Full wwPDB X-ray Structure Validation Report

Jun 17, 2024 – 12:20 PM EDT

PDB ID	:	8TXP
Title	:	Crystal structure of 05.GC.w13.01 Fab in complex with H1 HA from A/California/04/2009(H1N1)
Authors	:	Lin, T.H.; Moore, N.; Wilson, I.A.
Deposited on	:	2023-08-24
Resolution	:	2.75 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:

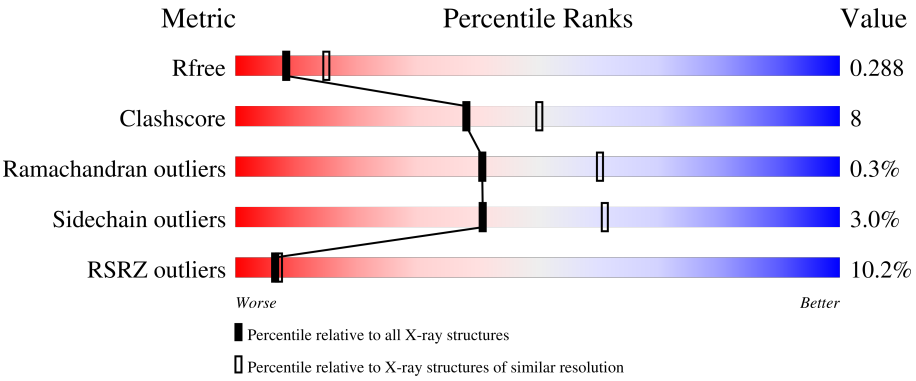
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	A	331	2% 76% 21%
2	B	177	86% 11%
3	H	225	14% 83% 17%
4	L	214	27% 78% 22%
5	C	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	D	2	100%
6	E	3	33% 67%
6	F	3	100%
6	G	3	100%

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
5	NAG	C	2	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7404 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2544	1610	438	485	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP C3W5S1
A	8	ASP	-	expression tag	UNP C3W5S1
A	9	PRO	-	expression tag	UNP C3W5S1
A	10	GLY	-	expression tag	UNP C3W5S1

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP I1ZFF9
B	176	GLY	-	expression tag	UNP I1ZFF9
B	177	ARG	-	expression tag	UNP I1ZFF9

- Molecule 3 is a protein called GC_w13_A, Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	224	Total	C	N	O	S	0	0	0
			1644	1037	277	322	8			

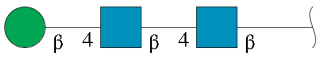
- Molecule 4 is a protein called GC_w13_A, Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1637	1019	276	337	5			

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

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

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



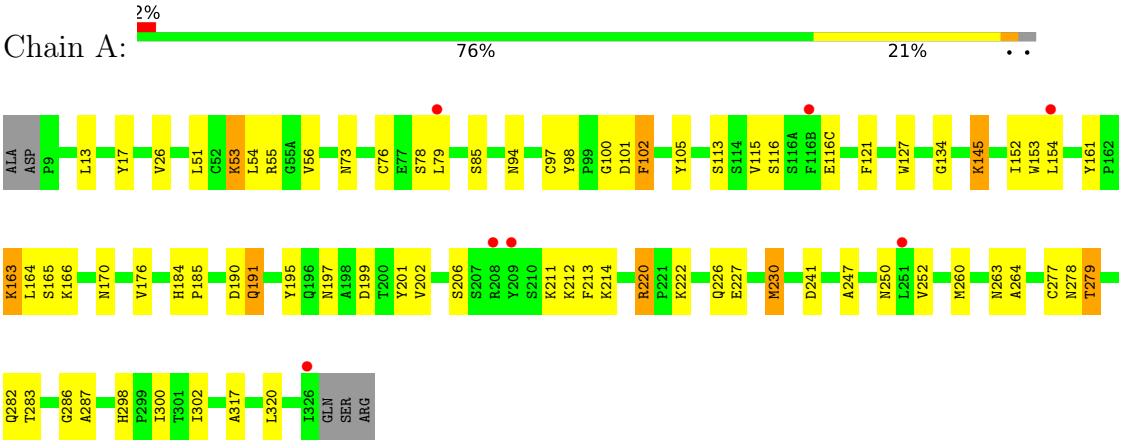
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

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.

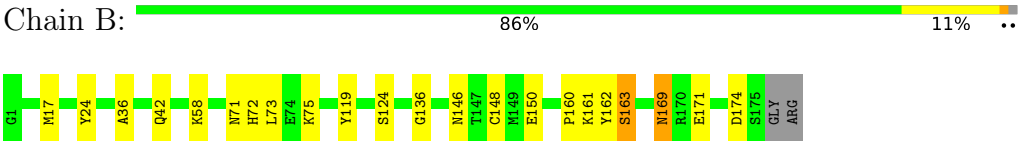
• Molecule 1: Hemagglutinin

Chain A:



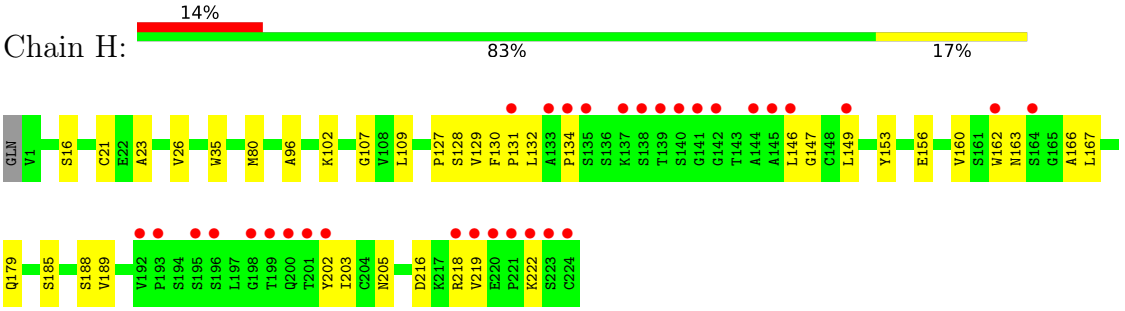
• Molecule 2: Hemagglutinin

Chain B:



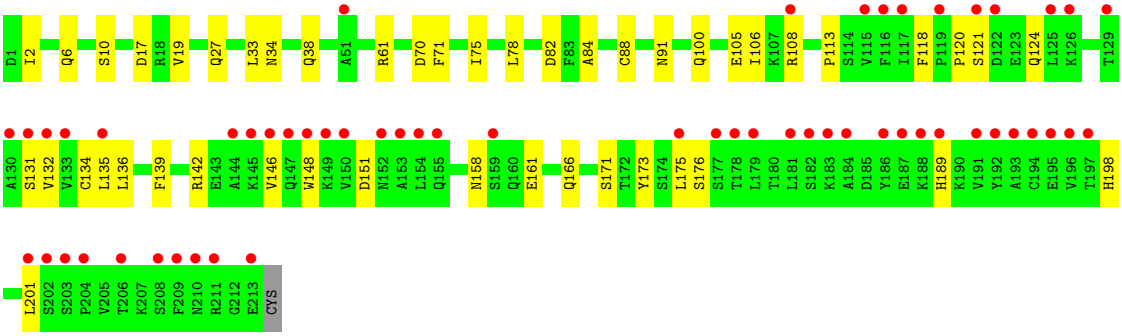
• Molecule 3: GC_w13_A, Fab heavy chain

Chain H:



• Molecule 4: GC_w13_A, Fab light chain

Chain L:

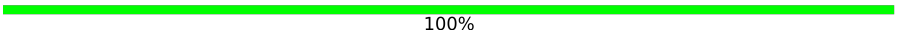


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain D:

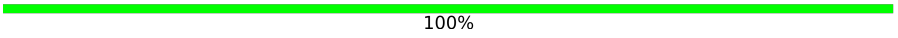


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

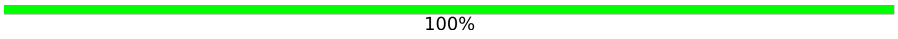
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.35Å 128.35Å 155.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.24 – 2.75 49.53 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.24-2.75) 99.8 (49.53-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.250 , 0.292 0.246 , 0.288	Depositor DCC
R_{free} test set	1963 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	77.8	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7404	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, 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	A	0.26	0/2609	0.52	0/3546
2	B	0.25	0/1434	0.42	0/1932
3	H	0.26	0/1680	0.53	0/2289
4	L	0.26	0/1671	0.51	0/2269
All	All	0.26	0/7394	0.50	0/10036

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2544	0	2494	48	0
2	B	1406	0	1327	11	0
3	H	1644	0	1643	25	0
4	L	1637	0	1584	32	0
5	C	28	0	25	0	0
5	D	28	0	25	0	0
6	E	39	0	34	3	0
6	F	39	0	34	0	0
6	G	39	0	34	0	0
All	All	7404	0	7200	111	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 (111) 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:L:105:GLU:OE2	4:L:142:ARG:NH2	2.04	0.90
1:A:98:TYR:CE2	1:A:226:GLN:HG2	2.15	0.81
4:L:108:ARG:HG3	4:L:171:SER:HB2	1.67	0.76
1:A:97:CYS:HB3	6:E:1:NAG:H81	1.70	0.74
3:H:203:ILE:HG22	3:H:218:ARG:HG2	1.72	0.71
2:B:171:GLU:HA	2:B:174:ASP:HB2	1.77	0.66
3:H:127:PRO:HB3	3:H:153:TYR:HB3	1.78	0.66
3:H:163:ASN:HB3	3:H:166:ALA:HB3	1.80	0.64
1:A:164:LEU:HB3	1:A:247:ALA:H	1.60	0.64
4:L:151:ASP:OD2	4:L:189:HIS:ND1	2.33	0.62
1:A:184:HIS:HB3	1:A:220:ARG:HH22	1.64	0.62
4:L:120:PRO:HD3	4:L:132:VAL:HG22	1.84	0.60
1:A:94:ASN:HD22	6:E:1:NAG:H83	1.66	0.60
3:H:162:TRP:HE1	3:H:202:TYR:HB3	1.67	0.59
1:A:282:GLN:NE2	1:A:286:GLY:O	2.36	0.59
1:A:222:LYS:HG3	1:A:227:GLU:HG3	1.84	0.59
1:A:56:VAL:O	1:A:85:SER:OG	2.21	0.59
1:A:230:MET:SD	1:A:252:VAL:HG21	2.43	0.59
4:L:19:VAL:HG21	4:L:78:LEU:HD23	1.83	0.58
3:H:160:VAL:HG21	3:H:188:SER:HB2	1.84	0.57
1:A:185:PRO:HG2	1:A:191:GLN:HG2	1.85	0.57
6:E:2:NAG:H83	6:E:2:NAG:H3	1.86	0.56
3:H:203:ILE:CG2	3:H:218:ARG:HG2	2.34	0.56
4:L:106:ILE:HG13	4:L:166:GLN:NE2	2.21	0.55
4:L:61:ARG:NE	4:L:82:ASP:OD2	2.32	0.55
3:H:134:PRO:HB3	3:H:146:LEU:HB3	1.90	0.54
1:A:98:TYR:HE2	1:A:226:GLN:HG2	1.67	0.54
1:A:278:ASN:O	1:A:279:THR:HG22	2.07	0.54
3:H:23:ALA:HB3	3:H:26:VAL:HG21	1.89	0.53
3:H:146:LEU:HD13	3:H:219:VAL:HG11	1.90	0.52
3:H:162:TRP:HB3	3:H:167:LEU:HB3	1.89	0.52
3:H:189:VAL:HG11	4:L:135:LEU:HD22	1.90	0.52
1:A:53:LYS:HG2	1:A:277:CYS:O	2.11	0.51
1:A:115:VAL:HG11	1:A:260:MET:HE2	1.92	0.51
1:A:76:CYS:HB3	1:A:79:LEU:HD12	1.93	0.51
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.93	0.51
1:A:127:TRP:CZ3	1:A:164:LEU:HD21	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:35:TRP:CE2	3:H:80:MET:HB2	2.46	0.51
3:H:96:ALA:HB1	3:H:109:LEU:HB3	1.93	0.51
2:B:161:LYS:HD3	2:B:162:TYR:CE2	2.46	0.50
1:A:26:VAL:HG21	1:A:317:ALA:HB2	1.92	0.50
1:A:13:LEU:HD11	2:B:24:TYR:HB3	1.92	0.50
1:A:145:LYS:N	1:A:145:LYS:HD2	2.27	0.50
4:L:105:GLU:OE2	4:L:173:TYR:OH	2.29	0.50
4:L:161:GLU:HB3	4:L:175:LEU:HD11	1.93	0.50
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.52	0.49
3:H:107:GLY:HA3	4:L:91:ASN:HB2	1.93	0.49
1:A:202:VAL:HG13	1:A:247:ALA:HB2	1.94	0.49
1:A:206:SER:OG	1:A:241:ASP:OD2	2.31	0.49
3:H:131:PRO:O	4:L:121:SER:OG	2.31	0.48
4:L:108:ARG:HG3	4:L:171:SER:CB	2.40	0.48
3:H:205:ASN:ND2	3:H:216:ASP:OD2	2.45	0.48
4:L:113:PRO:HD2	4:L:201:LEU:HD13	1.96	0.48
4:L:2:ILE:HG12	4:L:27:GLN:HG2	1.95	0.48
4:L:113:PRO:HD3	4:L:198:HIS:ND1	2.29	0.48
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.49	0.48
4:L:136:LEU:HD13	4:L:175:LEU:HG	1.96	0.48
4:L:6:GLN:O	4:L:100:GLN:NE2	2.44	0.47
1:A:214:LYS:HB3	1:A:214:LYS:HE3	1.57	0.47
1:A:199:ASP:OD1	1:A:214:LYS:NZ	2.44	0.47
3:H:128:SER:HB3	3:H:130:PHE:CE1	2.50	0.47
4:L:33:LEU:HD11	4:L:88:CYS:HB2	1.97	0.47
4:L:33:LEU:HD22	4:L:71:PHE:CG	2.50	0.47
3:H:179:GLN:NE2	3:H:185:SER:OG	2.47	0.46
4:L:124:GLN:OE1	4:L:131:SER:HB2	2.15	0.46
3:H:162:TRP:CD1	3:H:167:LEU:HD23	2.50	0.46
1:A:102:PHE:HB3	1:A:105:TYR:HB2	1.98	0.45
2:B:71:ASN:OD1	2:B:73:LEU:N	2.46	0.45
3:H:129:VAL:C	3:H:130:PHE:HD1	2.20	0.45
1:A:100:GLY:HA3	1:A:230:MET:O	2.16	0.45
4:L:19:VAL:HB	4:L:75:ILE:HB	1.99	0.45
1:A:51:LEU:HD23	1:A:282:GLN:NE2	2.32	0.44
1:A:121:PHE:CE1	1:A:166:LYS:HG3	2.53	0.44
1:A:283:THR:OG1	1:A:298:HIS:HB3	2.17	0.44
1:A:211:LYS:HG3	1:A:213:PHE:CE1	2.52	0.44
4:L:33:LEU:HG	4:L:34:ASN:N	2.33	0.44
2:B:169:ASN:OD1	2:B:169:ASN:N	2.51	0.44
3:H:132:LEU:HD21	3:H:149:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:HG22	1:A:154:LEU:HD22	2.00	0.44
1:A:195:TYR:O	1:A:197:ASN:N	2.49	0.43
1:A:191:GLN:NE2	1:A:250:ASN:OD1	2.51	0.43
2:B:17:MET:CE	2:B:36:ALA:HA	2.48	0.43
3:H:130:PHE:CE2	4:L:124:GLN:HA	2.54	0.43
1:A:116:SER:OG	1:A:263:ASN:HB2	2.18	0.43
2:B:146:ASN:O	2:B:150:GLU:HG2	2.18	0.43
4:L:38:GLN:O	4:L:84:ALA:HB1	2.18	0.43
3:H:132:LEU:HB3	4:L:118:PHE:CD1	2.53	0.43
4:L:166:GLN:HG3	4:L:173:TYR:CZ	2.53	0.43
4:L:136:LEU:HD11	4:L:146:VAL:HG21	1.99	0.43
1:A:54:LEU:HG	1:A:55:ARG:HG3	2.01	0.42
1:A:201:TYR:HB2	1:A:212:LYS:HE3	2.01	0.42
4:L:17:ASP:N	4:L:17:ASP:OD1	2.52	0.42
1:A:164:LEU:HD13	1:A:165:SER:N	2.35	0.42
4:L:175:LEU:HD12	4:L:176:SER:N	2.35	0.42
1:A:279:THR:HG21	1:A:287:ALA:HB1	2.02	0.42
2:B:58:LYS:HD3	2:B:58:LYS:HA	1.61	0.42
3:H:156:GLU:N	3:H:156:GLU:OE1	2.52	0.42
2:B:75:LYS:HB2	2:B:75:LYS:HE3	1.90	0.42
1:A:170:ASN:ND2	1:A:176:VAL:HG23	2.35	0.41
4:L:139:PHE:HB2	4:L:198:HIS:CE1	2.55	0.41
1:A:51:LEU:HD23	1:A:282:GLN:HE21	1.85	0.41
1:A:298:HIS:CE1	1:A:300:ILE:HB	2.55	0.41
1:A:320:LEU:HD12	1:A:320:LEU:H	1.86	0.41
1:A:163:LYS:HE3	1:A:163:LYS:HB3	1.84	0.41
1:A:127:TRP:HZ3	1:A:164:LEU:HD21	1.85	0.41
2:B:160:PRO:HA	2:B:163:SER:HB3	2.02	0.41
1:A:17:TYR:HB2	1:A:320:LEU:HD22	2.02	0.40
1:A:116(C):GLU:HA	1:A:116(C):GLU:OE2	2.21	0.40
3:H:147:GLY:HA2	3:H:162:TRP:CH2	2.56	0.40
4:L:134:CYS:HB2	4:L:148:TRP:CH2	2.56	0.40
1:A:54:LEU:HD13	1:A:302:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	324/331 (98%)	311 (96%)	11 (3%)	2 (1%)	25 42
2	B	173/177 (98%)	169 (98%)	4 (2%)	0	100 100
3	H	222/225 (99%)	213 (96%)	8 (4%)	1 (0%)	29 47
4	L	211/214 (99%)	207 (98%)	4 (2%)	0	100 100
All	All	930/947 (98%)	900 (97%)	27 (3%)	3 (0%)	41 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	ALA
1	A	279	THR
3	H	222	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	286/290 (99%)	274 (96%)	12 (4%)	30 49
2	B	150/151 (99%)	144 (96%)	6 (4%)	31 51
3	H	185/186 (100%)	182 (98%)	3 (2%)	62 77
4	L	189/190 (100%)	186 (98%)	3 (2%)	62 77
All	All	810/817 (99%)	786 (97%)	24 (3%)	41 61

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	78	SER
1	A	101	ASP
1	A	102	PHE
1	A	113	SER
1	A	145	LYS
1	A	161	TYR
1	A	163	LYS
1	A	190	ASP
1	A	191	GLN
1	A	220	ARG
1	A	230	MET
2	B	42	GLN
2	B	72	HIS
2	B	124	SER
2	B	148	CYS
2	B	163	SER
2	B	169	ASN
3	H	16	SER
3	H	21	CYS
3	H	102	LYS
4	L	10	SER
4	L	70	ASP
4	L	158	ASN

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)

13 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	$\#\|Z\| > 2$
5	NAG	C	1	5,1	14,14,15	0.34	0	17,19,21	0.56	0
5	NAG	C	2	5	14,14,15	0.79	1 (7%)	17,19,21	0.61	0
5	NAG	D	1	5,1	14,14,15	0.39	0	17,19,21	0.44	0
5	NAG	D	2	5	14,14,15	0.25	0	17,19,21	0.39	0
6	NAG	E	1	6,1	14,14,15	0.45	0	17,19,21	0.72	1 (5%)
6	NAG	E	2	6	14,14,15	0.41	0	17,19,21	1.47	2 (11%)
6	BMA	E	3	6	11,11,12	0.58	0	15,15,17	0.72	0
6	NAG	F	1	6,1	14,14,15	0.27	0	17,19,21	0.40	0
6	NAG	F	2	6	14,14,15	0.25	0	17,19,21	0.40	0
6	BMA	F	3	6	11,11,12	0.46	0	15,15,17	0.76	0
6	NAG	G	1	6,1	14,14,15	0.37	0	17,19,21	0.40	0
6	NAG	G	2	6	14,14,15	0.24	0	17,19,21	0.47	0
6	BMA	G	3	6	11,11,12	0.54	0	15,15,17	0.77	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
5	NAG	C	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	NAG	D	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
6	NAG	E	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	5/6/23/26	0/1/1/1
6	BMA	E	3	6	-	0/2/19/22	0/1/1/1
6	NAG	F	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	1/2/19/22	0/1/1/1
6	NAG	G	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	NAG	C1-C2	2.47	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	2	NAG	C2-N2-C7	4.43	129.21	122.90
6	E	2	NAG	C1-C2-N2	2.93	115.49	110.49
6	E	1	NAG	C1-O5-C5	2.13	115.08	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

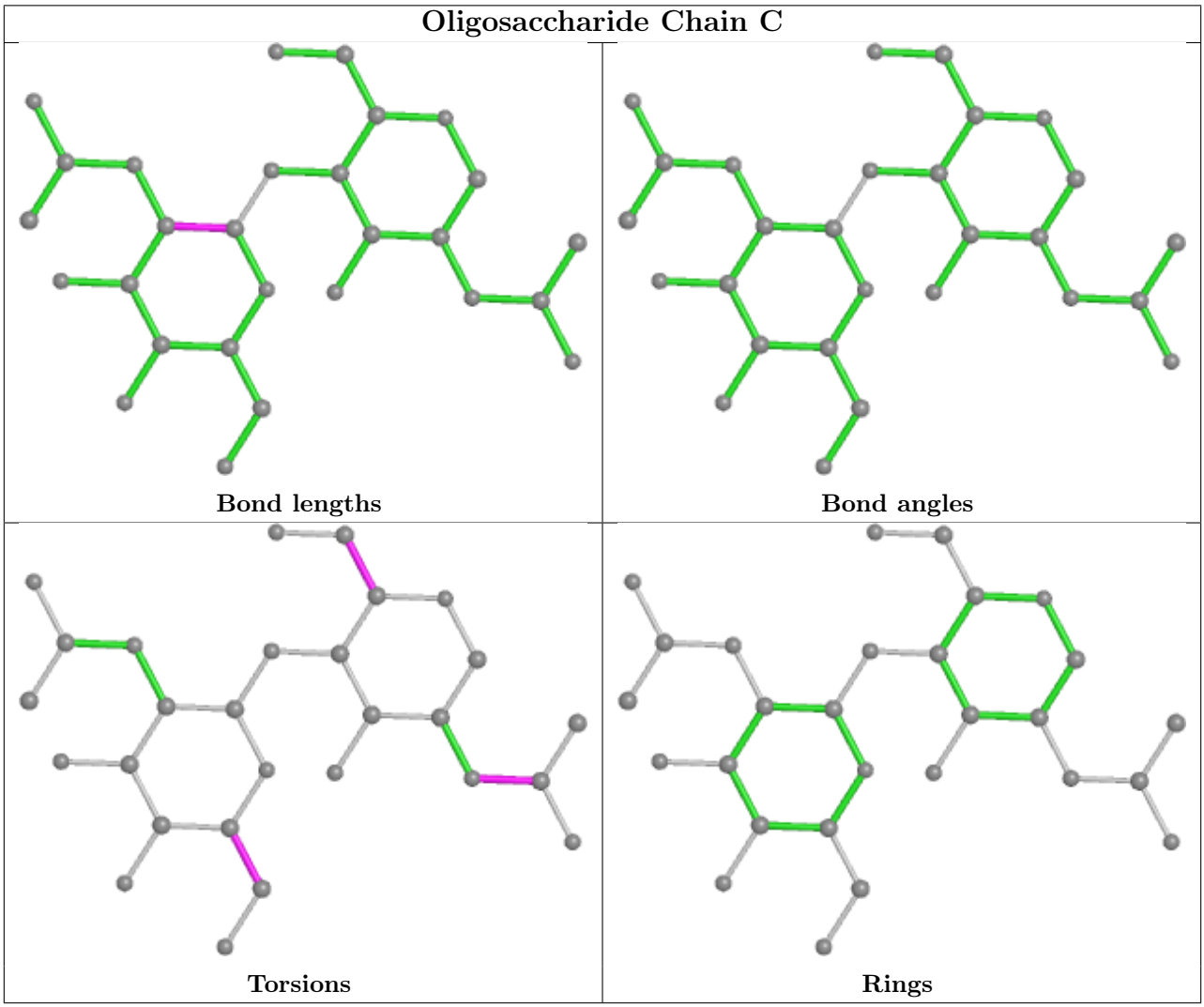
Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C8-C7-N2-C2
5	C	1	NAG	O7-C7-N2-C2
6	E	1	NAG	C8-C7-N2-C2
6	E	1	NAG	O7-C7-N2-C2
6	E	2	NAG	C8-C7-N2-C2
6	E	2	NAG	O7-C7-N2-C2
6	G	1	NAG	C8-C7-N2-C2
6	G	1	NAG	O7-C7-N2-C2
5	C	2	NAG	O5-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
6	E	2	NAG	C4-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
5	D	1	NAG	O5-C5-C6-O6
5	D	1	NAG	C4-C5-C6-O6
6	E	2	NAG	O5-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
6	E	2	NAG	C3-C2-N2-C7
6	F	2	NAG	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

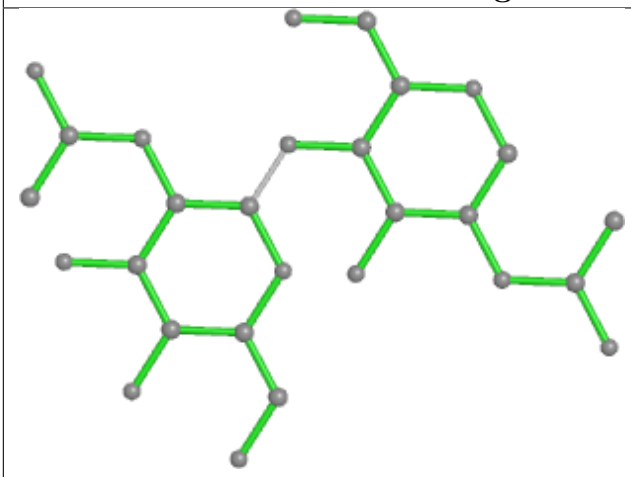
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1	NAG	2	0
6	E	2	NAG	1	0

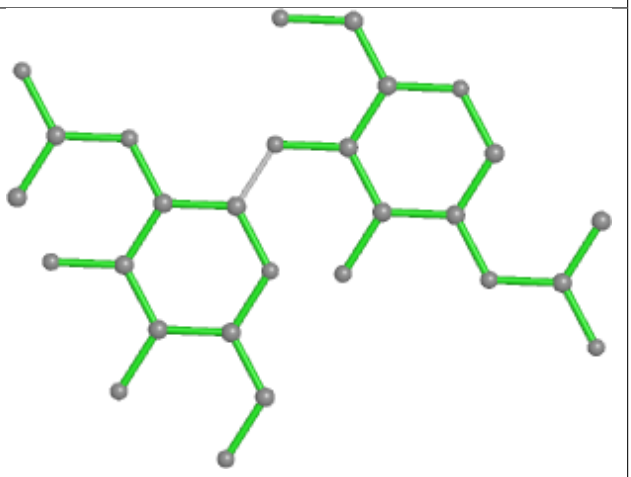
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



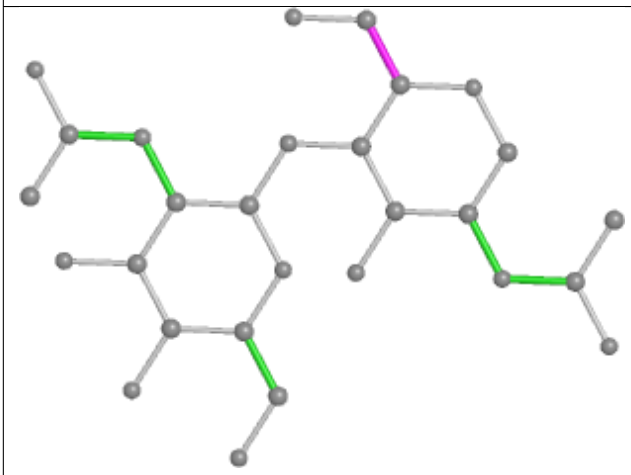
Oligosaccharide Chain D



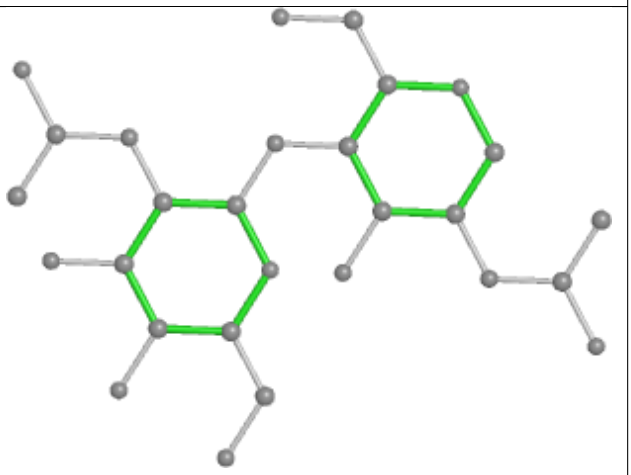
Bond lengths



Bond angles

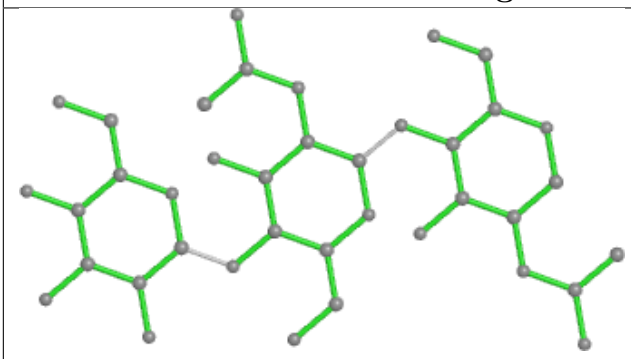


Torsions

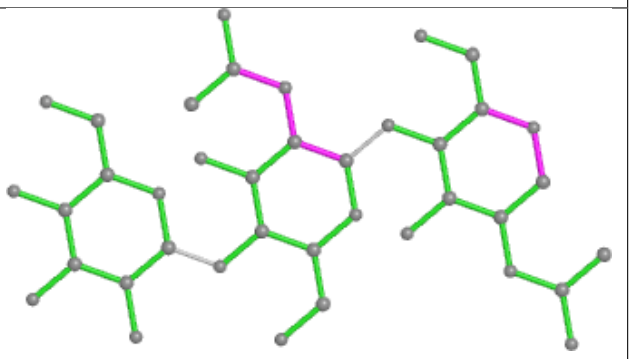


Rings

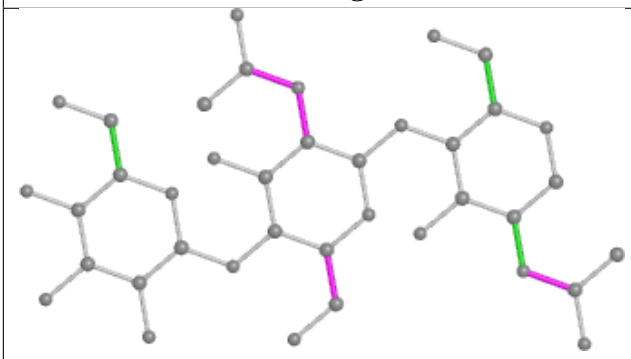
Oligosaccharide Chain E



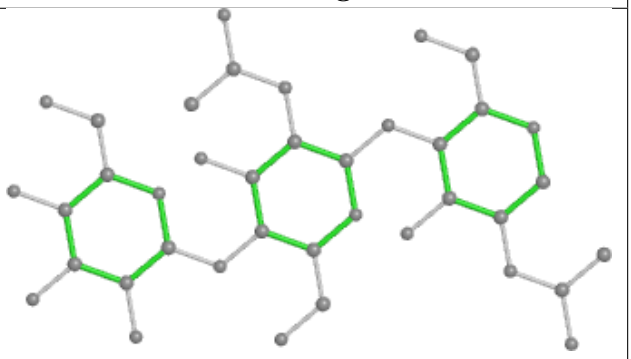
Bond lengths



Bond angles

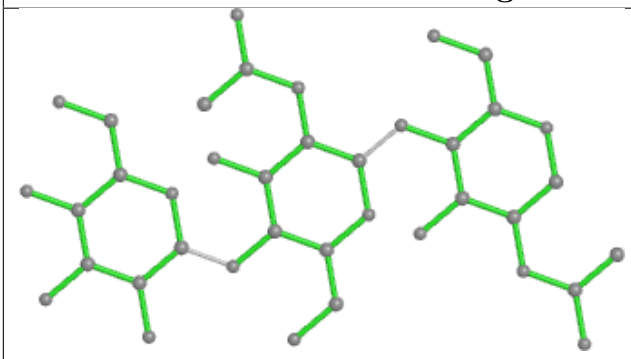


Torsions

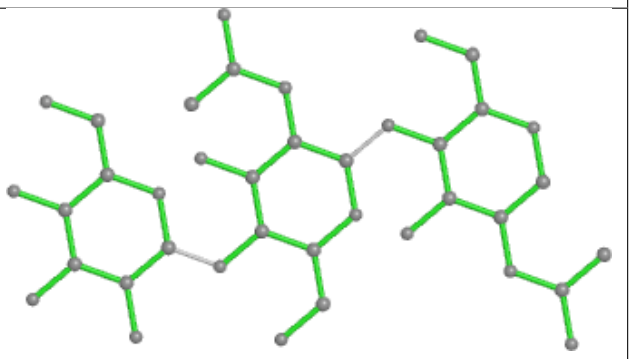


Rings

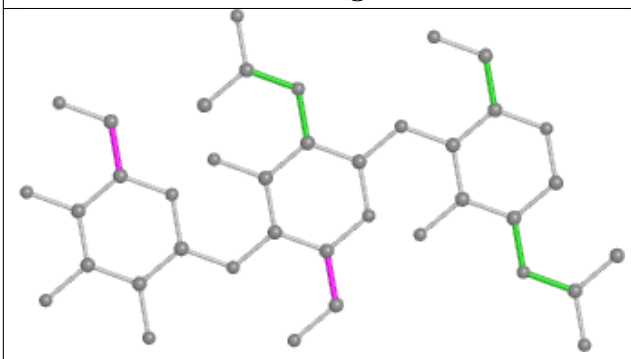
Oligosaccharide Chain F



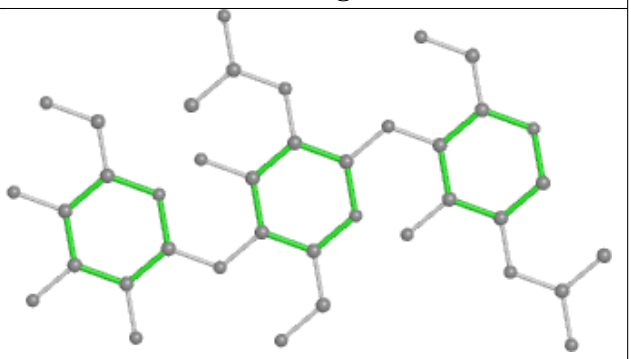
Bond lengths



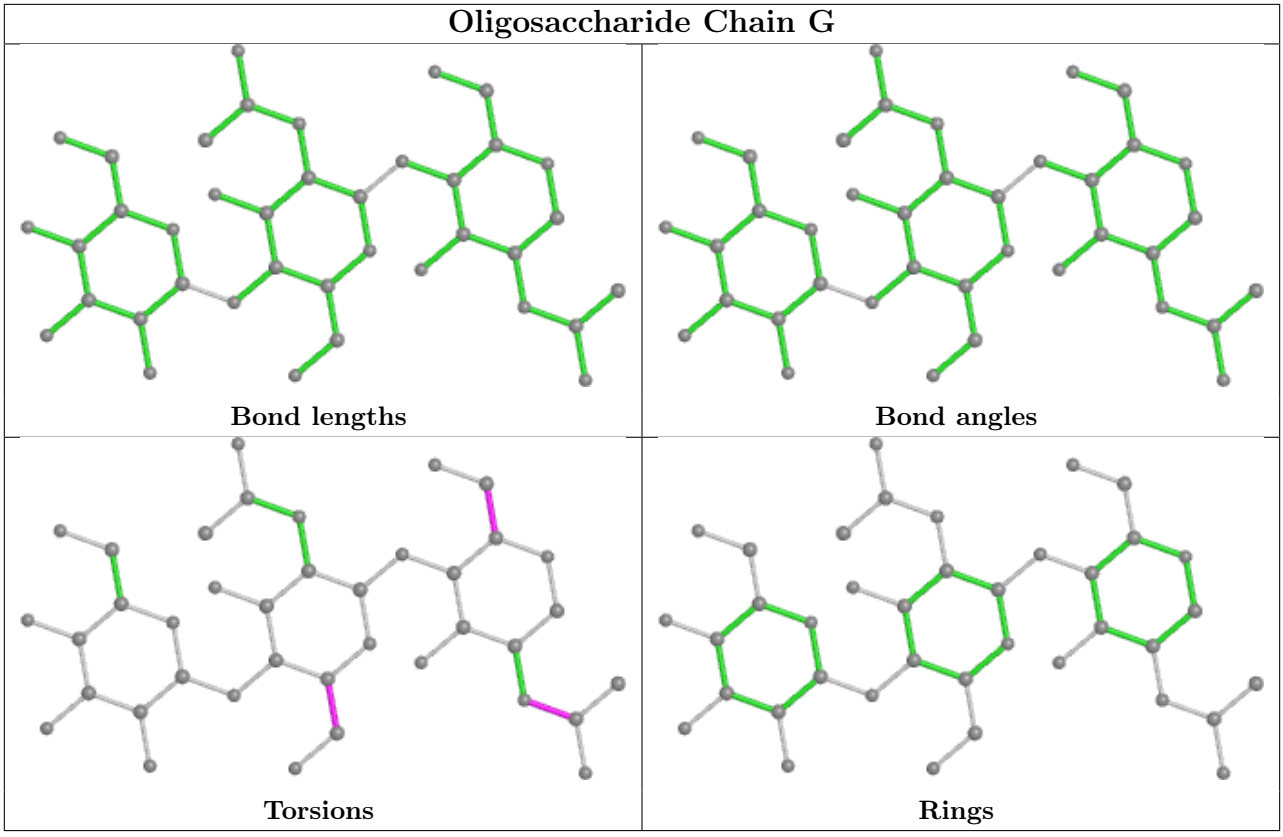
Bond angles



Torsions



Rings



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	326/331 (98%)	0.15	7 (2%) 63 72	38, 93, 119, 132	0
2	B	175/177 (98%)	0.18	0 100 100	37, 65, 99, 126	0
3	H	224/225 (99%)	0.77	32 (14%) 2 2	43, 88, 178, 197	0
4	L	213/214 (99%)	1.31	57 (26%) 0 0	60, 121, 187, 218	0
All	All	938/947 (99%)	0.57	96 (10%) 6 7	37, 87, 170, 218	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	193	PRO	13.2
3	H	223	SER	11.4
4	L	208	SER	10.0
4	L	181	LEU	9.1
3	H	134	PRO	8.7
3	H	224	CYS	8.2
4	L	130	ALA	8.0
3	H	222	LYS	7.7
4	L	149	LYS	7.5
4	L	182	SER	7.4
4	L	154	LEU	7.2
4	L	133	VAL	7.1
4	L	119	PRO	6.6
4	L	131	SER	6.6
4	L	209	PHE	6.5
3	H	146	LEU	6.4
3	H	218	ARG	6.2
3	H	201	THR	6.0
3	H	202	TYR	5.6
3	H	140	SER	5.5
4	L	196	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
4	L	192	TYR	5.3
3	H	135	SER	5.2
4	L	195	GLU	5.1
4	L	108	ARG	5.1
4	L	191	VAL	5.0
4	L	122	ASP	4.9
3	H	141	GLY	4.8
3	H	220	GLU	4.8
3	H	139	THR	4.7
4	L	148	TRP	4.7
4	L	125	LEU	4.5
4	L	152	ASN	4.5
4	L	184	ALA	4.5
4	L	186	TYR	4.4
3	H	200	GLN	4.4
4	L	210	ASN	4.3
3	H	138	SER	4.3
3	H	221	PRO	4.2
4	L	183	LYS	4.1
4	L	117	ILE	4.0
4	L	187	GLU	4.0
3	H	195	SER	3.9
3	H	133	ALA	3.9
3	H	192	VAL	3.9
3	H	164	SER	3.8
4	L	178	THR	3.8
4	L	147	GLN	3.6
4	L	211	ARG	3.6
3	H	131	PRO	3.6
4	L	121	SER	3.6
4	L	135	LEU	3.5
4	L	193	ALA	3.5
4	L	155	GLN	3.3
4	L	146	VAL	3.3
4	L	150	VAL	3.2
3	H	162	TRP	3.2
1	A	79	LEU	3.1
1	A	208	ARG	3.1
4	L	202	SER	3.1
4	L	203	SER	3.0
4	L	188	LYS	3.0
4	L	175	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
4	L	194	CYS	3.0
3	H	199	THR	2.9
4	L	132	VAL	2.9
4	L	115	VAL	2.9
3	H	145	ALA	2.9
3	H	137	LYS	2.9
4	L	179	LEU	2.9
4	L	116	PHE	2.8
4	L	189	HIS	2.7
4	L	145	LYS	2.7
3	H	144	ALA	2.7
3	H	219	VAL	2.7
3	H	142	GLY	2.6
4	L	204	PRO	2.6
4	L	126	LYS	2.5
4	L	159	SER	2.5
4	L	197	THR	2.4
4	L	201	LEU	2.4
4	L	213	GLU	2.4
1	A	251	LEU	2.4
1	A	326	ILE	2.4
1	A	209	TYR	2.3
3	H	149	LEU	2.3
1	A	116(B)	PHE	2.3
3	H	196	SER	2.2
4	L	144	ALA	2.2
4	L	206	THR	2.2
4	L	177	SER	2.2
3	H	198	GLY	2.2
4	L	129	THR	2.2
4	L	51	ALA	2.1
1	A	154	LEU	2.1
4	L	153	ALA	2.1

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)

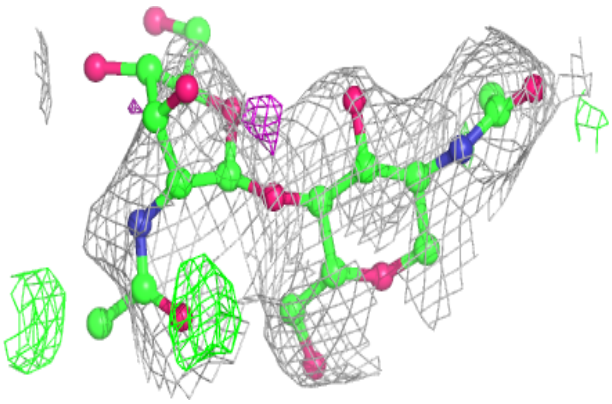
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

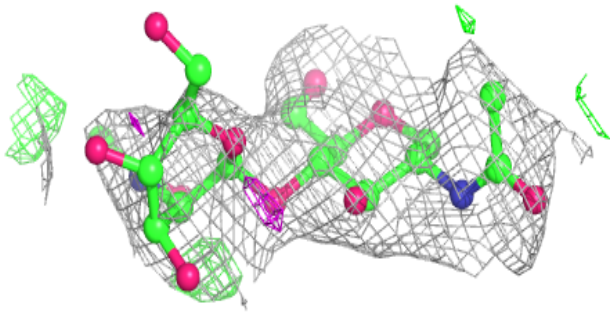
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	E	3	11/12	0.59	0.19	126,155,166,182	0
5	NAG	C	2	14/15	0.63	0.41	112,153,162,165	0
6	NAG	F	2	14/15	0.65	0.36	154,185,191,195	0
6	NAG	F	1	14/15	0.69	0.20	116,139,167,191	0
5	NAG	D	2	14/15	0.69	0.24	107,133,162,168	0
6	BMA	G	3	11/12	0.73	0.30	104,137,146,147	0
6	BMA	F	3	11/12	0.75	0.39	151,171,180,183	0
6	NAG	G	1	14/15	0.81	0.19	83,110,123,126	0
6	NAG	G	2	14/15	0.84	0.26	114,136,148,151	0
6	NAG	E	1	14/15	0.86	0.14	98,109,124,134	0
5	NAG	D	1	14/15	0.88	0.21	53,79,88,116	0
6	NAG	E	2	14/15	0.90	0.11	135,142,154,164	0
5	NAG	C	1	14/15	0.91	0.14	72,98,114,133	0

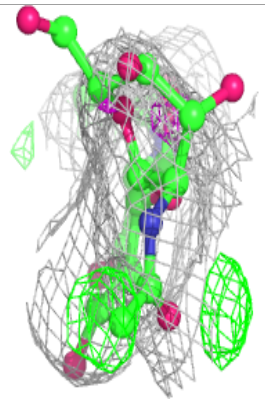
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

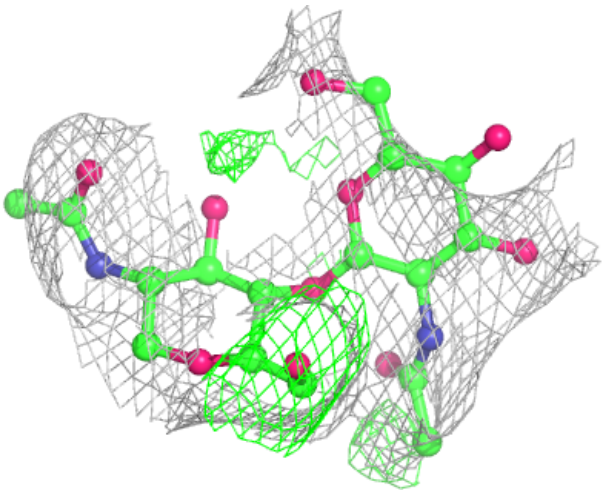


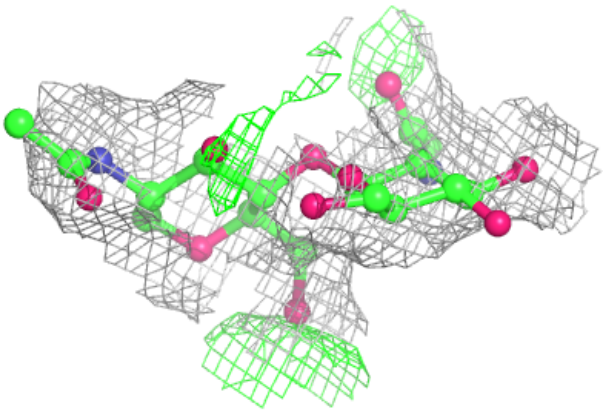


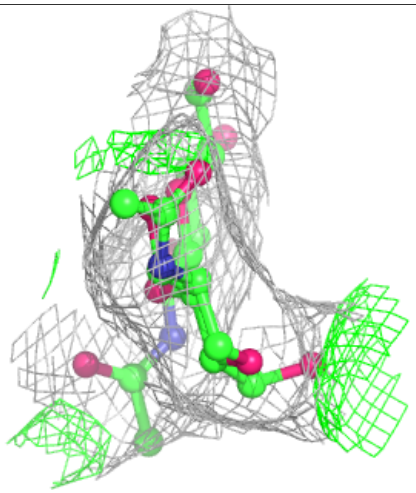


Electron density around Chain D:

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

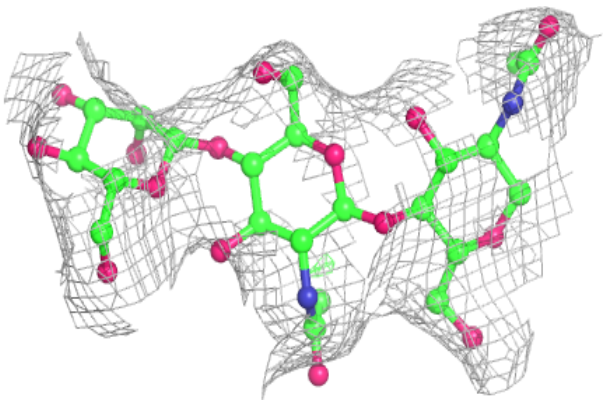


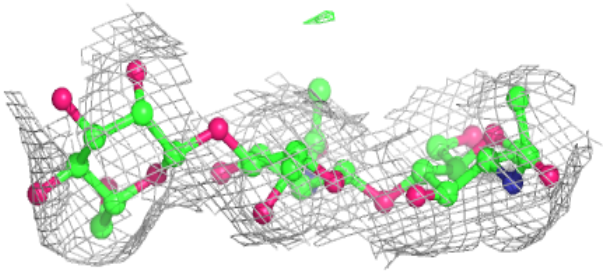


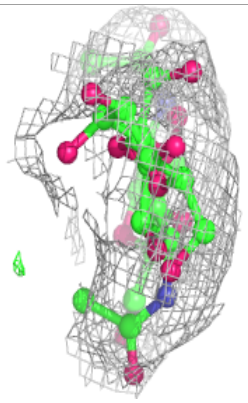


Electron density around Chain E:

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

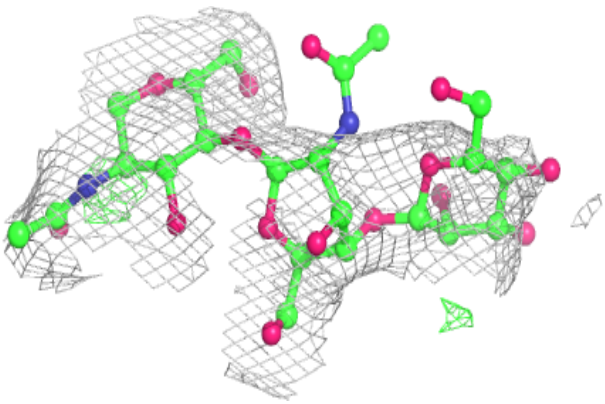


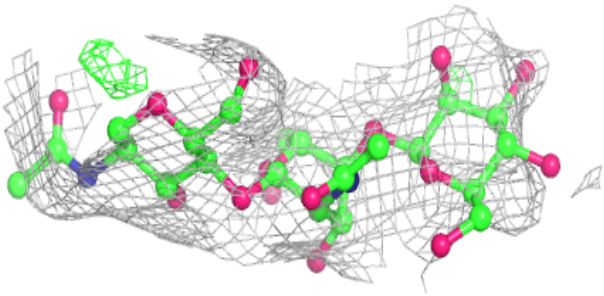


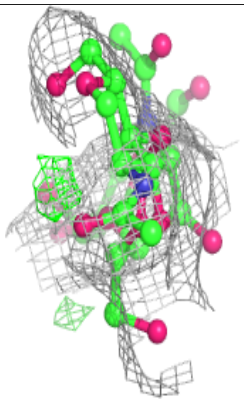


Electron density around Chain F:

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

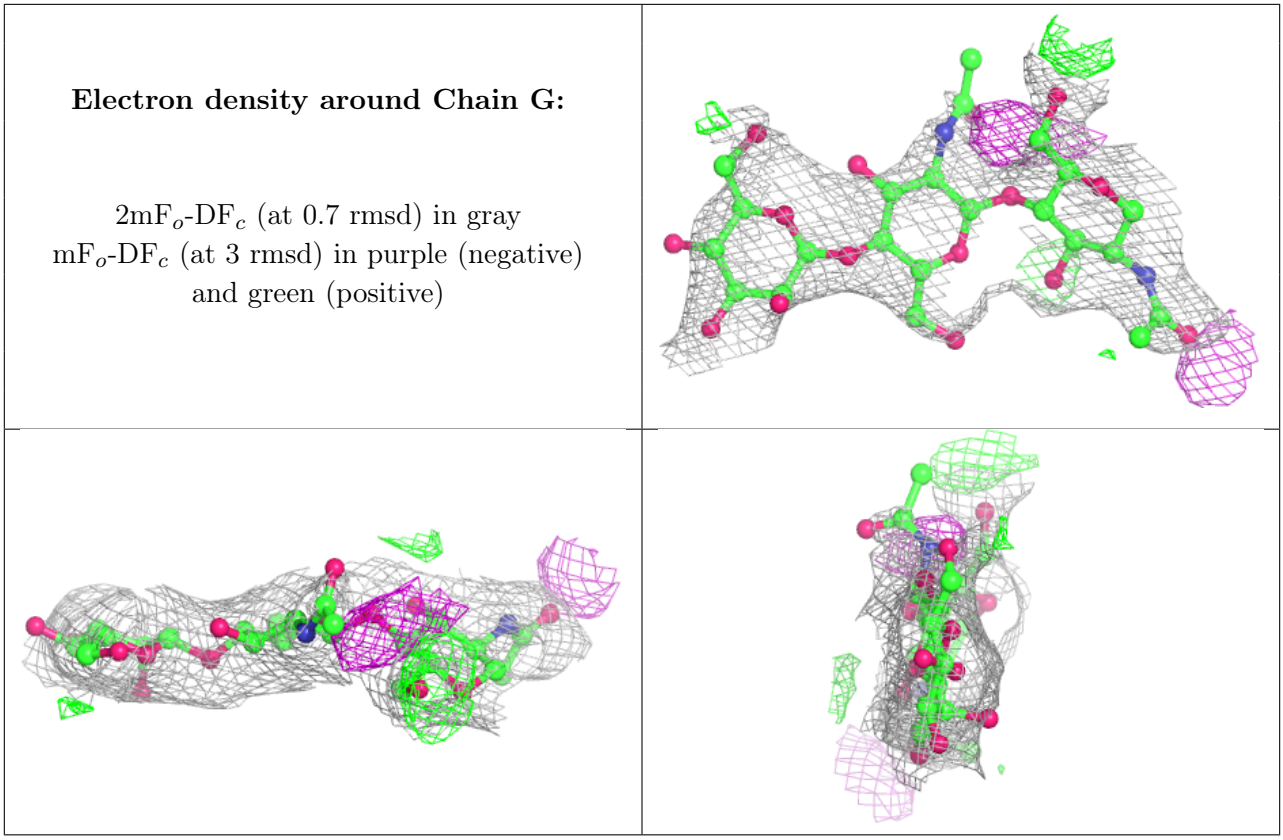






Electron density around Chain G:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.