Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:06 PM BST

PDB ID	:	4OQT
Title	:	LINGO-1/Li81 Fab complex
Authors	:	Pepinsky, R.B.; Arndt, J.W.; Quan, C.; Gao, Y.; Quintero-Monzon, O.; Lee, X.; Mi, S.
Deposited on	:	2014-02-10
Resolution	:	3.23 Å(reported)

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

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

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

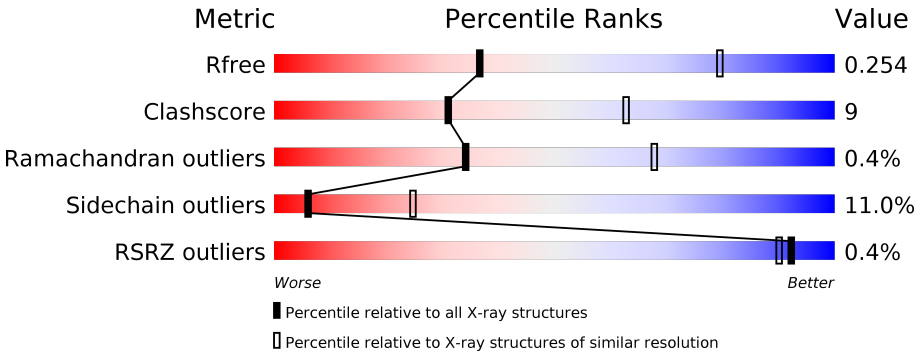
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.23 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	478	76% 21%
2	L	215	69% 28%
3	H	235	% 70% 20% 6%
4	B	3	33% 67%
4	D	3	67% 33%
4	F	3	33% 67%

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Mol	Chain	Length	Quality of chain
5	C	2	100%
5	E	2	50% 50%

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
6	NAG	A	506	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7257 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 Leucine-rich repeat and immunoglobulin-like domain-containing nogo receptor-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	475	3795	2415	679	684	17	0	0	0

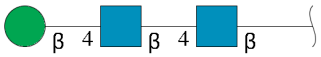
- Molecule 2 is a protein called Light Chain of Li81 Fab, kappa 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1643	1025	278	334	6	0	0	0

- Molecule 3 is a protein called Heavy Chain of Li81 Fab, VH3-23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	221	1618	1019	268	324	7	0	0	0

- Molecule 4 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.



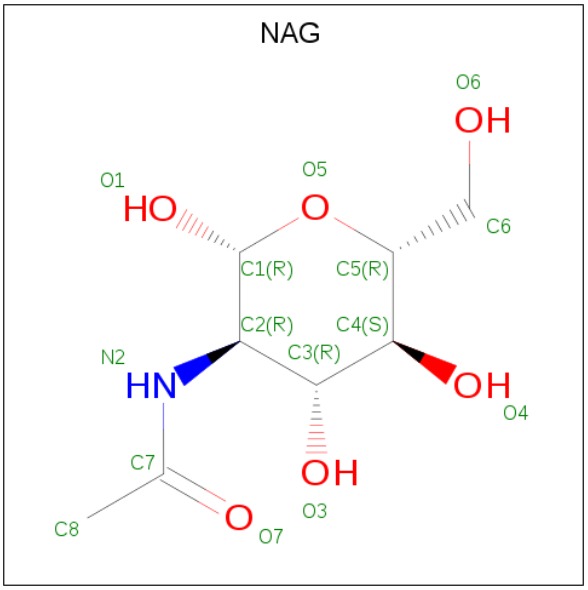
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	3	39	22	2	15	0	0	0
4	D	3	39	22	2	15	0	0	0
4	F	3	39	22	2	15	0	0	0

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

cetamido-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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



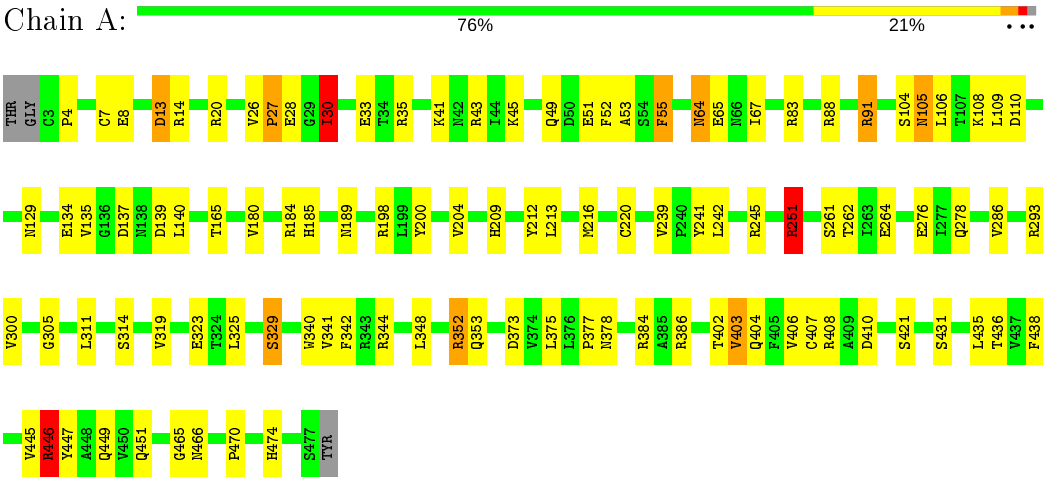
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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.

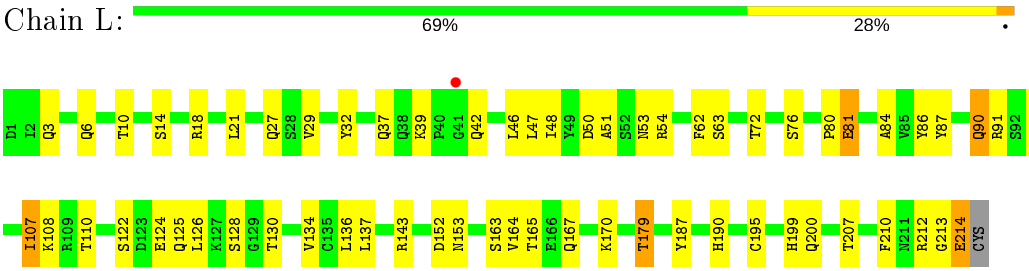
• Molecule 1: Leucine-rich repeat and immunoglobulin-like domain-containing nogo receptor-interacting protein 1

Chain A:



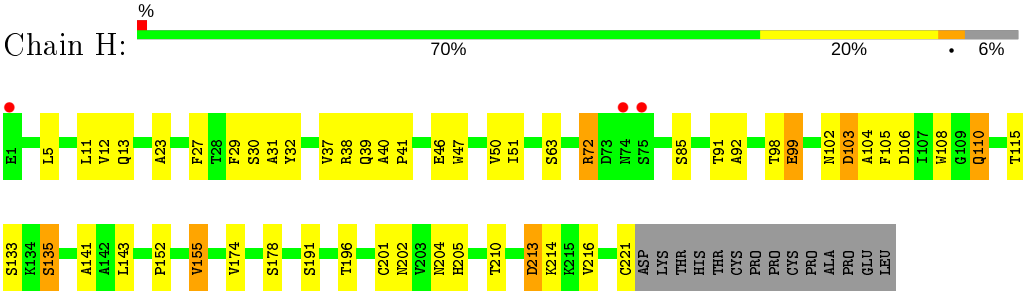
• Molecule 2: Light Chain of Li81 Fab, kappa 3

Chain L:



• Molecule 3: Heavy Chain of Li81 Fab, VH3-23

Chain H:

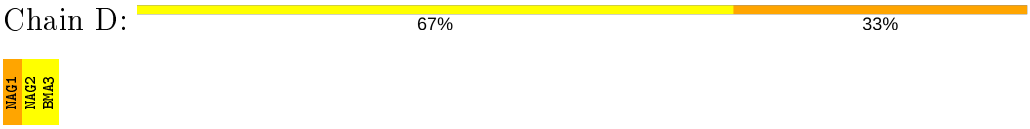


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

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

Chain D:

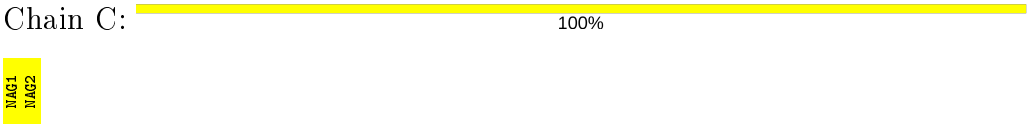


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• 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 E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	207.47Å 207.47Å 140.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.23 20.00 – 3.23	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.23) 100.0 (20.00-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.78 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.192 , 0.256 0.200 , 0.254	Depositor DCC
R_{free} test set	1479 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	99.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 72.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7257	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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: BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.59	0/3877	0.88	5/5272 (0.1%)
2	L	0.60	0/1680	0.78	0/2286
3	H	0.55	0/1656	0.77	0/2259
All	All	0.58	0/7213	0.83	5/9817 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	VAL	C-N-CD	6.41	141.86	128.40
1	A	30	ILE	C-N-CD	5.77	140.52	128.40
1	A	352	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	446	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	251	ARG	NE-CZ-NH1	5.46	123.03	120.30

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	3795	0	3799	56	0
2	L	1643	0	1568	43	0
3	H	1618	0	1550	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	39	0	34	3	0
4	D	39	0	34	1	0
4	F	39	0	34	2	0
5	C	28	0	25	0	0
5	E	28	0	25	1	0
6	A	28	0	26	0	0
All	All	7257	0	7095	130	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 9.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:CG2	1:A:55:PHE:CE1	2.22	1.22
1:A:30:ILE:HG21	1:A:55:PHE:CE1	1.81	1.15
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.25	1.13
1:A:30:ILE:HG22	1:A:55:PHE:CE1	1.89	1.05
3:H:37:VAL:HG22	3:H:47:TRP:CE3	1.91	1.05
3:H:37:VAL:CG2	3:H:47:TRP:CZ3	2.48	0.96
1:A:30:ILE:CG2	1:A:55:PHE:CD1	2.55	0.90
2:L:37:GLN:CB	2:L:47:LEU:HD11	2.01	0.90
1:A:43:ARG:CZ	1:A:67:ILE:HD11	2.02	0.89
3:H:37:VAL:HG22	3:H:47:TRP:CZ3	2.05	0.88
2:L:47:LEU:O	2:L:48:ILE:HD13	1.79	0.81
2:L:37:GLN:HB2	2:L:47:LEU:CD1	2.11	0.81
1:A:30:ILE:HG21	1:A:55:PHE:CD1	2.17	0.77
1:A:402:THR:HB	1:A:446:ARG:O	1.86	0.76
2:L:134:VAL:HG22	2:L:179:THR:HG23	1.67	0.74
4:F:2:NAG:H4	4:F:3:BMA:O2	1.87	0.74
2:L:91:ARG:NH1	3:H:103:ASP:O	2.20	0.74
2:L:137:LEU:HD12	2:L:137:LEU:N	2.04	0.72
1:A:406:VAL:HG11	1:A:408:ARG:HE	1.54	0.72
1:A:30:ILE:HG22	1:A:55:PHE:CD1	2.20	0.71
1:A:440:ASP:OD1	1:A:442:THR:HG23	1.93	0.68
1:A:198:ARG:NH2	2:L:50:ASP:OD1	2.26	0.67
2:L:213:GLY:O	2:L:214:GLU:HB3	1.94	0.67
1:A:438:PHE:HB3	1:A:439:PRO:HD2	1.76	0.67
1:A:30:ILE:HG22	1:A:55:PHE:HE1	1.51	0.67
1:A:446:ARG:HH21	1:A:446:ARG:HG3	1.60	0.66
2:L:124:GLU:OE1	3:H:214:LYS:NZ	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:54:ARG:NH1	2:L:62:PHE:O	2.29	0.65
1:A:239:VAL:HB	1:A:241:TYR:CE1	2.32	0.65
1:A:180:VAL:HG22	1:A:204:VAL:HB	1.81	0.63
3:H:102:ASN:C	3:H:104:ALA:H	2.02	0.62
1:A:83:ARG:NH2	1:A:105:ASN:OD1	2.33	0.61
1:A:30:ILE:HG21	1:A:55:PHE:CZ	2.35	0.61
1:A:340:TRP:CE2	1:A:341:VAL:HG23	2.39	0.58
1:A:4:PRO:HG2	1:A:7:CYS:SG	2.44	0.57
2:L:6:GLN:HE22	2:L:87:TYR:HA	1.69	0.57
2:L:46:LEU:HD22	3:H:105:PHE:CG	2.39	0.57
1:A:377:PRO:O	1:A:378:ASN:HB2	2.04	0.57
2:L:124:GLU:CD	3:H:214:LYS:NZ	2.58	0.57
3:H:124:PRO:HD2	3:H:210:THR:HG21	1.85	0.56
1:A:403:VAL:HG13	1:A:445:VAL:HB	1.86	0.56
4:B:1:NAG:O4	4:B:2:NAG:H83	2.06	0.55
2:L:91:ARG:HA	2:L:97:TYR:CD1	2.41	0.55
1:A:117:VAL:HA	1:A:139:ASP:O	2.07	0.55
2:L:91:ARG:NH2	3:H:106:ASP:OD1	2.40	0.55
1:A:4:PRO:HB3	1:A:28:GLU:O	2.08	0.54
3:H:11:LEU:HB2	3:H:152:PRO:HG3	1.89	0.54
3:H:132:SER:O	3:H:135:SER:OG	2.20	0.54
2:L:190:HIS:O	2:L:212:ARG:HD3	2.08	0.54
3:H:102:ASN:O	3:H:104:ALA:N	2.41	0.54
2:L:39:LYS:NZ	2:L:81:GLU:O	2.42	0.53
3:H:5:LEU:HD13	3:H:110:GLN:OE1	2.08	0.53
3:H:30:SER:O	3:H:31:ALA:HB3	2.09	0.53
1:A:104:SER:O	1:A:129:ASN:HB2	2.09	0.53
3:H:40:ALA:HB1	3:H:41:PRO:HD2	1.90	0.52
2:L:124:GLU:OE2	3:H:214:LYS:NZ	2.43	0.52
2:L:137:LEU:N	2:L:137:LEU:CD1	2.73	0.52
2:L:29:VAL:HG11	2:L:90:GLN:HG3	1.93	0.51
1:A:216:MET:HB3	1:A:220:CYS:SG	2.51	0.51
2:L:136:LEU:C	2:L:137:LEU:HD12	2.30	0.51
1:A:83:ARG:C	1:A:106:LEU:HD12	2.32	0.51
3:H:116:VAL:O	3:H:116:VAL:HG22	2.11	0.50
1:A:67:ILE:O	1:A:67:ILE:HG22	2.12	0.49
1:A:319:VAL:HG12	1:A:344:ARG:HH12	1.78	0.49
3:H:143:LEU:HB2	3:H:216:VAL:HG11	1.93	0.49
2:L:126:LEU:HD11	2:L:187:TYR:CE2	2.46	0.49
1:A:342:PHE:CE2	1:A:375:LEU:HD11	2.48	0.49
1:A:27:PRO:O	1:A:30:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLY:HA2	1:A:329:SER:HB3	1.95	0.49
1:A:13:ASP:OD1	1:A:13:ASP:N	2.44	0.48
3:H:155:VAL:HG13	3:H:205:HIS:HD2	1.77	0.48
2:L:47:LEU:CD2	2:L:62:PHE:CD1	2.97	0.48
3:H:5:LEU:HB2	3:H:23:ALA:HB3	1.96	0.48
3:H:32:TYR:CD2	3:H:99:GLU:O	2.67	0.48
2:L:50:ASP:O	2:L:51:ALA:HB3	2.15	0.47
1:A:384:ARG:HG3	1:A:465:GLY:HA3	1.97	0.47
2:L:152:ASP:O	2:L:153:ASN:HB2	2.16	0.46
1:A:276:GLU:HG3	1:A:300:VAL:HB	1.96	0.46
1:A:109:LEU:HD12	1:A:110:ASP:H	1.80	0.46
3:H:32:TYR:HD2	3:H:99:GLU:O	1.97	0.46
2:L:48:ILE:HA	2:L:53:ASN:O	2.16	0.46
1:A:67:ILE:HG23	1:A:91:ARG:CZ	2.46	0.46
3:H:37:VAL:HG21	3:H:47:TRP:CZ3	2.46	0.46
3:H:201:CYS:O	3:H:213:ASP:HA	2.16	0.46
3:H:51:ILE:HD13	3:H:72:ARG:HG2	1.99	0.45
2:L:37:GLN:CB	2:L:47:LEU:CD1	2.84	0.45
2:L:199:HIS:CG	2:L:200:GLN:H	2.34	0.45
1:A:406:VAL:HG12	1:A:407:CYS:N	2.31	0.45
1:A:67:ILE:CG2	1:A:91:ARG:NH1	2.80	0.45
2:L:164:VAL:HG12	2:L:165:THR:O	2.16	0.45
2:L:14:SER:HA	2:L:108:LYS:HB2	1.99	0.45
2:L:84:ALA:HB3	2:L:86:TYR:CE1	2.52	0.45
4:F:2:NAG:C4	4:F:3:BMA:O2	2.61	0.44
1:A:43:ARG:NE	1:A:67:ILE:HD11	2.32	0.44
2:L:210:PHE:CD1	2:L:210:PHE:O	2.70	0.44
1:A:185:HIS:HA	1:A:209:HIS:O	2.17	0.44
1:A:299:ARG:NH1	1:A:299:ARG:HB3	2.31	0.44
1:A:200:TYR:HD2	2:L:32:TYR:CE1	2.35	0.44
1:A:438:PHE:HB3	1:A:439:PRO:CD	2.47	0.44
1:A:278:GLN:HG3	4:B:1:NAG:H82	2.00	0.44
3:H:39:GLN:O	3:H:92:ALA:HB1	2.18	0.43
1:A:14:ARG:HB2	1:A:35:ARG:HB2	2.00	0.43
3:H:108:TRP:N	3:H:108:TRP:CD1	2.87	0.43
2:L:125:GLN:O	2:L:128:SER:HB3	2.17	0.43
1:A:189:ASN:HA	1:A:213:LEU:HA	1.99	0.43
3:H:110:GLN:HE21	3:H:110:GLN:HB3	1.69	0.43
3:H:141:ALA:HB2	3:H:191:SER:HB3	2.01	0.43
3:H:37:VAL:HG12	3:H:38:ARG:N	2.32	0.43
2:L:48:ILE:HG23	2:L:53:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLU:O	1:A:348:LEU:HA	2.19	0.43
1:A:212:TYR:CD1	4:D:1:NAG:H81	2.55	0.42
1:A:20:ARG:NH1	1:A:41:LYS:HB3	2.34	0.42
3:H:214:LYS:HD2	3:H:214:LYS:HA	1.89	0.42
2:L:95:PRO:HB2	3:H:50:VAL:HG21	2.01	0.42
2:L:80:PRO:HA	2:L:107:ILE:HG21	2.02	0.41
3:H:91:THR:HG23	3:H:115:THR:HA	2.00	0.41
1:A:474:HIS:CE1	5:E:1:NAG:H5	2.55	0.41
4:B:2:NAG:O3	4:B:3:BMA:H2	2.21	0.41
1:A:311:LEU:CD2	1:A:325:LEU:HD11	2.49	0.41
2:L:195:CYS:O	2:L:207:THR:HA	2.21	0.41
2:L:214:GLU:HG2	3:H:221:CYS:O	2.21	0.41
1:A:251:ARG:HH11	1:A:251:ARG:HB3	1.85	0.41
1:A:447:TYR:O	1:A:449:GLN:OE1	2.39	0.41
2:L:107:ILE:H	2:L:167:GLN:HE22	1.67	0.41
1:A:51:GLU:HB3	1:A:52:PHE:CD2	2.56	0.40
2:L:21:LEU:N	2:L:21:LEU:HD12	2.36	0.40
1:A:64:ASN:ND2	1:A:64:ASN:H	2.19	0.40
3:H:12:VAL:HG13	3:H:116:VAL:HB	2.03	0.40
3:H:27:PHE:CE2	3:H:29:PHE:HA	2.56	0.40
2:L:199:HIS:CG	2:L:200:GLN:N	2.89	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	473/478 (99%)	419 (89%)	52 (11%)	2 (0%)	34 68
2	L	212/215 (99%)	196 (92%)	16 (8%)	0	100 100
3	H	219/235 (93%)	206 (94%)	11 (5%)	2 (1%)	17 52
All	All	904/928 (97%)	821 (91%)	79 (9%)	4 (0%)	34 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ALA
3	H	178	SER
3	H	103	ASP
1	A	470	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/428 (99%)	375 (89%)	48 (11%)	6	24
2	L	183/187 (98%)	162 (88%)	21 (12%)	5	23
3	H	177/196 (90%)	160 (90%)	17 (10%)	8	30
All	All	783/811 (96%)	697 (89%)	86 (11%)	6	25

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	13	ASP
1	A	27	PRO
1	A	30	ILE
1	A	33	GLU
1	A	45	LYS
1	A	49	GLN
1	A	55	PHE
1	A	64	ASN
1	A	65	GLU
1	A	88	ARG
1	A	91	ARG
1	A	105	ASN
1	A	108	LYS
1	A	115	LYS
1	A	118	ILE
1	A	134	GLU

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Mol	Chain	Res	Type
1	A	135	VAL
1	A	137	ASP
1	A	140	LEU
1	A	165	THR
1	A	184	ARG
1	A	242	LEU
1	A	245	ARG
1	A	251	ARG
1	A	261	SER
1	A	262	THR
1	A	264	GLU
1	A	286	VAL
1	A	293	ARG
1	A	296	ASN
1	A	314	SER
1	A	329	SER
1	A	352	ARG
1	A	353	GLN
1	A	373	ASP
1	A	386	ARG
1	A	403	VAL
1	A	404	GLN
1	A	410	ASP
1	A	421	SER
1	A	431	SER
1	A	435	LEU
1	A	436	THR
1	A	442	THR
1	A	446	ARG
1	A	451	GLN
1	A	466	ASN
2	L	3	GLN
2	L	10	THR
2	L	18	ARG
2	L	27	GLN
2	L	42	GLN
2	L	63	SER
2	L	72	THR
2	L	76	SER
2	L	81	GLU
2	L	90	GLN
2	L	93	ASN

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Mol	Chain	Res	Type
2	L	96	MET
2	L	107	ILE
2	L	110	THR
2	L	122	SER
2	L	130	THR
2	L	143	ARG
2	L	163	SER
2	L	170	LYS
2	L	179	THR
2	L	214	GLU
3	H	13	GLN
3	H	46	GLU
3	H	63	SER
3	H	72	ARG
3	H	85	SER
3	H	98	THR
3	H	99	GLU
3	H	110	GLN
3	H	116	VAL
3	H	133	SER
3	H	135	SER
3	H	155	VAL
3	H	174	VAL
3	H	196	THR
3	H	202	ASN
3	H	204	ASN
3	H	213	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	349	ASN
1	A	394	GLN
2	L	6	GLN
2	L	139	ASN
2	L	167	GLN

5.3.3 RNA

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	$\#\|Z\| > 2$
4	NAG	B	1	1,4	14,14,15	0.75	0	17,19,21	2.04	4 (23%)
4	NAG	B	2	4	14,14,15	0.80	0	17,19,21	1.19	0
4	BMA	B	3	4	11,11,12	0.54	0	15,15,17	1.86	4 (26%)
5	NAG	C	1	1,5	14,14,15	0.68	0	17,19,21	1.25	1 (5%)
5	NAG	C	2	5	14,14,15	0.72	0	17,19,21	1.83	4 (23%)
4	NAG	D	1	1,4	14,14,15	0.70	0	17,19,21	1.92	4 (23%)
4	NAG	D	2	4	14,14,15	0.92	0	17,19,21	2.48	8 (47%)
4	BMA	D	3	4	11,11,12	0.65	0	15,15,17	2.11	4 (26%)
5	NAG	E	1	1,5	14,14,15	0.51	0	17,19,21	1.68	3 (17%)
5	NAG	E	2	5	14,14,15	0.49	0	17,19,21	2.96	6 (35%)
4	NAG	F	1	1,4	14,14,15	0.67	0	17,19,21	1.66	3 (17%)
4	NAG	F	2	4	14,14,15	0.67	0	17,19,21	2.53	7 (41%)
4	BMA	F	3	4	11,11,12	0.60	0	15,15,17	1.22	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	4/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C1-O5-C5	8.77	124.07	112.19
4	B	1	NAG	C1-O5-C5	6.22	120.61	112.19
4	D	2	NAG	C8-C7-N2	5.67	125.70	116.10
4	B	3	BMA	O5-C1-C2	-5.00	103.06	110.77
5	E	1	NAG	C1-O5-C5	4.74	118.62	112.19
4	F	2	NAG	C4-C3-C2	4.68	117.87	111.02
4	F	2	NAG	O5-C1-C2	-4.61	104.00	111.29
5	C	2	NAG	C3-C4-C5	4.61	118.46	110.24
4	D	3	BMA	C1-O5-C5	4.47	118.25	112.19
4	D	1	NAG	C1-C2-N2	-4.45	102.88	110.49
4	D	3	BMA	C1-C2-C3	4.22	114.86	109.67
4	D	2	NAG	C4-C3-C2	4.11	117.04	111.02
5	E	2	NAG	C1-C2-N2	-3.74	104.09	110.49
5	E	2	NAG	O5-C5-C4	3.70	119.83	110.83
4	F	1	NAG	C1-C2-N2	3.70	116.80	110.49
4	F	2	NAG	C8-C7-N2	3.67	122.31	116.10
4	D	2	NAG	O5-C1-C2	-3.64	105.55	111.29
5	E	2	NAG	C4-C3-C2	3.59	116.27	111.02
4	F	2	NAG	C1-O5-C5	3.58	117.05	112.19
4	D	3	BMA	O5-C1-C2	3.39	116.00	110.77
4	F	2	NAG	O4-C4-C3	-3.24	102.85	110.35
4	D	2	NAG	C1-O5-C5	3.13	116.44	112.19
4	D	1	NAG	C1-O5-C5	3.10	116.39	112.19
5	E	1	NAG	C1-C2-N2	-3.09	105.20	110.49
4	B	1	NAG	O7-C7-C8	-3.09	116.31	122.06
5	C	2	NAG	O5-C5-C4	3.08	118.33	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C8-C7-N2	3.05	121.26	116.10
5	C	2	NAG	C1-O5-C5	3.01	116.27	112.19
5	C	1	NAG	C1-C2-N2	-3.01	105.35	110.49
4	F	1	NAG	O5-C1-C2	-2.92	106.67	111.29
4	D	1	NAG	C8-C7-N2	-2.84	111.29	116.10
4	D	2	NAG	O7-C7-C8	-2.77	116.91	122.06
4	D	1	NAG	O7-C7-N2	2.74	126.98	121.95
4	F	2	NAG	O3-C3-C2	-2.69	103.90	109.47
4	B	3	BMA	C1-O5-C5	2.55	115.64	112.19
4	D	2	NAG	O4-C4-C3	-2.52	104.52	110.35
4	F	3	BMA	C2-C3-C4	2.50	115.22	110.89
4	D	2	NAG	O7-C7-N2	-2.48	117.39	121.95
4	B	1	NAG	C1-C2-N2	2.42	114.62	110.49
4	B	3	BMA	C1-C2-C3	-2.41	106.71	109.67
4	B	3	BMA	O2-C2-C3	-2.40	105.32	110.14
4	B	1	NAG	O7-C7-N2	2.39	126.35	121.95
4	F	3	BMA	O5-C5-C4	-2.35	105.11	110.83
5	E	1	NAG	O4-C4-C5	2.33	115.08	109.30
4	F	1	NAG	O3-C3-C2	-2.26	104.80	109.47
4	D	2	NAG	O3-C3-C2	-2.14	105.05	109.47
5	C	2	NAG	C4-C3-C2	2.13	114.14	111.02
5	E	2	NAG	O7-C7-N2	-2.11	118.08	121.95
4	D	3	BMA	O2-C2-C3	-2.10	105.93	110.14
4	F	2	NAG	O7-C7-C8	-2.07	118.22	122.06
4	F	3	BMA	C1-C2-C3	2.03	112.16	109.67

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2

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

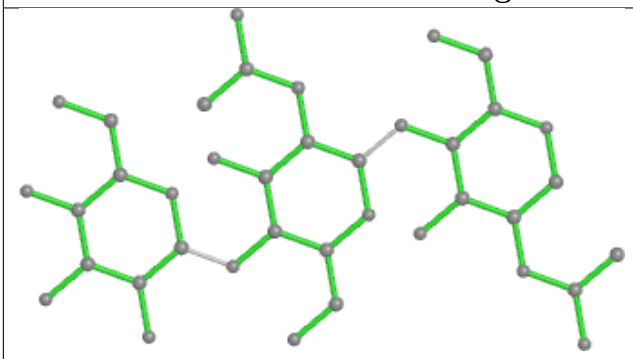
There are no ring outliers.

7 monomers are involved in 7 short contacts:

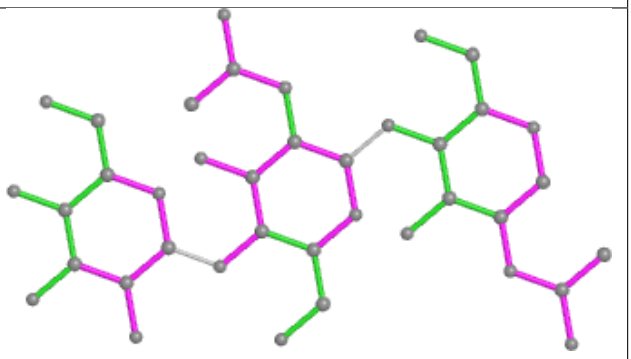
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	2	0
4	B	2	NAG	2	0
4	D	1	NAG	1	0
4	B	3	BMA	1	0
4	F	3	BMA	2	0
4	B	1	NAG	2	0
5	E	1	NAG	1	0

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

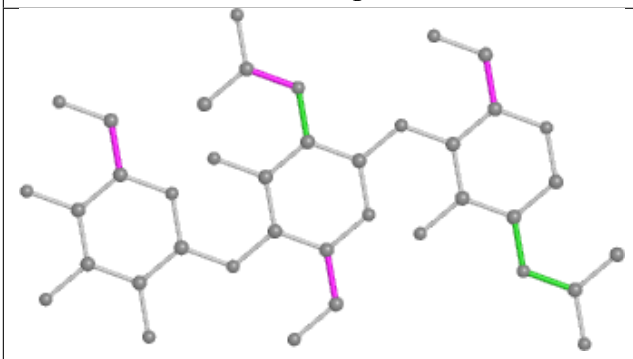
Oligosaccharide Chain D



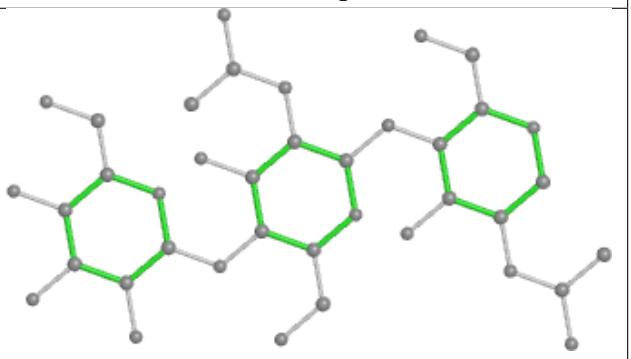
Bond lengths



Bond angles

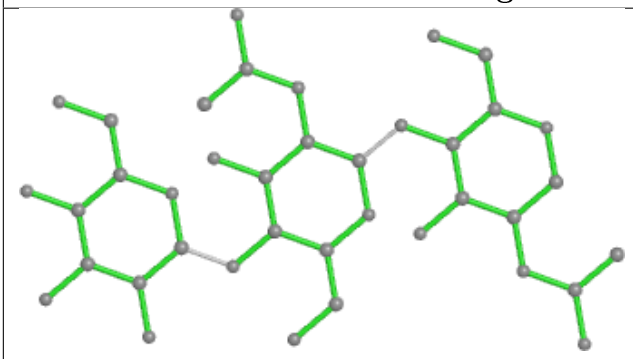


Torsions

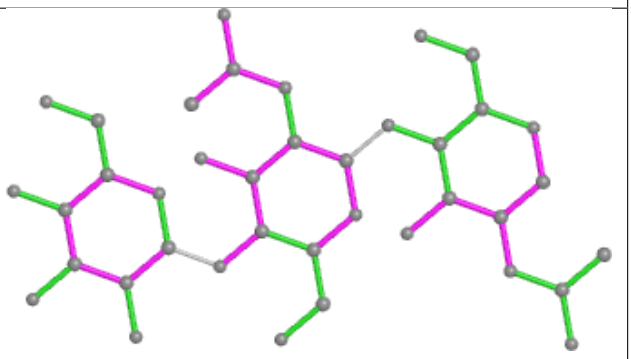


Rings

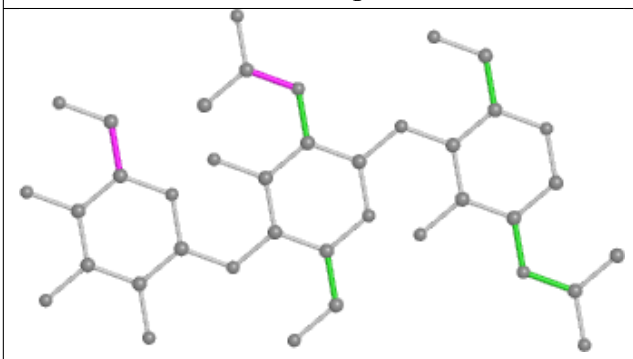
Oligosaccharide Chain F



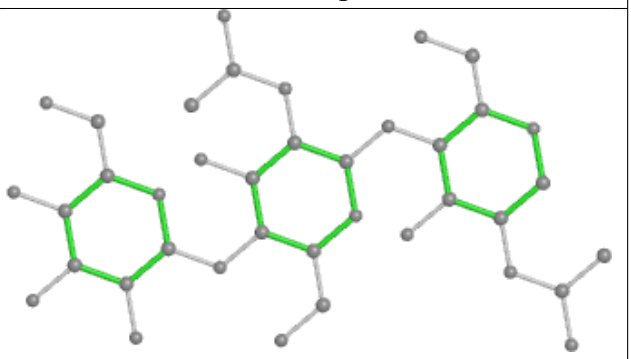
Bond lengths



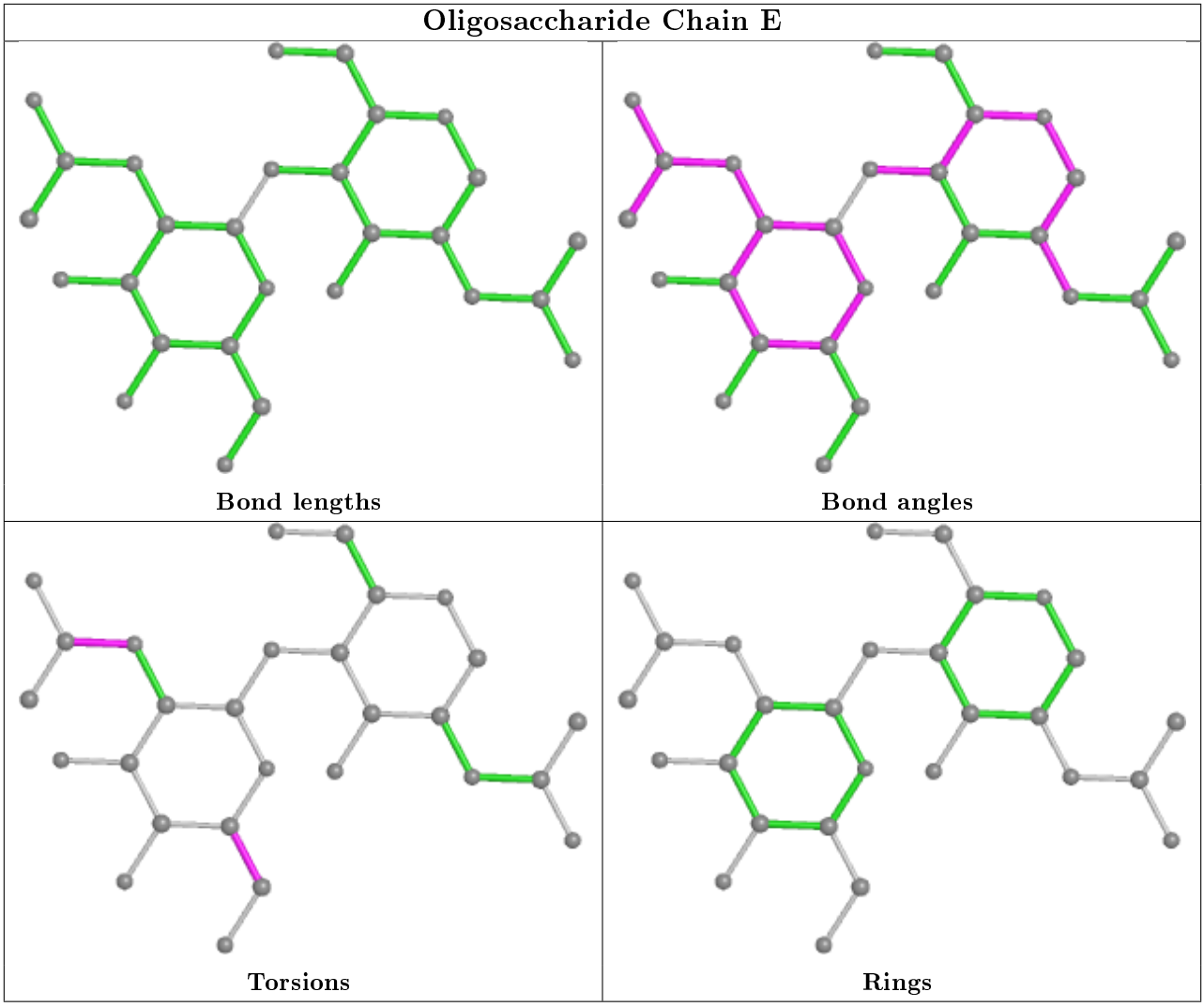
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
6	NAG	A	510	1	14,14,15	0.99	1 (7%)	17,19,21	2.65	6 (35%)
6	NAG	A	506	1	14,14,15	0.74	0	17,19,21	2.35	4 (23%)

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
6	NAG	A	510	1	-	1/6/23/26	0/1/1/1
6	NAG	A	506	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	510	NAG	C1-C2	2.68	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	506	NAG	C1-C2-N2	6.08	120.87	110.49
6	A	510	NAG	C1-O5-C5	5.25	119.30	112.19
6	A	510	NAG	O4-C4-C3	5.18	122.34	110.35
6	A	510	NAG	O5-C5-C6	5.13	115.25	107.20
6	A	506	NAG	C2-N2-C7	4.78	129.71	122.90
6	A	506	NAG	C1-O5-C5	3.76	117.29	112.19
6	A	506	NAG	O7-C7-C8	-3.31	115.90	122.06
6	A	510	NAG	C4-C3-C2	-2.96	106.69	111.02
6	A	510	NAG	C6-C5-C4	-2.95	106.10	113.00
6	A	510	NAG	O7-C7-C8	-2.92	116.64	122.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	506	NAG	C1-C2-N2-C7
6	A	506	NAG	C4-C5-C6-O6
6	A	506	NAG	O5-C5-C6-O6
6	A	510	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	475/478 (99%)	-0.55	0 100 100	66, 88, 132, 164	0
2	L	214/215 (99%)	-0.42	1 (0%) 91 87	68, 93, 123, 138	0
3	H	221/235 (94%)	-0.29	3 (1%) 75 66	59, 103, 130, 152	0
All	All	910/928 (98%)	-0.45	4 (0%) 92 90	59, 93, 128, 164	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	74	ASN	2.7
3	H	1	GLU	2.3
2	L	41	GLY	2.1
3	H	75	SER	2.1

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

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

6.3 Carbohydrates

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
4	BMA	B	3	11/12	0.67	0.31	98,121,155,176	0
4	BMA	F	3	11/12	0.81	0.30	95,114,126,135	0
5	NAG	C	2	14/15	0.83	0.31	114,131,145,155	0
4	BMA	D	3	11/12	0.91	0.22	100,112,125,131	0

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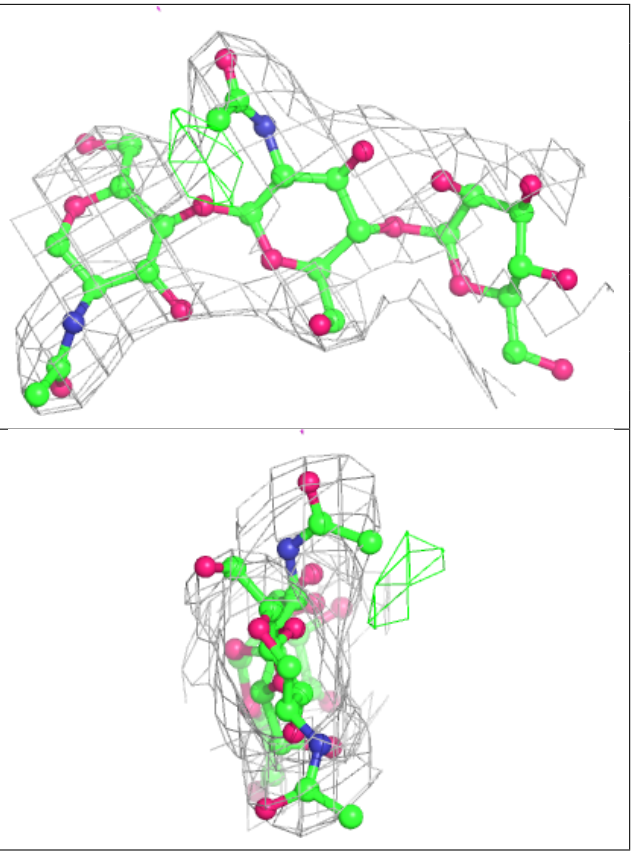
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	2	14/15	0.92	0.33	74,98,107,127	0
5	NAG	E	2	14/15	0.93	0.29	97,129,142,157	0
4	NAG	D	2	14/15	0.93	0.19	76,84,100,127	0
5	NAG	E	1	14/15	0.93	0.15	90,98,105,106	0
4	NAG	F	2	14/15	0.94	0.28	70,81,90,101	0
4	NAG	B	1	14/15	0.95	0.14	73,77,85,87	0
4	NAG	D	1	14/15	0.97	0.12	78,89,98,106	0
5	NAG	C	1	14/15	0.97	0.14	75,84,90,95	0
4	NAG	F	1	14/15	0.98	0.11	65,73,78,78	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.

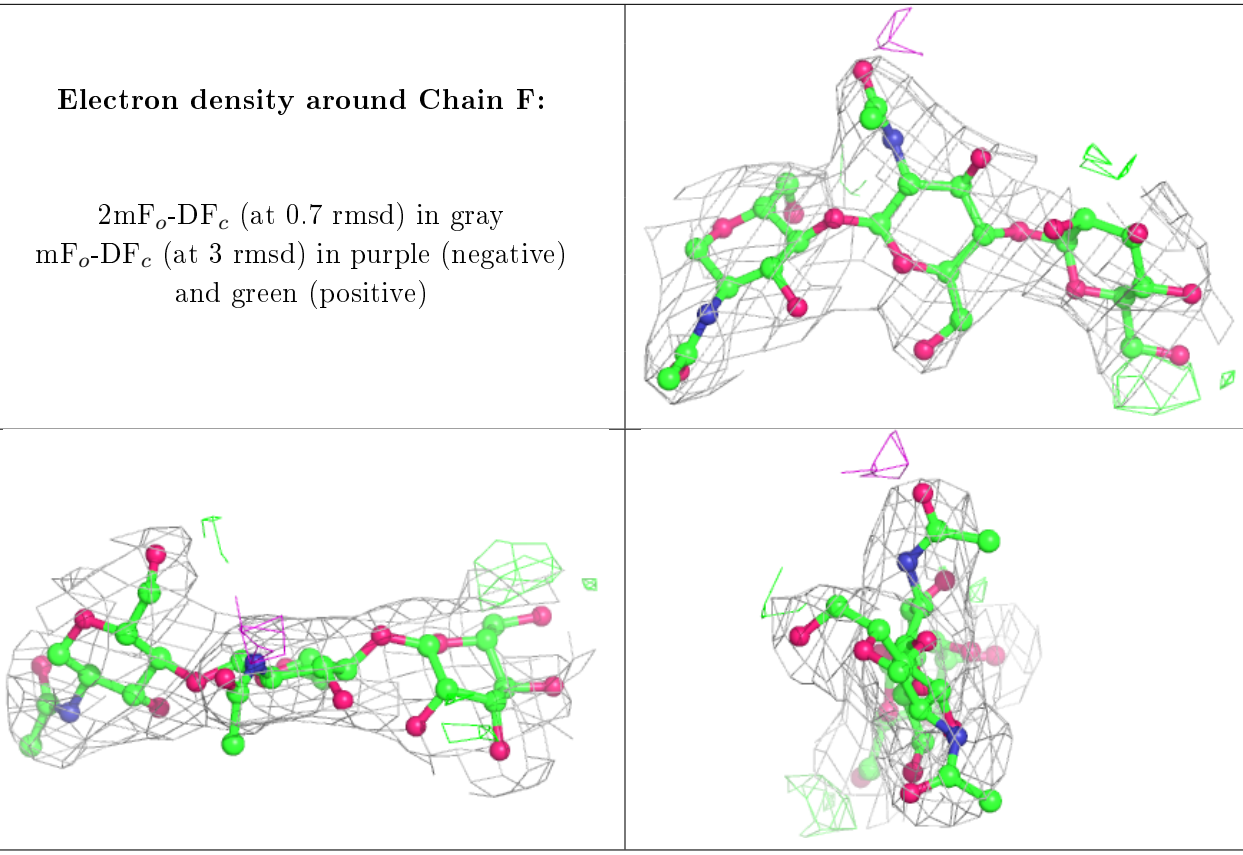
Electron density around Chain D:

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



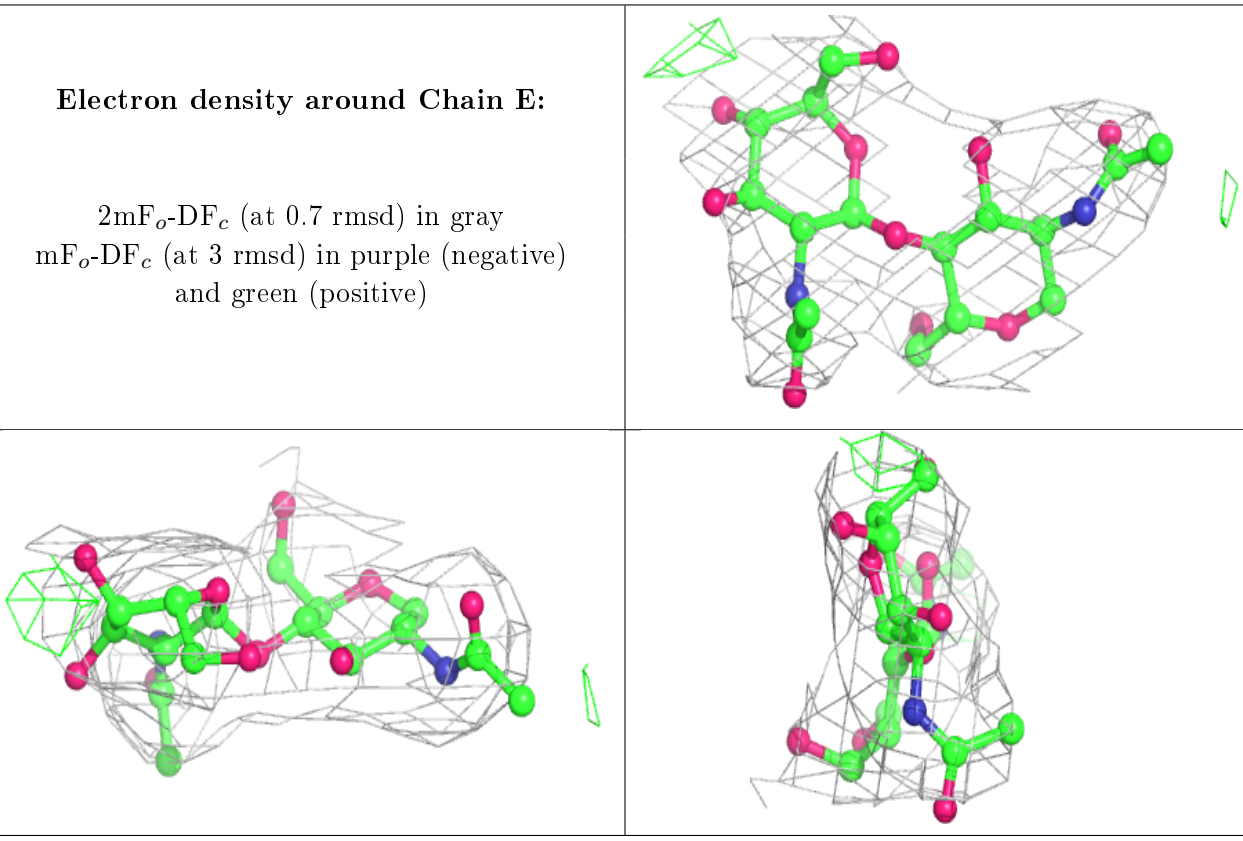
Electron density around Chain F:

$2mF_o$-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 E:

$2mF_o$-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
6	NAG	A	506	14/15	0.76	0.48	114,138,156,159	0
6	NAG	A	510	14/15	0.82	0.31	113,142,163,171	0

6.5 Other polymers

There are no such residues in this entry.