Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 11:27 PM JST

PDB ID	:	6IEQ
Title	:	Crystal Structure of HIV-1 Env ConM SOSIP.v7 in Complex with bNAb PGT124 and 35O22
Authors	:	Han, B.W.; Wilson, I.A.
Deposited on	:	2018-09-16
Resolution	:	3.90 Å(reported)

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

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

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

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

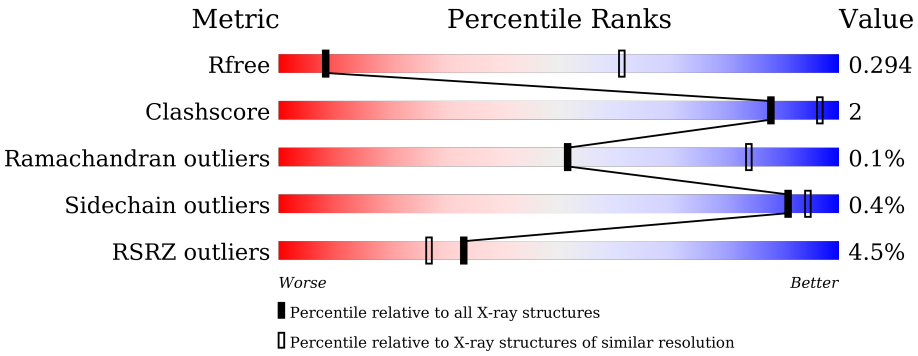
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	G	497	2% 82% 6% 12%
2	B	153	% 80% 5% 14%
3	L	214	2% 93% 5% •
4	H	236	8% 94% • •
5	D	240	5% 94% • 5%
6	E	216	8% 95% • •

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Mol	Chain	Length	Quality of chain
7	A	6	83% 17%
8	C	4	25% 75%
9	F	2	50% 50%
9	M	2	50% 50%
9	O	2	50% 50%
10	I	5	20% 60% 20%
10	K	5	100%
10	N	5	100%
11	J	2	100%
12	P	8	12% 62% 25%

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
7	MAN	A	4	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 11846 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	439	Total	C	N	O	S	0	0	0
			3483	2188	612	657	26			

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			1043	656	176	204	7			

- Molecule 3 is a protein called PGT124 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			

- Molecule 4 is a protein called PGT124 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	231	Total	C	N	O	S	0	0	0
			1754	1111	293	345	5			

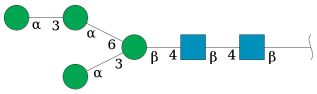
- Molecule 5 is a protein called 35O22 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	229	Total	C	N	O	S	0	0	0
			1731	1100	290	334	7			

- Molecule 6 is a protein called 35O22 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 7 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			
7	A	6	72	40	2	30	0	0	0

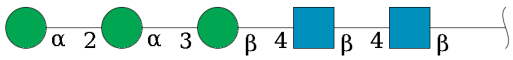
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

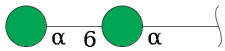
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	F	2	28	16	2	10	0	0	0
			Total	C	N	O			
9	M	2	28	16	2	10	0	0	0
			Total	C	N	O			
9	O	2	28	16	2	10	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



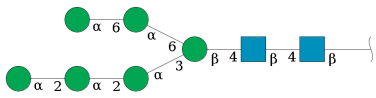
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	I	5	Total C N O 61 34 2 25	0	0	0
10	K	5	Total C N O 61 34 2 25	0	0	0
10	N	5	Total C N O 61 34 2 25	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



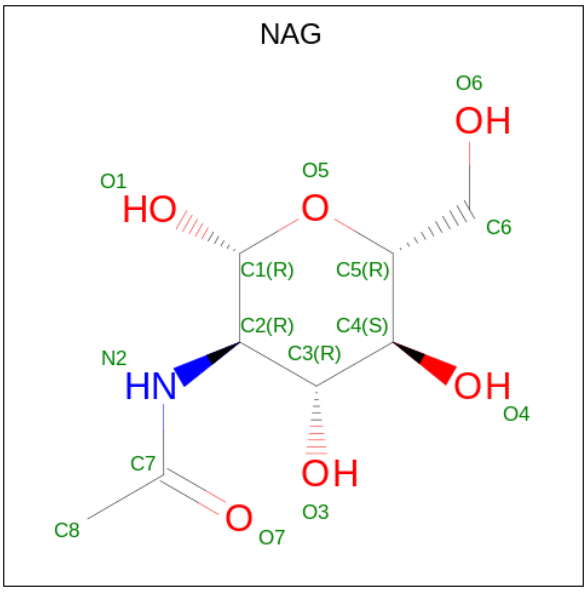
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	J	2	Total C O 22 12 10	0	0	0

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



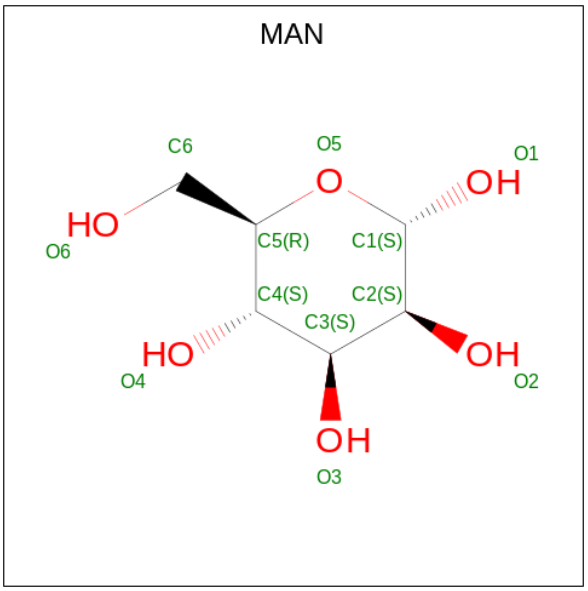
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	P	8	Total C N O 94 52 2 40	0	0	0

- 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
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0

- Molecule 14 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



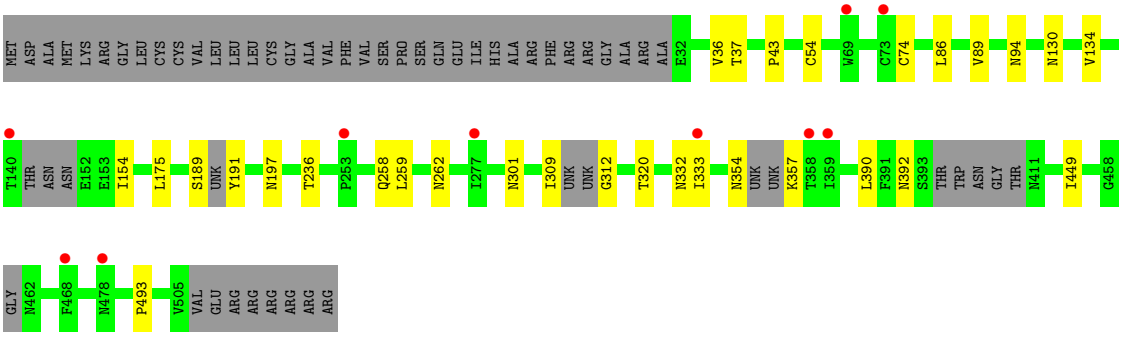
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	L	1	Total C O 11 6 5	0	0
14	H	1	Total C O 11 6 5	0	0

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.

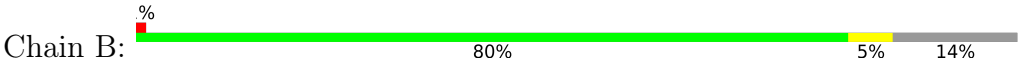
• Molecule 1: Envelope glycoprotein gp160

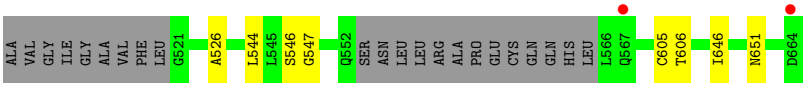
Chain G:



• Molecule 2: Envelope glycoprotein gp160

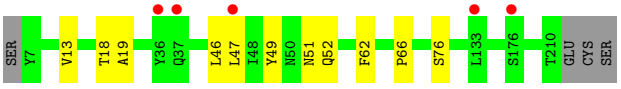
Chain B:





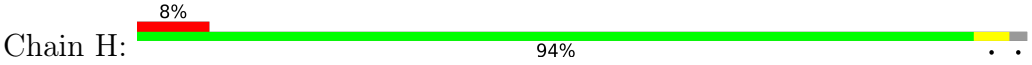
• Molecule 3: PGT124 Fab Light Chain

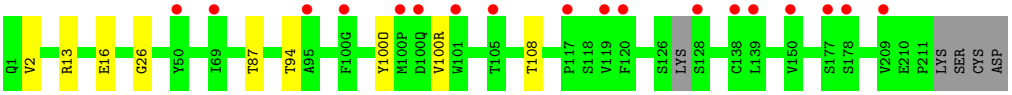
Chain L:



• Molecule 4: PGT124 Fab Heavy Chain

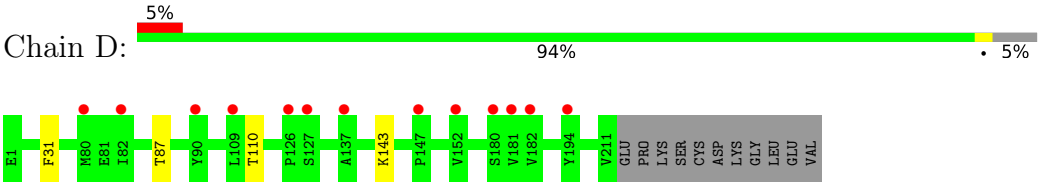
Chain H:





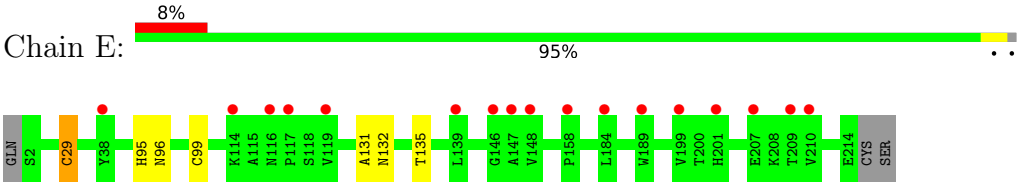
• Molecule 5: 35O22 Fab Heavy Chain

Chain D:



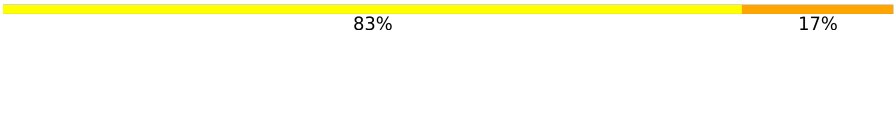
• Molecule 6: 35O22 Fab Light Chain

Chain E:



• Molecule 7: 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 A:

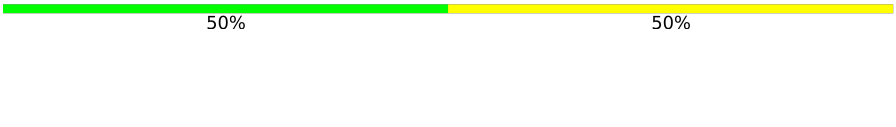


• Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain F:



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

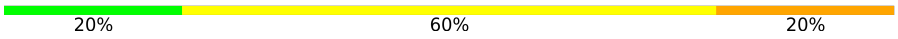
Chain M:

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

Chain O:

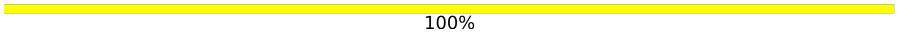
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



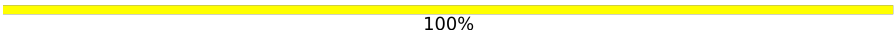
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



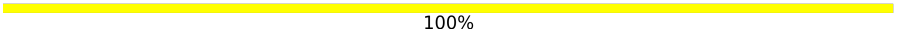
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



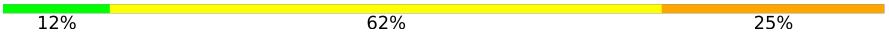
• Molecule 11: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose

Chain J:



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

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	127.59Å 127.59Å 315.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 3.90 49.60 – 3.90	Depositor EDS
% Data completeness (in resolution range)	88.9 (50.01-3.90) 88.9 (49.60-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.247 , 0.296 0.249 , 0.294	Depositor DCC
R_{free} test set	1193 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	132.8	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 176.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.105 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11846	wwPDB-VP
Average B, all atoms (Å^2)	256.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	G	0.36	0/3550	0.58	0/4815
2	B	0.38	0/1060	0.56	0/1436
3	L	0.34	0/1638	0.56	1/2238 (0.0%)
4	H	0.37	0/1797	0.60	0/2453
5	D	0.36	0/1777	0.53	0/2422
6	E	0.36	0/1659	0.53	0/2269
All	All	0.36	0/11481	0.56	1/15633 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	46	LEU	CA-CB-CG	5.25	127.37	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	E	29	CYS	Peptide

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	G	3483	0	3432	23	0
2	B	1043	0	1013	6	0
3	L	1595	0	1541	8	0
4	H	1754	0	1719	5	0
5	D	1731	0	1702	4	0
6	E	1615	0	1544	4	0
7	A	72	0	61	1	0
8	C	50	0	43	0	0
9	F	28	0	25	0	0
9	M	28	0	25	2	0
9	O	28	0	25	1	0
10	I	61	0	52	1	0
10	K	61	0	52	0	0
10	N	61	0	52	0	0
11	J	22	0	19	0	0
12	P	94	0	79	4	0
13	B	28	0	26	0	0
13	G	70	0	65	1	0
14	H	11	0	9	5	0
14	L	11	0	10	5	0
All	All	11846	0	11494	47	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 2.

All (47) 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)
14:L:301:MAN:O2	14:H:309:MAN:C1	2.11	0.98
14:L:301:MAN:C2	14:H:309:MAN:C1	2.52	0.85
14:L:301:MAN:HO2	14:H:309:MAN:C1	1.97	0.73
1:G:189:SER:O	1:G:191:TYR:N	2.26	0.69
1:G:262:ASN:HD21	10:I:1:NAG:C1	2.14	0.60
1:G:36:VAL:HG21	2:B:646:ILE:HD11	1.83	0.59
14:L:301:MAN:H2	14:H:309:MAN:C1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:301:ASN:HD21	9:M:1:NAG:C2	2.16	0.58
1:G:333:ILE:HD11	1:G:390:LEU:HD22	1.86	0.58
1:G:130:ASN:HA	1:G:189:SER:HA	1.86	0.56
4:H:94:THR:HG22	4:H:100(R):VAL:HB	1.92	0.52
1:G:43:PRO:HB2	2:B:526:ALA:HA	1.92	0.51
3:L:52:GLN:HE21	3:L:66:PRO:HB3	1.76	0.51
1:G:37:THR:HG22	2:B:605:CYS:HA	1.93	0.51
3:L:52:GLN:NE2	12:P:5:MAN:O3	2.44	0.50
3:L:52:GLN:HE22	12:P:5:MAN:H4	1.77	0.49
1:G:175:LEU:O	1:G:320:THR:OG1	2.30	0.49
5:D:31:PHE:HA	7:A:1:NAG:H62	1.94	0.49
1:G:309:ILE:C	1:G:312:GLY:N	2.66	0.49
1:G:301:ASN:HD21	9:M:1:NAG:H2	1.78	0.49
1:G:197:ASN:HD21	13:G:609:NAG:H2	1.78	0.49
1:G:333:ILE:HD11	1:G:390:LEU:CD2	2.43	0.48
6:E:131:ALA:N	6:E:132:ASN:HA	2.28	0.48
3:L:13:VAL:HG11	3:L:19:ALA:HB2	1.96	0.48
5:D:87:THR:HG23	5:D:110:THR:HA	1.98	0.46
14:L:301:MAN:O2	14:H:309:MAN:O5	2.15	0.46
5:D:143:LYS:HE3	6:E:135:THR:HG21	1.97	0.46
3:L:52:GLN:NE2	12:P:5:MAN:O2	2.49	0.45
4:H:13:ARG:HB2	4:H:16:GLU:HG3	1.97	0.45
1:G:36:VAL:HG23	2:B:606:THR:OG1	2.17	0.44
1:G:189:SER:C	1:G:191:TYR:N	2.71	0.43
3:L:18:THR:HG22	3:L:76:SER:HA	2.00	0.43
4:H:2:VAL:HA	4:H:26:GLY:HA3	2.01	0.43
1:G:354:ASN:O	1:G:357:LYS:N	2.53	0.42
1:G:94:ASN:HA	1:G:236:THR:HG22	2.01	0.42
5:D:143:LYS:CE	6:E:135:THR:HG21	2.50	0.42
1:G:332:ASN:HD21	12:P:1:NAG:C6	2.33	0.42
1:G:86:LEU:HB3	1:G:89:VAL:HG21	2.01	0.42
1:G:493:PRO:HG3	2:B:544:LEU:HD21	2.01	0.42
6:E:95:HIS:CE1	6:E:96:ASN:HD22	2.38	0.41
1:G:134:VAL:HB	1:G:154:ILE:HG23	2.01	0.41
3:L:47:LEU:HD13	3:L:62:PHE:CD1	2.55	0.41
1:G:259:LEU:HD13	1:G:449:ILE:HD13	2.02	0.41
3:L:49:TYR:HB2	4:H:100(O):TYR:CD2	2.55	0.41
1:G:392:ASN:ND2	9:O:1:NAG:O7	2.53	0.41
4:H:87:THR:HG23	4:H:108:THR:HA	2.02	0.41
2:B:546:SER:HA	2:B:547:GLY:HA3	1.81	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	G	425/497 (86%)	406 (96%)	18 (4%)	1 (0%)	47 79
2	B	127/153 (83%)	120 (94%)	7 (6%)	0	100 100
3	L	208/214 (97%)	201 (97%)	6 (3%)	1 (0%)	29 67
4	H	227/236 (96%)	221 (97%)	6 (3%)	0	100 100
5	D	227/240 (95%)	220 (97%)	7 (3%)	0	100 100
6	E	211/216 (98%)	205 (97%)	6 (3%)	0	100 100
All	All	1425/1556 (92%)	1373 (96%)	50 (4%)	2 (0%)	51 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	258	GLN
3	L	51	ASN

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	G	397/440 (90%)	395 (100%)	2 (0%)	88 93
2	B	114/131 (87%)	113 (99%)	1 (1%)	78 87
3	L	176/180 (98%)	176 (100%)	0	100 100
4	H	199/204 (98%)	199 (100%)	0	100 100
5	D	193/203 (95%)	193 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	E	186/189 (98%)	184 (99%)	2 (1%)	73 84
All	All	1265/1347 (94%)	1260 (100%)	5 (0%)	91 94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	54	CYS
1	G	74	CYS
2	B	651	ASN
6	E	29	CYS
6	E	99	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	197	ASN
1	G	246	GLN
1	G	262	ASN
1	G	301	ASN
1	G	377	ASN
1	G	386	ASN
1	G	432	GLN
1	G	448	ASN
2	B	651	ASN
3	L	52	GLN
3	L	170	ASN
4	H	31	ASN
4	H	81	GLN
6	E	95	HIS
6	E	112	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

41 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	7,1	14,14,15	0.50	0	17,19,21	1.43	3 (17%)
7	NAG	A	2	7	14,14,15	0.57	0	17,19,21	2.17	4 (23%)
7	BMA	A	3	7	11,11,12	0.51	0	15,15,17	1.30	2 (13%)
7	MAN	A	4	7	11,11,12	0.65	0	15,15,17	2.30	3 (20%)
7	MAN	A	5	7	11,11,12	0.67	0	15,15,17	1.99	2 (13%)
7	MAN	A	6	7	11,11,12	0.26	0	15,15,17	0.89	1 (6%)
8	NAG	C	1	8,1	14,14,15	0.62	0	17,19,21	2.29	4 (23%)
8	NAG	C	2	8	14,14,15	0.62	0	17,19,21	2.26	6 (35%)
8	BMA	C	3	8	11,11,12	0.51	0	15,15,17	0.74	0
8	MAN	C	4	8	11,11,12	0.44	0	15,15,17	1.15	2 (13%)
9	NAG	F	1	9,1	14,14,15	0.65	0	17,19,21	1.46	4 (23%)
9	NAG	F	2	9	14,14,15	0.35	0	17,19,21	0.88	0
10	NAG	I	1	10	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
10	NAG	I	2	10	14,14,15	0.36	0	17,19,21	0.84	0
10	BMA	I	3	10	11,11,12	0.59	0	15,15,17	1.65	3 (20%)
10	MAN	I	4	10	11,11,12	0.56	0	15,15,17	1.64	4 (26%)
10	MAN	I	5	10	11,11,12	0.41	0	15,15,17	1.38	1 (6%)
11	MAN	J	1	11	11,11,12	0.49	0	15,15,17	1.59	3 (20%)
11	MAN	J	2	11	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
10	NAG	K	1	10	14,14,15	0.50	0	17,19,21	1.56	3 (17%)
10	NAG	K	2	10	14,14,15	0.69	0	17,19,21	1.37	1 (5%)
10	BMA	K	3	10	11,11,12	0.72	0	15,15,17	1.85	4 (26%)
10	MAN	K	4	10	11,11,12	0.32	0	15,15,17	0.95	1 (6%)
10	MAN	K	5	10	11,11,12	0.37	0	15,15,17	1.59	2 (13%)
9	NAG	M	1	9	14,14,15	0.43	0	17,19,21	1.14	1 (5%)
9	NAG	M	2	9	14,14,15	0.49	0	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	N	1	10	14,14,15	0.45	0	17,19,21	1.45	4 (23%)
10	NAG	N	2	10	14,14,15	0.57	0	17,19,21	0.95	2 (11%)
10	BMA	N	3	10	11,11,12	0.55	0	15,15,17	1.27	3 (20%)
10	MAN	N	4	10	11,11,12	0.33	0	15,15,17	0.99	1 (6%)
10	MAN	N	5	10	11,11,12	0.45	0	15,15,17	1.90	3 (20%)
9	NAG	O	1	9	14,14,15	0.46	0	17,19,21	0.89	1 (5%)
9	NAG	O	2	9	14,14,15	0.45	0	17,19,21	1.42	2 (11%)
12	NAG	P	1	12	14,14,15	0.55	0	17,19,21	2.12	6 (35%)
12	NAG	P	2	12	14,14,15	0.34	0	17,19,21	1.23	3 (17%)
12	BMA	P	3	12	11,11,12	0.44	0	15,15,17	1.09	2 (13%)
12	MAN	P	4	12	11,11,12	0.32	0	15,15,17	1.66	3 (20%)
12	MAN	P	5	12	11,11,12	0.48	0	15,15,17	0.88	1 (6%)
12	MAN	P	6	12	11,11,12	0.57	0	15,15,17	1.71	4 (26%)
12	MAN	P	7	12	11,11,12	0.35	0	15,15,17	0.81	0
12	MAN	P	8	12	11,11,12	0.52	0	15,15,17	1.28	2 (13%)

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	7,1	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	2/2/19/22	0/1/1/1
7	MAN	A	6	7	-	1/2/19/22	0/1/1/1
8	NAG	C	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	1/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	MAN	C	4	8	-	1/2/19/22	0/1/1/1
9	NAG	F	1	9,1	-	4/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
10	NAG	I	1	10	-	1/6/23/26	0/1/1/1
10	NAG	I	2	10	-	0/6/23/26	0/1/1/1
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
10	MAN	I	4	10	-	2/2/19/22	0/1/1/1

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

There are no bond length outliers.

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1	NAG	C1-O5-C5	7.44	122.28	112.19
7	A	4	MAN	C1-O5-C5	6.92	121.57	112.19
7	A	5	MAN	C1-C2-C3	6.28	117.39	109.67
10	N	5	MAN	C1-O5-C5	6.01	120.33	112.19
7	A	2	NAG	C2-N2-C7	5.84	131.22	122.90
8	C	2	NAG	C1-O5-C5	5.60	119.78	112.19
12	P	1	NAG	C1-O5-C5	5.47	119.61	112.19
10	K	5	MAN	C1-O5-C5	5.18	119.22	112.19
12	P	4	MAN	C1-O5-C5	4.75	118.63	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2	NAG	C8-C7-N2	4.65	123.97	116.10
10	K	3	BMA	C1-C2-C3	4.63	115.36	109.67
10	I	3	BMA	C3-C4-C5	4.35	117.99	110.24
7	A	4	MAN	C3-C4-C5	4.27	117.86	110.24
10	I	4	MAN	C3-C4-C5	4.14	117.63	110.24
8	C	2	NAG	O5-C1-C2	-4.08	104.84	111.29
11	J	1	MAN	C1-O5-C5	4.01	117.62	112.19
9	O	2	NAG	C1-O5-C5	3.98	117.58	112.19
10	I	5	MAN	C1-O5-C5	3.96	117.56	112.19
10	K	1	NAG	O5-C1-C2	-3.84	105.22	111.29
12	P	1	NAG	C3-C4-C5	3.81	117.04	110.24
10	I	1	NAG	O5-C1-C2	-3.78	105.32	111.29
10	K	2	NAG	C4-C3-C2	3.75	116.51	111.02
12	P	6	MAN	C1-C2-C3	3.57	114.05	109.67
10	K	1	NAG	C3-C4-C5	3.44	116.38	110.24
12	P	6	MAN	C3-C4-C5	3.44	116.38	110.24
12	P	8	MAN	C1-C2-C3	3.41	113.86	109.67
9	M	2	NAG	C4-C3-C2	3.40	116.00	111.02
11	J	2	MAN	C1-C2-C3	3.33	113.75	109.67
10	N	5	MAN	C1-C2-C3	3.27	113.69	109.67
7	A	1	NAG	C4-C3-C2	3.23	115.76	111.02
8	C	4	MAN	C1-C2-C3	3.23	113.64	109.67
9	M	1	NAG	C4-C3-C2	3.22	115.73	111.02
10	N	1	NAG	C4-C3-C2	3.20	115.71	111.02
12	P	6	MAN	C2-C3-C4	3.10	116.25	110.89
8	C	1	NAG	O5-C5-C4	3.10	118.36	110.83
9	F	1	NAG	C4-C3-C2	3.07	115.52	111.02
10	K	3	BMA	C3-C4-C5	3.07	115.71	110.24
10	I	3	BMA	O5-C1-C2	-2.96	106.20	110.77
7	A	3	BMA	C6-C5-C4	2.94	119.90	113.00
7	A	5	MAN	C2-C3-C4	2.88	115.88	110.89
7	A	2	NAG	C3-C4-C5	2.88	115.38	110.24
10	K	3	BMA	C2-C3-C4	2.88	115.88	110.89
11	J	1	MAN	O5-C5-C6	2.88	111.72	107.20
10	K	3	BMA	O5-C5-C6	2.86	111.69	107.20
8	C	2	NAG	C1-C2-N2	2.76	115.20	110.49
12	P	2	NAG	C3-C4-C5	2.76	115.16	110.24
12	P	2	NAG	O5-C1-C2	-2.74	106.97	111.29
10	I	4	MAN	C1-O5-C5	2.72	115.87	112.19
12	P	4	MAN	C1-C2-C3	2.69	112.97	109.67
8	C	2	NAG	O5-C5-C4	2.66	117.31	110.83
8	C	2	NAG	C2-N2-C7	2.64	126.66	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	2	NAG	C2-N2-C7	2.60	126.60	122.90
7	A	1	NAG	C3-C4-C5	2.57	114.83	110.24
11	J	1	MAN	C1-C2-C3	2.57	112.82	109.67
7	A	2	NAG	O7-C7-C8	-2.56	117.30	122.06
10	K	4	MAN	C1-O5-C5	2.52	115.61	112.19
10	N	3	BMA	O5-C1-C2	-2.52	106.89	110.77
8	C	1	NAG	C3-C4-C5	2.51	114.71	110.24
12	P	1	NAG	C8-C7-N2	2.49	120.32	116.10
12	P	1	NAG	O5-C5-C4	2.49	116.89	110.83
10	K	5	MAN	C1-C2-C3	2.48	112.72	109.67
10	I	3	BMA	C2-C3-C4	2.46	115.15	110.89
7	A	3	BMA	C1-C2-C3	-2.46	106.64	109.67
10	I	1	NAG	C4-C3-C2	-2.40	107.50	111.02
10	N	3	BMA	C3-C4-C5	2.38	114.49	110.24
10	I	1	NAG	C3-C4-C5	2.37	114.47	110.24
12	P	3	BMA	O3-C3-C2	-2.34	105.52	109.99
10	N	1	NAG	O5-C1-C2	-2.33	107.61	111.29
12	P	5	MAN	O5-C5-C6	2.32	110.84	107.20
12	P	3	BMA	C3-C4-C5	2.31	114.36	110.24
10	N	2	NAG	O5-C1-C2	-2.27	107.70	111.29
9	F	1	NAG	C1-O5-C5	-2.27	109.12	112.19
9	M	2	NAG	C3-C4-C5	2.25	114.25	110.24
8	C	2	NAG	C3-C4-C5	2.25	114.24	110.24
7	A	4	MAN	O5-C5-C4	2.24	116.28	110.83
7	A	6	MAN	C1-O5-C5	2.23	115.22	112.19
10	K	1	NAG	O5-C5-C4	2.23	116.25	110.83
12	P	1	NAG	O4-C4-C5	-2.22	103.77	109.30
12	P	4	MAN	O2-C2-C1	-2.22	104.61	109.15
10	N	4	MAN	C1-O5-C5	2.19	115.16	112.19
10	I	4	MAN	C2-C3-C4	2.19	114.68	110.89
12	P	8	MAN	C2-C3-C4	2.18	114.67	110.89
9	F	1	NAG	C2-N2-C7	2.18	126.00	122.90
10	N	3	BMA	O5-C5-C6	2.15	110.57	107.20
10	N	5	MAN	O5-C1-C2	2.12	114.04	110.77
10	I	4	MAN	O5-C1-C2	-2.12	107.50	110.77
9	O	1	NAG	O5-C1-C2	-2.09	107.98	111.29
9	F	1	NAG	O5-C5-C6	2.09	110.48	107.20
8	C	1	NAG	C1-C2-N2	2.09	114.06	110.49
7	A	1	NAG	O4-C4-C5	-2.09	104.11	109.30
12	P	2	NAG	O4-C4-C5	-2.09	104.11	109.30
10	N	1	NAG	C3-C4-C5	2.07	113.94	110.24
12	P	6	MAN	C1-O5-C5	2.04	114.95	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	1	NAG	C2-N2-C7	2.03	125.80	122.90
8	C	4	MAN	C1-O5-C5	2.03	114.94	112.19
10	N	1	NAG	C1-O5-C5	-2.02	109.45	112.19
10	N	2	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	3	BMA	C4-C5-C6-O6
11	J	2	MAN	O5-C5-C6-O6
12	P	8	MAN	O5-C5-C6-O6
10	N	2	NAG	O5-C5-C6-O6
9	O	1	NAG	C4-C5-C6-O6
9	O	2	NAG	O5-C5-C6-O6
12	P	8	MAN	C4-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
7	A	4	MAN	O5-C5-C6-O6
10	I	5	MAN	O5-C5-C6-O6
12	P	1	NAG	O5-C5-C6-O6
12	P	2	NAG	O5-C5-C6-O6
7	A	5	MAN	O5-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
12	P	5	MAN	O5-C5-C6-O6
11	J	1	MAN	O5-C5-C6-O6
11	J	2	MAN	C4-C5-C6-O6
9	O	1	NAG	O5-C5-C6-O6
10	I	4	MAN	O5-C5-C6-O6
10	N	3	BMA	C4-C5-C6-O6
12	P	5	MAN	C4-C5-C6-O6
7	A	4	MAN	C4-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
9	O	2	NAG	C4-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
12	P	1	NAG	C8-C7-N2-C2
12	P	1	NAG	O7-C7-N2-C2
7	A	5	MAN	C4-C5-C6-O6
11	J	1	MAN	C4-C5-C6-O6
12	P	2	NAG	C4-C5-C6-O6
12	P	4	MAN	O5-C5-C6-O6
10	N	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	I	5	MAN	C4-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
9	M	2	NAG	C4-C5-C6-O6
9	F	1	NAG	C1-C2-N2-C7
10	N	5	MAN	O5-C5-C6-O6
12	P	6	MAN	O5-C5-C6-O6
12	P	4	MAN	C4-C5-C6-O6
9	M	1	NAG	O5-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
10	K	5	MAN	O5-C5-C6-O6
8	C	4	MAN	O5-C5-C6-O6
10	K	4	MAN	O5-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
9	O	2	NAG	C3-C2-N2-C7
9	M	2	NAG	O5-C5-C6-O6
12	P	1	NAG	C4-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7
8	C	1	NAG	C3-C2-N2-C7
9	F	2	NAG	O5-C5-C6-O6
10	I	4	MAN	C4-C5-C6-O6
10	I	1	NAG	O5-C5-C6-O6
8	C	2	NAG	C3-C2-N2-C7
9	F	1	NAG	C3-C2-N2-C7
7	A	6	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

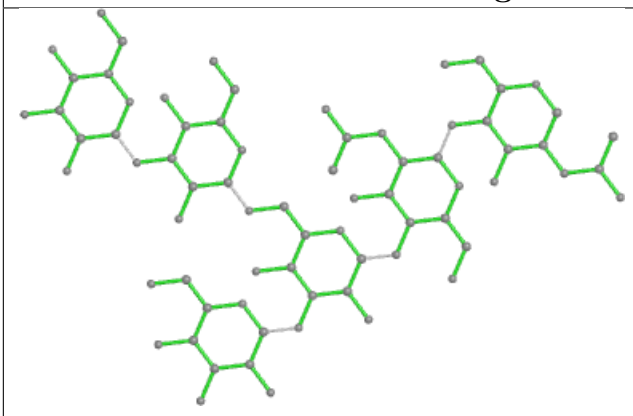
Mol	Chain	Res	Type	Atoms
11	J	1	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 9 short contacts:

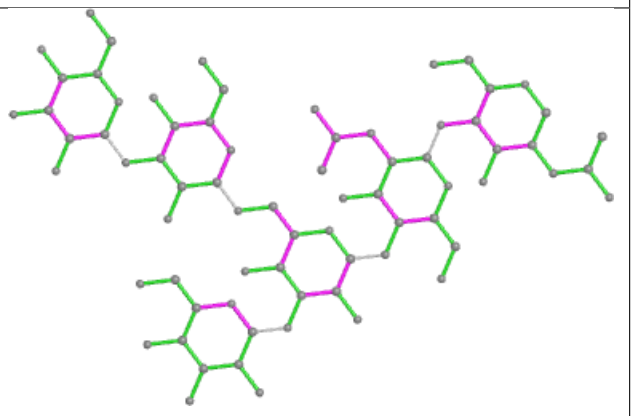
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	1	NAG	1	0
9	O	1	NAG	1	0
9	M	1	NAG	2	0
12	P	5	MAN	3	0
12	P	1	NAG	1	0
7	A	1	NAG	1	0

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

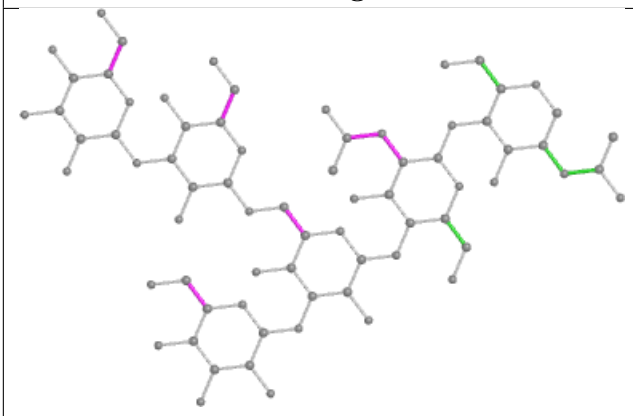
Oligosaccharide Chain A



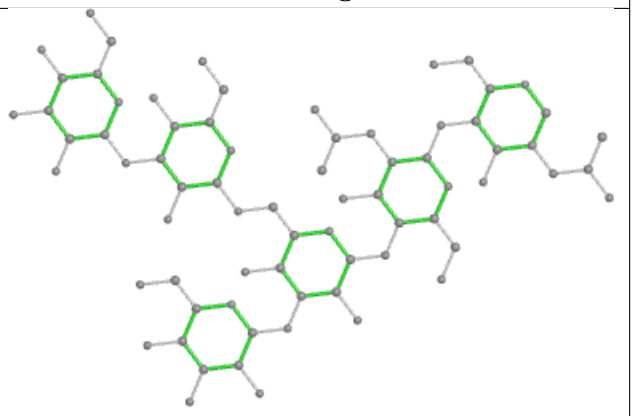
Bond lengths



Bond angles

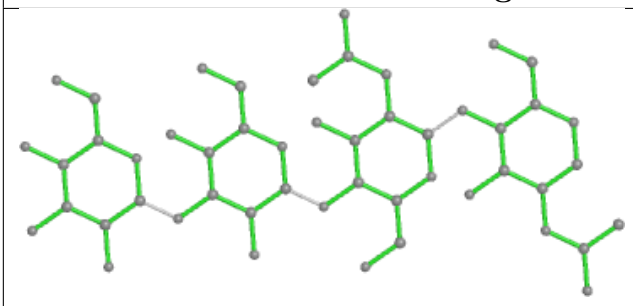


Torsions

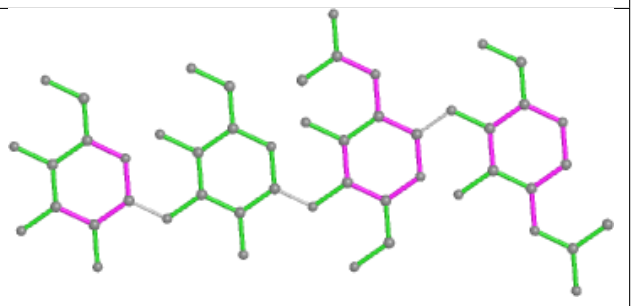


Rings

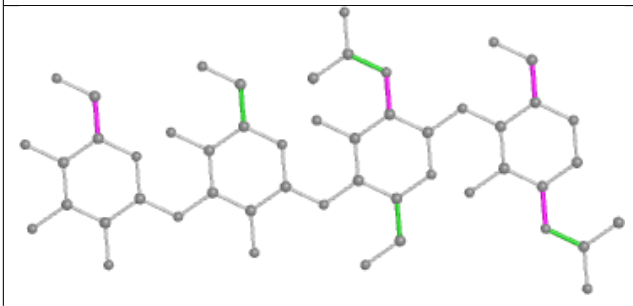
Oligosaccharide Chain C



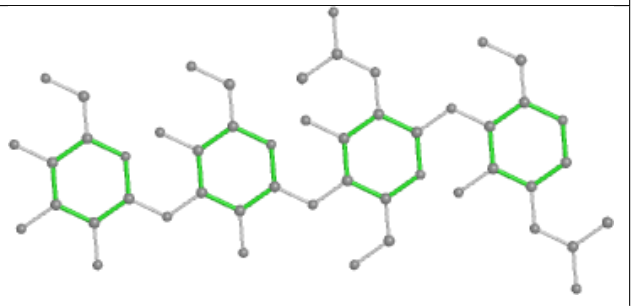
Bond lengths



Bond angles

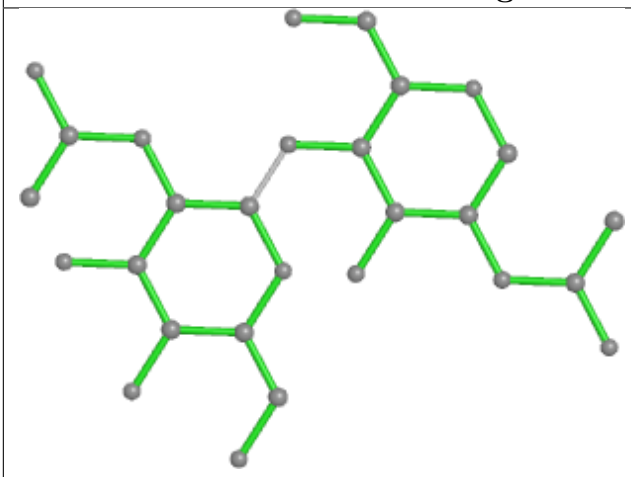


Torsions

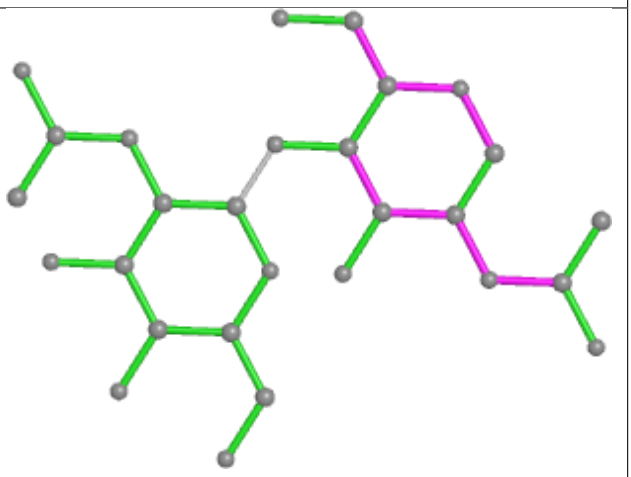


Rings

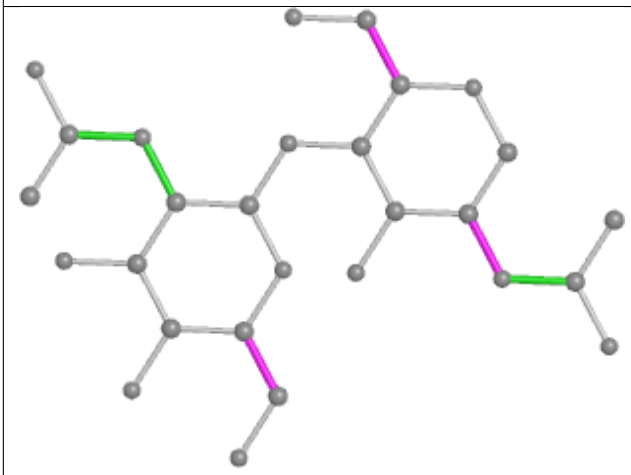
Oligosaccharide Chain F



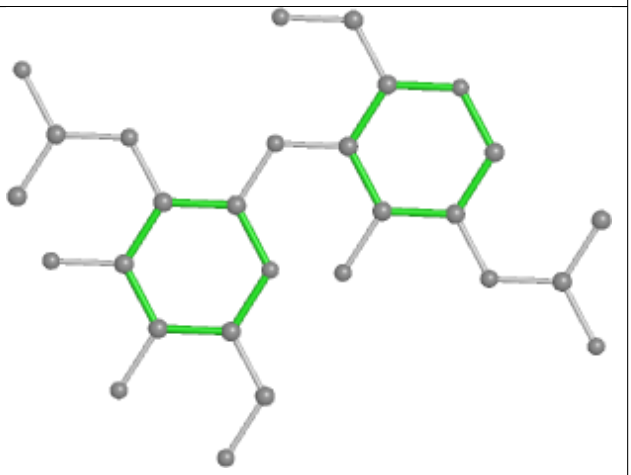
Bond lengths



Bond angles

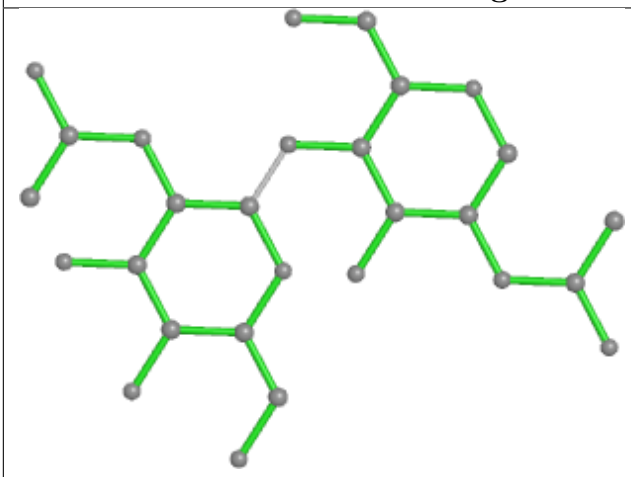


Torsions

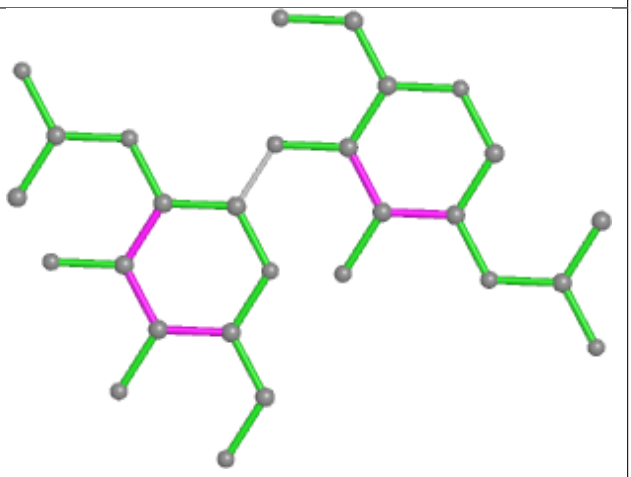


Rings

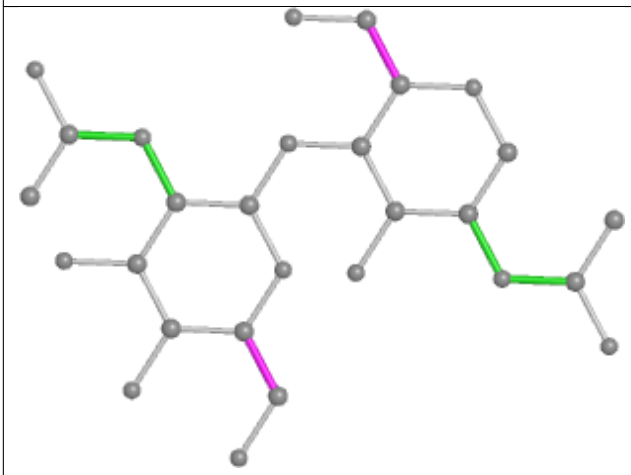
Oligosaccharide Chain M



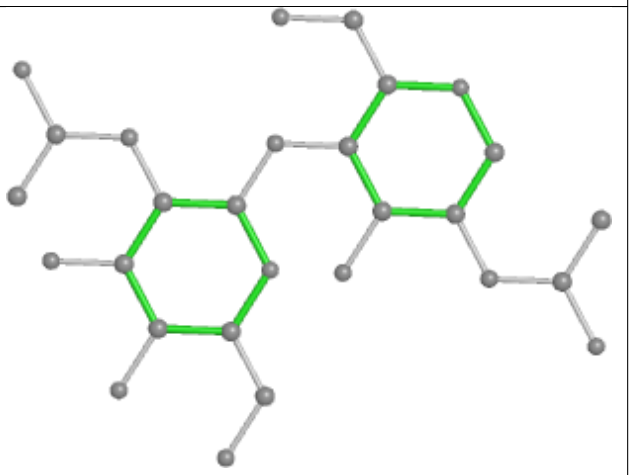
Bond lengths



Bond angles

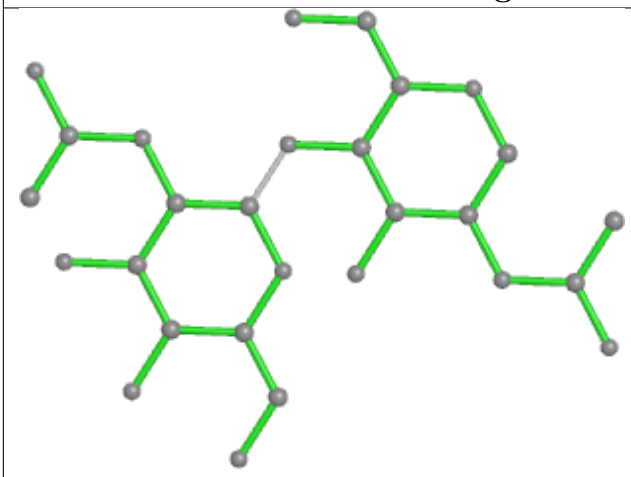


Torsions

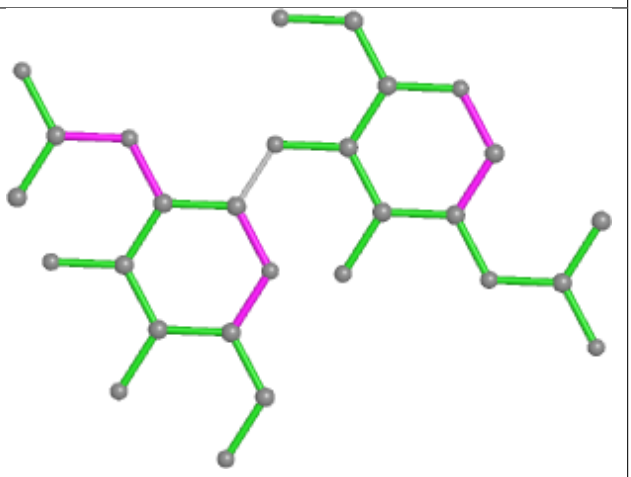


Rings

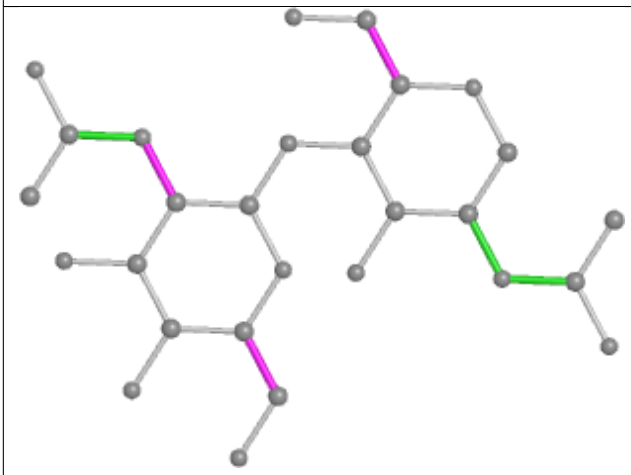
Oligosaccharide Chain O



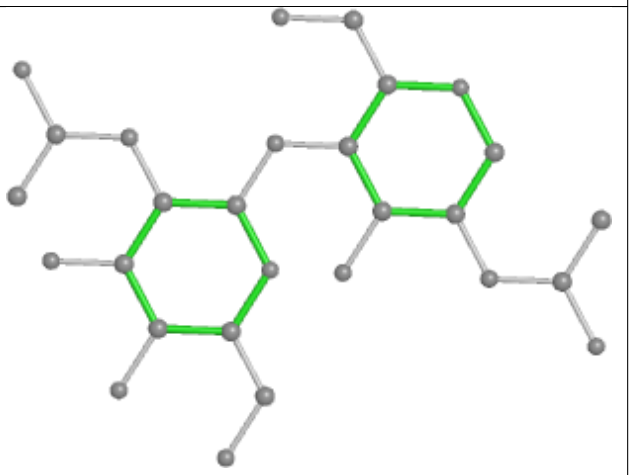
Bond lengths



Bond angles

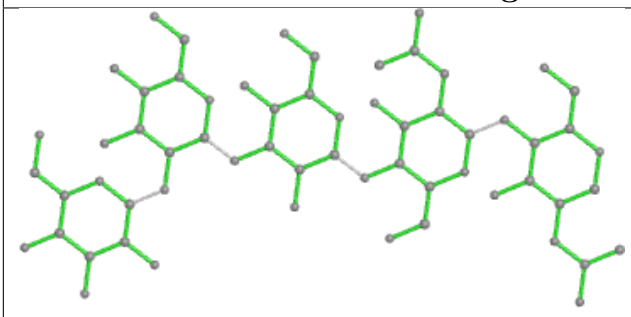


Torsions

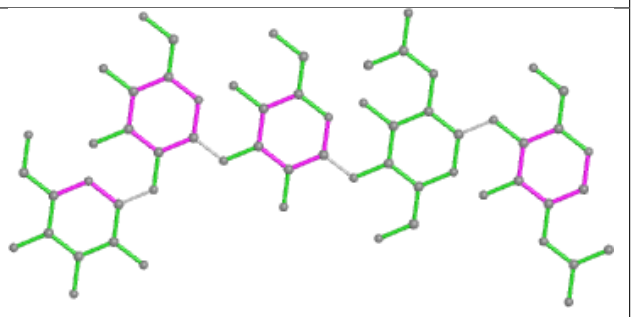


Rings

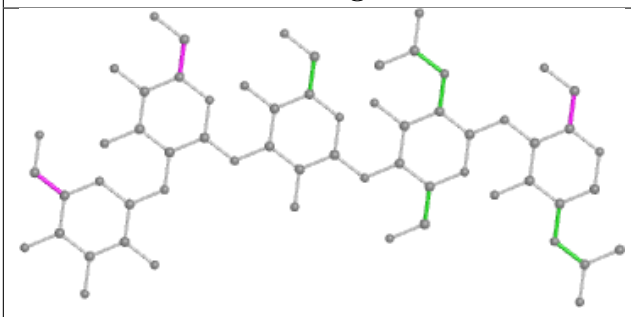
Oligosaccharide Chain I



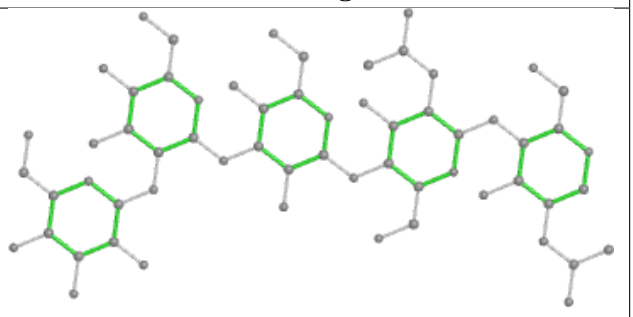
Bond lengths



Bond angles

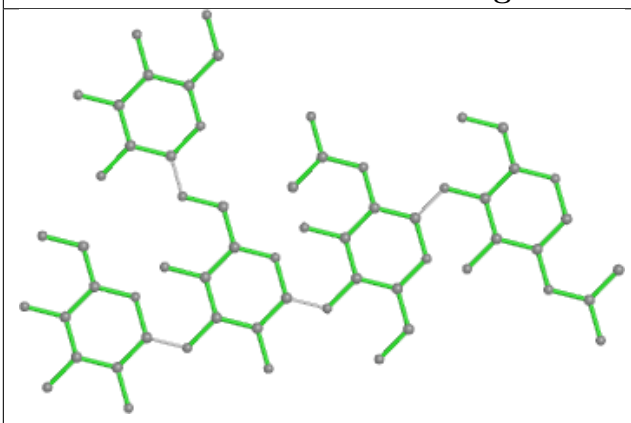


Torsions

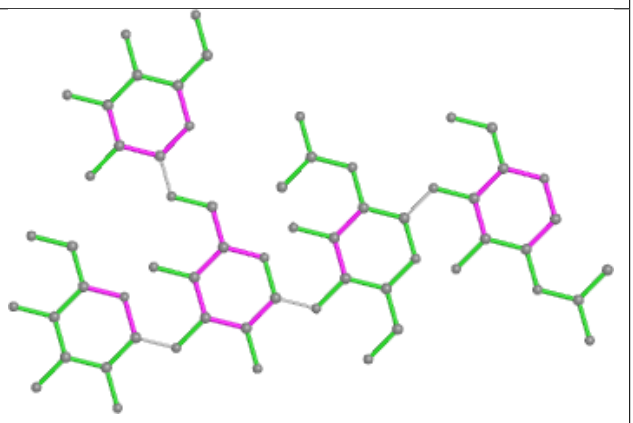


Rings

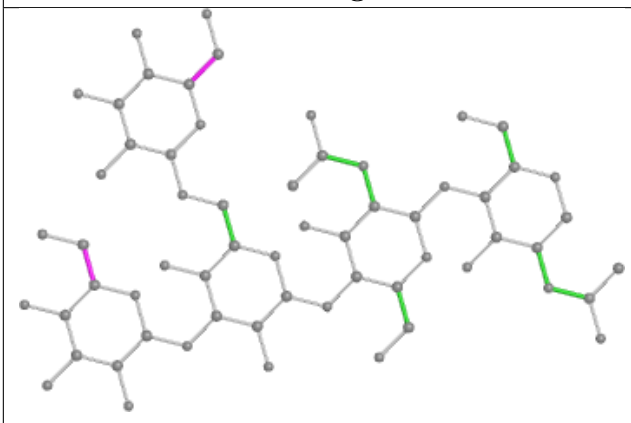
Oligosaccharide Chain K



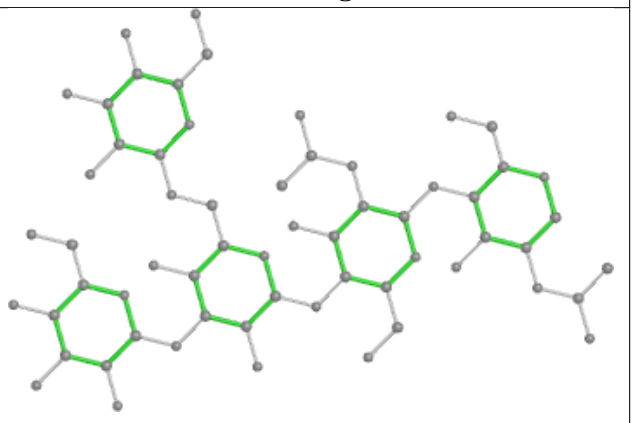
Bond lengths



Bond angles

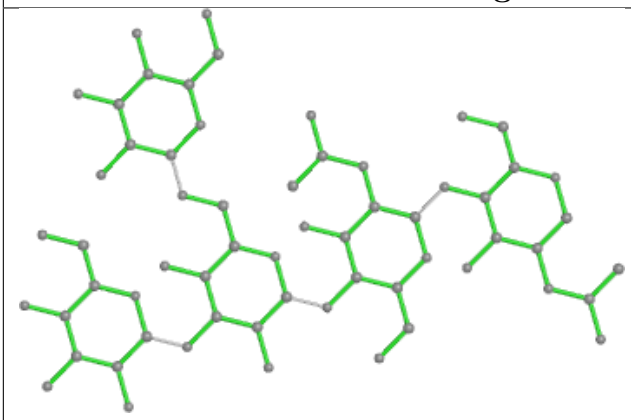


Torsions

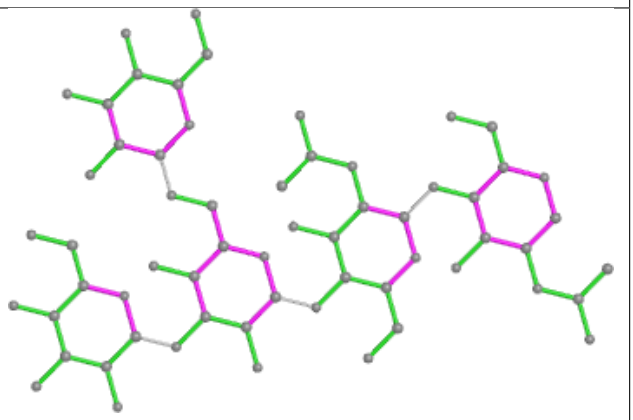


Rings

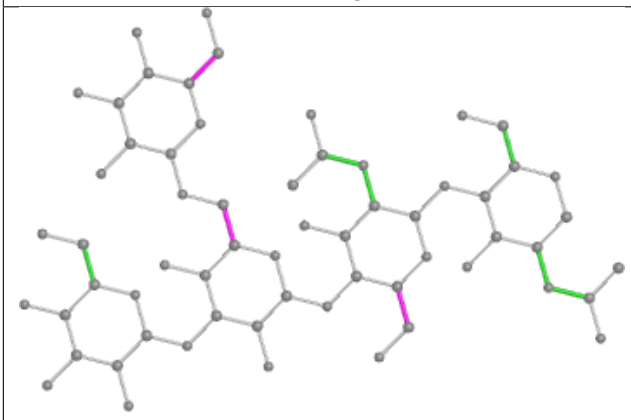
Oligosaccharide Chain N



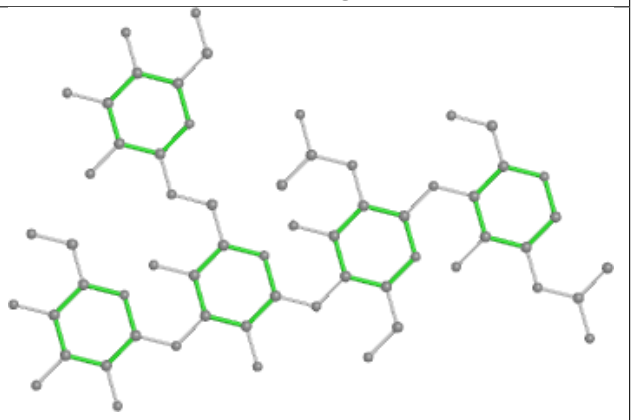
Bond lengths



Bond angles

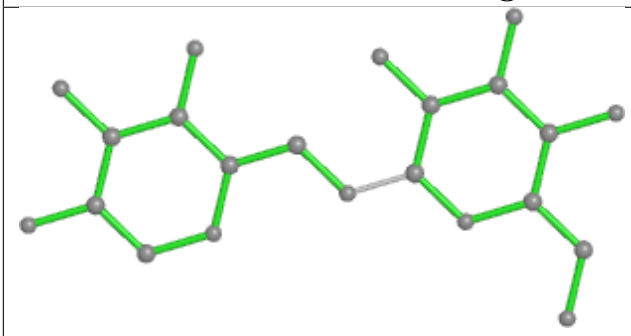


Torsions

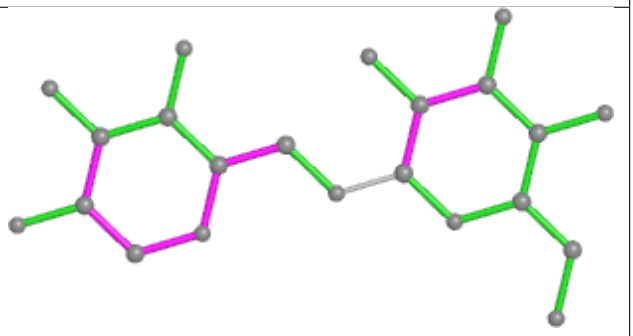


Rings

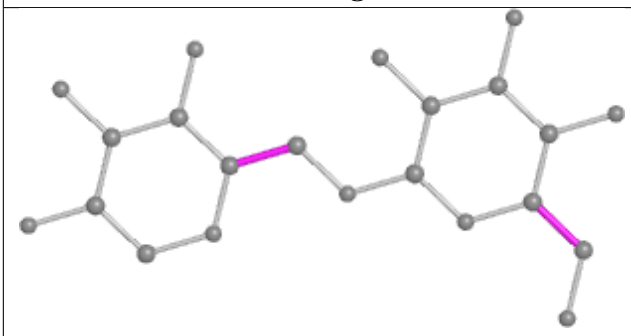
Oligosaccharide Chain J



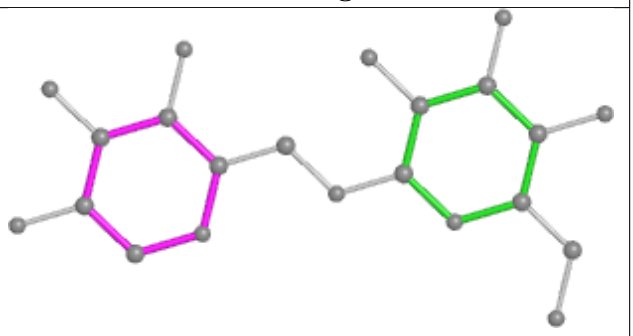
Bond lengths



Bond angles

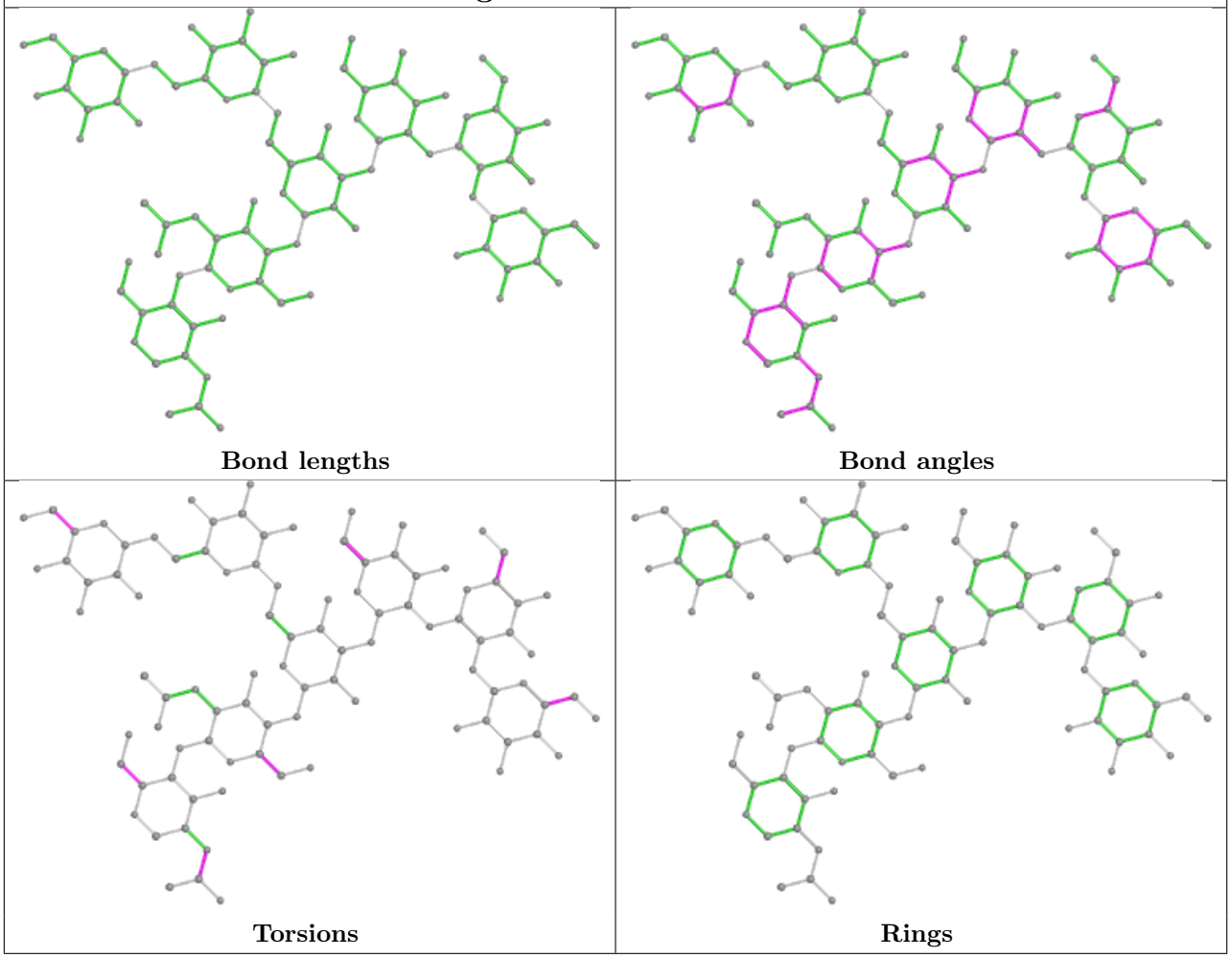


Torsions



Rings

Oligosaccharide Chain P



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	607	1	14,14,15	0.28	0	17,19,21	1.11	1 (5%)
13	NAG	G	608	1	14,14,15	0.34	0	17,19,21	0.68	0
13	NAG	G	609	-	14,14,15	0.57	0	17,19,21	1.53	2 (11%)
14	MAN	H	309	-	11,11,12	0.72	0	15,15,17	2.78	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	G	638	-	14,14,15	0.46	0	17,19,21	1.71	3 (17%)
13	NAG	B	702	2	14,14,15	0.41	0	17,19,21	0.96	1 (5%)
14	MAN	L	301	-	11,11,12	0.27	0	15,15,17	0.64	0
13	NAG	G	623	1	14,14,15	0.27	0	17,19,21	2.04	1 (5%)
13	NAG	B	701	2	14,14,15	0.32	0	17,19,21	1.24	3 (17%)

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	607	1	-	2/6/23/26	0/1/1/1
13	NAG	G	608	1	-	0/6/23/26	0/1/1/1
13	NAG	G	609	-	-	4/6/23/26	0/1/1/1
14	MAN	H	309	-	-	1/2/19/22	0/1/1/1
13	NAG	G	638	-	-	4/6/23/26	0/1/1/1
13	NAG	B	702	2	-	1/6/23/26	0/1/1/1
14	MAN	L	301	-	-	0/2/19/22	0/1/1/1
13	NAG	G	623	1	-	0/6/23/26	0/1/1/1
13	NAG	B	701	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	623	NAG	C1-O5-C5	7.35	122.15	112.19
14	H	309	MAN	C1-O5-C5	6.21	120.61	112.19
14	H	309	MAN	C3-C4-C5	4.85	118.89	110.24
14	H	309	MAN	C1-C2-C3	3.86	114.42	109.67
13	G	638	NAG	C8-C7-N2	3.77	122.48	116.10
13	G	638	NAG	C2-N2-C7	3.77	128.27	122.90
13	G	607	NAG	C1-O5-C5	3.77	117.29	112.19
14	H	309	MAN	C2-C3-C4	3.61	117.14	110.89
13	G	609	NAG	C4-C3-C2	3.43	116.04	111.02
13	G	609	NAG	O5-C1-C2	3.40	116.65	111.29
14	H	309	MAN	O5-C1-C2	3.14	115.61	110.77
13	B	702	NAG	C1-O5-C5	3.12	116.42	112.19
13	B	701	NAG	O5-C1-C2	-3.02	106.52	111.29
14	H	309	MAN	O5-C5-C4	2.77	117.58	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	638	NAG	C1-C2-N2	-2.58	106.07	110.49
13	B	701	NAG	C1-O5-C5	2.23	115.22	112.19
13	B	701	NAG	C3-C4-C5	2.20	114.16	110.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	609	NAG	O5-C5-C6-O6
13	G	638	NAG	O5-C5-C6-O6
13	G	638	NAG	C8-C7-N2-C2
13	G	638	NAG	O7-C7-N2-C2
14	H	309	MAN	O5-C5-C6-O6
13	G	607	NAG	C4-C5-C6-O6
13	G	609	NAG	C4-C5-C6-O6
13	G	607	NAG	O5-C5-C6-O6
13	G	638	NAG	C4-C5-C6-O6
13	G	609	NAG	C1-C2-N2-C7
13	B	702	NAG	O5-C5-C6-O6
13	G	609	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	609	NAG	1	0
14	H	309	MAN	5	0
14	L	301	MAN	5	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	G	439/497 (88%)	0.13	10 (2%)	60	50	141, 227, 301, 363	0
2	B	131/153 (85%)	0.14	2 (1%)	73	64	149, 207, 302, 318	0
3	L	210/214 (98%)	-0.01	5 (2%)	59	48	204, 251, 289, 313	0
4	H	231/236 (97%)	0.25	18 (7%)	13	10	194, 267, 332, 358	0
5	D	229/240 (95%)	0.31	13 (5%)	23	19	189, 275, 369, 419	0
6	E	213/216 (98%)	0.19	17 (7%)	12	10	209, 282, 373, 405	0
All	All	1453/1556 (93%)	0.17	65 (4%)	33	27	141, 250, 346, 419	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	178	SER	6.1
6	E	148	VAL	5.4
6	E	147	ALA	5.3
4	H	119	VAL	5.2
5	D	90	TYR	4.3
4	H	101	TRP	4.3
6	E	184	LEU	4.3
4	H	100(P)	MET	4.3
6	E	210	VAL	4.1
2	B	567	GLN	4.0
3	L	176	SER	3.9
1	G	253	PRO	3.8
4	H	177	SER	3.6
5	D	182	VAL	3.6
4	H	138	CYS	3.6
5	D	80	MET	3.5
1	G	468	PHE	3.4
4	H	117	PRO	3.4
3	L	47	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	73	CYS	3.2
4	H	95	ALA	3.2
6	E	116	ASN	3.2
5	D	180	SER	3.1
5	D	109	LEU	3.1
4	H	139	LEU	3.0
6	E	38	TYR	3.0
5	D	152	VAL	3.0
5	D	137	ALA	2.9
5	D	194	TYR	2.9
1	G	333	ILE	2.9
4	H	105	THR	2.8
6	E	207	GLU	2.8
3	L	37	GLN	2.8
6	E	119	VAL	2.8
1	G	358	THR	2.7
1	G	69	TRP	2.7
4	H	128	SER	2.7
5	D	127	SER	2.7
6	E	117	PRO	2.6
4	H	150	VAL	2.6
6	E	201	HIS	2.6
3	L	36	TYR	2.6
5	D	181	VAL	2.5
4	H	120	PHE	2.5
6	E	209	THR	2.5
5	D	147	PRO	2.5
3	L	133	LEU	2.4
5	D	82	ILE	2.4
1	G	140	THR	2.3
1	G	277	ILE	2.3
4	H	50	TYR	2.3
1	G	359	ILE	2.2
6	E	199	VAL	2.2
6	E	189	TRP	2.2
5	D	126	PRO	2.1
6	E	114	LYS	2.1
1	G	478	ASN	2.1
6	E	146	GLY	2.1
4	H	100(Q)	ASP	2.1
6	E	139	LEU	2.1
2	B	664	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
4	H	69	ILE	2.0
4	H	100(G)	PHE	2.0
6	E	158	PRO	2.0
4	H	209	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BMA	C	3	11/12	0.27	0.24	342,370,383,396	0
7	MAN	A	4	11/12	0.68	0.72	251,273,279,289	0
9	NAG	F	1	14/15	0.70	0.35	216,239,282,283	0
8	MAN	C	4	11/12	0.74	0.30	287,316,336,348	0
9	NAG	F	2	14/15	0.76	0.27	264,279,298,300	0
10	BMA	K	3	11/12	0.79	0.15	342,352,360,363	0
10	MAN	I	5	11/12	0.81	0.17	300,309,314,315	0
7	NAG	A	2	14/15	0.82	0.46	193,203,211,212	0
10	MAN	K	4	11/12	0.83	0.21	314,335,343,351	0
8	NAG	C	2	14/15	0.84	0.23	292,309,328,347	0
10	MAN	K	5	11/12	0.84	0.21	334,339,344,347	0
10	MAN	N	5	11/12	0.84	0.18	304,312,322,328	0
9	NAG	M	1	14/15	0.85	0.23	231,252,266,278	0
10	BMA	N	3	11/12	0.86	0.07	299,307,324,329	0
10	NAG	K	1	14/15	0.86	0.21	225,244,263,273	0
10	NAG	K	2	14/15	0.87	0.25	294,312,331,347	0
11	MAN	J	2	11/12	0.87	0.11	308,319,330,331	0
10	NAG	N	2	14/15	0.88	0.13	277,305,312,322	0
10	MAN	N	4	11/12	0.88	0.12	297,314,317,319	0
9	NAG	O	2	14/15	0.89	0.12	265,292,305,307	0
7	BMA	A	3	11/12	0.89	0.37	192,212,234,238	0
8	NAG	C	1	14/15	0.89	0.21	242,274,293,299	0
12	MAN	P	8	11/12	0.89	0.42	218,247,254,264	0
12	NAG	P	1	14/15	0.90	0.24	199,221,236,240	0

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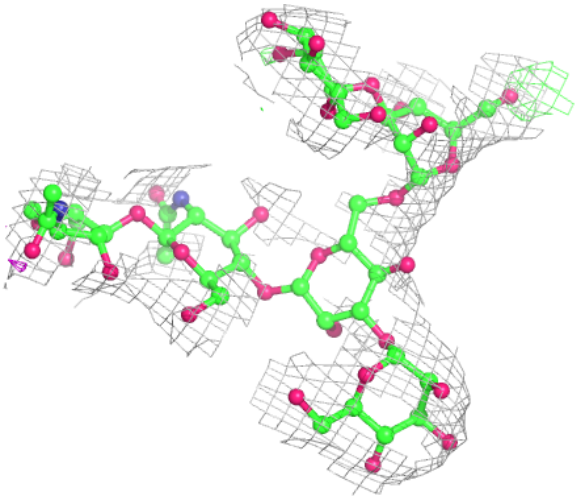
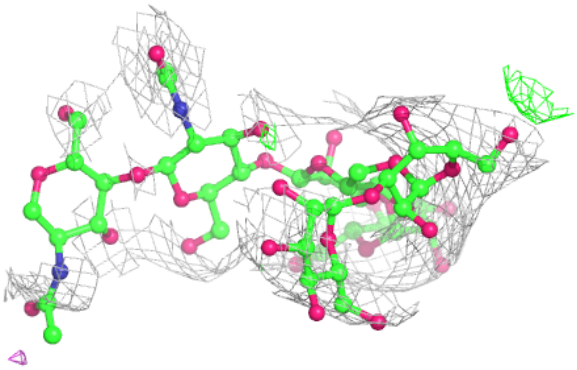
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	M	2	14/15	0.90	0.25	270,286,300,307	0
7	NAG	A	1	14/15	0.91	0.35	170,187,196,197	0
11	MAN	J	1	11/12	0.92	0.10	292,311,325,332	0
10	BMA	I	3	11/12	0.92	0.12	297,306,317,325	0
10	NAG	N	1	14/15	0.92	0.22	218,242,251,270	0
12	MAN	P	5	11/12	0.92	0.14	207,219,228,232	0
7	MAN	A	5	11/12	0.92	0.75	258,292,302,319	0
12	MAN	P	6	11/12	0.93	0.18	227,229,235,240	0
12	MAN	P	7	11/12	0.94	0.20	246,254,259,267	0
10	NAG	I	1	14/15	0.94	0.24	159,212,239,243	0
12	MAN	P	4	11/12	0.95	0.18	188,197,207,214	0
10	MAN	I	4	11/12	0.95	0.08	287,303,311,320	0
9	NAG	O	1	14/15	0.95	0.13	289,295,310,314	0
7	MAN	A	6	11/12	0.95	0.43	223,225,234,237	0
12	BMA	P	3	11/12	0.95	0.21	207,215,231,235	0
10	NAG	I	2	14/15	0.96	0.16	246,261,274,291	0
12	NAG	P	2	14/15	0.96	0.17	188,207,219,222	0

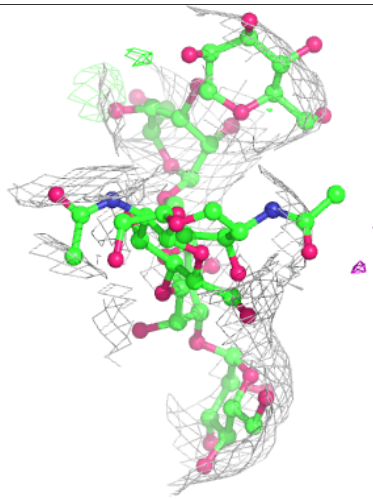
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

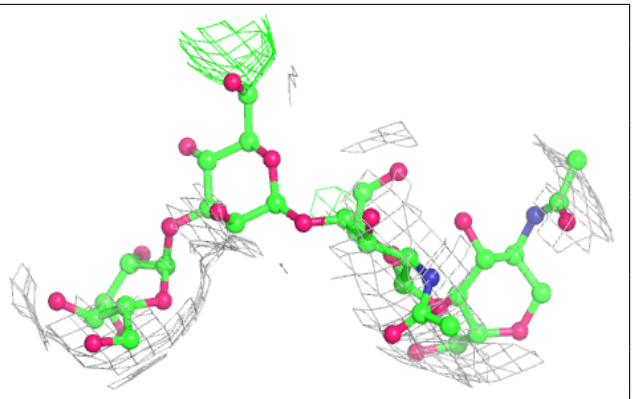


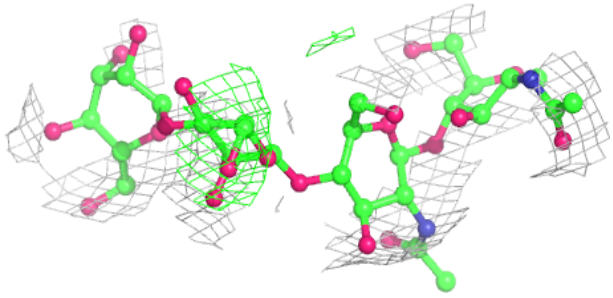


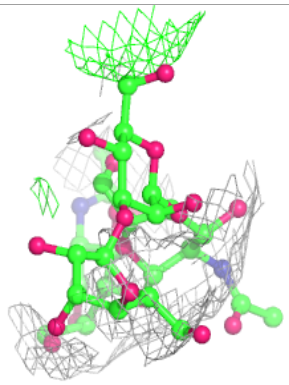


Electron density around Chain C:

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

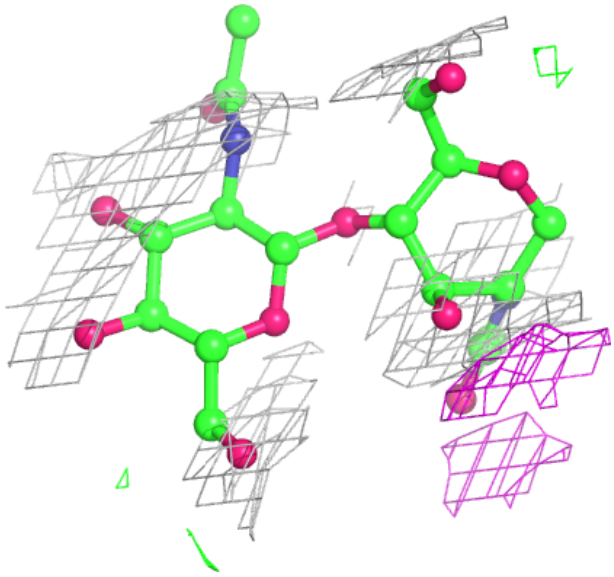


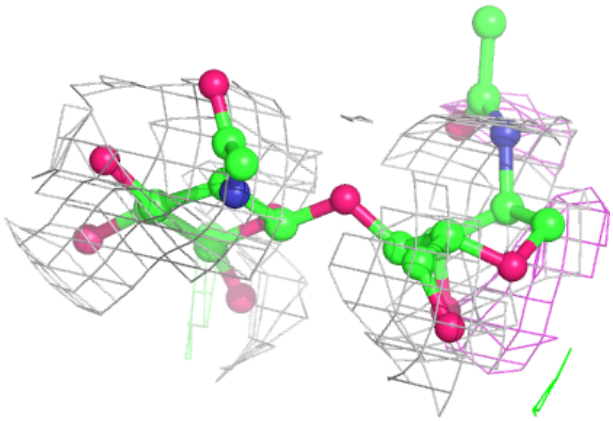


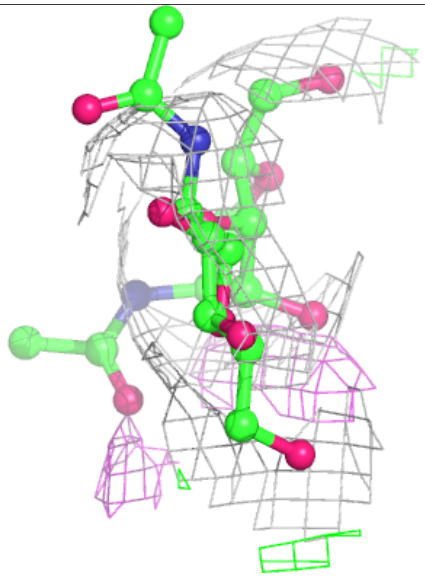


Electron density around Chain F:

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

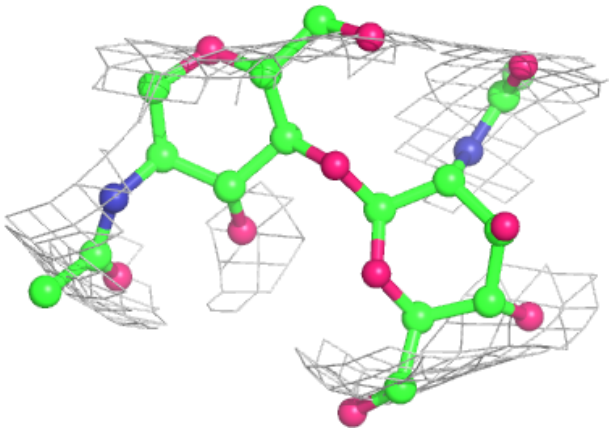


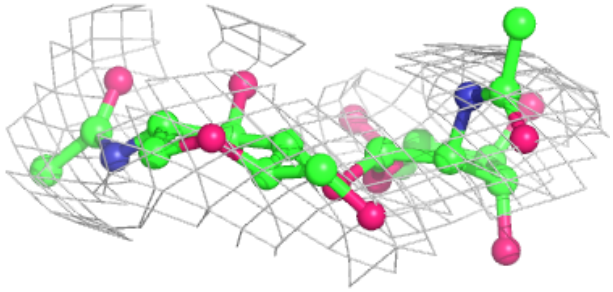


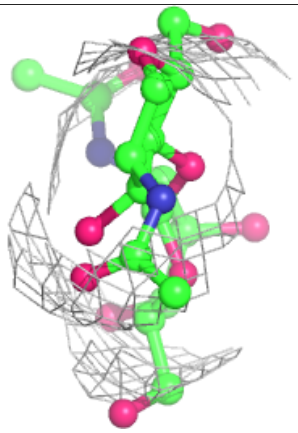


Electron density around Chain M:

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

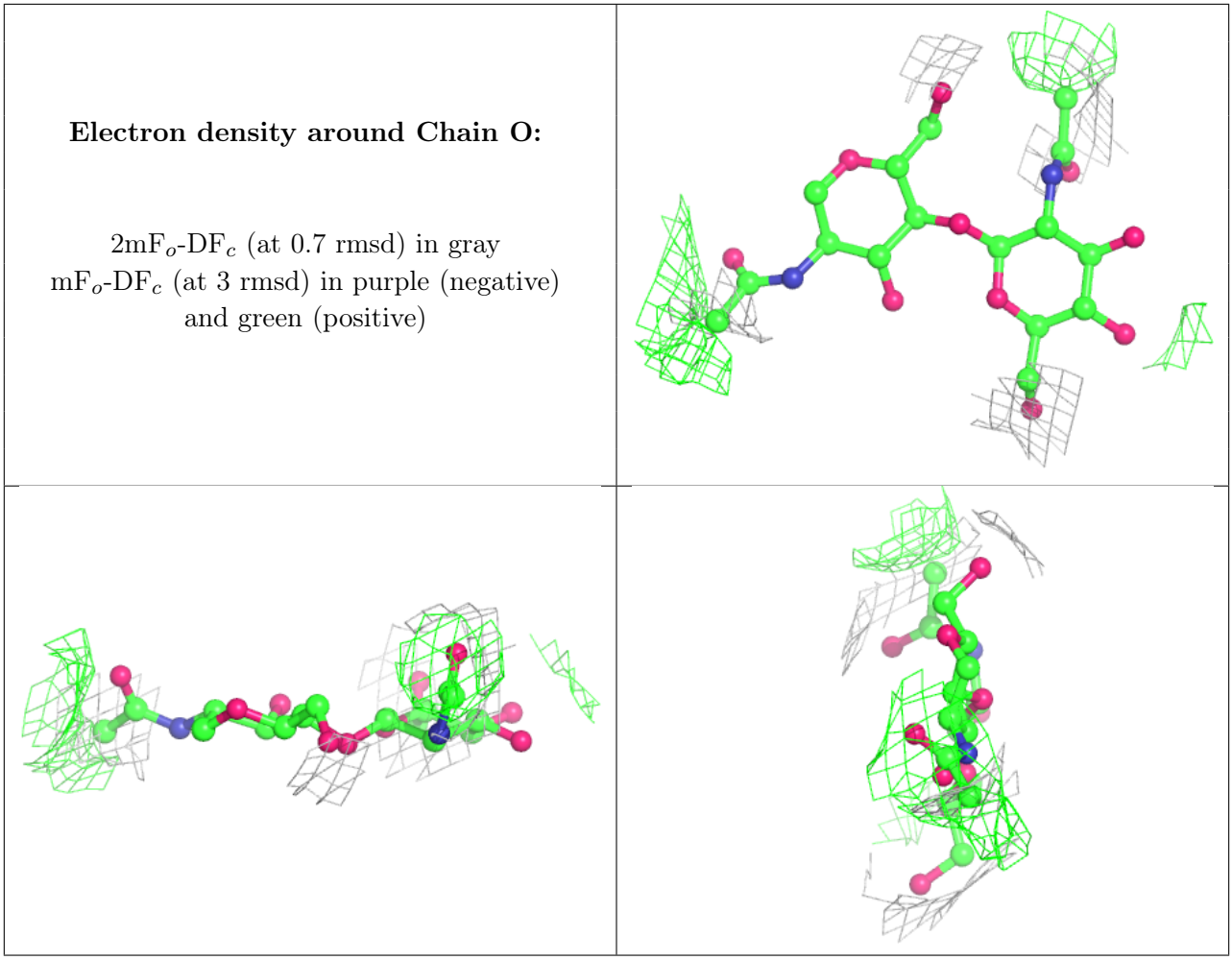






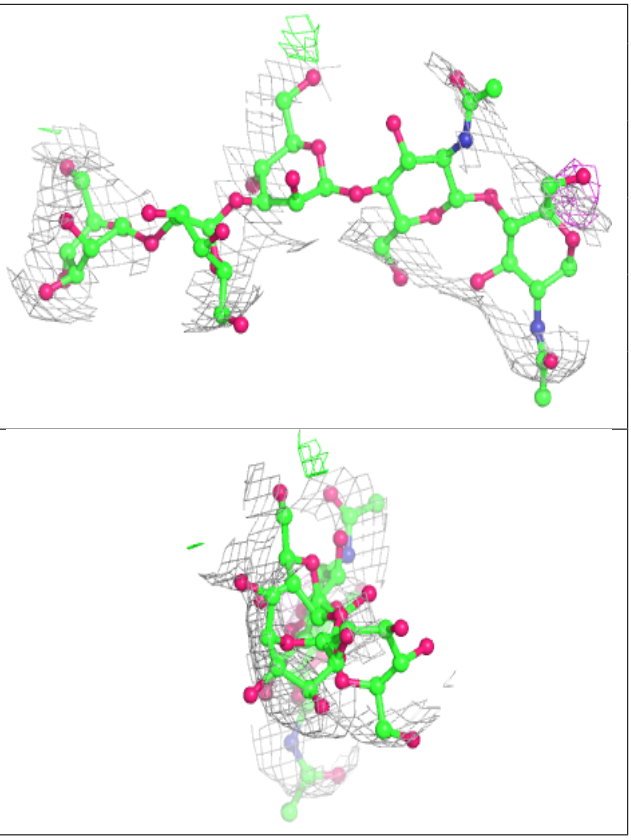
Electron density around Chain O:

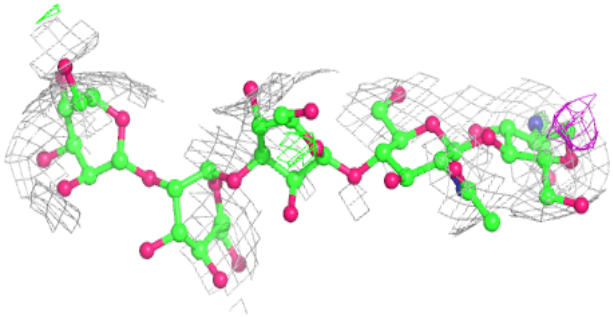
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain I:

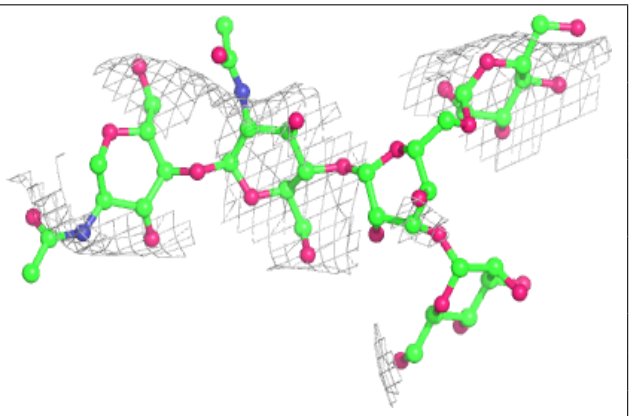
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

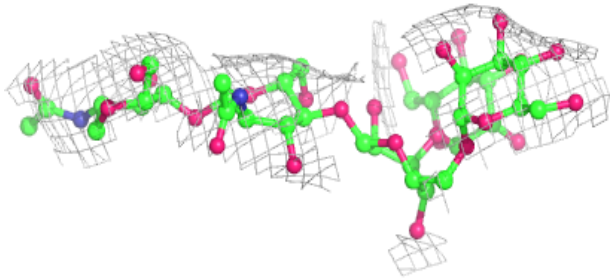


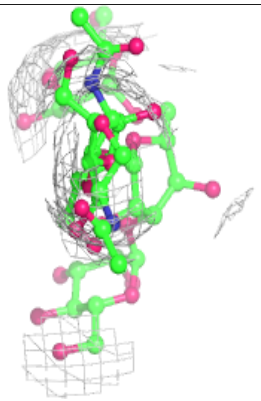


Electron density around Chain K:

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

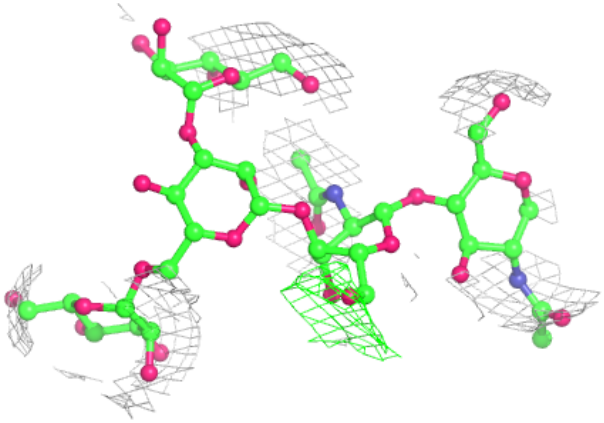


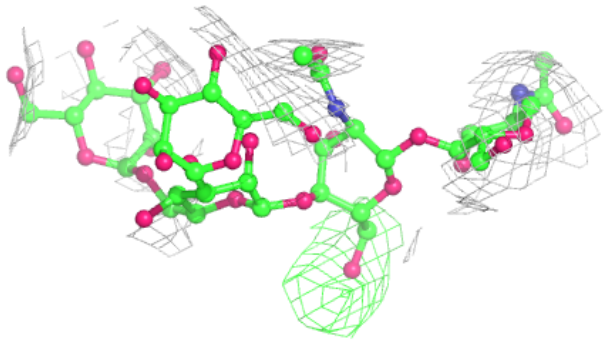


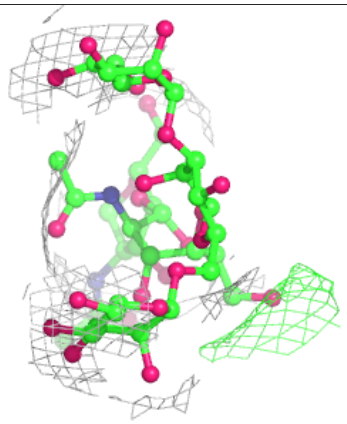


Electron density around Chain N:

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

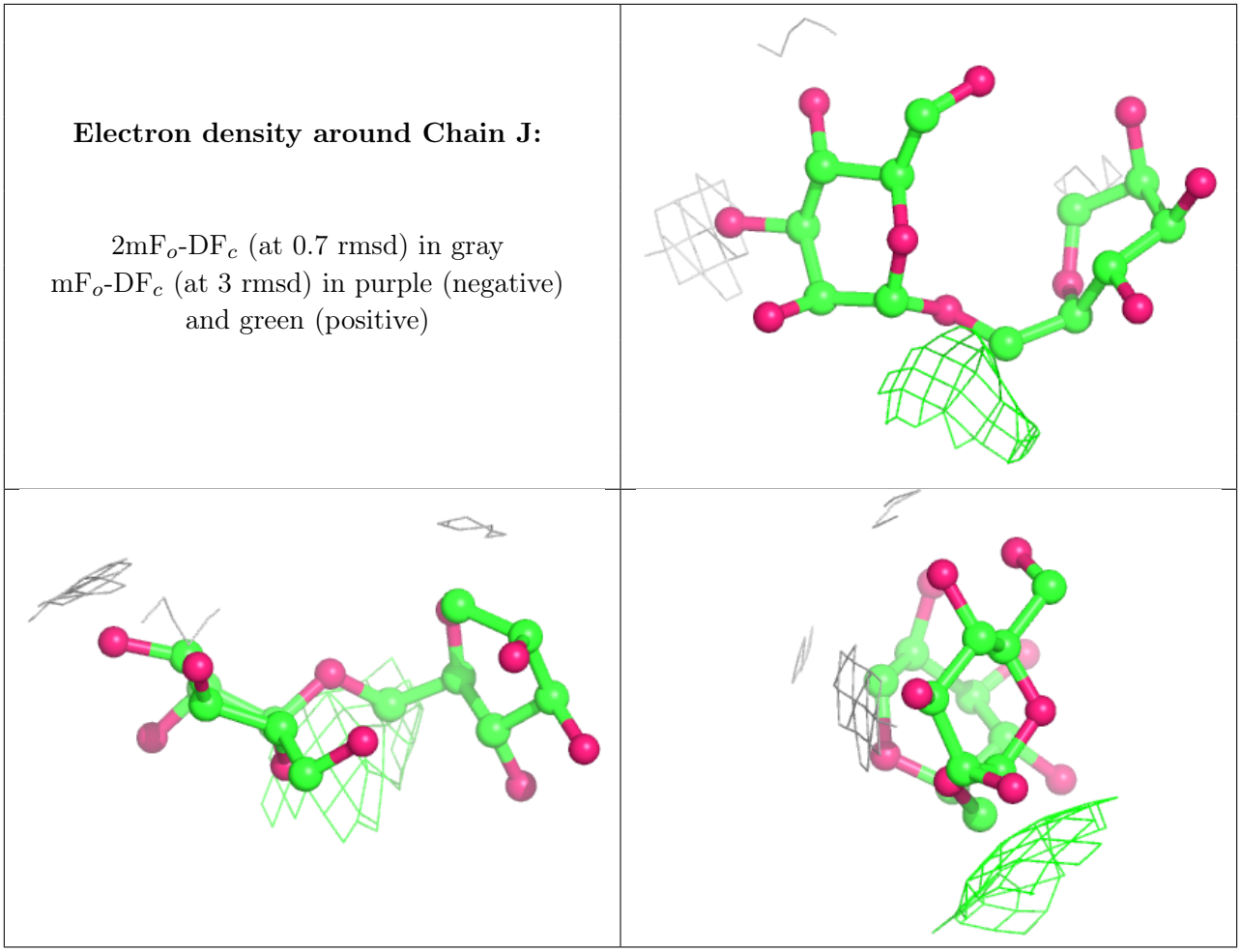






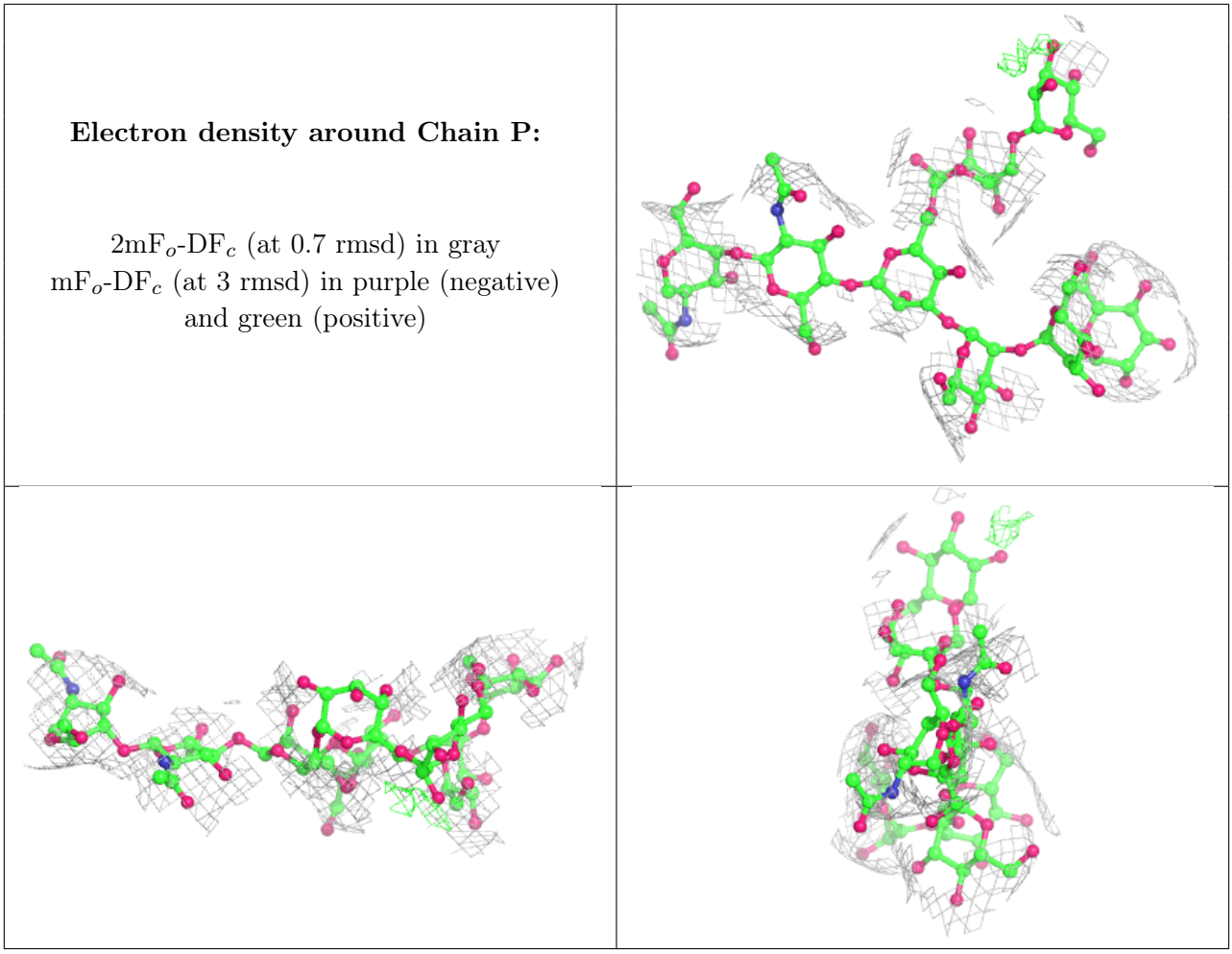
Electron density around Chain J:

$2mF_o$-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 P:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	NAG	B	702	14/15	0.51	0.30	289,323,338,343	0
13	NAG	G	608	14/15	0.81	0.16	245,264,284,288	0
14	MAN	H	309	11/12	0.81	0.21	248,257,279,287	0
13	NAG	G	638	14/15	0.86	0.32	209,222,231,235	0
13	NAG	G	609	14/15	0.88	0.20	218,245,253,254	0
14	MAN	L	301	11/12	0.89	0.27	283,290,296,300	0
13	NAG	B	701	14/15	0.90	0.28	269,284,294,301	0
13	NAG	G	607	14/15	0.91	0.18	253,262,281,306	0
13	NAG	G	623	14/15	0.93	0.28	263,292,303,308	0

6.5 Other polymers (i)

There are no such residues in this entry.