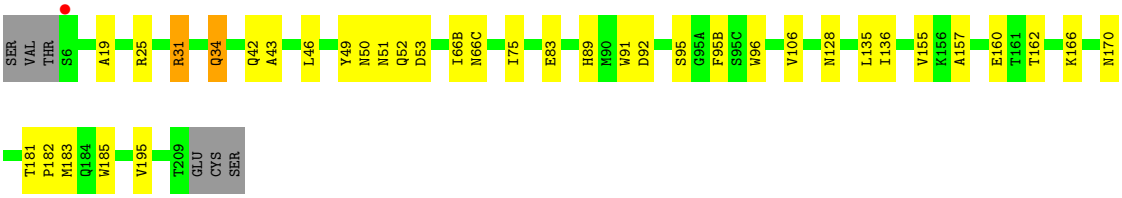
• Molecule 5: 3H109L Fab heavy chain

Chain H:



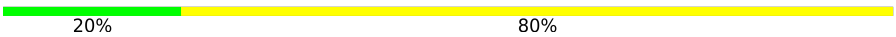
• Molecule 6: 3H109L Fab light chain

Chain L:



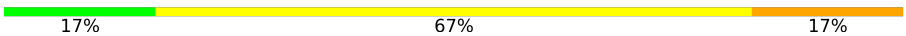
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



• Molecule 8: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%

NAG1 NAG2 BMA3 MAN4

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

NAG1 NAG2

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%

NAG1 NAG2

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%

NAG1 NAG2

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 100%

NAG1 NAG2

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 100%

NAG1 NAG2

• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%

• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	131.90Å 131.90Å 314.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.17 – 2.71 43.17 – 2.71	Depositor EDS
% Data completeness (in resolution range)	35.5 (43.17-2.71) 35.5 (43.17-2.71)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.248 , 0.288 0.248 , 0.286	Depositor DCC
R_{free} test set	1472 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 13.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.076 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	10056	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	B	0.23	0/1049	0.38	0/1423
2	D	0.24	0/1021	0.45	0/1390
3	E	0.24	0/784	0.43	0/1070
4	G	0.24	0/3471	0.44	0/4708
5	H	0.25	0/1711	0.46	0/2330
6	L	0.24	0/1647	0.44	0/2247
All	All	0.24	0/9683	0.44	0/13168

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	B	1030	0	1005	20	0
2	D	994	0	958	15	0
3	E	762	0	712	8	0
4	G	3403	0	3355	79	0
5	H	1670	0	1637	25	0
6	L	1604	0	1553	22	0
7	A	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	72	0	61	2	0
9	F	50	0	43	1	0
10	I	28	0	25	0	0
10	K	28	0	25	0	0
10	M	28	0	25	0	0
10	O	28	0	25	0	0
10	P	28	0	25	0	0
11	J	28	0	25	1	0
12	N	116	0	97	2	0
13	B	28	0	26	0	0
13	G	98	0	91	3	0
All	All	10056	0	9740	158	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 8.

All (158) 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)
4:G:378:CYS:SG	4:G:379:ARG:N	2.52	0.83
4:G:71:THR:HG21	4:G:213:ILE:HD11	1.67	0.76
4:G:169:LYS:HB2	13:G:1601:NAG:H82	1.68	0.74
6:L:46:LEU:HD21	6:L:49:TYR:HB3	1.68	0.74
2:D:35:ASN:HB2	2:D:93:ALA:HB3	1.71	0.73
4:G:101:VAL:HG13	4:G:479:TRP:HB2	1.72	0.71
6:L:50:ASN:O	6:L:52:GLN:N	2.23	0.71
5:H:169:VAL:HB	6:L:162:THR:HG22	1.72	0.70
4:G:192:ARG:NH2	4:G:197:ASN:OD1	2.25	0.70
4:G:294:ILE:HG23	4:G:447:SER:HB2	1.72	0.69
4:G:349:LEU:HB3	4:G:359:ILE:HD12	1.76	0.68
5:H:51:ILE:HG22	5:H:57:THR:HG22	1.76	0.66
5:H:203:SER:O	5:H:204:ASN:ND2	2.30	0.65
4:G:212:PRO:HB2	4:G:252:LYS:HB3	1.80	0.63
5:H:159:LEU:HD21	5:H:182:VAL:HG11	1.81	0.62
3:E:4:LEU:HB3	3:E:99:GLY:HA2	1.81	0.62
4:G:257:THR:HG22	4:G:258:GLN:HG3	1.83	0.61
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.82	0.61
1:B:605:CYS:HA	4:G:37:THR:HG22	1.83	0.61
4:G:101:VAL:HG21	4:G:480:ARG:HG2	1.84	0.60
4:G:219:ALA:O	4:G:246:GLN:NE2	2.34	0.60
4:G:165:ILE:HD11	4:G:313:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:240:ASN:N	4:G:240:ASN:OD1	2.34	0.60
4:G:454:LEU:HD23	4:G:468:PHE:HB3	1.84	0.60
4:G:54:CYS:SG	4:G:55:ALA:N	2.75	0.59
4:G:477:ASP:OD1	4:G:480:ARG:NH1	2.36	0.59
5:H:11:LEU:HB2	5:H:147:PRO:HG3	1.83	0.58
3:E:37:GLN:HB2	3:E:47:ILE:HD11	1.85	0.58
8:C:2:NAG:H3	8:C:2:NAG:H83	1.86	0.58
3:E:31:LYS:O	3:E:66:LYS:NZ	2.29	0.58
2:D:83:THR:OG1	2:D:86:ASP:OD1	2.22	0.58
4:G:303:THR:HB	4:G:322:ASP:H	1.69	0.56
2:D:96:LEU:HG	2:D:97:LEU:HG	1.87	0.56
6:L:34:GLN:HB2	6:L:89:HIS:HB3	1.88	0.56
2:D:11:THR:HG22	2:D:110:THR:H	1.71	0.55
4:G:201:ILE:HA	4:G:433:ALA:HB3	1.87	0.55
2:D:80:MET:HE3	2:D:82:ILE:HB	1.89	0.55
1:B:582:ALA:HB1	4:G:221:ALA:HB3	1.88	0.55
4:G:359:ILE:HG12	4:G:466:GLU:HB2	1.88	0.55
4:G:114:GLN:HA	4:G:117:LYS:HE2	1.88	0.54
1:B:597:GLY:HA3	4:G:503:ARG:HH12	1.72	0.54
1:B:569:THR:HA	1:B:573:PHE:HB3	1.89	0.54
4:G:363:PRO:O	4:G:469:ARG:NH1	2.38	0.54
2:D:19:LYS:HG2	2:D:81:GLU:HB2	1.89	0.54
4:G:163:THR:OG1	4:G:168:LYS:O	2.23	0.54
4:G:289:ASN:OD1	13:G:2891:NAG:N2	2.41	0.54
2:D:108:LEU:H	2:D:108:LEU:HD23	1.72	0.54
11:J:1:NAG:H83	11:J:2:NAG:H82	1.91	0.53
4:G:131:CYS:HA	4:G:157:CYS:HA	1.90	0.53
4:G:292:VAL:HG22	4:G:337:LYS:HG3	1.91	0.53
2:D:43:ARG:HG3	2:D:44:GLY:H	1.74	0.53
6:L:66(B):ILE:HG13	6:L:66(C):ASN:H	1.74	0.53
5:H:150:VAL:HG22	5:H:200:HIS:HD2	1.74	0.53
4:G:98:ASN:ND2	4:G:486:TYR:O	2.43	0.52
6:L:136:ILE:HG12	6:L:195:VAL:HG11	1.91	0.52
4:G:390:LEU:HD11	4:G:416:LEU:HD11	1.91	0.52
5:H:100(P):MET:N	5:H:100(P):MET:SD	2.83	0.52
6:L:50:ASN:O	6:L:53:ASP:N	2.31	0.52
5:H:40:SER:HB3	5:H:43:LYS:HB2	1.92	0.52
4:G:288:LEU:HD23	4:G:451:GLY:HA2	1.91	0.52
4:G:369:LEU:O	4:G:373:THR:OG1	2.28	0.51
4:G:286:VAL:HB	4:G:452:LEU:HB2	1.93	0.50
4:G:446:LYS:HB2	7:A:2:NAG:H83	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:50:THR:OG1	4:G:51:THR:N	2.45	0.50
5:H:6:GLU:N	5:H:6:GLU:OE1	2.45	0.49
4:G:116:LEU:HD21	4:G:204:ILE:HG22	1.94	0.49
2:D:94:LYS:HB3	2:D:102:LEU:HB3	1.95	0.49
5:H:82:LEU:HD22	5:H:82(C):VAL:HG12	1.93	0.49
5:H:195:ILE:HG12	5:H:210:LYS:HG2	1.94	0.48
1:B:589:VAL:HG13	4:G:494:LEU:HG	1.95	0.48
1:B:635:ILE:O	1:B:638:TYR:N	2.45	0.48
1:B:597:GLY:N	1:B:650:GLN:HG3	2.28	0.48
4:G:155:LYS:NZ	4:G:191:TYR:OH	2.43	0.48
5:H:117:LYS:HD3	5:H:175:LEU:HD21	1.96	0.48
3:E:7:SER:HB3	3:E:22:SER:H	1.78	0.48
4:G:260:LEU:HD12	4:G:451:GLY:HA3	1.96	0.47
4:G:258:GLN:NE2	4:G:371:ILE:O	2.47	0.47
1:B:520:LEU:HD11	1:B:536:THR:HB	1.96	0.47
5:H:166:PHE:CE1	6:L:135:LEU:HD23	2.49	0.47
2:D:18:VAL:HG11	2:D:109:LEU:HD11	1.96	0.47
6:L:83:GLU:HB2	6:L:106:VAL:HG23	1.97	0.47
8:C:1:NAG:H61	8:C:2:NAG:C7	2.44	0.47
5:H:14:PRO:HA	5:H:82(C):VAL:HG23	1.95	0.47
6:L:34:GLN:HG3	6:L:49:TYR:HA	1.96	0.47
1:B:587:LEU:O	1:B:591:GLN:N	2.47	0.47
2:D:83:THR:OG1	2:D:85:ASP:OD1	2.22	0.47
6:L:31:ARG:HA	6:L:92:ASP:HA	1.96	0.47
6:L:128:ASN:HA	6:L:182:PRO:HG2	1.97	0.47
3:E:47:ILE:HG22	3:E:48:ILE:HG13	1.97	0.46
4:G:370:GLU:HG3	4:G:384:TYR:HE2	1.80	0.46
6:L:42:GLN:HG2	6:L:43:ALA:H	1.79	0.46
6:L:92:ASP:OD1	6:L:95:SER:N	2.40	0.46
6:L:155:VAL:HG12	6:L:157:ALA:H	1.79	0.46
5:H:47:TRP:HZ3	6:L:91:TRP:HZ2	1.64	0.46
6:L:66(B):ILE:O	12:N:4:MAN:O4	2.28	0.46
4:G:39:TYR:O	4:G:495:GLY:N	2.44	0.46
4:G:120:VAL:HG13	4:G:315:GLN:HG3	1.98	0.46
4:G:344:ARG:HD2	13:G:2891:NAG:H5	1.98	0.46
6:L:181:THR:HG22	6:L:183:MET:H	1.81	0.46
1:B:618:SER:HB3	1:B:621:ASP:HB2	1.98	0.45
4:G:385:CYS:HA	4:G:418:CYS:HA	1.97	0.45
4:G:160:ASN:OD1	4:G:171:LYS:HD2	2.16	0.45
4:G:258:GLN:HG2	4:G:470:PRO:HB2	1.98	0.45
3:E:38:TRP:CG	3:E:44:PRO:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:11:LEU:HD22	5:H:147:PRO:HD3	1.98	0.45
2:D:105:GLN:HE21	2:D:106:GLY:N	2.15	0.45
4:G:97:LYS:HD3	4:G:97:LYS:HA	1.80	0.45
1:B:547:GLY:O	1:B:549:VAL:N	2.49	0.45
4:G:198:THR:OG1	4:G:199:SER:N	2.50	0.45
5:H:36:TRP:CD2	5:H:80:LEU:HD23	2.52	0.44
4:G:71:THR:HA	4:G:74:CYS:SG	2.57	0.44
4:G:456:ARG:HD2	4:G:468:PHE:HE1	1.82	0.44
4:G:69:TRP:HZ3	4:G:108:ILE:HG23	1.83	0.44
4:G:175:LEU:HD11	9:F:1:NAG:H82	2.00	0.44
5:H:93:ALA:HB1	5:H:100(P):MET:HB3	2.00	0.43
1:B:534:SER:HA	1:B:537:LEU:HD23	2.00	0.43
4:G:223:TYR:HA	4:G:490:GLU:HA	2.00	0.43
4:G:265:LEU:HD21	4:G:291:SER:HB3	2.01	0.43
5:H:100:ARG:NH1	6:L:31:ARG:O	2.52	0.43
1:B:610:TRP:HE3	4:G:36:VAL:HG12	1.83	0.43
4:G:98:ASN:OD1	4:G:99:ASP:N	2.52	0.43
2:D:72:ASP:OD2	2:D:79:TYR:OH	2.36	0.43
4:G:116:LEU:HD11	4:G:434:MET:HG2	1.99	0.43
3:E:27(C):CYS:HA	3:E:28:CYS:HA	1.67	0.43
3:E:35:TRP:CE2	3:E:73:LEU:HB2	2.53	0.43
5:H:151:THR:OG1	5:H:199:ASN:HB3	2.19	0.43
4:G:386:ASN:HB3	4:G:417:PRO:HG2	2.00	0.43
6:L:166:LYS:HE2	6:L:170:ASN:HA	2.01	0.43
4:G:45:TRP:HB2	4:G:489:VAL:HB	2.01	0.43
5:H:146:PHE:HA	5:H:147:PRO:HA	1.80	0.42
4:G:285:ILE:HD11	4:G:477:ASP:HB3	2.00	0.42
1:B:664:ASP:N	1:B:664:ASP:OD1	2.53	0.42
4:G:307:ILE:HD11	4:G:317:PHE:HD2	1.84	0.42
1:B:614:TRP:HA	1:B:638:TYR:CD2	2.55	0.42
1:B:597:GLY:HA3	4:G:503:ARG:HH22	1.85	0.42
5:H:29:ILE:HG13	5:H:34:TRP:NE1	2.35	0.42
5:H:60:ASN:ND2	6:L:96:TRP:HB3	2.35	0.42
1:B:640:ASP:OD1	1:B:640:ASP:N	2.49	0.42
4:G:272:ILE:HD11	4:G:348:LYS:HB3	2.01	0.42
1:B:608:VAL:HB	4:G:36:VAL:HG22	2.02	0.41
4:G:305:LYS:HG3	4:G:321:GLY:HA2	2.02	0.41
4:G:429:GLU:HB2	4:G:432:ARG:HB3	2.02	0.41
4:G:257:THR:C	4:G:259:LEU:H	2.23	0.41
2:D:19:LYS:HA	2:D:80:MET:O	2.21	0.41
6:L:19:ALA:HB3	6:L:75:ILE:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:PHE:HE1	2:D:66:ARG:HH21	1.68	0.41
5:H:119:PRO:HB3	5:H:145:TYR:HB3	2.02	0.41
1:B:619:GLN:HE22	4:G:499:THR:HA	1.86	0.41
4:G:377:ASN:HB2	4:G:382:PHE:HD1	1.86	0.41
4:G:167:ASP:HB3	4:G:168:LYS:H	1.52	0.41
4:G:223:TYR:CE2	4:G:490:GLU:HB3	2.55	0.41
4:G:333:ILE:O	4:G:414:ILE:HG22	2.21	0.41
5:H:100:ARG:HA	5:H:100:ARG:HD2	1.94	0.41
4:G:487:LYS:HE3	4:G:487:LYS:HB2	1.95	0.41
4:G:225:ILE:HG13	4:G:245:VAL:HG23	2.04	0.40
1:B:610:TRP:CE3	4:G:36:VAL:HG12	2.57	0.40
4:G:265:LEU:HD11	4:G:291:SER:HB3	2.02	0.40
4:G:297:THR:HG21	12:N:1:NAG:H81	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	125/153 (82%)	114 (91%)	9 (7%)	2 (2%)	9 23
2	D	126/134 (94%)	110 (87%)	16 (13%)	0	100 100
3	E	96/114 (84%)	82 (85%)	13 (14%)	1 (1%)	15 35
4	G	418/463 (90%)	359 (86%)	57 (14%)	2 (0%)	29 53
5	H	213/244 (87%)	194 (91%)	17 (8%)	2 (1%)	17 38
6	L	209/217 (96%)	191 (91%)	16 (8%)	2 (1%)	15 35
All	All	1187/1325 (90%)	1050 (88%)	128 (11%)	9 (1%)	19 41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	51	ASN
6	L	25	ARG
5	H	144	ASP
1	B	548	ILE
1	B	625	ASN
3	E	51	ASP
4	G	165	ILE
4	G	321	GLY
5	H	149	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	111/129 (86%)	109 (98%)	2 (2%)	59	82
2	D	107/112 (96%)	104 (97%)	3 (3%)	43	71
3	E	87/100 (87%)	81 (93%)	6 (7%)	15	34
4	G	389/421 (92%)	371 (95%)	18 (5%)	27	52
5	H	190/212 (90%)	189 (100%)	1 (0%)	88	95
6	L	175/181 (97%)	170 (97%)	5 (3%)	42	70
All	All	1059/1155 (92%)	1024 (97%)	35 (3%)	38	66

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	535	ASN
1	B	585	ARG
2	D	19	LYS
2	D	79	TYR
2	D	105	GLN
3	E	27(C)	CYS
3	E	28	CYS
3	E	74	THR
3	E	89	CYS
3	E	92	THR

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Mol	Chain	Res	Type
3	E	96	CYS
4	G	67	ASN
4	G	112	TRP
4	G	125	LEU
4	G	136	VAL
4	G	217	TYR
4	G	240	ASN
4	G	287	HIS
4	G	289	ASN
4	G	296	CYS
4	G	316	THR
4	G	322	ASP
4	G	331	CYS
4	G	350	LYS
4	G	357	LYS
4	G	368	ASP
4	G	377	ASN
4	G	426	MET
4	G	456	ARG
5	H	204	ASN
6	L	31	ARG
6	L	34	GLN
6	L	95(B)	PHE
6	L	160	GLU
6	L	185	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

37 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	$\#\|Z\| > 2$
7	NAG	A	1	4,7	14,14,15	0.98	1 (7%)	17,19,21	1.96	3 (17%)
7	NAG	A	2	7	14,14,15	0.28	0	17,19,21	0.53	0
7	BMA	A	3	7	11,11,12	0.67	0	15,15,17	0.94	0
7	MAN	A	4	7	11,11,12	0.73	0	15,15,17	0.90	1 (6%)
7	MAN	A	5	7	11,11,12	0.68	0	15,15,17	1.10	2 (13%)
8	NAG	C	1	4,8	14,14,15	0.32	0	17,19,21	0.43	0
8	NAG	C	2	8	14,14,15	0.45	0	17,19,21	1.27	1 (5%)
8	BMA	C	3	8	11,11,12	0.59	0	15,15,17	0.75	0
8	MAN	C	4	8	11,11,12	0.58	0	15,15,17	1.15	2 (13%)
8	MAN	C	5	8	11,11,12	0.75	0	15,15,17	1.28	2 (13%)
8	MAN	C	6	8	11,11,12	0.73	0	15,15,17	1.00	2 (13%)
9	NAG	F	1	4,9	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	F	2	9	14,14,15	0.26	0	17,19,21	0.41	0
9	BMA	F	3	9	11,11,12	0.62	0	15,15,17	0.88	0
9	MAN	F	4	9	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
10	NAG	I	1	4,10	14,14,15	0.36	0	17,19,21	0.54	0
10	NAG	I	2	10	14,14,15	0.29	0	17,19,21	0.35	0
11	NAG	J	1	4,11	14,14,15	0.39	0	17,19,21	0.45	0
11	NAG	J	2	11	14,14,15	0.27	0	17,19,21	0.53	0
10	NAG	K	1	4,10	14,14,15	0.23	0	17,19,21	0.41	0
10	NAG	K	2	10	14,14,15	0.29	0	17,19,21	0.47	0
10	NAG	M	1	4,10	14,14,15	0.22	0	17,19,21	0.38	0
10	NAG	M	2	10	14,14,15	0.24	0	17,19,21	0.45	0
12	NAG	N	1	4,12	14,14,15	0.30	0	17,19,21	0.59	0
12	MAN	N	10	12	11,11,12	0.71	0	15,15,17	0.97	2 (13%)
12	NAG	N	2	12	14,14,15	0.22	0	17,19,21	0.42	0
12	BMA	N	3	12	11,11,12	0.73	0	15,15,17	1.04	0
12	MAN	N	4	12	11,11,12	0.76	1 (9%)	15,15,17	1.32	2 (13%)
12	MAN	N	5	12	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
12	MAN	N	6	12	11,11,12	1.09	2 (18%)	15,15,17	2.11	5 (33%)
12	MAN	N	7	12	11,11,12	1.13	0	15,15,17	1.33	3 (20%)
12	MAN	N	8	12	11,11,12	0.92	1 (9%)	15,15,17	1.21	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	MAN	N	9	12	11,11,12	0.90	1 (9%)	15,15,17	1.42	2 (13%)
10	NAG	O	1	4,10	14,14,15	0.33	0	17,19,21	0.47	0
10	NAG	O	2	10	14,14,15	0.20	0	17,19,21	0.46	0
10	NAG	P	1	4,10	14,14,15	0.28	0	17,19,21	0.48	0
10	NAG	P	2	10	14,14,15	0.27	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	4,7	-	5/6/23/26	0/1/1/1
7	NAG	A	2	7	-	1/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	1/2/19/22	0/1/1/1
8	NAG	C	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	5/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
8	MAN	C	4	8	-	0/2/19/22	0/1/1/1
8	MAN	C	5	8	-	2/2/19/22	1/1/1/1
8	MAN	C	6	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	4,9	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	2/2/19/22	0/1/1/1
9	MAN	F	4	9	-	1/2/19/22	0/1/1/1
10	NAG	I	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	I	2	10	-	0/6/23/26	0/1/1/1
11	NAG	J	1	4,11	-	2/6/23/26	0/1/1/1
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1
10	NAG	K	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
10	NAG	M	1	4,10	-	0/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
12	NAG	N	1	4,12	-	3/6/23/26	0/1/1/1
12	MAN	N	10	12	-	0/2/19/22	0/1/1/1
12	NAG	N	2	12	-	2/6/23/26	0/1/1/1
12	BMA	N	3	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	N	4	12	-	2/2/19/22	0/1/1/1
12	MAN	N	5	12	-	2/2/19/22	0/1/1/1
12	MAN	N	6	12	-	0/2/19/22	0/1/1/1
12	MAN	N	7	12	-	1/2/19/22	0/1/1/1
12	MAN	N	8	12	-	0/2/19/22	0/1/1/1
12	MAN	N	9	12	-	0/2/19/22	0/1/1/1
10	NAG	O	1	4,10	-	1/6/23/26	0/1/1/1
10	NAG	O	2	10	-	0/6/23/26	0/1/1/1
10	NAG	P	1	4,10	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1	NAG	O5-C1	3.46	1.49	1.43
12	N	9	MAN	C1-C2	2.75	1.58	1.52
12	N	6	MAN	C1-C2	2.39	1.57	1.52
12	N	4	MAN	C1-C2	2.27	1.57	1.52
12	N	6	MAN	C2-C3	2.17	1.55	1.52
12	N	8	MAN	C1-C2	2.02	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1	NAG	C1-O5-C5	5.89	120.17	112.19
12	N	6	MAN	C1-C2-C3	4.53	115.24	109.67
7	A	1	NAG	C2-N2-C7	4.41	129.18	122.90
8	C	2	NAG	C2-N2-C7	4.29	129.01	122.90
12	N	6	MAN	C1-O5-C5	4.15	117.82	112.19
12	N	9	MAN	C1-O5-C5	4.00	117.61	112.19
8	C	5	MAN	C1-O5-C5	3.90	117.48	112.19
12	N	4	MAN	C1-O5-C5	3.48	116.91	112.19
12	N	8	MAN	C1-O5-C5	3.48	116.90	112.19
12	N	6	MAN	O5-C1-C2	2.97	115.36	110.77
12	N	6	MAN	O2-C2-C3	-2.86	104.42	110.14
7	A	5	MAN	C1-O5-C5	2.71	115.86	112.19
8	C	4	MAN	C1-O5-C5	2.71	115.86	112.19
12	N	5	MAN	O2-C2-C3	-2.62	104.89	110.14
12	N	7	MAN	O3-C3-C4	2.52	116.16	110.35
9	F	4	MAN	C1-O5-C5	2.41	115.46	112.19
12	N	6	MAN	C2-C3-C4	2.34	114.94	110.89
12	N	10	MAN	O2-C2-C3	-2.33	105.47	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	6	MAN	C1-O5-C5	2.33	115.35	112.19
12	N	5	MAN	C1-O5-C5	2.32	115.34	112.19
12	N	7	MAN	O3-C3-C2	2.31	114.41	109.99
8	C	4	MAN	O2-C2-C3	-2.29	105.56	110.14
9	F	4	MAN	O2-C2-C3	-2.22	105.70	110.14
7	A	1	NAG	C1-C2-N2	2.21	114.27	110.49
12	N	7	MAN	C3-C4-C5	-2.21	106.30	110.24
12	N	9	MAN	O2-C2-C3	-2.21	105.72	110.14
7	A	5	MAN	O2-C2-C3	-2.20	105.73	110.14
7	A	4	MAN	O2-C2-C3	-2.20	105.73	110.14
12	N	4	MAN	O2-C2-C3	-2.17	105.79	110.14
8	C	5	MAN	O2-C2-C3	-2.16	105.80	110.14
12	N	10	MAN	C1-O5-C5	2.16	115.12	112.19
12	N	8	MAN	O3-C3-C2	2.13	114.07	109.99
8	C	6	MAN	O2-C2-C3	-2.10	105.93	110.14

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	3	BMA	O5-C5-C6-O6
8	C	5	MAN	O5-C5-C6-O6
9	F	3	BMA	C4-C5-C6-O6
10	K	1	NAG	O5-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
8	C	2	NAG	O5-C5-C6-O6
10	I	1	NAG	O5-C5-C6-O6
8	C	3	BMA	C4-C5-C6-O6
9	F	3	BMA	O5-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6
12	N	2	NAG	O5-C5-C6-O6
8	C	5	MAN	C4-C5-C6-O6
12	N	2	NAG	C4-C5-C6-O6
7	A	1	NAG	C8-C7-N2-C2
7	A	1	NAG	O7-C7-N2-C2
8	C	2	NAG	C8-C7-N2-C2
8	C	2	NAG	O7-C7-N2-C2
10	M	2	NAG	O5-C5-C6-O6
8	C	2	NAG	C4-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
11	J	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	N	4	MAN	O5-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
10	M	2	NAG	C4-C5-C6-O6
7	A	5	MAN	O5-C5-C6-O6
12	N	4	MAN	C4-C5-C6-O6
10	I	1	NAG	C4-C5-C6-O6
11	J	1	NAG	O5-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
9	F	4	MAN	O5-C5-C6-O6
12	N	5	MAN	O5-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
12	N	5	MAN	C4-C5-C6-O6
12	N	1	NAG	C4-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
10	O	1	NAG	O5-C5-C6-O6
12	N	1	NAG	O5-C5-C6-O6
7	A	1	NAG	C3-C2-N2-C7
7	A	2	NAG	C3-C2-N2-C7
12	N	7	MAN	C4-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
11	J	1	NAG	C4-C5-C6-O6
8	C	2	NAG	C3-C2-N2-C7
12	N	1	NAG	C3-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	5	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	1	NAG	1	0
12	N	1	NAG	1	0
8	C	1	NAG	1	0
11	J	1	NAG	1	0
12	N	4	MAN	1	0
8	C	2	NAG	2	0
7	A	2	NAG	1	0

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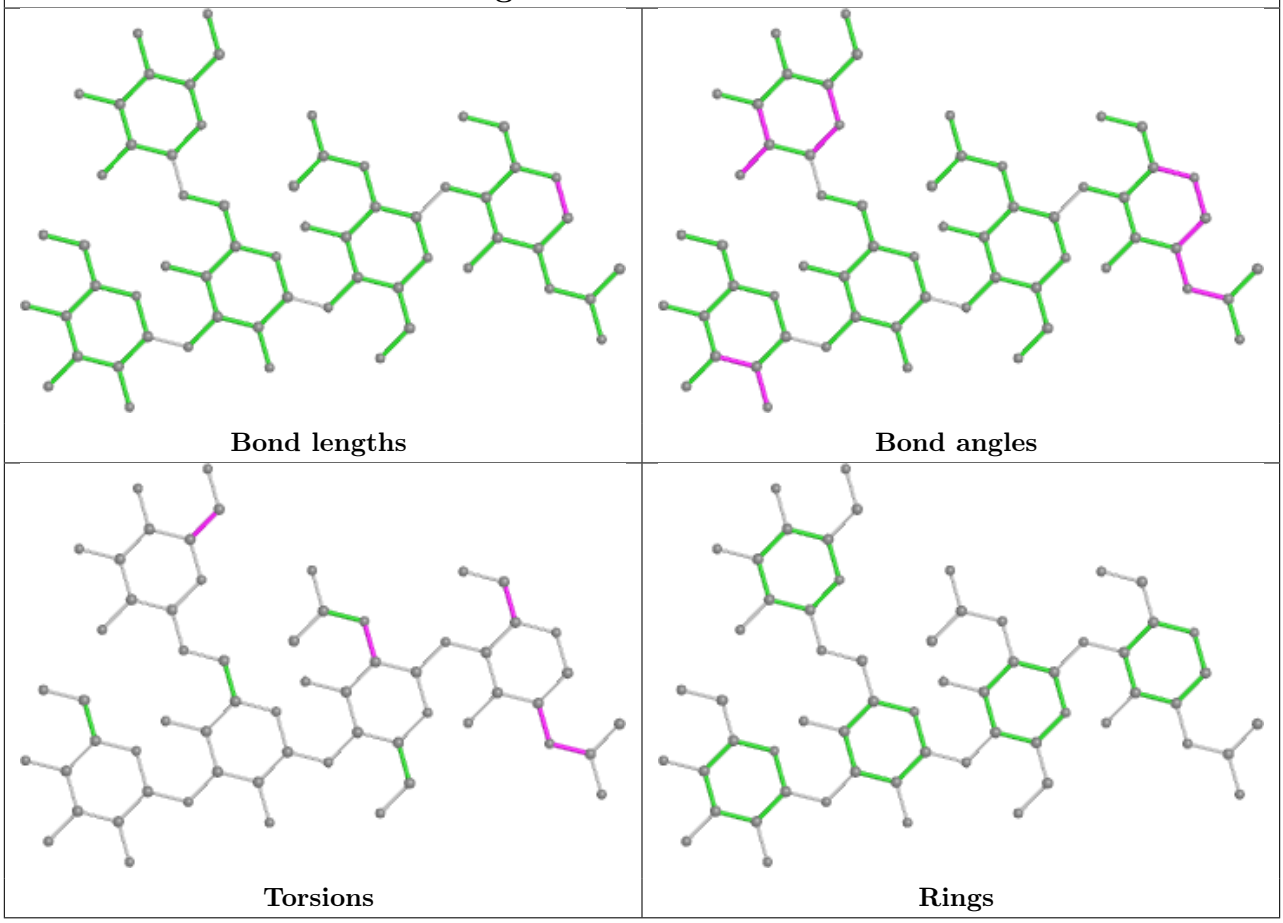
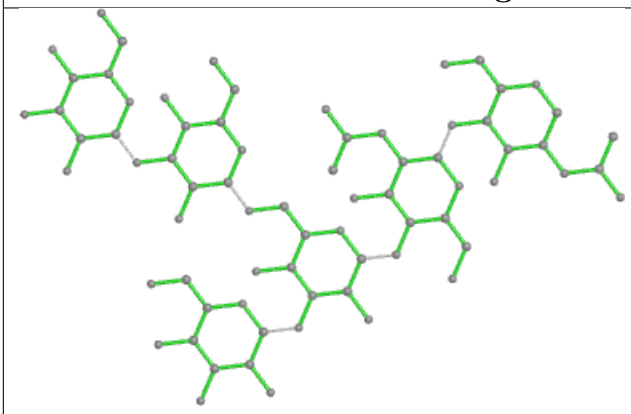
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	J	2	NAG	1	0

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

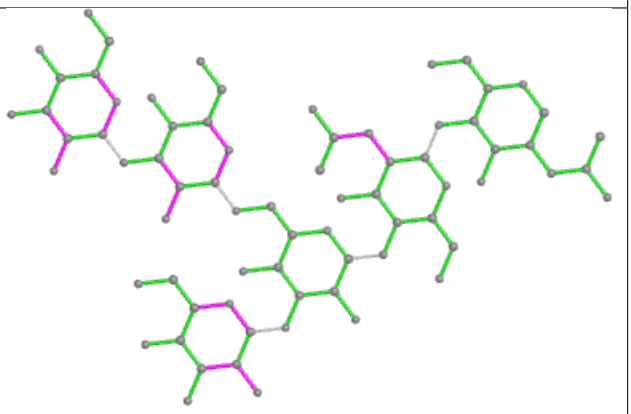
Oligosaccharide Chain A



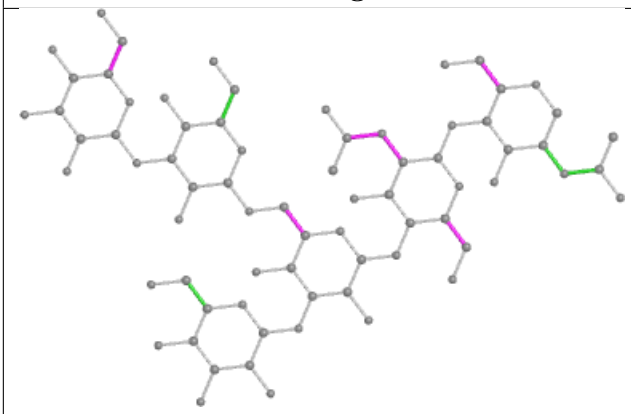
Oligosaccharide Chain C



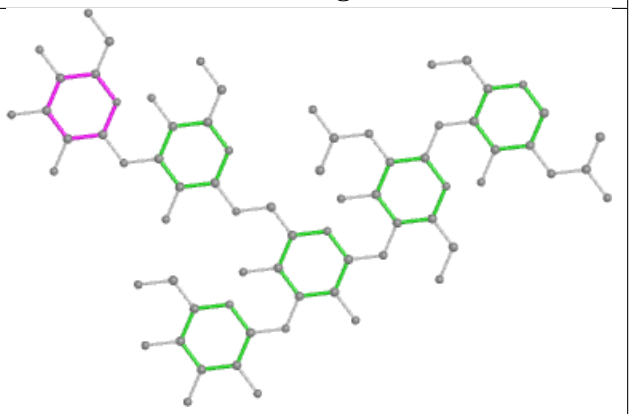
Bond lengths



Bond angles

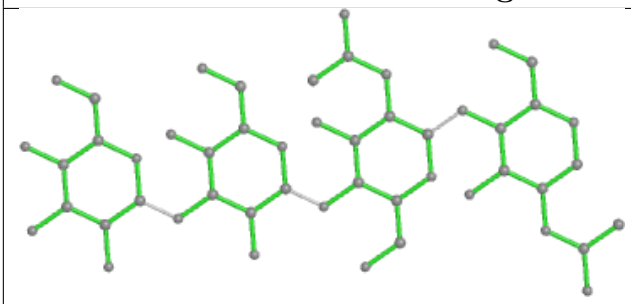


Torsions

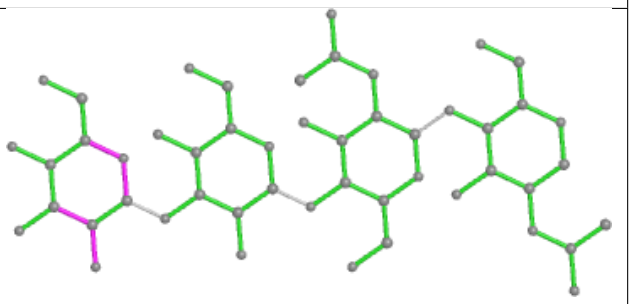


Rings

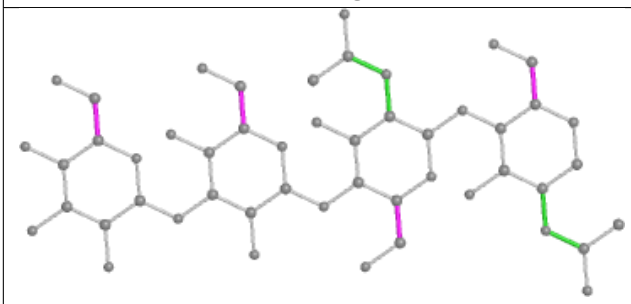
Oligosaccharide Chain F



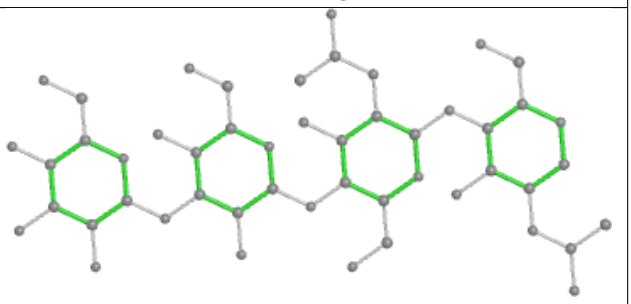
Bond lengths



Bond angles

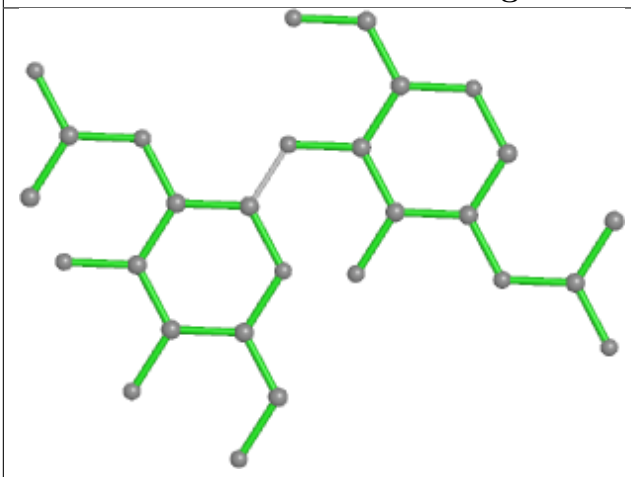


Torsions

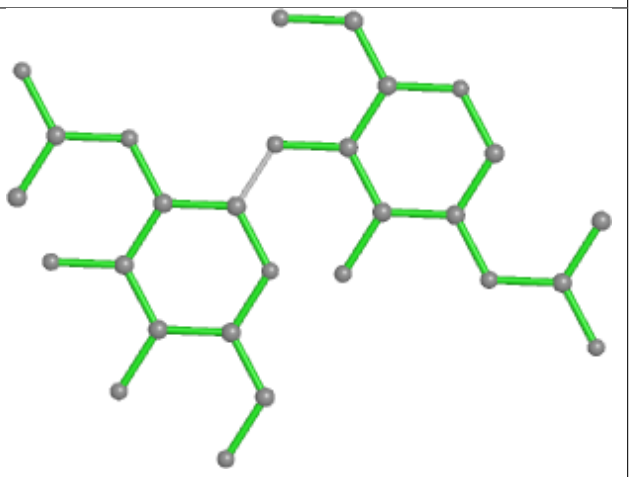


Rings

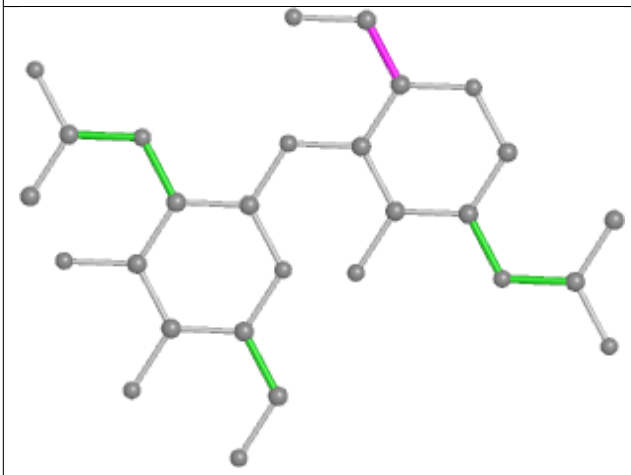
Oligosaccharide Chain I



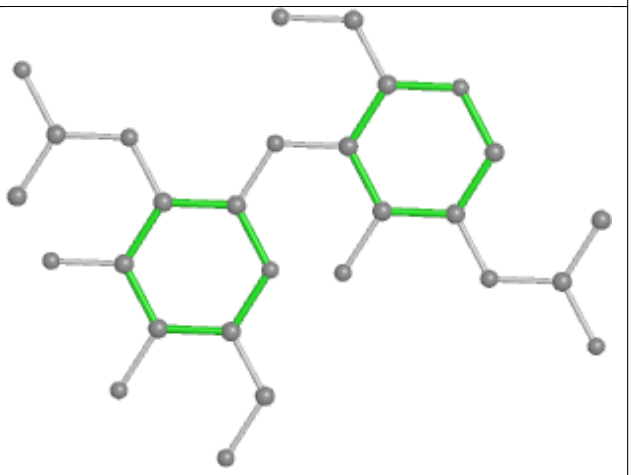
Bond lengths



Bond angles

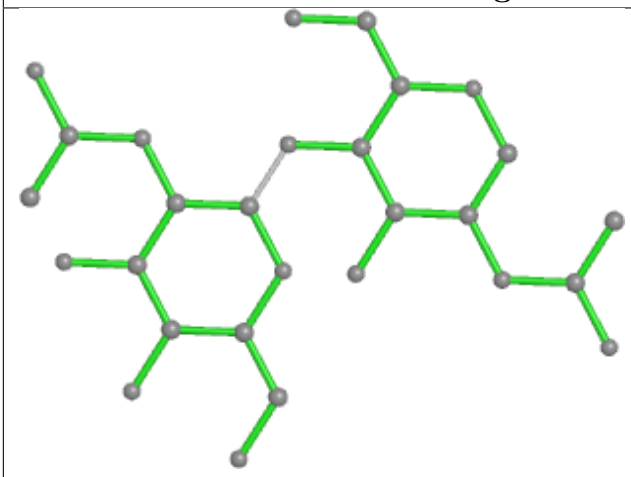


Torsions

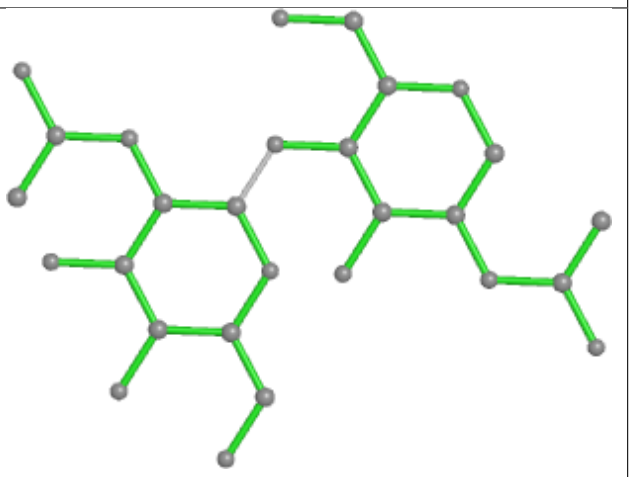


Rings

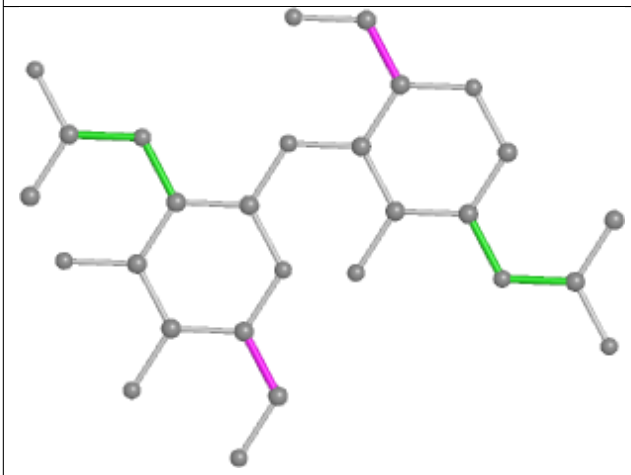
Oligosaccharide Chain K



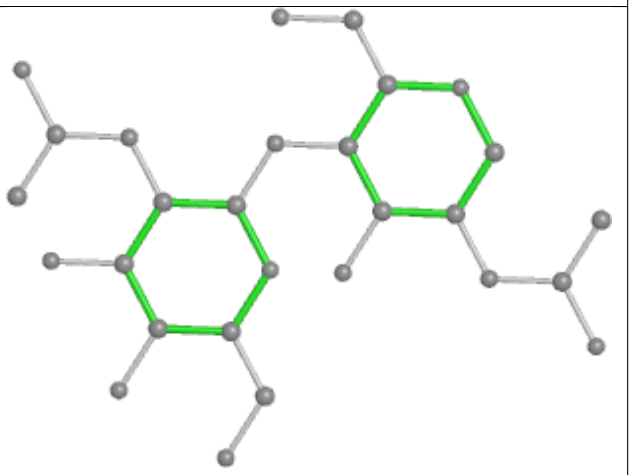
Bond lengths



Bond angles

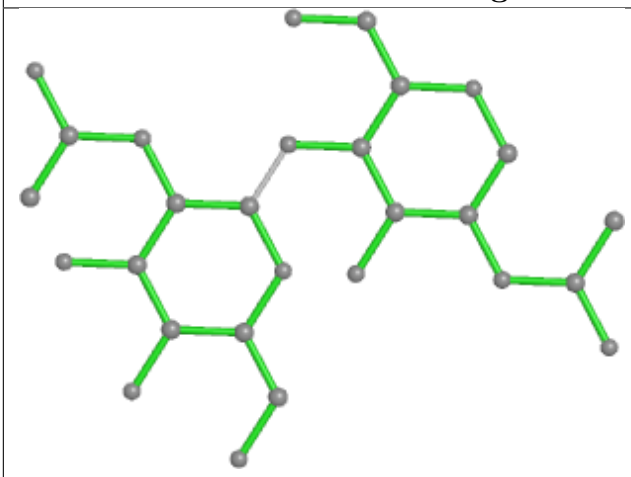


Torsions

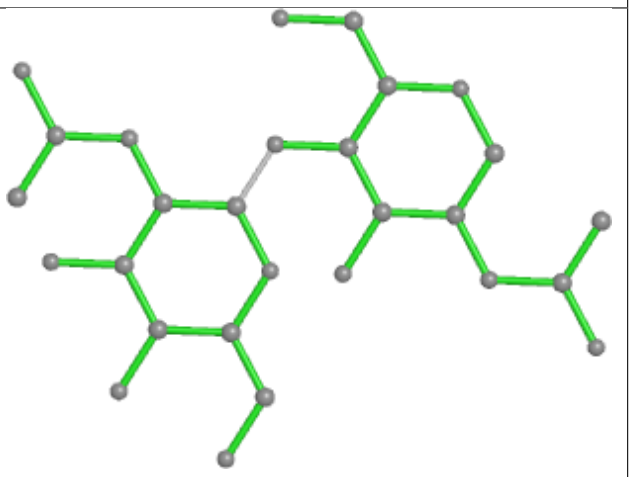


Rings

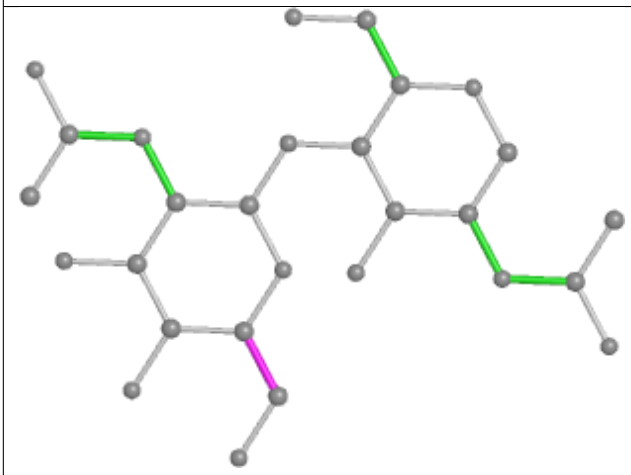
Oligosaccharide Chain M



Bond lengths



Bond angles



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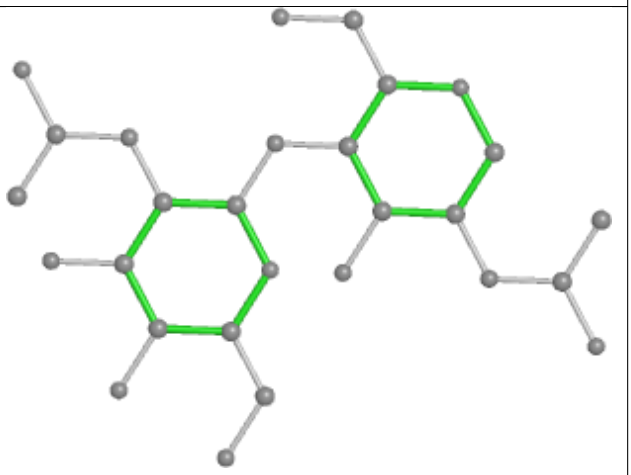
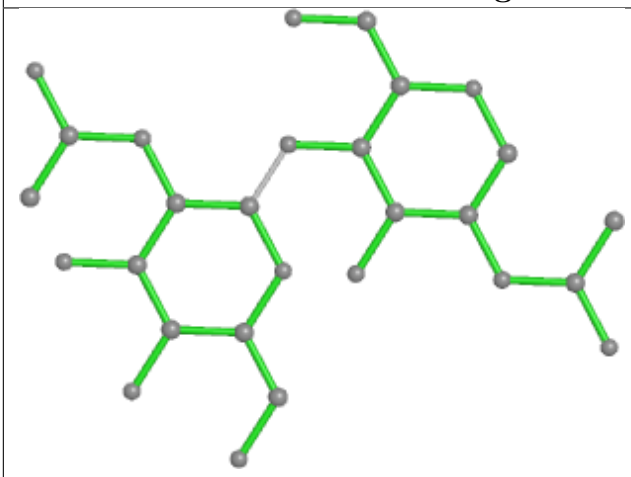
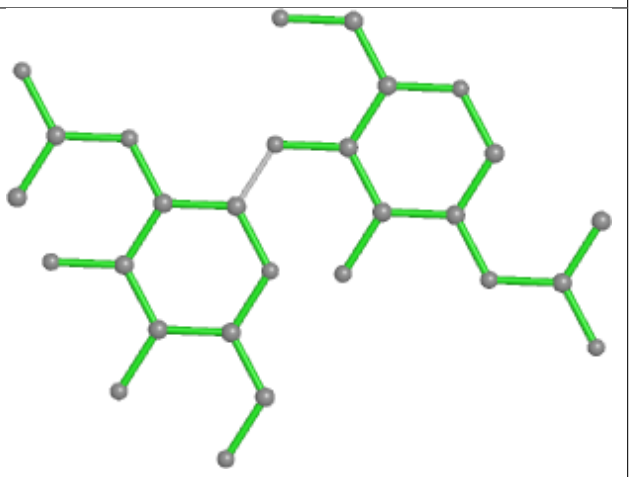


Rings

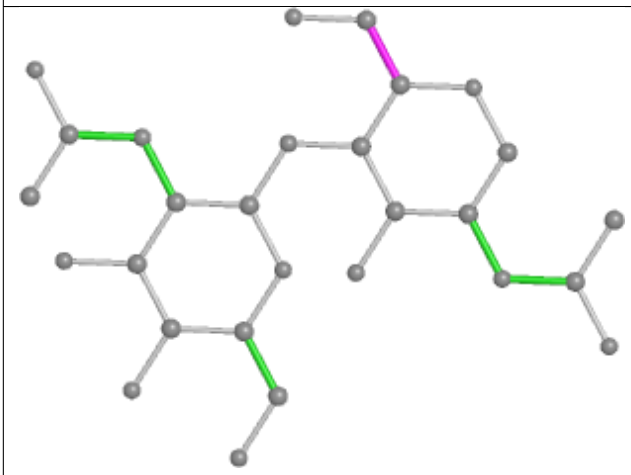
Oligosaccharide Chain O



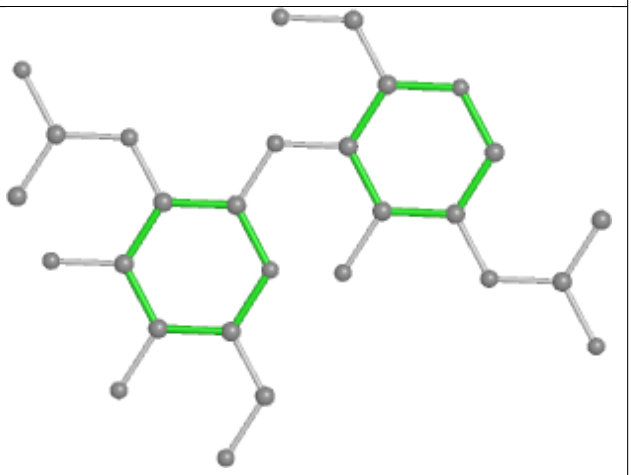
Bond lengths



Bond angles

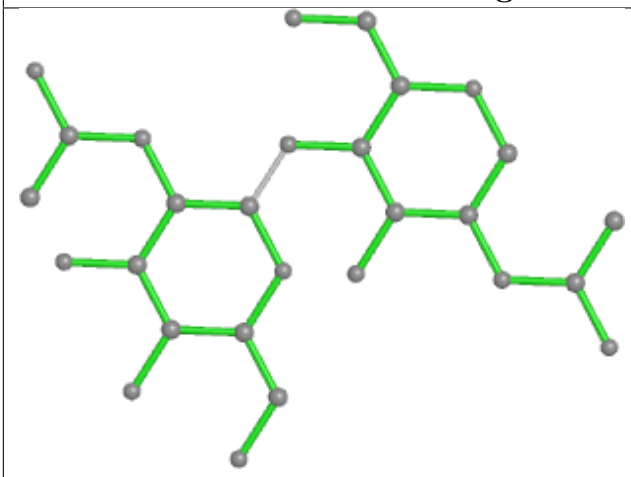


Torsions

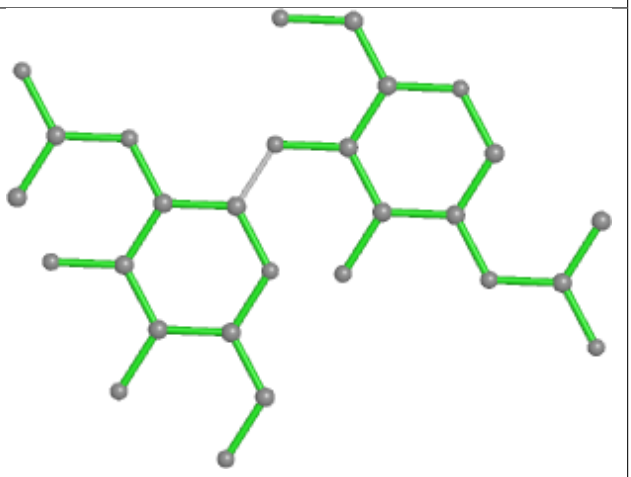


Rings

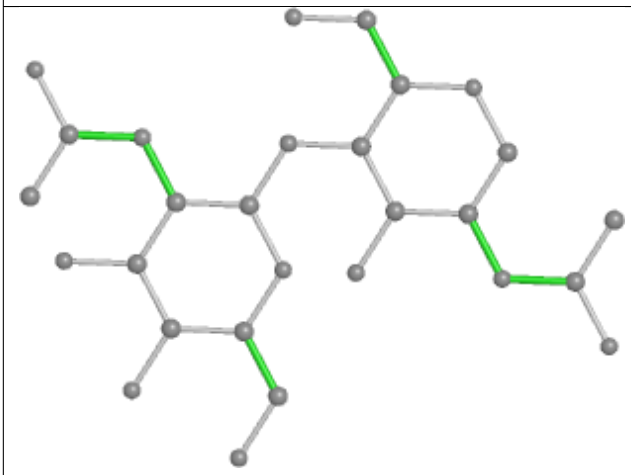
Oligosaccharide Chain P



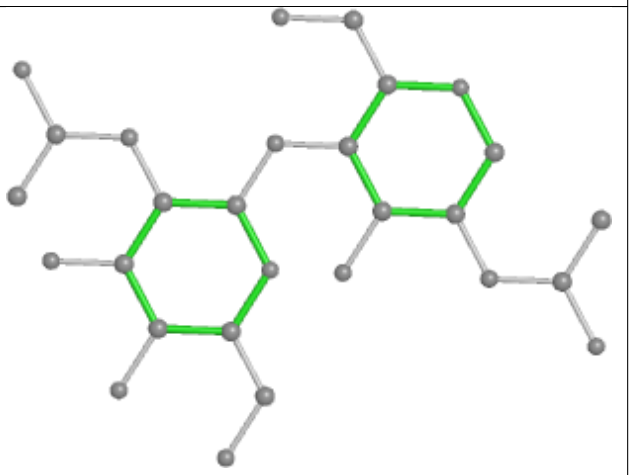
Bond lengths



Bond angles

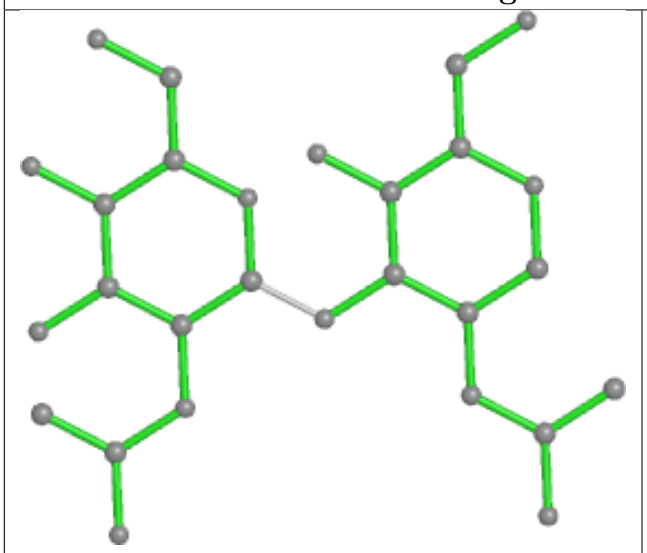


Torsions

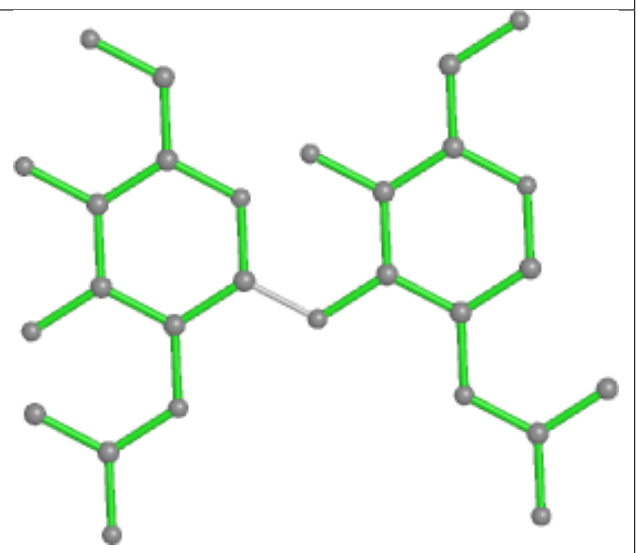


Rings

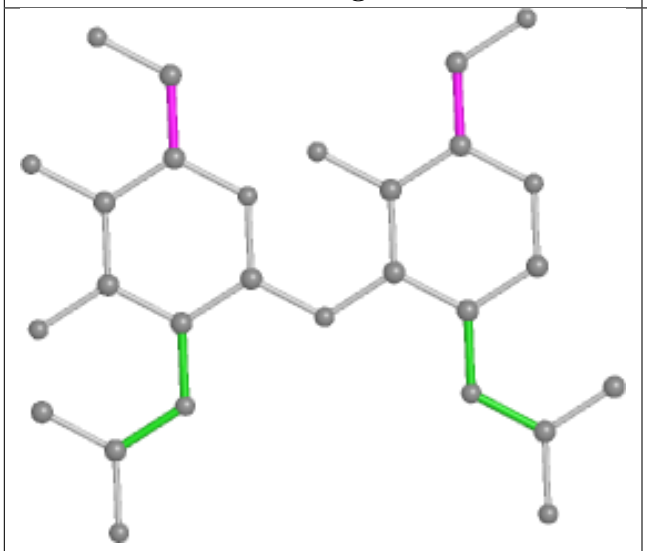
Oligosaccharide Chain J



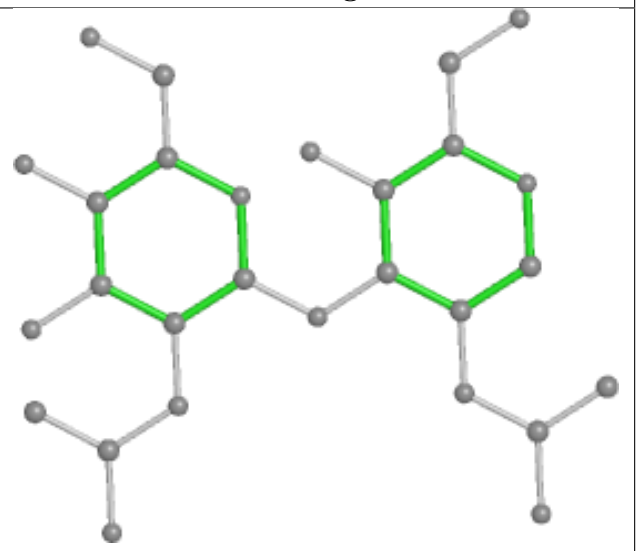
Bond lengths



Bond angles

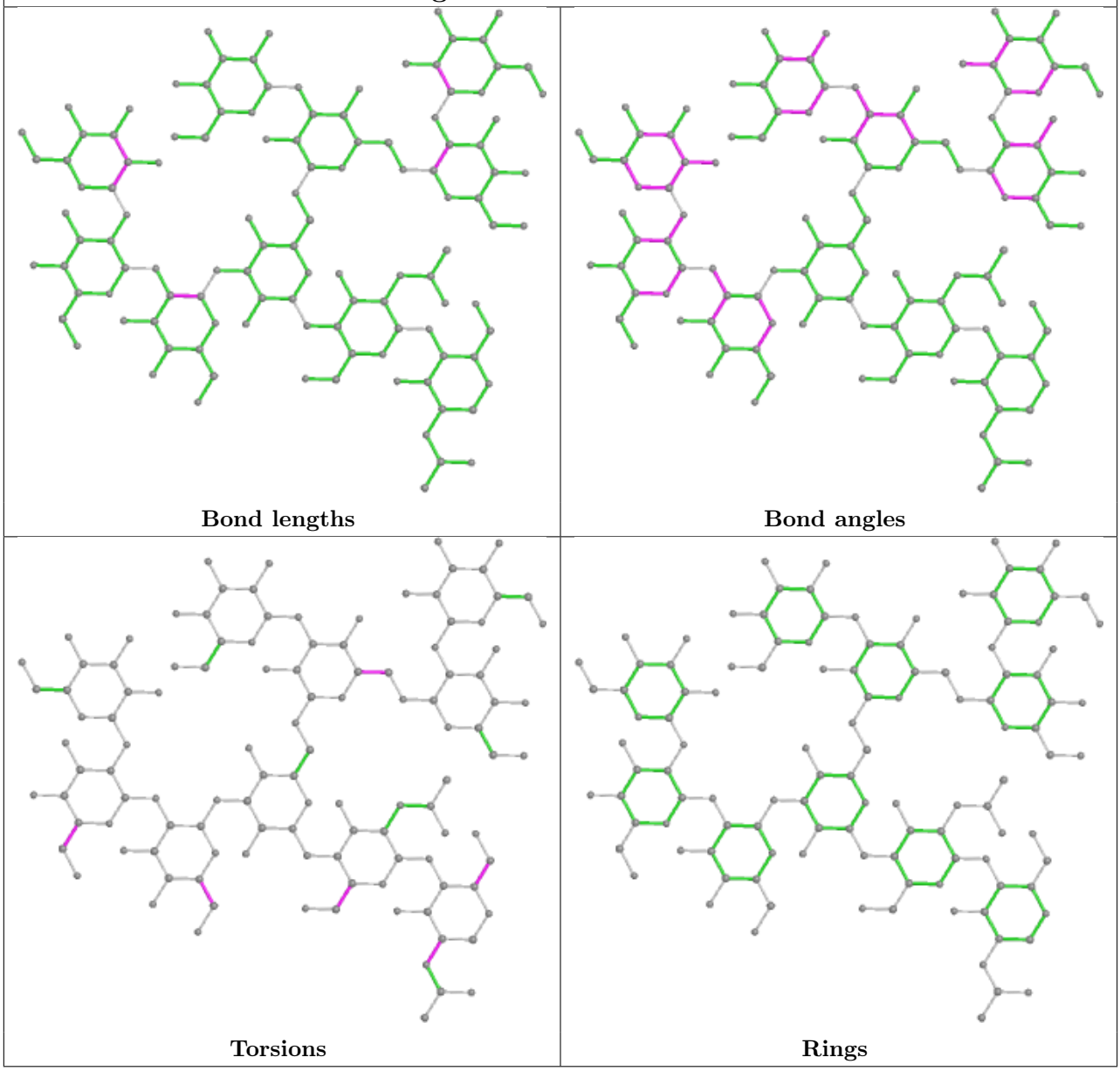


Torsions



Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
13	NAG	G	1601	4	14,14,15	0.31	0	17,19,21	0.37	0
13	NAG	G	617	4	14,14,15	0.27	0	17,19,21	0.41	0
13	NAG	G	4421	4	14,14,15	0.20	0	17,19,21	0.41	0
13	NAG	G	2761	4	14,14,15	0.26	0	17,19,21	0.44	0
13	NAG	G	2891	4	14,14,15	0.45	0	17,19,21	0.58	0
13	NAG	G	2411	4	14,14,15	0.23	0	17,19,21	0.37	0
13	NAG	B	6371	1	14,14,15	0.25	0	17,19,21	0.46	0
13	NAG	B	6111	1	14,14,15	0.27	0	17,19,21	0.47	0
13	NAG	G	1301	4	14,14,15	0.28	0	17,19,21	0.45	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
13	NAG	G	1601	4	-	2/6/23/26	0/1/1/1
13	NAG	G	617	4	-	1/6/23/26	0/1/1/1
13	NAG	G	4421	4	-	2/6/23/26	0/1/1/1
13	NAG	G	2761	4	-	2/6/23/26	0/1/1/1
13	NAG	G	2891	4	-	2/6/23/26	0/1/1/1
13	NAG	G	2411	4	-	1/6/23/26	0/1/1/1
13	NAG	B	6371	1	-	0/6/23/26	0/1/1/1
13	NAG	B	6111	1	-	2/6/23/26	0/1/1/1
13	NAG	G	1301	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	1601	NAG	O5-C5-C6-O6
13	B	6111	NAG	O5-C5-C6-O6
13	G	1601	NAG	C4-C5-C6-O6
13	B	6111	NAG	C4-C5-C6-O6
13	G	2761	NAG	C4-C5-C6-O6
13	G	1301	NAG	O5-C5-C6-O6
13	G	2761	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	G	1301	NAG	C4-C5-C6-O6
13	G	617	NAG	O5-C5-C6-O6
13	G	2891	NAG	C4-C5-C6-O6
13	G	2411	NAG	O5-C5-C6-O6
13	G	2891	NAG	O5-C5-C6-O6
13	G	4421	NAG	C4-C5-C6-O6
13	G	4421	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	1601	NAG	1	0
13	G	2891	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	129/153 (84%)	-0.36	1 (0%)	86	87	14, 32, 63, 100	0
2	D	128/134 (95%)	0.23	8 (6%)	20	19	47, 82, 122, 136	0
3	E	100/114 (87%)	0.27	7 (7%)	16	15	64, 79, 107, 116	0
4	G	430/463 (92%)	-0.37	6 (1%)	75	77	21, 42, 87, 113	0
5	H	219/244 (89%)	0.12	9 (4%)	37	36	48, 68, 98, 111	0
6	L	211/217 (97%)	-0.43	1 (0%)	91	92	36, 50, 69, 95	0
All	All	1217/1325 (91%)	-0.17	32 (2%)	56	57	14, 55, 101, 136	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	18	VAL	4.9
4	G	367	GLY	4.5
5	H	30	SER	4.0
3	E	15	LEU	3.8
2	D	82(A)	ARG	3.6
2	D	110	THR	3.3
3	E	84	THR	3.1
5	H	125	ALA	3.1
1	B	664	ASP	2.9
5	H	71	VAL	2.8
4	G	166	ARG	2.6
4	G	457	ASP	2.6
3	E	14	SER	2.6
3	E	11	VAL	2.6
3	E	18	SER	2.6
2	D	17	SER	2.5
2	D	70	THR	2.5
3	E	17	GLN	2.5
6	L	6	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	19	VAL	2.5
4	G	366	GLY	2.4
5	H	138	LEU	2.4
5	H	195	ILE	2.2
5	H	211	VAL	2.2
4	G	80	ASN	2.2
5	H	11	LEU	2.2
2	D	10	THR	2.2
5	H	17	THR	2.1
5	H	210	LYS	2.1
2	D	1	GLN	2.0
2	D	67	VAL	2.0
4	G	79	PRO	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MAN	F	4	11/12	0.72	0.31	116,125,135,136	0
7	MAN	A	4	11/12	0.73	0.21	95,102,107,111	0
8	MAN	C	5	11/12	0.76	0.33	107,116,122,127	0
9	BMA	F	3	11/12	0.77	0.28	106,115,129,131	0
10	NAG	K	2	14/15	0.78	0.42	117,136,159,162	0
10	NAG	O	2	14/15	0.78	0.40	108,121,130,132	0
7	BMA	A	3	11/12	0.79	0.17	103,115,125,127	0
7	MAN	A	5	11/12	0.81	0.23	69,88,102,108	0
10	NAG	M	2	14/15	0.82	0.34	93,112,125,127	0
8	MAN	C	4	11/12	0.85	0.17	86,98,107,109	0
10	NAG	I	2	14/15	0.86	0.27	82,102,110,111	0
11	NAG	J	2	14/15	0.88	0.26	102,107,115,115	0
11	NAG	J	1	14/15	0.90	0.19	38,89,105,106	0
10	NAG	I	1	14/15	0.90	0.17	44,69,92,102	0
12	MAN	N	9	11/12	0.90	0.29	86,98,106,108	0

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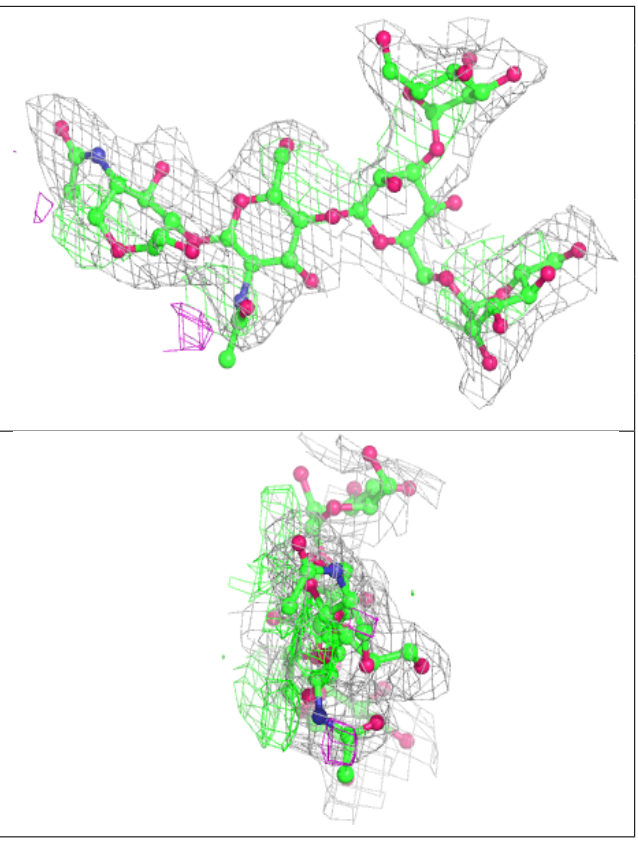
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	MAN	N	8	11/12	0.91	0.15	58,68,78,90	0
7	NAG	A	2	14/15	0.92	0.17	50,63,93,93	0
10	NAG	P	2	14/15	0.92	0.22	53,101,112,112	0
12	MAN	N	10	11/12	0.92	0.13	71,84,99,108	0
12	MAN	N	6	11/12	0.93	0.17	41,60,67,76	0
10	NAG	O	1	14/15	0.93	0.15	63,71,92,104	0
8	NAG	C	1	14/15	0.94	0.16	30,35,63,75	0
12	MAN	N	7	11/12	0.95	0.11	78,87,97,105	0
9	NAG	F	2	14/15	0.95	0.14	57,73,93,97	0
12	NAG	N	1	14/15	0.95	0.10	37,51,67,68	0
10	NAG	P	1	14/15	0.95	0.11	54,63,88,101	0
12	NAG	N	2	14/15	0.96	0.14	41,47,61,71	0
8	BMA	C	3	11/12	0.96	0.10	32,34,48,69	0
10	NAG	M	1	14/15	0.96	0.11	32,72,86,92	0
8	MAN	C	6	11/12	0.96	0.10	30,39,59,62	0
9	NAG	F	1	14/15	0.96	0.13	39,51,57,65	0
8	NAG	C	2	14/15	0.96	0.15	32,40,63,70	0
12	BMA	N	3	11/12	0.97	0.11	40,41,60,73	0
10	NAG	K	1	14/15	0.97	0.08	38,50,69,91	0
7	NAG	A	1	14/15	0.97	0.12	30,36,55,56	0
12	MAN	N	5	11/12	0.98	0.10	39,40,51,62	0
12	MAN	N	4	11/12	0.98	0.09	38,43,49,65	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

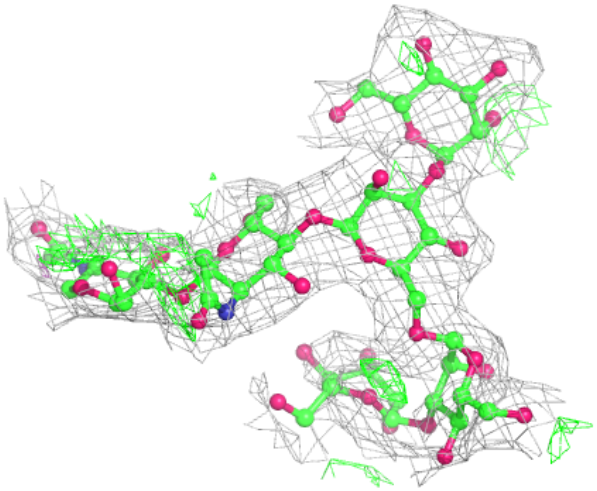
Electron density around Chain A:

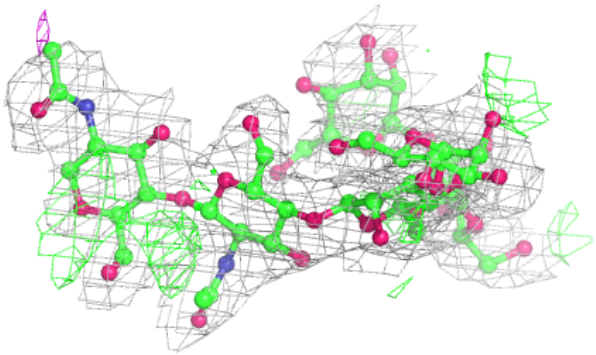
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

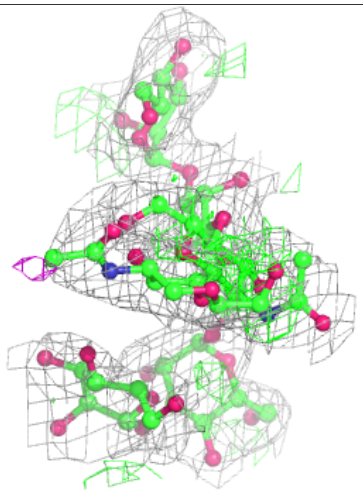


Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

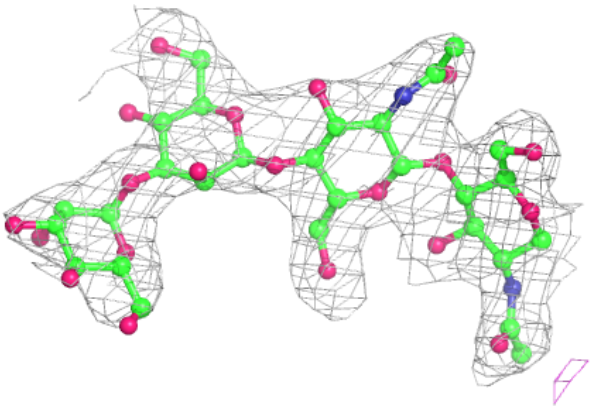


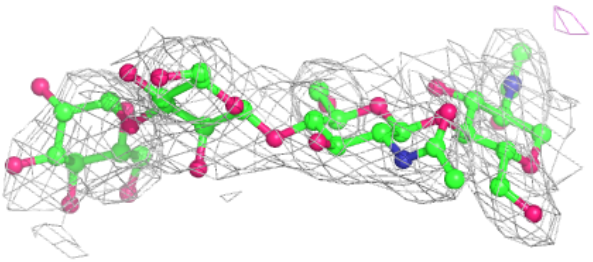


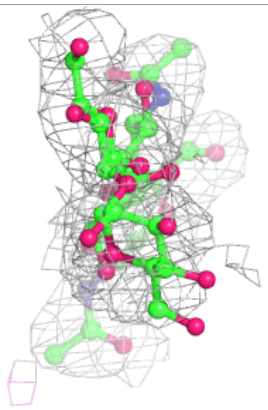


Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

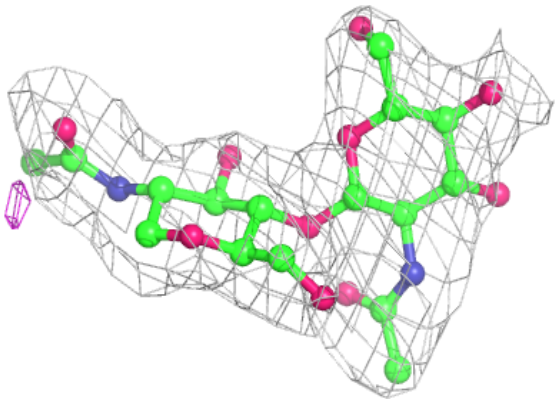


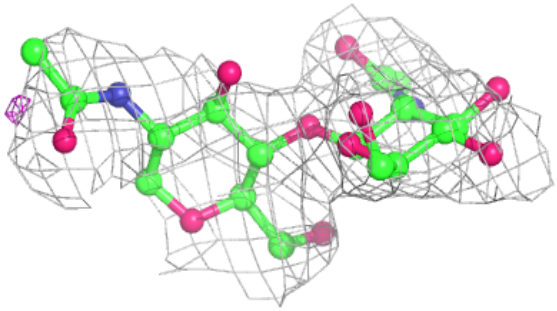


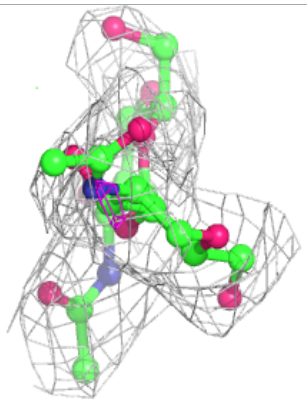


Electron density around Chain I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

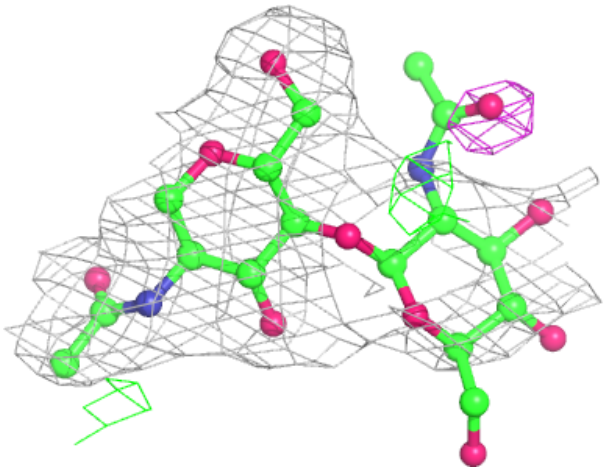


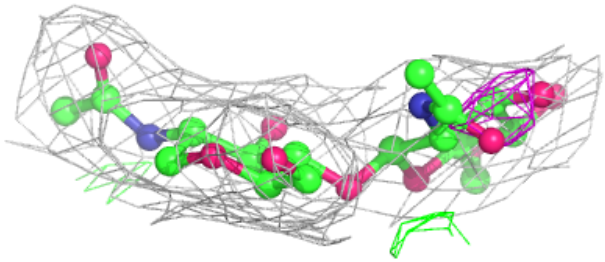


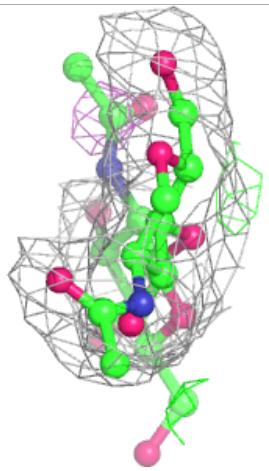


Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

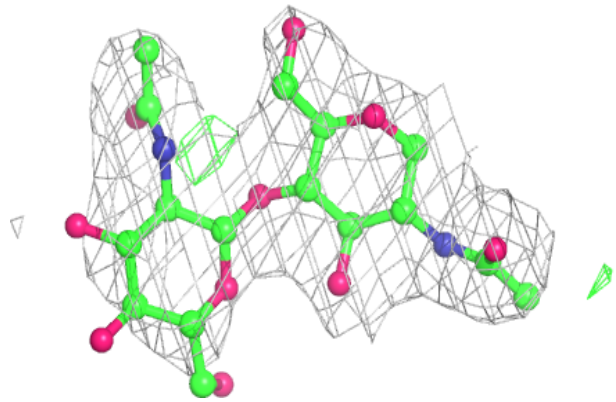


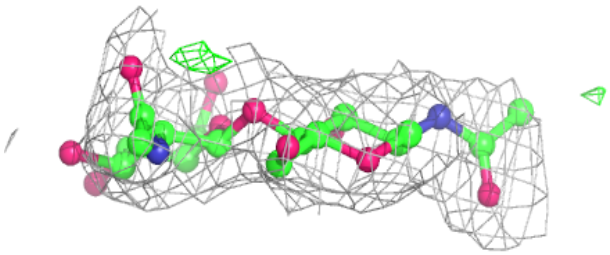


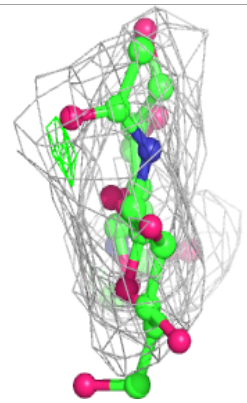


Electron density around Chain M:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

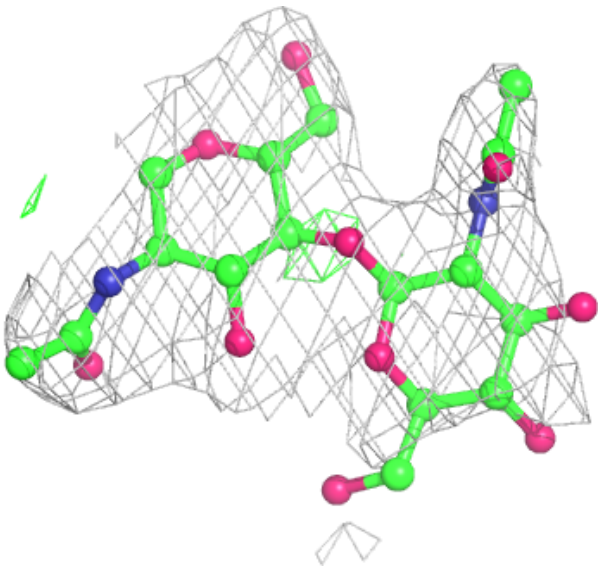


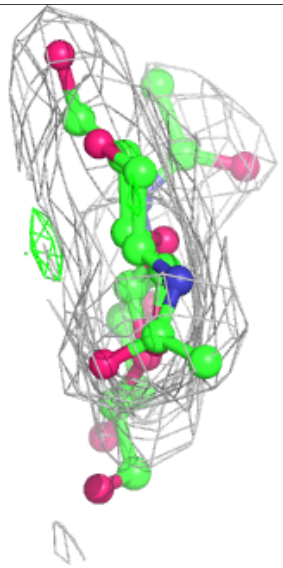




Electron density around Chain O:

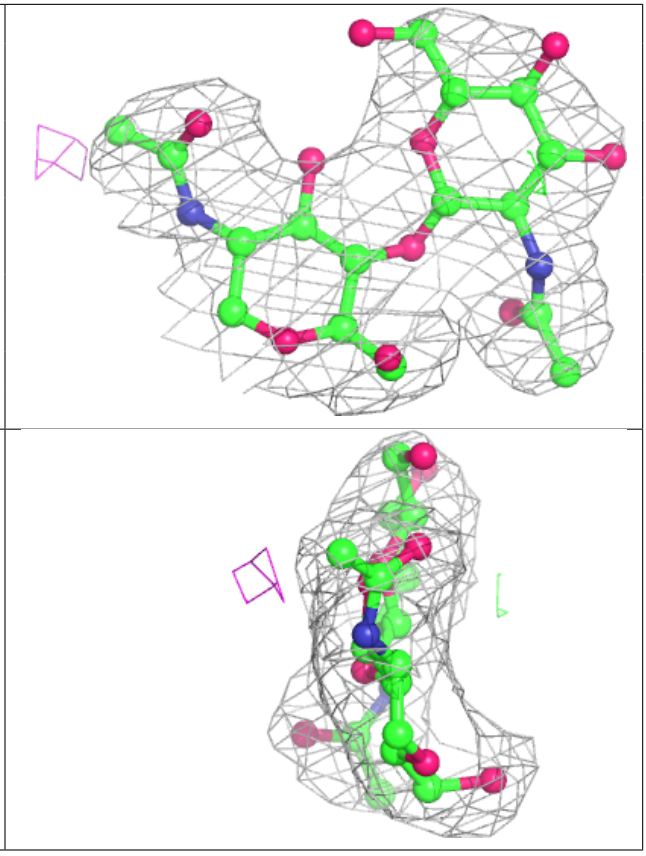
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





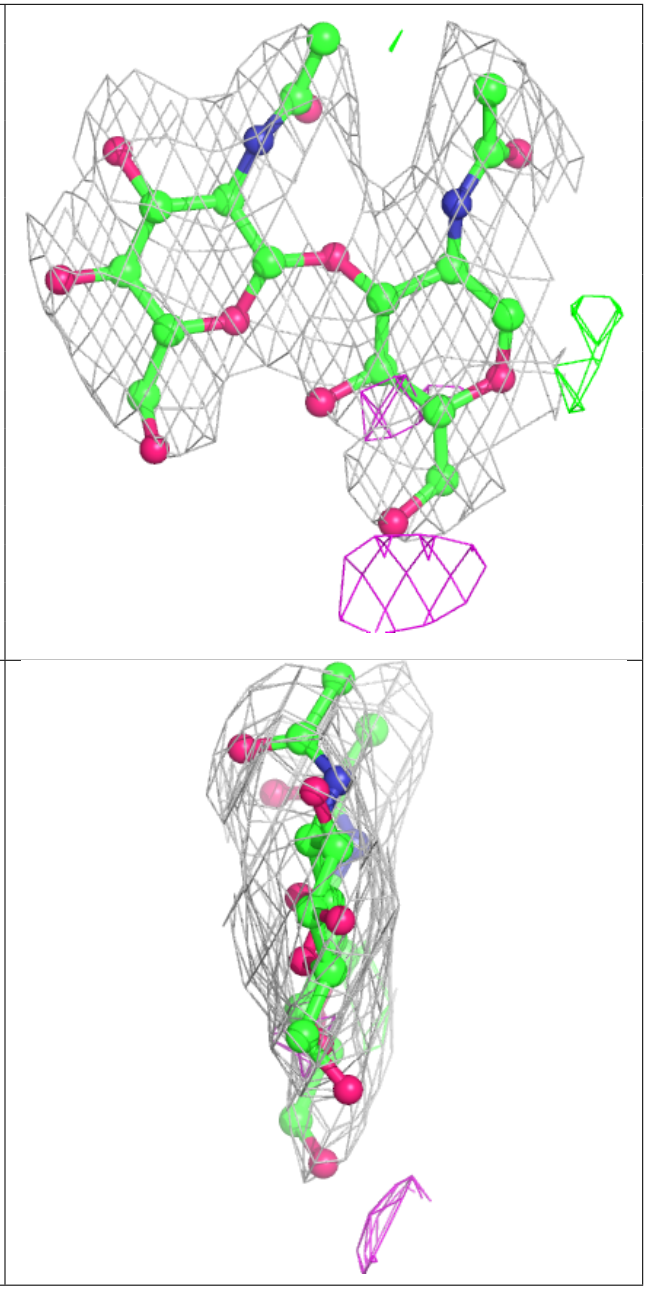
Electron density around Chain P:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



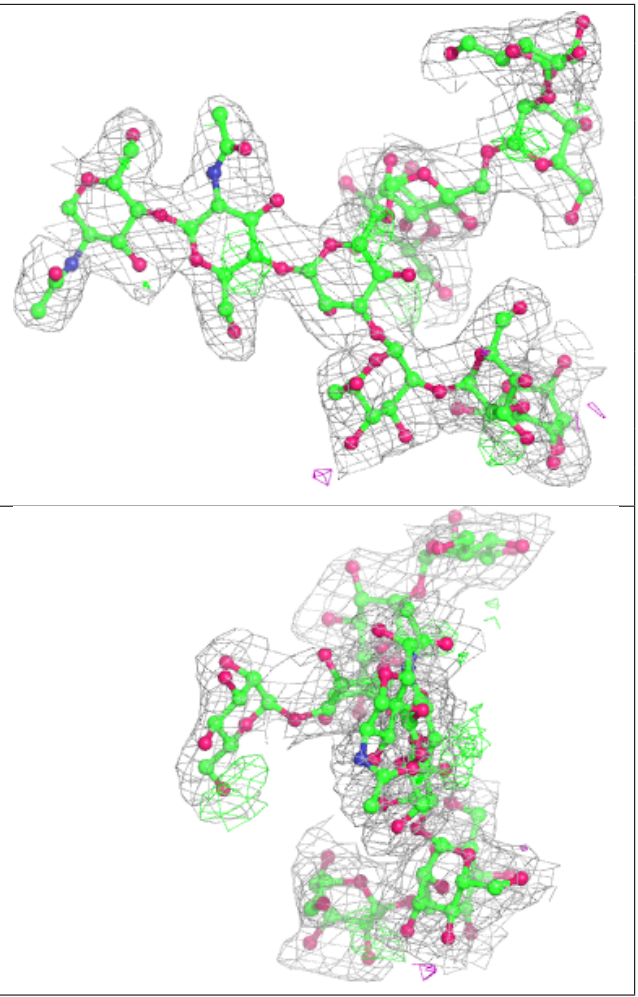
Electron density around Chain J:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	NAG	G	4421	14/15	0.83	0.46	105,117,125,130	0
13	NAG	G	1601	14/15	0.86	0.19	72,91,97,97	0
13	NAG	B	6111	14/15	0.87	0.28	48,72,85,96	0
13	NAG	G	2411	14/15	0.91	0.19	56,74,97,103	0
13	NAG	G	1301	14/15	0.91	0.19	86,89,96,98	0
13	NAG	G	2761	14/15	0.92	0.34	86,101,118,118	0
13	NAG	G	617	14/15	0.94	0.14	56,68,72,80	0
13	NAG	B	6371	14/15	0.94	0.28	79,91,98,106	0
13	NAG	G	2891	14/15	0.95	0.14	41,45,75,78	0

6.5 Other polymers (i)

There are no such residues in this entry.