



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:03 AM EDT

PDB ID : 5L56 / pdb_00005l56
Title : Plexin A1 full extracellular region, domains 1 to 10, to 4 angstrom
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.
Deposited on : 2016-05-28
Resolution : 4.00 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:

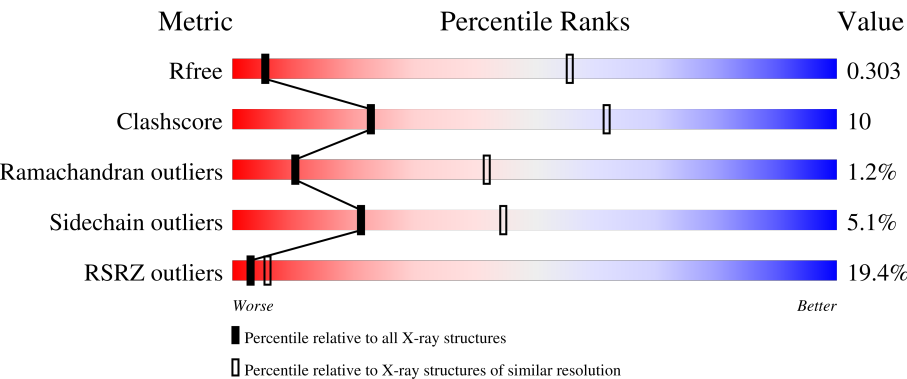
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.00 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.



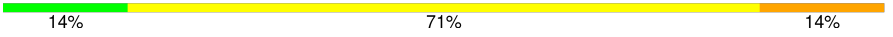
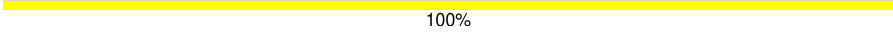
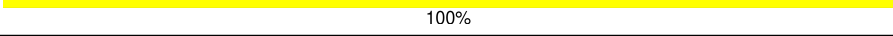
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 $\leq 5\%$. 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	1212	19% 71% 24% • •
2	B	4	25% 50% 25%
2	D	4	100%
3	C	6	17% 83%
3	I	6	17% 83%

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Mol	Chain	Length	Quality of chain
4	E	7	 71%29%
4	F	7	 29%71%
4	J	7	 14%71%14%
5	G	5	 100%
6	H	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
3	NAG	I	1	-	-	-	X
4	NAG	J	1	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9692 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.

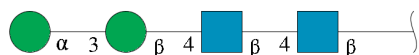
- Molecule 1 is a protein called Plexin-A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1171	9085	5719	1593	1715	58	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

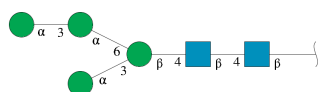
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLU	-	expression tag	UNP P70206
A	35	THR	-	expression tag	UNP P70206
A	36	GLY	-	expression tag	UNP P70206
A	1237	ARG	-	expression tag	UNP P70206
A	1238	THR	-	expression tag	UNP P70206
A	1239	LYS	-	expression tag	UNP P70206
A	1240	HIS	-	expression tag	UNP P70206
A	1241	HIS	-	expression tag	UNP P70206
A	1242	HIS	-	expression tag	UNP P70206
A	1243	HIS	-	expression tag	UNP P70206
A	1244	HIS	-	expression tag	UNP P70206
A	1245	HIS	-	expression tag	UNP P70206

- Molecule 2 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.



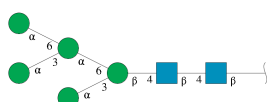
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0
2	D	4	50	28	2	20	0	0	0

- Molecule 3 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.



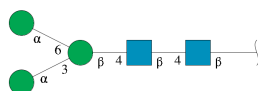
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
4	E	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	F	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

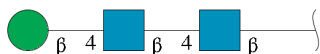
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

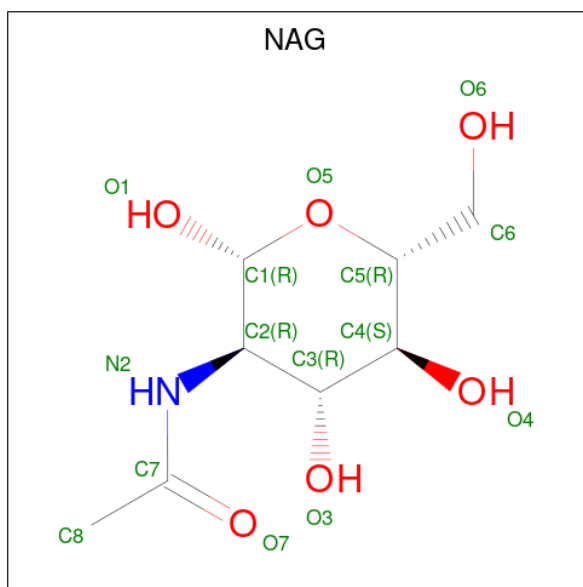
- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

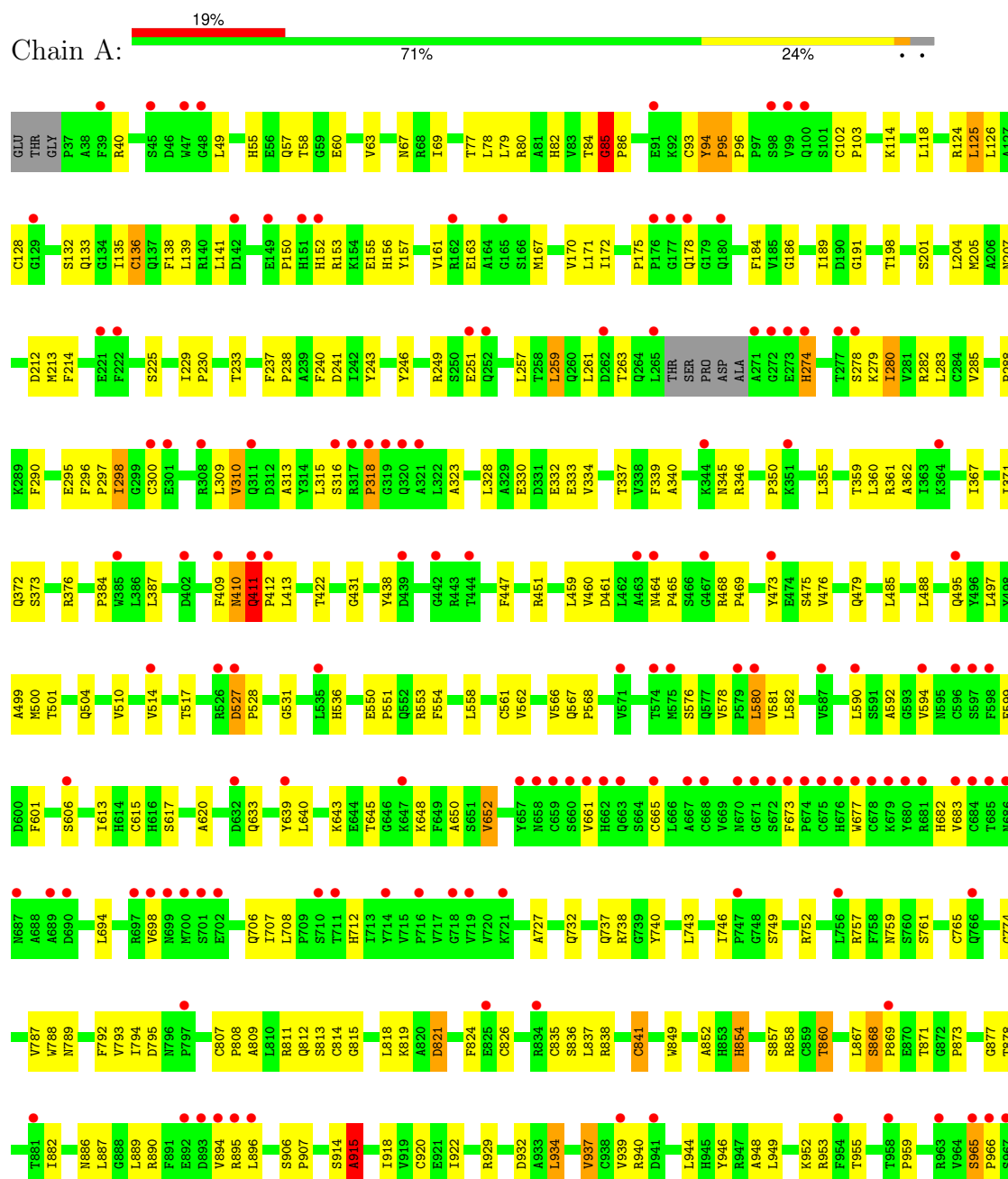


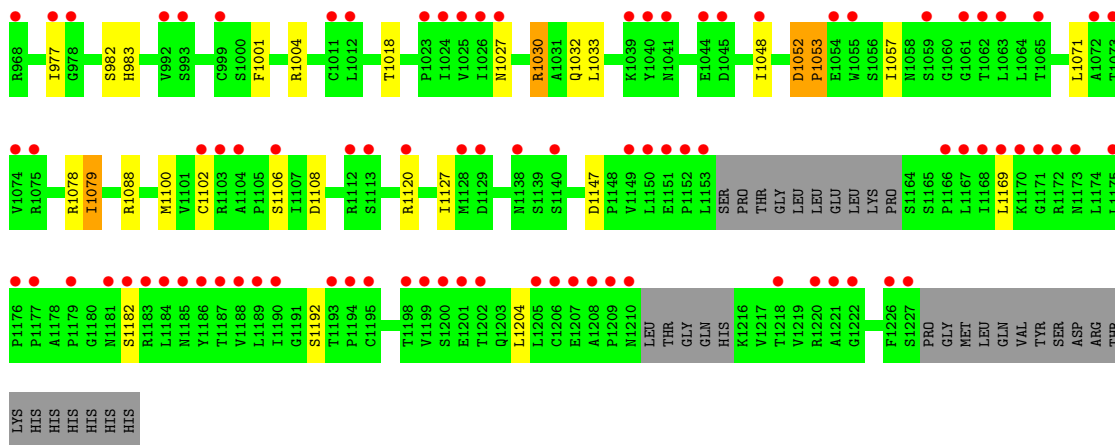
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

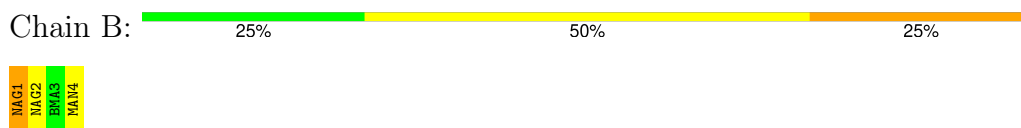
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Plexin-A1





- Molecule 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



- Molecule 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



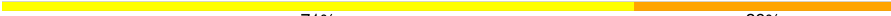
- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 E:  71% 29%

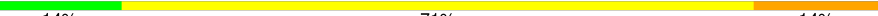
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain F:  29% 71%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  14% 71% 14%

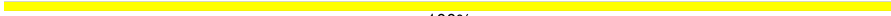
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain G:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain H:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	195.34Å 195.34Å 176.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.51 – 4.00 87.51 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (87.51-4.00) 98.6 (87.51-4.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.257 , 0.308 0.253 , 0.303	Depositor DCC
R_{free} test set	1471 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	117.4	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 310.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	9692	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MAN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/9297	0.88	19/12642 (0.2%)

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
1	A	0	8

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	ASP	CA-C-N	8.15	127.80	119.82
1	A	527	ASP	C-N-CA	8.15	127.80	119.82
1	A	1052	ASP	N-CA-C	7.65	123.63	110.02
1	A	868	SER	CA-C-N	7.44	129.14	119.84
1	A	868	SER	C-N-CA	7.44	129.14	119.84
1	A	809	ALA	N-CA-C	-5.93	105.70	113.17
1	A	841	CYS	CA-C-N	5.76	125.70	119.76
1	A	841	CYS	C-N-CA	5.76	125.70	119.76
1	A	712	HIS	N-CA-C	5.76	118.42	110.35
1	A	85	GLY	CA-C-N	5.76	127.04	119.84
1	A	85	GLY	C-N-CA	5.76	127.04	119.84
1	A	965	SER	CA-C-N	-5.73	112.68	119.84
1	A	965	SER	C-N-CA	-5.73	112.68	119.84
1	A	854	HIS	N-CA-C	-5.70	105.72	114.16
1	A	965	SER	N-CA-C	5.49	121.94	109.81
1	A	1053	PRO	N-CA-C	-5.10	101.97	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	GLU	N-CA-C	5.08	115.84	107.20
1	A	316	SER	N-CA-C	5.08	114.85	108.45
1	A	915	ALA	N-CA-C	5.02	121.50	110.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	ASP	Peptide
1	A	410	ASN	Peptide
1	A	527	ASP	Peptide
1	A	807	CYS	Peptide
1	A	85	GLY	Peptide
1	A	868	SER	Peptide
1	A	94	TYR	Peptide
1	A	965	SER	Peptide

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	9085	0	8879	196	0
2	B	50	0	43	1	0
2	D	50	0	43	0	0
3	C	72	0	60	0	0
3	I	72	0	61	0	0
4	E	83	0	70	1	0
4	F	83	0	70	0	0
4	J	83	0	70	1	0
5	G	61	0	52	0	0
6	H	39	0	34	0	0
7	A	14	0	13	0	0
All	All	9692	0	9395	198	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 10.

All (198) 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:411:GLN:HG2	1:A:412:PRO:HD2	1.35	1.06
1:A:860:THR:HA	1:A:946:TYR:CE1	1.93	1.01
1:A:860:THR:HA	1:A:946:TYR:HE1	1.29	0.91
1:A:468:ARG:HG2	1:A:469:PRO:HD2	1.51	0.89
1:A:94:TYR:CD2	1:A:95:PRO:HD3	2.08	0.89
1:A:189:ILE:HD12	1:A:198:THR:HG23	1.52	0.88
1:A:808:PRO:HD2	1:A:835:CYS:O	1.76	0.85
1:A:567:GLN:HB3	1:A:568:PRO:HD3	1.61	0.81
1:A:280:ILE:HB	1:A:298:ILE:HD12	1.64	0.80
1:A:818:LEU:HB3	1:A:852:ALA:HB2	1.62	0.80
1:A:153:ARG:H	1:A:156:HIS:HD2	1.30	0.79
1:A:789:ASN:HD22	1:A:792:PHE:HE2	1.31	0.78
1:A:259:LEU:HD23	1:A:346:ARG:HG3	1.66	0.78
1:A:895:ARG:O	1:A:896:LEU:HB2	1.85	0.76
1:A:411:GLN:CG	1:A:412:PRO:HD2	2.14	0.75
1:A:230:PRO:O	1:A:233:THR:HG22	1.86	0.74
1:A:743:LEU:HD22	1:A:752:ARG:HG2	1.70	0.74
1:A:860:THR:CA	1:A:946:TYR:HE1	2.03	0.71
1:A:82:HIS:HD2	1:A:84:THR:HG22	1.55	0.70
1:A:171:LEU:HD22	1:A:204:LEU:HD11	1.72	0.70
1:A:852:ALA:HA	1:A:857:SER:OG	1.91	0.70
1:A:1079:ILE:HD11	1:A:1102:CYS:HB3	1.73	0.70
1:A:606:SER:HB3	1:A:615:CYS:HB3	1.74	0.69
1:A:310:VAL:HG22	1:A:339:PHE:CE1	2.28	0.69
1:A:345:ASN:HD22	1:A:1120:ARG:NH2	1.90	0.69
1:A:813:SER:HB2	1:A:886:ASN:OD1	1.93	0.69
1:A:55:HIS:HE2	1:A:141:LEU:HD21	1.57	0.68
1:A:895:ARG:HA	1:A:907:PRO:HG2	1.76	0.68
1:A:138:PHE:CZ	1:A:213:MET:HE2	2.28	0.68
1:A:468:ARG:CG	1:A:469:PRO:HD2	2.24	0.68
1:A:114:LYS:HE2	1:A:167:MET:HE3	1.75	0.67
1:A:818:LEU:HB2	1:A:889:LEU:HD11	1.75	0.67
1:A:746:ILE:HB	1:A:749:SER:O	1.95	0.67
1:A:566:VAL:HG22	1:A:582:LEU:HD23	1.76	0.66
1:A:175:PRO:HG2	1:A:178:GLN:HG3	1.77	0.66
1:A:315:LEU:HD11	1:A:333:GLU:HB3	1.78	0.66
1:A:1057:ILE:HD12	1:A:1147:ASP:OD1	1.97	0.65
1:A:887:LEU:HB2	1:A:915:ALA:HA	1.80	0.63
1:A:69:ILE:HD12	1:A:84:THR:HG21	1.79	0.63
1:A:550:GLU:HB3	1:A:551:PRO:HD2	1.80	0.63
1:A:345:ASN:HD22	1:A:1120:ARG:HH21	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:OG1	1:A:60:GLU:HG2	1.99	0.61
1:A:939:VAL:HG22	1:A:946:TYR:HB3	1.82	0.61
1:A:639:TYR:CD2	1:A:648:LYS:HD2	2.36	0.61
1:A:740:TYR:CD1	1:A:788:TRP:HB3	2.36	0.60
1:A:732:GLN:HG2	1:A:757:ARG:HH22	1.66	0.60
1:A:819:LYS:NZ	1:A:914:SER:O	2.26	0.60
1:A:578:VAL:H	1:A:617:SER:HB3	1.66	0.60
1:A:55:HIS:NE2	1:A:141:LEU:HD21	2.17	0.59
1:A:858:ARG:HB3	1:A:940:ARG:NH2	2.17	0.59
1:A:259:LEU:HD23	1:A:346:ARG:CG	2.31	0.59
1:A:153:ARG:N	1:A:156:HIS:HD2	1.99	0.58
1:A:246:TYR:CD2	1:A:313:ALA:HB3	2.39	0.58
1:A:447:PHE:HZ	1:A:510:VAL:HG23	1.69	0.58
1:A:878:THR:HB	1:A:922:ILE:HD12	1.84	0.57
1:A:485:LEU:HD12	1:A:500:MET:HG2	1.86	0.57
1:A:132:SER:HB2	1:A:135:ILE:HG12	1.87	0.57
1:A:531:GLY:HA3	1:A:554:PHE:CZ	2.40	0.57
1:A:172:ILE:HG22	1:A:249:ARG:HD2	1.87	0.56
1:A:808:PRO:HG3	1:A:835:CYS:HB3	1.87	0.56
1:A:732:GLN:HG2	1:A:757:ARG:NH2	2.20	0.56
1:A:337:THR:O	1:A:355:LEU:HD12	2.05	0.56
1:A:153:ARG:H	1:A:156:HIS:CD2	2.18	0.56
1:A:789:ASN:HB3	1:A:792:PHE:CD2	2.41	0.56
1:A:738:ARG:HB2	1:A:789:ASN:HA	1.89	0.55
1:A:682:HIS:HB3	1:A:792:PHE:CD1	2.41	0.55
1:A:279:LYS:HG2	1:A:297:PRO:HA	1.87	0.55
1:A:737:GLN:HG2	1:A:789:ASN:ND2	2.22	0.55
1:A:318:PRO:HG2	1:A:323:ALA:HB2	1.89	0.55
1:A:282:ARG:HG3	1:A:283:LEU:N	2.22	0.55
1:A:296:PHE:CE1	1:A:367:ILE:HG12	2.41	0.55
1:A:567:GLN:HB2	1:A:581:VAL:HG22	1.87	0.55
1:A:488:LEU:HD12	1:A:499:ALA:HA	1.89	0.54
1:A:93:CYS:O	1:A:133:GLN:NE2	2.40	0.54
1:A:877:GLY:HA3	1:A:1030:ARG:HG3	1.89	0.54
1:A:464:ASN:CG	1:A:465:PRO:HD2	2.32	0.53
1:A:789:ASN:HB3	1:A:792:PHE:HD2	1.73	0.53
1:A:205:MET:HG3	1:A:212:ASP:HB3	1.90	0.53
1:A:566:VAL:HG22	1:A:582:LEU:CD2	2.37	0.53
1:A:332:GLU:OE2	1:A:361:ARG:NH2	2.41	0.53
1:A:310:VAL:HG22	1:A:339:PHE:HE1	1.72	0.53
1:A:278:SER:HB3	1:A:310:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LEU:HD21	1:A:528:PRO:HG3	1.91	0.53
1:A:536:HIS:HA	1:A:645:THR:HG21	1.90	0.53
1:A:821:ASP:HB2	1:A:824:PHE:CD2	2.44	0.53
1:A:170:VAL:HG11	1:A:249:ARG:HB2	1.91	0.52
1:A:58:THR:CB	1:A:60:GLU:HG2	2.39	0.52
1:A:126:LEU:HD11	1:A:136:CYS:SG	2.49	0.52
1:A:124:ARG:HD2	1:A:138:PHE:HD2	1.74	0.52
1:A:640:LEU:HD12	1:A:650:ALA:HB3	1.91	0.52
1:A:461:ASP:HA	1:A:464:ASN:HB3	1.92	0.52
1:A:447:PHE:CZ	1:A:510:VAL:HG23	2.45	0.52
1:A:677:TRP:HB3	1:A:698:VAL:HB	1.92	0.51
1:A:153:ARG:NH2	1:A:212:ASP:HA	2.26	0.51
1:A:229:ILE:HD12	1:A:240:PHE:HE2	1.76	0.51
1:A:345:ASN:ND2	1:A:1120:ARG:HH21	2.08	0.51
1:A:55:HIS:CE1	1:A:57:GLN:HB2	2.46	0.50
1:A:438:TYR:CE1	1:A:510:VAL:HG21	2.46	0.50
1:A:323:ALA:HA	1:A:328:LEU:HD12	1.94	0.50
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.77	0.50
1:A:186:GLY:HA2	1:A:198:THR:O	2.12	0.50
1:A:431:GLY:HA3	1:A:451:ARG:HD2	1.93	0.50
1:A:939:VAL:CG2	1:A:946:TYR:HB3	2.42	0.49
1:A:708:LEU:H	1:A:727:ALA:HA	1.77	0.49
1:A:172:ILE:HD11	1:A:184:PHE:HE2	1.77	0.49
1:A:153:ARG:HB2	1:A:156:HIS:CD2	2.48	0.48
1:A:495:GLN:O	1:A:510:VAL:HG12	2.13	0.48
1:A:1027:ASN:HB3	1:A:1032:GLN:HG3	1.95	0.48
1:A:40:ARG:NH2	2:B:1:NAG:O3	2.47	0.48
1:A:907:PRO:HA	1:A:920:CYS:HA	1.96	0.48
1:A:63:VAL:HG13	1:A:500:MET:HE1	1.96	0.47
1:A:96:PRO:HD2	1:A:157:TYR:CZ	2.48	0.47
1:A:447:PHE:CD2	1:A:497:LEU:HD22	2.50	0.47
1:A:821:ASP:HB2	1:A:824:PHE:CE2	2.50	0.47
1:A:372:GLN:O	1:A:376:ARG:HD3	2.15	0.47
1:A:460:VAL:HA	1:A:469:PRO:HB3	1.96	0.47
1:A:461:ASP:CA	1:A:464:ASN:HB3	2.45	0.47
1:A:567:GLN:CB	1:A:581:VAL:HG22	2.44	0.47
1:A:934:LEU:HD23	1:A:953:ARG:HB3	1.97	0.46
1:A:566:VAL:CG2	1:A:652:VAL:HG21	2.45	0.46
1:A:665:CYS:HB3	1:A:795:ASP:OD2	2.15	0.46
1:A:818:LEU:HD22	1:A:852:ALA:H	1.80	0.46
1:A:172:ILE:HD13	1:A:285:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LEU:HD12	1:A:561:CYS:SG	2.56	0.46
1:A:79:LEU:O	1:A:80:ARG:HG3	2.17	0.45
1:A:860:THR:HG22	1:A:946:TYR:OH	2.16	0.45
1:A:932:ASP:N	1:A:932:ASP:OD1	2.50	0.45
1:A:937:VAL:HG23	1:A:948:ALA:HB3	1.98	0.45
1:A:566:VAL:HG23	1:A:652:VAL:HG21	1.98	0.45
1:A:102:CYS:HA	1:A:103:PRO:HD3	1.87	0.45
1:A:125:LEU:HD23	1:A:139:LEU:HB2	1.99	0.44
1:A:201:SER:HB2	1:A:290:PHE:HE1	1.81	0.44
1:A:501:THR:OG1	1:A:504:GLN:N	2.44	0.44
1:A:550:GLU:HB2	1:A:553:ARG:HG3	2.00	0.44
1:A:576:SER:OG	1:A:620:ALA:N	2.51	0.44
1:A:887:LEU:HD23	1:A:918:ILE:HD11	1.98	0.44
1:A:67:ASN:CB	1:A:85:GLY:HA3	2.48	0.44
1:A:261:LEU:HD11	1:A:274:HIS:CB	2.48	0.44
1:A:682:HIS:CB	1:A:792:PHE:CD1	3.01	0.44
1:A:815:GLY:O	1:A:819:LYS:HB2	2.17	0.44
1:A:740:TYR:HE1	1:A:794:ILE:HD11	1.83	0.44
1:A:359:THR:HG23	1:A:362:ALA:CB	2.48	0.44
1:A:161:VAL:HG12	1:A:163:GLU:H	1.83	0.43
1:A:906:SER:HA	1:A:907:PRO:HD3	1.77	0.43
1:A:952:LYS:HA	1:A:952:LYS:HD2	1.70	0.43
1:A:150:PRO:HB2	1:A:156:HIS:ND1	2.34	0.43
1:A:706:GLN:O	1:A:727:ALA:HB1	2.19	0.43
1:A:1088:ARG:HD2	1:A:1106:SER:O	2.18	0.43
1:A:155:GLU:N	1:A:155:GLU:OE1	2.51	0.43
1:A:808:PRO:HB2	1:A:811:ARG:H	1.82	0.43
1:A:959:PRO:HA	1:A:983:HIS:HB2	2.01	0.43
1:A:132:SER:CB	1:A:135:ILE:HG12	2.47	0.43
1:A:789:ASN:ND2	1:A:792:PHE:HE2	2.09	0.43
1:A:838:ARG:NH1	1:A:841:CYS:O	2.51	0.43
1:A:894:VAL:HG11	1:A:918:ILE:HD13	1.99	0.43
1:A:309:LEU:O	1:A:339:PHE:HA	2.19	0.43
1:A:639:TYR:HD2	1:A:648:LYS:HD2	1.84	0.43
1:A:1078:ARG:HG3	1:A:1127:ILE:HB	1.99	0.43
1:A:58:THR:HB	1:A:60:GLU:HG2	2.01	0.42
1:A:410:ASN:O	1:A:411:GLN:O	2.37	0.42
1:A:633:GLN:OE1	1:A:673:PHE:CE1	2.72	0.42
4:J:1:NAG:H83	4:J:1:NAG:H2	1.87	0.42
1:A:818:LEU:HD22	1:A:852:ALA:N	2.34	0.42
1:A:1071:LEU:HD13	1:A:1100:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PHE:HA	1:A:238:PRO:HD3	1.89	0.42
1:A:599:GLU:C	1:A:601:PHE:H	2.28	0.42
1:A:787:VAL:HG22	1:A:793:VAL:HG22	2.01	0.42
1:A:371:ILE:C	1:A:373:SER:H	2.28	0.42
1:A:476:VAL:HB	1:A:479:GLN:HG2	2.01	0.42
1:A:1001:PHE:HZ	1:A:1004:ARG:HB2	1.85	0.42
1:A:49:LEU:HD13	1:A:500:MET:HE2	2.02	0.42
1:A:818:LEU:HB3	1:A:852:ALA:CB	2.41	0.42
1:A:944:LEU:HD12	1:A:944:LEU:H	1.85	0.42
1:A:468:ARG:HG2	1:A:469:PRO:CD	2.36	0.41
1:A:682:HIS:HB3	1:A:792:PHE:CE1	2.55	0.41
1:A:871:THR:HG22	1:A:955:THR:HB	2.02	0.41
1:A:813:SER:HB2	1:A:886:ASN:CG	2.45	0.41
1:A:340:ALA:HB1	1:A:350:PRO:HG2	2.02	0.41
1:A:643:LYS:HE3	1:A:643:LYS:HB3	1.98	0.41
1:A:568:PRO:HG2	1:A:580:LEU:HD23	2.01	0.41
1:A:824:PHE:C	1:A:826:CYS:H	2.27	0.41
1:A:582:LEU:HB2	1:A:613:ILE:HB	2.02	0.41
1:A:69:ILE:CD1	1:A:84:THR:HG21	2.48	0.41
1:A:136:CYS:HB3	1:A:214:PHE:CZ	2.56	0.41
1:A:189:ILE:HG22	1:A:191:GLY:H	1.86	0.41
1:A:225:SER:HB3	1:A:288:PRO:O	2.20	0.41
1:A:873:PRO:HD2	1:A:878:THR:OG1	2.21	0.41
1:A:1169:LEU:HB2	1:A:1204:LEU:HB2	2.02	0.41
1:A:836:SER:O	1:A:849:TRP:NE1	2.54	0.41
1:A:241:ASP:HB3	1:A:243:TYR:CZ	2.56	0.40
1:A:263:THR:HB	1:A:384:PRO:HB2	2.01	0.40
1:A:461:ASP:CB	1:A:464:ASN:HB3	2.50	0.40
1:A:590:LEU:C	1:A:592:ALA:N	2.79	0.40
1:A:473:TYR:CE2	1:A:475:SER:HB2	2.56	0.40
1:A:488:LEU:HG	1:A:497:LEU:HD11	2.02	0.40
1:A:409:PHE:C	1:A:411:GLN:H	2.29	0.40
1:A:606:SER:CB	1:A:615:CYS:HB3	2.48	0.40
1:A:759:ASN:C	1:A:761:SER:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1163/1212 (96%)	1056 (91%)	93 (8%)	14 (1%)	10	42

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	A	95	PRO
1	A	411	GLN
1	A	869	PRO
1	A	915	ALA
1	A	1192	SER
1	A	251	GLU
1	A	1053	PRO
1	A	1182	SER
1	A	694	LEU
1	A	966	PRO
1	A	318	PRO
1	A	1108	ASP
1	A	774	GLY

5.3.2 Protein sidechains

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	1015/1051 (97%)	963 (95%)	52 (5%)	21	45

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	78	LEU
1	A	118	LEU
1	A	125	LEU
1	A	128	CYS
1	A	136	CYS
1	A	152	HIS
1	A	207	ASN
1	A	257	LEU
1	A	259	LEU
1	A	274	HIS
1	A	280	ILE
1	A	298	ILE
1	A	300	CYS
1	A	310	VAL
1	A	330	GLU
1	A	334	VAL
1	A	360	LEU
1	A	387	LEU
1	A	411	GLN
1	A	413	LEU
1	A	422	THR
1	A	514	VAL
1	A	517	THR
1	A	562	VAL
1	A	580	LEU
1	A	594	VAL
1	A	652	VAL
1	A	661	VAL
1	A	683	VAL
1	A	707	ILE
1	A	765	CYS
1	A	812	GLN
1	A	814	CYS
1	A	821	ASP
1	A	837	LEU
1	A	854	HIS
1	A	860	THR
1	A	867	LEU
1	A	882	ILE
1	A	890	ARG
1	A	929	ARG
1	A	934	LEU

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Mol	Chain	Res	Type
1	A	937	VAL
1	A	949	LEU
1	A	977	ILE
1	A	982	SER
1	A	1018	THR
1	A	1030	ARG
1	A	1033	LEU
1	A	1048	ILE
1	A	1079	ILE

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

Mol	Chain	Res	Type
1	A	57	GLN
1	A	156	HIS
1	A	260	GLN
1	A	345	ASN
1	A	536	HIS
1	A	563	GLN
1	A	616	HIS
1	A	706	GLN
1	A	729	ASN
1	A	764	GLN
1	A	766	GLN
1	A	840	HIS
1	A	899	HIS
1	A	931	HIS
1	A	1035	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

41 non-standard protein/DNA/RNA residues 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
3	MAN	I	5	3	11,11,12	0.60	0	15,15,17	1.01	2 (13%)
2	NAG	D	2	2	14,14,15	0.56	0	17,19,21	1.22	2 (11%)
5	MAN	G	5	5	11,11,12	0.52	0	15,15,17	1.42	2 (13%)
7	NAG	A	1334	1	14,14,15	0.53	0	17,19,21	0.97	1 (5%)
4	NAG	J	2	4	14,14,15	0.54	0	17,19,21	1.46	3 (17%)
3	NAG	I	2	3	14,14,15	0.57	0	17,19,21	1.13	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.64	0	17,19,21	1.05	1 (5%)
6	NAG	H	1	1,6	14,14,15	0.59	0	17,19,21	1.11	1 (5%)
3	MAN	C	6	3	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	MAN	E	5	4	11,11,12	0.53	0	15,15,17	1.23	1 (6%)
2	NAG	B	2	2	14,14,15	0.58	0	17,19,21	1.54	1 (5%)
3	NAG	C	1	1,3	14,14,15	0.64	0	17,19,21	1.20	1 (5%)
4	MAN	F	7	4	11,11,12	0.55	0	15,15,17	1.06	1 (6%)
4	MAN	F	4	4	11,11,12	0.63	0	15,15,17	0.78	0
3	MAN	I	4	3	11,11,12	0.73	0	15,15,17	1.18	2 (13%)
4	NAG	E	2	4	14,14,15	0.53	0	17,19,21	1.15	2 (11%)
4	MAN	J	5	4	11,11,12	0.62	0	15,15,17	1.14	1 (6%)
6	NAG	H	2	6	14,14,15	0.56	0	17,19,21	1.19	2 (11%)
4	MAN	E	7	4	11,11,12	0.57	0	15,15,17	0.83	1 (6%)
3	NAG	I	1	1,3	14,14,15	0.60	0	17,19,21	1.07	1 (5%)
3	MAN	I	6	3	11,11,12	0.63	0	15,15,17	0.80	0
5	NAG	G	2	5	14,14,15	0.66	0	17,19,21	1.11	1 (5%)
4	MAN	J	6	4	11,11,12	0.63	0	15,15,17	0.96	1 (6%)
3	MAN	C	4	3	11,11,12	0.65	0	15,15,17	0.88	1 (6%)
4	NAG	F	1	1,4	14,14,15	0.62	0	17,19,21	1.25	1 (5%)
4	MAN	F	5	4	11,11,12	0.62	0	15,15,17	1.14	2 (13%)
4	MAN	J	4	4	11,11,12	0.61	0	15,15,17	0.89	0
2	MAN	B	4	2	11,11,12	0.62	0	15,15,17	0.94	1 (6%)
4	NAG	F	2	4	14,14,15	0.54	0	17,19,21	1.08	1 (5%)
2	MAN	D	4	2	11,11,12	0.57	0	15,15,17	1.00	1 (6%)
4	MAN	J	7	4	11,11,12	0.60	0	15,15,17	1.04	2 (13%)
4	NAG	E	1	1,4	14,14,15	0.67	0	17,19,21	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	G	4	5	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.65	0	17,19,21	1.27	1 (5%)
3	NAG	C	2	3	14,14,15	0.50	0	17,19,21	1.25	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.40	0	17,19,21	1.50	3 (17%)
2	NAG	B	1	1,2	14,14,15	0.81	0	17,19,21	1.74	3 (17%)
3	MAN	C	5	3	11,11,12	0.57	0	15,15,17	1.18	2 (13%)
4	MAN	E	4	4	11,11,12	0.62	0	15,15,17	0.87	1 (6%)
4	MAN	E	6	4	11,11,12	0.55	0	15,15,17	1.28	2 (13%)
4	MAN	F	6	4	11,11,12	0.59	0	15,15,17	0.93	1 (6%)

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
3	MAN	I	5	3	-	1/2/19/22	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	1/1/1/1
7	NAG	A	1334	1	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
6	NAG	H	1	1,6	-	2/6/23/26	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
4	MAN	F	7	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	MAN	J	5	4	-	2/2/19/22	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
4	MAN	E	7	4	-	2/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	MAN	I	6	3	-	1/2/19/22	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	J	6	4	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
4	MAN	J	7	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
4	NAG	J	1	1,4	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	1/2/19/22	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C4-C3-C2	5.14	118.56	111.02
2	B	2	NAG	C4-C3-C2	4.88	118.17	111.02
5	G	5	MAN	C1-O5-C5	4.49	118.21	112.19
4	E	5	MAN	C1-O5-C5	4.28	117.92	112.19
2	D	1	NAG	C4-C3-C2	4.09	117.01	111.02
3	C	2	NAG	C1-O5-C5	4.03	117.58	112.19
4	E	1	NAG	C4-C3-C2	4.00	116.88	111.02
4	J	1	NAG	C1-O5-C5	3.78	117.25	112.19
4	F	2	NAG	C1-O5-C5	3.73	117.18	112.19
4	E	6	MAN	C1-O5-C5	3.70	117.15	112.19
3	I	4	MAN	C1-C2-C3	3.53	114.79	109.64
3	C	5	MAN	C1-O5-C5	3.45	116.81	112.19
3	I	1	NAG	C1-O5-C5	3.32	116.64	112.19
6	H	1	NAG	C4-C3-C2	3.32	115.88	111.02
4	F	1	NAG	C4-C3-C2	3.30	115.86	111.02
4	F	7	MAN	C1-O5-C5	3.29	116.59	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C4-C3-C2	3.04	115.48	111.02
5	G	2	NAG	C4-C3-C2	3.04	115.47	111.02
5	G	1	NAG	C4-C3-C2	3.03	115.45	111.02
2	B	1	NAG	C3-C4-C5	3.02	115.70	110.23
2	D	2	NAG	C1-O5-C5	3.01	116.21	112.19
6	H	2	NAG	C4-C3-C2	2.98	115.39	111.02
4	J	5	MAN	C1-C2-C3	2.90	113.87	109.64
4	J	2	NAG	C3-C4-C5	2.87	115.44	110.23
3	C	6	MAN	C1-O5-C5	2.85	116.00	112.19
3	C	1	NAG	C4-C3-C2	2.84	115.17	111.02
2	D	2	NAG	C4-C3-C2	2.68	114.94	111.02
5	G	4	MAN	C1-O5-C5	2.64	115.72	112.19
4	J	2	NAG	O5-C1-C2	-2.53	107.38	111.29
3	I	5	MAN	C1-O5-C5	2.52	115.56	112.19
4	F	5	MAN	C1-O5-C5	2.47	115.50	112.19
4	J	7	MAN	C1-C2-C3	2.46	113.22	109.64
4	E	6	MAN	C1-C2-C3	2.44	113.20	109.64
3	C	5	MAN	C1-C2-C3	2.44	113.20	109.64
2	B	1	NAG	C2-N2-C7	2.38	126.10	122.90
4	J	6	MAN	C1-C2-C3	2.34	113.06	109.64
4	F	6	MAN	C1-O5-C5	2.31	115.28	112.19
6	H	2	NAG	O5-C1-C2	-2.31	107.72	111.29
2	D	4	MAN	C1-O5-C5	2.30	115.26	112.19
4	J	1	NAG	O5-C1-C2	-2.29	107.74	111.29
4	J	7	MAN	C1-O5-C5	2.28	115.25	112.19
4	F	5	MAN	C3-C4-C5	2.23	114.28	110.23
7	A	1334	NAG	C4-C3-C2	2.23	114.28	111.02
3	I	5	MAN	C1-C2-C3	2.22	112.87	109.64
4	E	7	MAN	C1-O5-C5	2.20	115.13	112.19
3	C	4	MAN	C1-C2-C3	2.19	112.84	109.64
2	B	4	MAN	C1-C2-C3	2.17	112.80	109.64
4	E	2	NAG	C3-C4-C5	2.17	114.16	110.23
5	G	5	MAN	C1-C2-C3	2.09	112.69	109.64
4	E	2	NAG	O5-C1-C2	-2.09	108.06	111.29
3	I	2	NAG	C2-N2-C7	2.05	125.64	122.90
4	E	4	MAN	O5-C5-C6	2.02	111.59	107.66
4	J	1	NAG	O4-C4-C5	2.01	114.28	109.32
3	I	4	MAN	O5-C5-C6	2.01	111.57	107.66
3	C	6	MAN	C1-C2-C3	2.00	112.56	109.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	J	1	NAG	C1

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
4	F	7	MAN	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
4	F	6	MAN	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	F	6	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
4	J	7	MAN	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
4	E	7	MAN	C4-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6
4	J	5	MAN	C4-C5-C6-O6
4	J	7	MAN	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
4	J	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	I	5	MAN	C4-C5-C6-O6
4	E	7	MAN	O5-C5-C6-O6
7	A	1334	NAG	C4-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	I	6	MAN	C4-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
4	J	6	MAN	C4-C5-C6-O6
5	G	4	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

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

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0
4	E	1	NAG	1	0
4	J	1	NAG	1	0
2	B	1	NAG	1	0

5.5 Carbohydrates [i](#)

49 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	1,2	14,14,15	0.81	0	17,19,21	1.74	3 (17%)
2	NAG	B	2	2	14,14,15	0.58	0	17,19,21	1.54	1 (5%)
2	BMA	B	3	2	11,11,12	0.64	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	B	4	2	11,11,12	0.62	0	15,15,17	0.94	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.64	0	17,19,21	1.20	1 (5%)
3	NAG	C	2	3	14,14,15	0.50	0	17,19,21	1.25	1 (5%)
3	BMA	C	3	3	11,11,12	0.52	0	15,15,17	0.57	0
3	MAN	C	4	3	11,11,12	0.65	0	15,15,17	0.88	1 (6%)
3	MAN	C	5	3	11,11,12	0.57	0	15,15,17	1.18	2 (13%)
3	MAN	C	6	3	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
2	NAG	D	1	1,2	14,14,15	0.65	0	17,19,21	1.27	1 (5%)
2	NAG	D	2	2	14,14,15	0.56	0	17,19,21	1.22	2 (11%)
2	BMA	D	3	2	11,11,12	0.80	1 (9%)	15,15,17	1.92	3 (20%)
2	MAN	D	4	2	11,11,12	0.57	0	15,15,17	1.00	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.67	0	17,19,21	1.19	1 (5%)
4	NAG	E	2	4	14,14,15	0.53	0	17,19,21	1.15	2 (11%)
4	BMA	E	3	4	11,11,12	0.59	0	15,15,17	1.54	3 (20%)
4	MAN	E	4	4	11,11,12	0.62	0	15,15,17	0.87	1 (6%)
4	MAN	E	5	4	11,11,12	0.53	0	15,15,17	1.23	1 (6%)
4	MAN	E	6	4	11,11,12	0.55	0	15,15,17	1.28	2 (13%)
4	MAN	E	7	4	11,11,12	0.57	0	15,15,17	0.83	1 (6%)
4	NAG	F	1	1,4	14,14,15	0.62	0	17,19,21	1.25	1 (5%)
4	NAG	F	2	4	14,14,15	0.54	0	17,19,21	1.08	1 (5%)
4	BMA	F	3	4	11,11,12	0.53	0	15,15,17	0.80	0
4	MAN	F	4	4	11,11,12	0.63	0	15,15,17	0.78	0
4	MAN	F	5	4	11,11,12	0.62	0	15,15,17	1.14	2 (13%)
4	MAN	F	6	4	11,11,12	0.59	0	15,15,17	0.93	1 (6%)
4	MAN	F	7	4	11,11,12	0.55	0	15,15,17	1.06	1 (6%)
5	NAG	G	1	1,5	14,14,15	0.64	0	17,19,21	1.05	1 (5%)
5	NAG	G	2	5	14,14,15	0.66	0	17,19,21	1.11	1 (5%)
5	BMA	G	3	5	11,11,12	0.43	0	15,15,17	1.63	2 (13%)
5	MAN	G	4	5	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
5	MAN	G	5	5	11,11,12	0.52	0	15,15,17	1.42	2 (13%)
6	NAG	H	1	1,6	14,14,15	0.59	0	17,19,21	1.11	1 (5%)
6	NAG	H	2	6	14,14,15	0.56	0	17,19,21	1.19	2 (11%)
6	BMA	H	3	6	11,11,12	0.48	0	15,15,17	1.13	2 (13%)
3	NAG	I	1	1,3	14,14,15	0.60	0	17,19,21	1.07	1 (5%)
3	NAG	I	2	3	14,14,15	0.57	0	17,19,21	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	I	3	3	11,11,12	0.52	0	15,15,17	1.17	2 (13%)
3	MAN	I	4	3	11,11,12	0.73	0	15,15,17	1.18	2 (13%)
3	MAN	I	5	3	11,11,12	0.60	0	15,15,17	1.01	2 (13%)
3	MAN	I	6	3	11,11,12	0.63	0	15,15,17	0.80	0
4	NAG	J	1	1,4	14,14,15	0.40	0	17,19,21	1.50	3 (17%)
4	NAG	J	2	4	14,14,15	0.54	0	17,19,21	1.46	3 (17%)
4	BMA	J	3	4	11,11,12	0.38	0	15,15,17	0.74	1 (6%)
4	MAN	J	4	4	11,11,12	0.61	0	15,15,17	0.89	0
4	MAN	J	5	4	11,11,12	0.62	0	15,15,17	1.14	1 (6%)
4	MAN	J	6	4	11,11,12	0.63	0	15,15,17	0.96	1 (6%)
4	MAN	J	7	4	11,11,12	0.60	0	15,15,17	1.04	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	1/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
4	MAN	E	7	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	2/2/19/22	0/1/1/1
4	MAN	F	7	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	1/1/1/1
6	NAG	H	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
6	BMA	H	3	6	-	2/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
3	MAN	I	5	3	-	1/2/19/22	0/1/1/1
3	MAN	I	6	3	-	1/2/19/22	0/1/1/1
4	NAG	J	1	1,4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	2/2/19/22	0/1/1/1
4	MAN	J	6	4	-	1/2/19/22	0/1/1/1
4	MAN	J	7	4	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	C2-C3	2.07	1.55	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	BMA	C1-C2-C3	6.15	118.61	109.64
2	B	1	NAG	C4-C3-C2	5.14	118.56	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C4-C3-C2	4.88	118.17	111.02
5	G	3	BMA	C1-O5-C5	4.65	118.42	112.19
5	G	5	MAN	C1-O5-C5	4.49	118.21	112.19
4	E	5	MAN	C1-O5-C5	4.28	117.92	112.19
2	D	1	NAG	C4-C3-C2	4.09	117.01	111.02
3	C	2	NAG	C1-O5-C5	4.03	117.58	112.19
4	E	1	NAG	C4-C3-C2	4.00	116.88	111.02
4	J	1	NAG	C1-O5-C5	3.78	117.25	112.19
4	F	2	NAG	C1-O5-C5	3.73	117.18	112.19
4	E	6	MAN	C1-O5-C5	3.70	117.15	112.19
4	E	3	BMA	C3-C4-C5	3.69	116.92	110.23
3	I	4	MAN	C1-C2-C3	3.53	114.79	109.64
3	C	5	MAN	C1-O5-C5	3.45	116.81	112.19
3	I	1	NAG	C1-O5-C5	3.32	116.64	112.19
6	H	1	NAG	C4-C3-C2	3.32	115.88	111.02
4	F	1	NAG	C4-C3-C2	3.30	115.86	111.02
4	F	7	MAN	C1-O5-C5	3.29	116.59	112.19
6	H	3	BMA	C1-O5-C5	3.26	116.56	112.19
5	G	3	BMA	C1-C2-C3	3.18	114.27	109.64
4	J	2	NAG	C4-C3-C2	3.04	115.48	111.02
5	G	2	NAG	C4-C3-C2	3.04	115.47	111.02
5	G	1	NAG	C4-C3-C2	3.03	115.45	111.02
2	B	1	NAG	C3-C4-C5	3.02	115.70	110.23
2	D	2	NAG	C1-O5-C5	3.01	116.21	112.19
6	H	2	NAG	C4-C3-C2	2.98	115.39	111.02
4	E	3	BMA	C2-C3-C4	2.95	116.04	110.86
3	I	3	BMA	C3-C4-C5	2.94	115.56	110.23
4	J	5	MAN	C1-C2-C3	2.90	113.87	109.64
4	J	2	NAG	C3-C4-C5	2.87	115.44	110.23
3	C	6	MAN	C1-O5-C5	2.85	116.00	112.19
3	C	1	NAG	C4-C3-C2	2.84	115.17	111.02
2	D	2	NAG	C4-C3-C2	2.68	114.94	111.02
4	E	3	BMA	C1-C2-C3	2.68	113.54	109.64
5	G	4	MAN	C1-O5-C5	2.64	115.72	112.19
4	J	2	NAG	O5-C1-C2	-2.53	107.38	111.29
3	I	5	MAN	C1-O5-C5	2.52	115.56	112.19
4	F	5	MAN	C1-O5-C5	2.47	115.50	112.19
4	J	7	MAN	C1-C2-C3	2.46	113.22	109.64
4	E	6	MAN	C1-C2-C3	2.44	113.20	109.64
3	C	5	MAN	C1-C2-C3	2.44	113.20	109.64
2	B	1	NAG	C2-N2-C7	2.38	126.10	122.90
4	J	6	MAN	C1-C2-C3	2.34	113.06	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	BMA	C2-C3-C4	2.34	114.98	110.86
4	F	6	MAN	C1-O5-C5	2.31	115.28	112.19
6	H	2	NAG	O5-C1-C2	-2.31	107.72	111.29
2	D	4	MAN	C1-O5-C5	2.30	115.26	112.19
4	J	1	NAG	O5-C1-C2	-2.29	107.74	111.29
4	J	7	MAN	C1-O5-C5	2.28	115.25	112.19
4	F	5	MAN	C3-C4-C5	2.23	114.28	110.23
3	I	5	MAN	C1-C2-C3	2.22	112.87	109.64
6	H	3	BMA	C1-C2-C3	2.20	112.85	109.64
4	E	7	MAN	C1-O5-C5	2.20	115.13	112.19
3	C	4	MAN	C1-C2-C3	2.19	112.84	109.64
2	D	3	BMA	C1-O5-C5	2.18	115.11	112.19
2	B	4	MAN	C1-C2-C3	2.17	112.80	109.64
4	E	2	NAG	C3-C4-C5	2.17	114.16	110.23
3	I	3	BMA	C2-C3-C4	2.15	114.64	110.86
5	G	5	MAN	C1-C2-C3	2.09	112.69	109.64
4	E	2	NAG	O5-C1-C2	-2.09	108.06	111.29
4	J	3	BMA	C1-O5-C5	2.08	114.97	112.19
3	I	2	NAG	C2-N2-C7	2.05	125.64	122.90
4	E	4	MAN	O5-C5-C6	2.02	111.59	107.66
4	J	1	NAG	O4-C4-C5	2.01	114.28	109.32
3	I	4	MAN	O5-C5-C6	2.01	111.57	107.66
3	C	6	MAN	C1-C2-C3	2.00	112.56	109.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	J	1	NAG	C1

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	H	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
4	F	7	MAN	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
4	F	6	MAN	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	F	6	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	J	7	MAN	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
6	H	3	BMA	C4-C5-C6-O6
4	E	7	MAN	C4-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6
4	J	5	MAN	C4-C5-C6-O6
4	J	7	MAN	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
4	J	5	MAN	O5-C5-C6-O6
3	I	5	MAN	C4-C5-C6-O6
4	E	7	MAN	O5-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C4-C5-C6-O6
3	I	6	MAN	C4-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
4	J	6	MAN	C4-C5-C6-O6
5	G	4	MAN	C4-C5-C6-O6

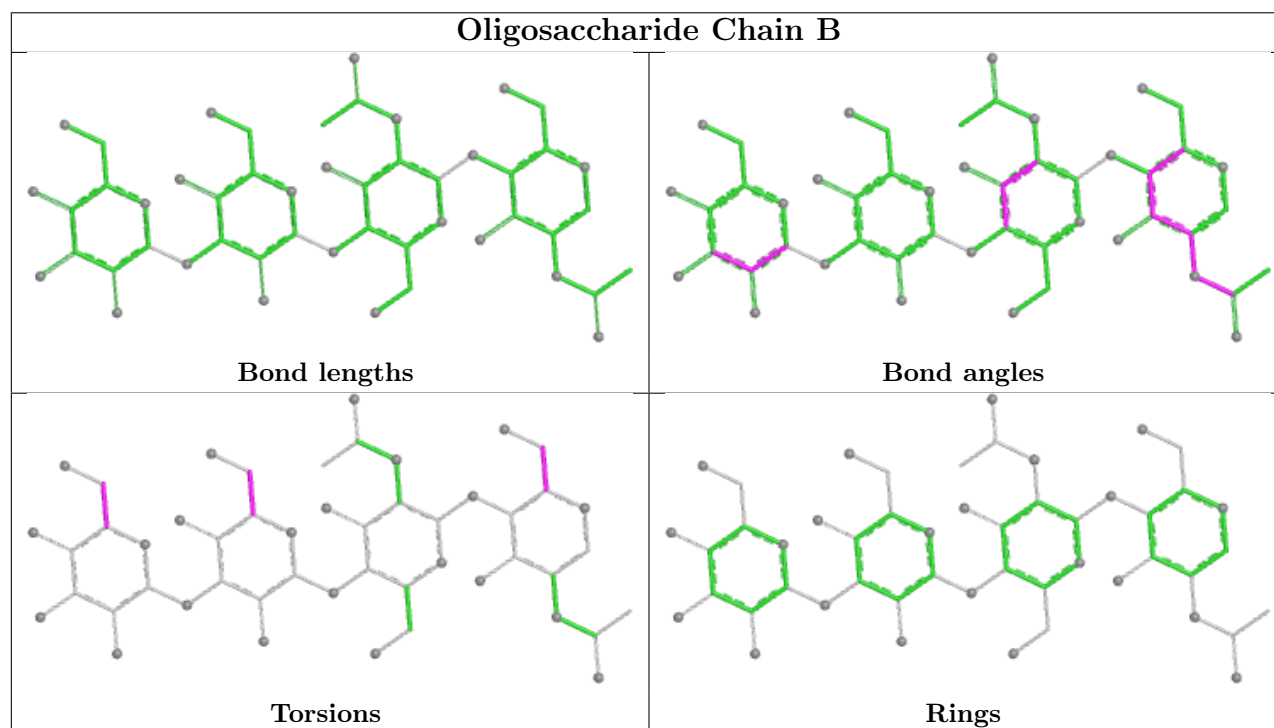
All (1) ring outliers are listed below:

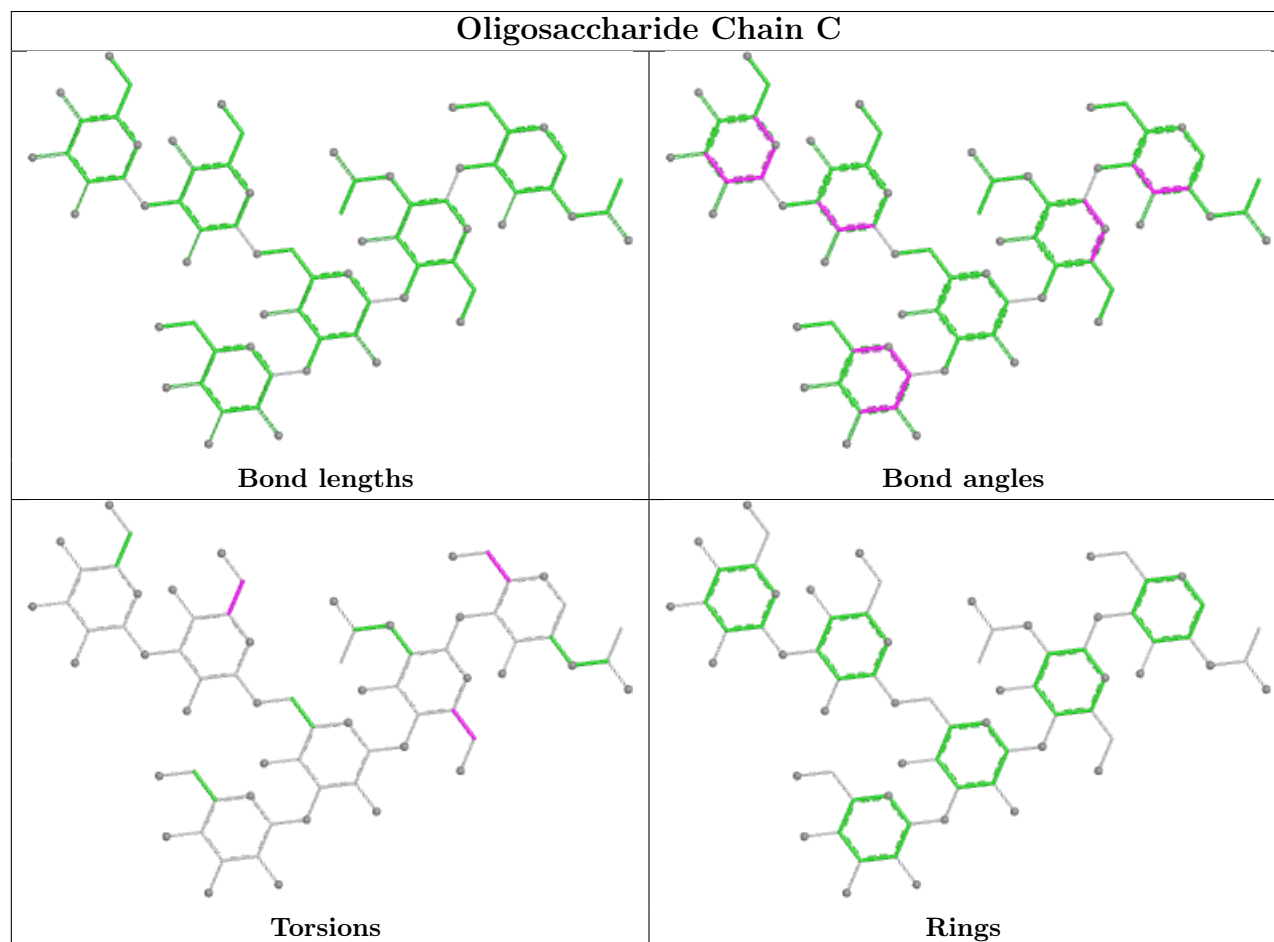
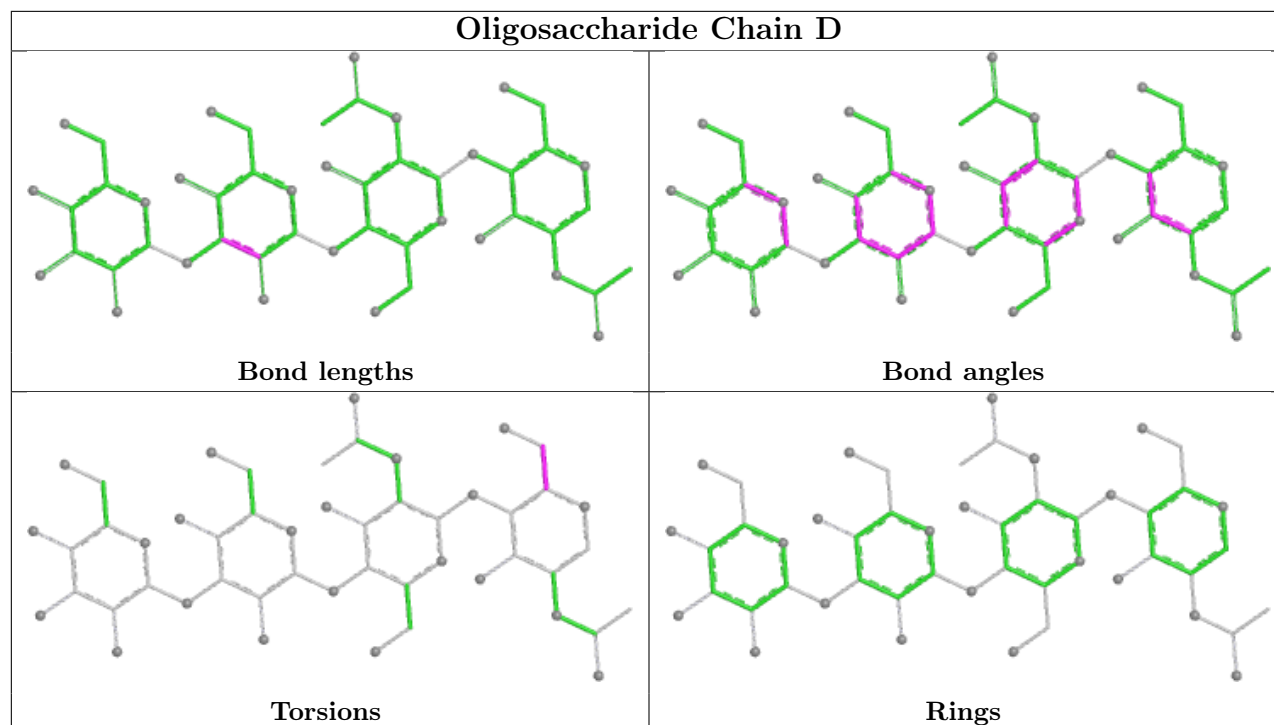
Mol	Chain	Res	Type	Atoms
5	G	5	MAN	C1-C2-C3-C4-C5-O5

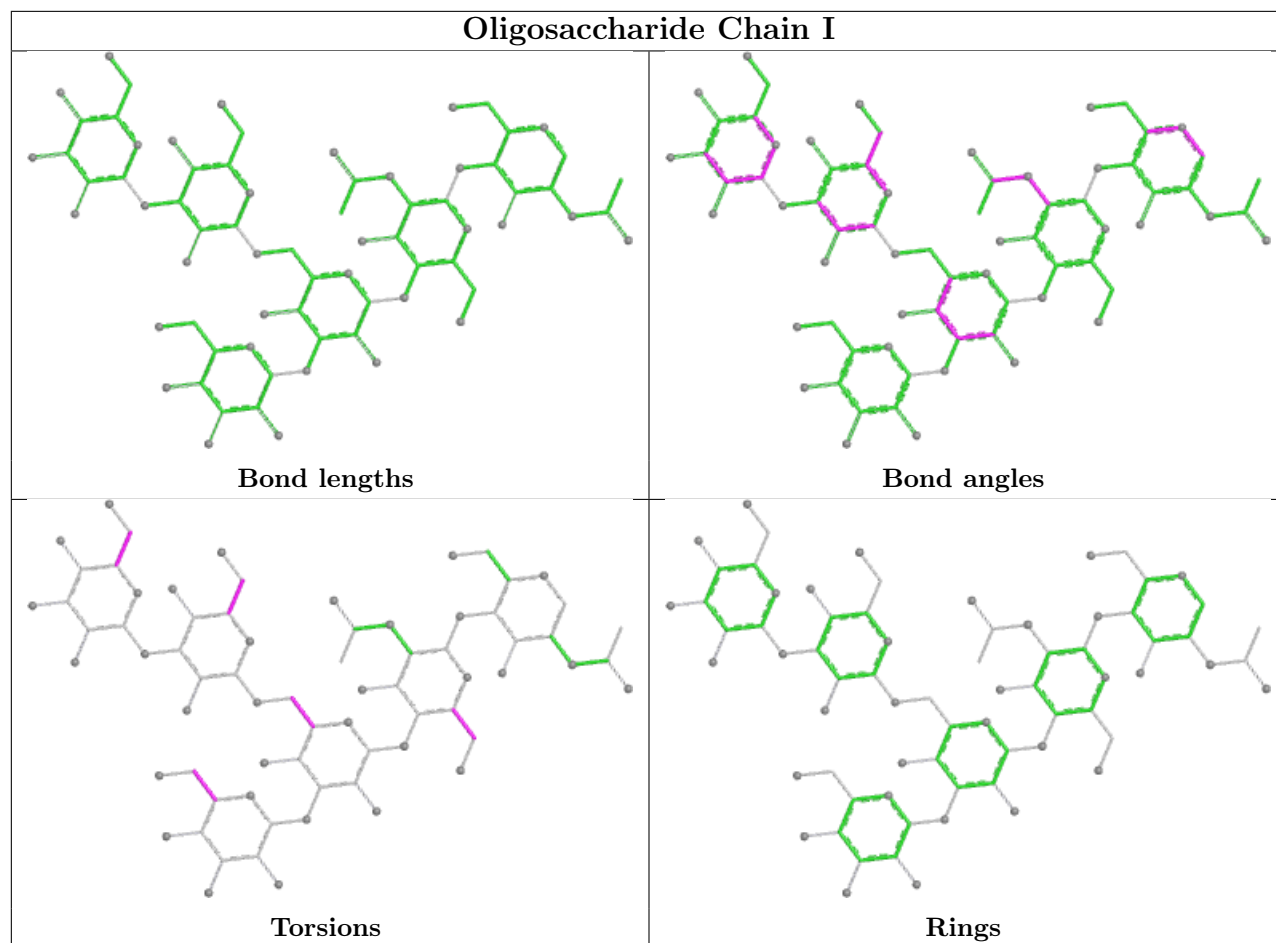
4 monomers are involved in 3 short contacts:

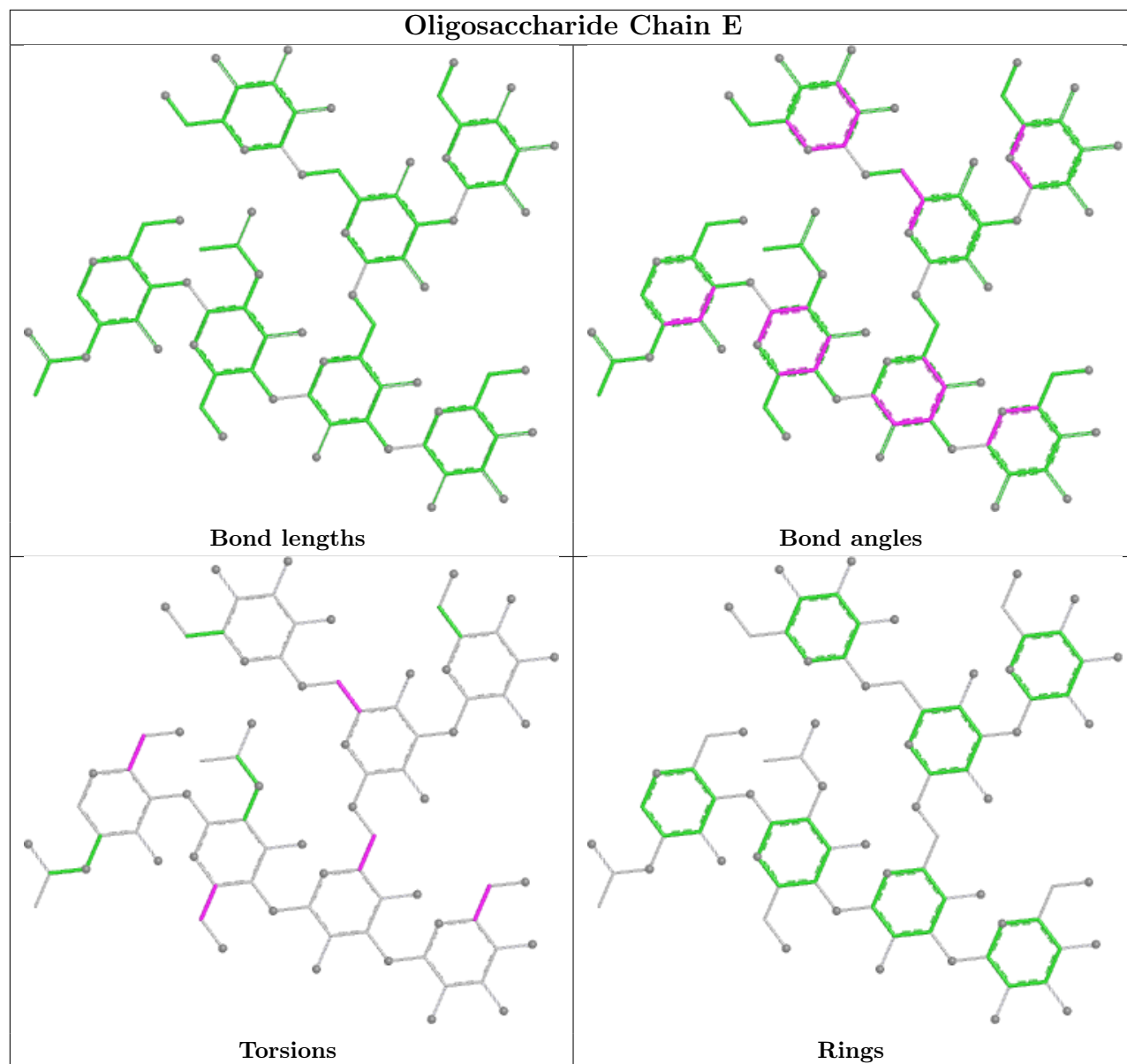
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0
4	E	1	NAG	1	0
4	J	1	NAG	1	0
2	B	1	NAG	1	0

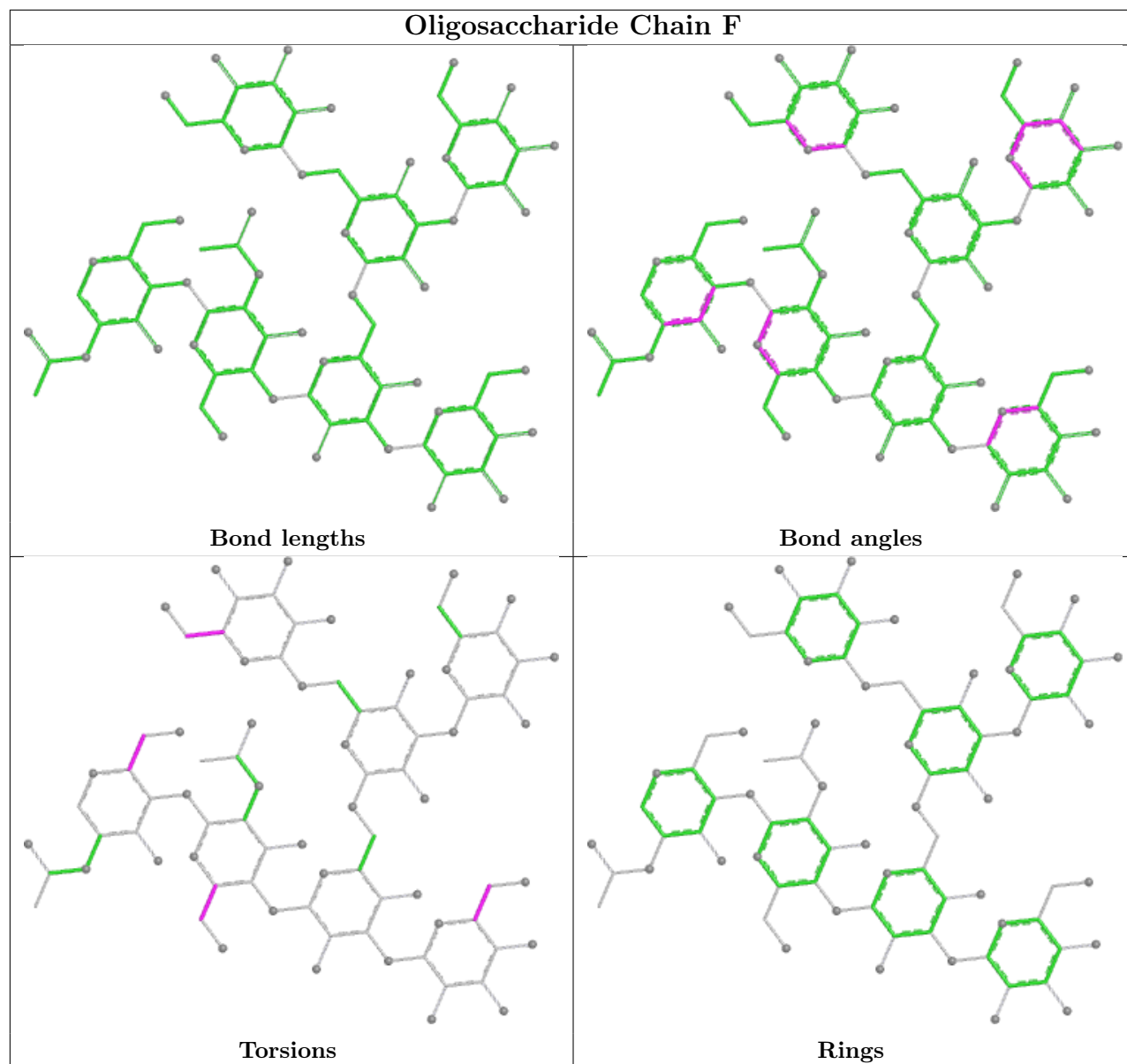
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

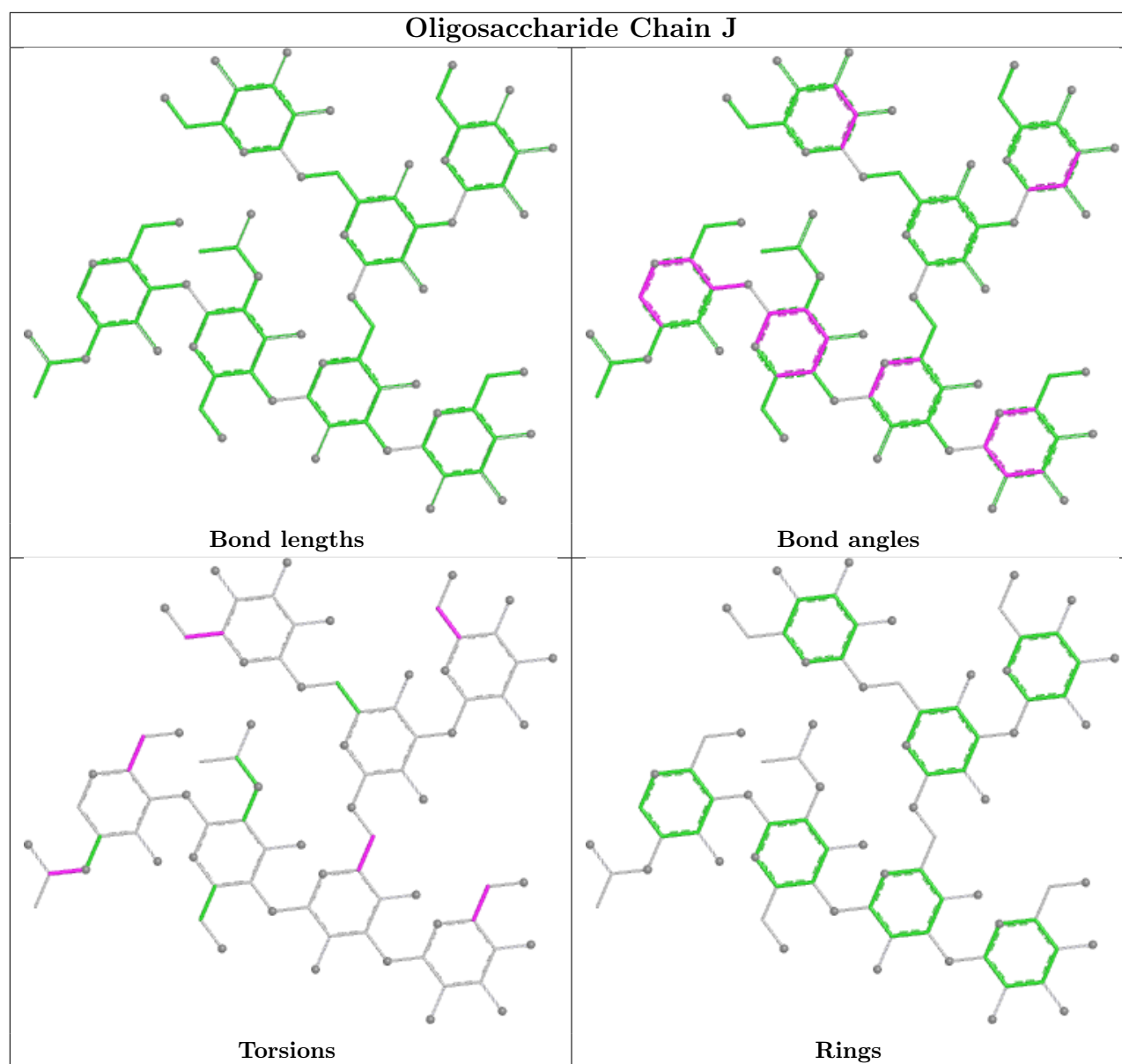




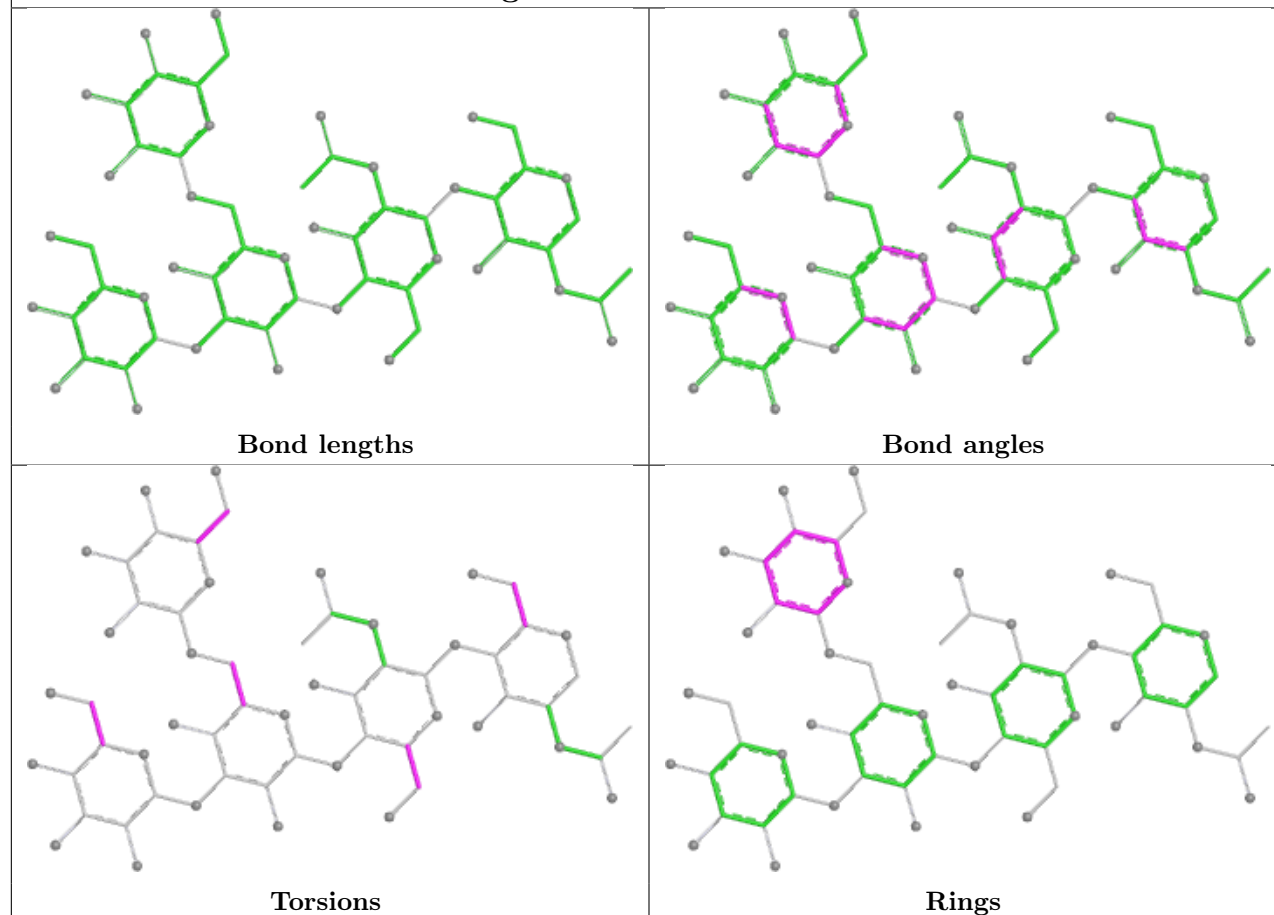




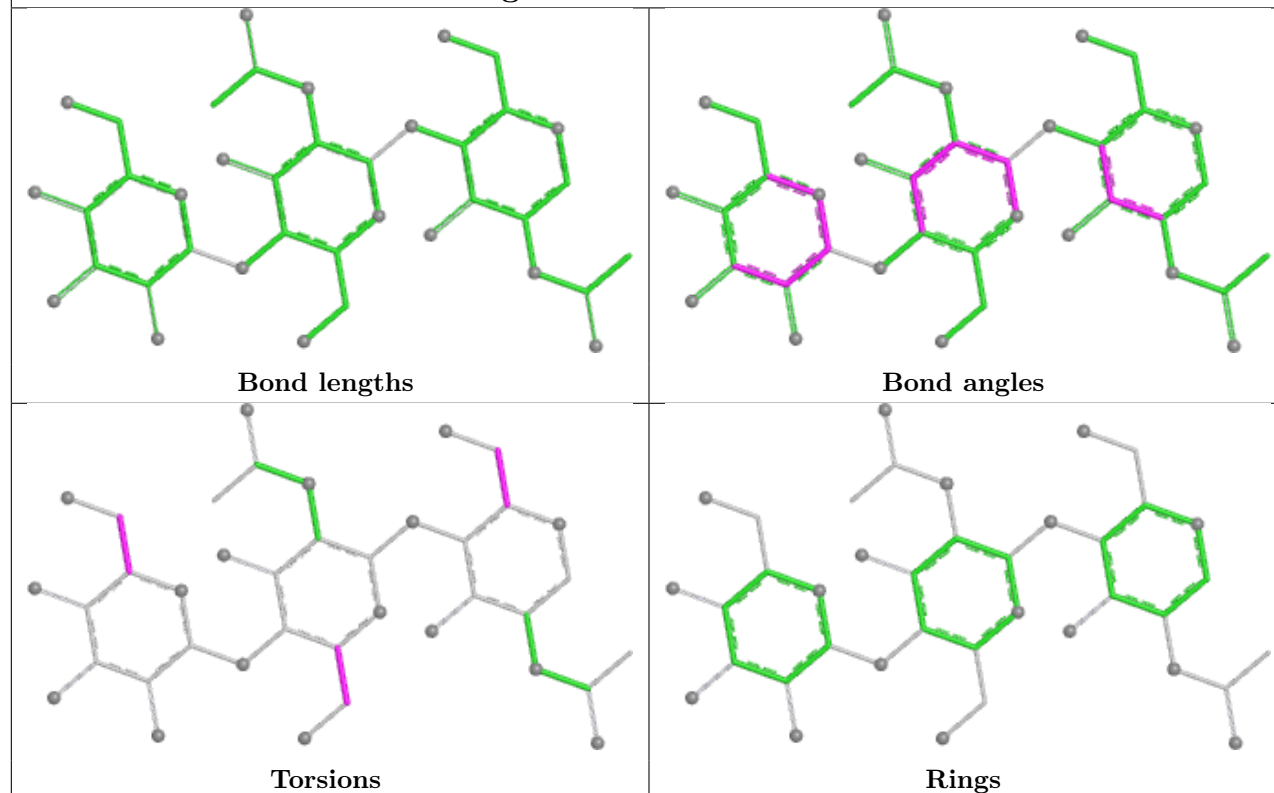




Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry

1 ligand is 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	1334	1	14,14,15	0.53	0	17,19,21	0.97	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1334	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1334	NAG	C4-C3-C2	2.23	114.28	111.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1334	NAG	C4-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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1171/1212 (96%)	1.13	227 (19%) 3 6	43, 122, 212, 302	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1222	GLY	10.7
1	A	686	ASN	9.8
1	A	1075	ARG	8.5
1	A	687	ASN	7.9
1	A	663	GLN	7.9
1	A	702	GLU	7.6
1	A	675	CYS	7.4
1	A	1187	THR	7.3
1	A	676	HIS	7.3
1	A	1168	ILE	6.8
1	A	674	PRO	6.8
1	A	1221	ALA	6.6
1	A	1208	ALA	6.4
1	A	968	ARG	5.9
1	A	965	SER	5.8
1	A	1207	GLU	5.7
1	A	671	GLY	5.6
1	A	1201	GLU	5.6
1	A	1185	ASN	5.5
1	A	1103	ARG	5.3
1	A	526	ARG	5.2
1	A	271	ALA	5.2
1	A	99	VAL	5.1
1	A	766	GLN	5.0
1	A	690	ASP	4.9
1	A	1186	TYR	4.9
1	A	660	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	670	ASN	4.8
1	A	1177	PRO	4.7
1	A	1167	LEU	4.7
1	A	48	GLY	4.6
1	A	574	THR	4.6
1	A	896	LEU	4.6
1	A	1202	THR	4.6
1	A	661	VAL	4.5
1	A	527	ASP	4.4
1	A	672	SER	4.4
1	A	1061	GLY	4.4
1	A	1152	PRO	4.3
1	A	662	HIS	4.3
1	A	1149	VAL	4.2
1	A	47	TRP	4.2
1	A	1063	LEU	4.2
1	A	177	GLY	4.1
1	A	699	ASN	4.1
1	A	596	CYS	4.1
1	A	1062	THR	4.0
1	A	277	THR	4.0
1	A	1209	PRO	4.0
1	A	402	ASP	3.9
1	A	659	CYS	3.9
1	A	176	PRO	3.8
1	A	575	MET	3.8
1	A	151	HIS	3.8
1	A	893	ASP	3.7
1	A	1166	PRO	3.7
1	A	178	GLN	3.7
1	A	1218	THR	3.6
1	A	1195	CYS	3.6
1	A	1074	VAL	3.6
1	A	1193	THR	3.6
1	A	308	ARG	3.6
1	A	1198	THR	3.6
1	A	1170	LYS	3.6
1	A	587	VAL	3.5
1	A	1059	SER	3.5
1	A	677	TRP	3.5
1	A	978	GLY	3.5
1	A	993	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1024	ILE	3.5
1	A	681	ARG	3.5
1	A	1025	VAL	3.5
1	A	892	GLU	3.4
1	A	685	THR	3.4
1	A	1026	ILE	3.4
1	A	1194	PRO	3.4
1	A	1173	ASN	3.4
1	A	1040	TYR	3.4
1	A	895	ARG	3.4
1	A	756	LEU	3.4
1	A	273	GLU	3.3
1	A	1176	PRO	3.3
1	A	1220	ARG	3.3
1	A	1153	LEU	3.3
1	A	317	ARG	3.2
1	A	665	CYS	3.2
1	A	668	CYS	3.2
1	A	684	CYS	3.2
1	A	714	TYR	3.2
1	A	1227	SER	3.2
1	A	321	ALA	3.2
1	A	495	GLN	3.1
1	A	1189	LEU	3.1
1	A	1206	CYS	3.1
1	A	834	ARG	3.1
1	A	1072	ALA	3.1
1	A	710	SER	3.1
1	A	1179	PRO	3.1
1	A	718	GLY	3.1
1	A	1226	PHE	3.1
1	A	598	PHE	3.1
1	A	719	VAL	3.1
1	A	1023	PRO	3.1
1	A	411	GLN	3.0
1	A	1175	LEU	3.0
1	A	251	GLU	3.0
1	A	272	GLY	3.0
1	A	941	ASP	2.9
1	A	1120	ARG	2.9
1	A	1054	GLU	2.9
1	A	1011	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	152	HIS	2.9
1	A	467	GLY	2.9
1	A	590	LEU	2.9
1	A	1104	ALA	2.8
1	A	149	GLU	2.8
1	A	881	THR	2.8
1	A	1039	LYS	2.8
1	A	689	ALA	2.8
1	A	721	LYS	2.8
1	A	91	GLU	2.8
1	A	1045	ASP	2.7
1	A	657	TYR	2.7
1	A	1140	SER	2.7
1	A	319	GLY	2.7
1	A	100	GLN	2.7
1	A	301	GLU	2.7
1	A	1182	SER	2.7
1	A	274	HIS	2.6
1	A	316	SER	2.6
1	A	463	ALA	2.6
1	A	967	SER	2.6
1	A	1205	LEU	2.6
1	A	747	PRO	2.6
1	A	966	PRO	2.6
1	A	1138	ASN	2.6
1	A	1065	THR	2.6
1	A	385	TRP	2.6
1	A	999	CYS	2.6
1	A	473	TYR	2.6
1	A	45	SER	2.6
1	A	1151	GLU	2.6
1	A	963	ARG	2.6
1	A	701	SER	2.5
1	A	129	GLY	2.5
1	A	265	LEU	2.5
1	A	1200	SER	2.5
1	A	165	GLY	2.5
1	A	825	GLU	2.5
1	A	1150	LEU	2.5
1	A	439	ASP	2.5
1	A	683	VAL	2.5
1	A	442	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	579	PRO	2.5
1	A	1102	CYS	2.5
1	A	444	THR	2.5
1	A	958	THR	2.5
1	A	1184	LEU	2.5
1	A	1199	VAL	2.5
1	A	700	MET	2.5
1	A	320	GLN	2.4
1	A	1169	LEU	2.4
1	A	39	PHE	2.4
1	A	939	VAL	2.4
1	A	464	ASN	2.4
1	A	667	ALA	2.4
1	A	673	PHE	2.4
1	A	680	TYR	2.4
1	A	679	LYS	2.4
1	A	1012	LEU	2.4
1	A	1041	ASN	2.4
1	A	1210	ASN	2.4
1	A	992	VAL	2.4
1	A	1188	VAL	2.4
1	A	318	PRO	2.3
1	A	1027	ASN	2.3
1	A	1183	ARG	2.3
1	A	180	GLN	2.3
1	A	1172	ARG	2.3
1	A	262	ASP	2.3
1	A	716	PRO	2.3
1	A	514	VAL	2.3
1	A	142	ASP	2.3
1	A	698	VAL	2.3
1	A	1112	ARG	2.3
1	A	977	ILE	2.3
1	A	344	LYS	2.3
1	A	311	GLN	2.2
1	A	409	PHE	2.2
1	A	639	TYR	2.2
1	A	797	PRO	2.2
1	A	98	SER	2.2
1	A	1181	ASN	2.2
1	A	412	PRO	2.2
1	A	869	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	647	LYS	2.2
1	A	894	VAL	2.2
1	A	1073	THR	2.2
1	A	1044	GLU	2.2
1	A	1128	MET	2.2
1	A	221	GLU	2.2
1	A	162	ARG	2.2
1	A	711	THR	2.1
1	A	300	CYS	2.1
1	A	1048	ILE	2.1
1	A	678	CYS	2.1
1	A	658	ASN	2.1
1	A	252	GLN	2.1
1	A	535	LEU	2.1
1	A	1055	TRP	2.1
1	A	954	PHE	2.1
1	A	1171	GLY	2.1
1	A	697	ARG	2.1
1	A	1129	ASP	2.1
1	A	278	SER	2.1
1	A	632	ASP	2.1
1	A	597	SER	2.1
1	A	1190	ILE	2.0
1	A	351	LYS	2.0
1	A	222	PHE	2.0
1	A	571	VAL	2.0
1	A	364	LYS	2.0
1	A	606	SER	2.0
1	A	594	VAL	2.0
1	A	580	LEU	2.0
1	A	1106	SER	2.0
1	A	1113	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	J	5	11/12	-0.06	0.26	263,278,284,287	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	C	4	11/12	0.18	0.19	230,242,254,256	0
4	MAN	J	4	11/12	0.22	0.21	282,295,299,300	0
3	MAN	I	5	11/12	0.26	0.26	225,241,245,246	0
2	MAN	B	4	11/12	0.41	0.20	262,282,287,288	0
4	MAN	F	7	11/12	0.42	0.30	230,245,248,256	0
6	NAG	H	2	14/15	0.47	0.12	224,240,248,256	0
6	NAG	H	1	14/15	0.51	0.19	192,213,227,237	0
4	MAN	J	7	11/12	0.54	0.19	244,272,282,284	0
7	NAG	A	1334	14/15	0.58	0.21	203,226,240,242	0
4	MAN	E	7	11/12	0.60	0.12	232,245,257,259	0
3	MAN	C	5	11/12	0.67	0.18	227,255,259,262	0
3	MAN	I	4	11/12	0.68	0.19	229,248,250,253	0
3	NAG	I	2	14/15	0.69	0.31	227,255,266,272	0
4	MAN	E	5	11/12	0.69	0.27	197,204,207,215	0
4	MAN	J	6	11/12	0.71	0.31	264,275,278,279	0
2	MAN	D	4	11/12	0.74	0.10	210,234,236,238	0
5	MAN	G	5	11/12	0.75	0.19	229,246,253,254	0
4	MAN	E	4	11/12	0.76	0.13	208,222,237,250	0
2	NAG	D	2	14/15	0.76	0.18	206,233,247,257	0
3	MAN	C	6	11/12	0.77	0.21	247,257,267,268	0
2	NAG	B	1	14/15	0.77	0.25	143,163,173,182	0
3	MAN	I	6	11/12	0.77	0.15	236,244,249,250	0
3	NAG	I	1	14/15	0.79	0.40	230,258,278,292	0
3	NAG	C	2	14/15	0.82	0.17	184,202,222,233	0
5	MAN	G	4	11/12	0.82	0.18	189,227,234,237	0
4	MAN	E	6	11/12	0.82	0.35	246,255,269,271	0
4	NAG	F	1	14/15	0.83	0.15	166,190,206,218	0
4	NAG	J	1	14/15	0.83	0.25	186,212,241,250	0
4	NAG	F	2	14/15	0.83	0.15	206,226,233,240	0
4	MAN	F	4	11/12	0.85	0.25	235,258,264,269	0
2	NAG	D	1	14/15	0.85	0.20	170,185,213,214	0
5	NAG	G	1	14/15	0.86	0.17	112,127,138,142	0
2	NAG	B	2	14/15	0.86	0.20	192,203,221,240	0
4	NAG	J	2	14/15	0.87	0.28	253,275,297,308	0
4	MAN	F	6	11/12	0.89	0.17	246,253,256,257	0
4	NAG	E	2	14/15	0.89	0.19	182,208,219,230	0
4	NAG	E	1	14/15	0.93	0.23	171,181,191,194	0
3	NAG	C	1	14/15	0.93	0.16	130,149,159,165	0
4	MAN	F	5	11/12	0.94	0.16	250,253,259,261	0
5	NAG	G	2	14/15	0.94	0.20	148,161,174,195	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

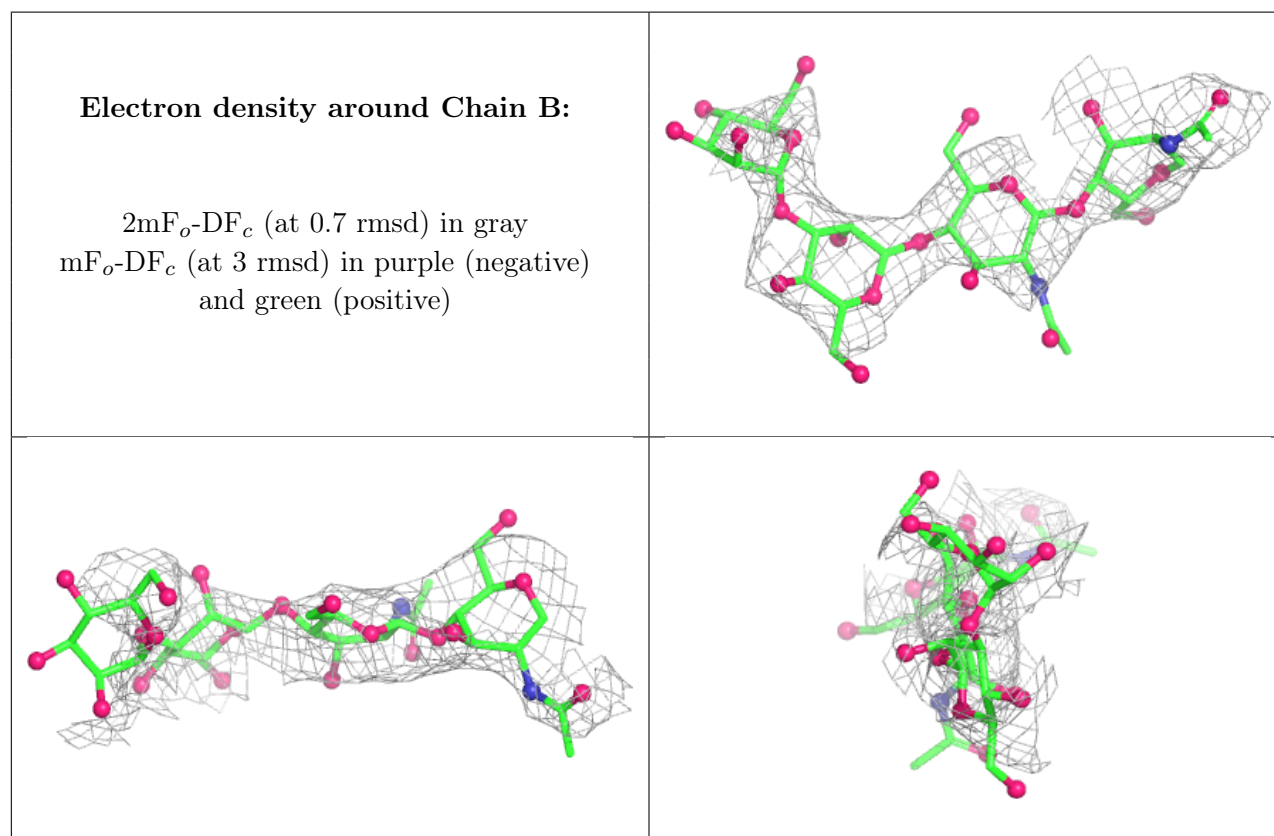
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	J	5	11/12	-0.06	0.26	263,278,284,287	0
4	BMA	E	3	11/12	0.13	0.18	232,248,259,265	0
3	MAN	C	4	11/12	0.18	0.19	230,242,254,256	0
4	MAN	J	4	11/12	0.22	0.21	282,295,299,300	0
2	BMA	D	3	11/12	0.22	0.18	202,234,254,265	0
3	MAN	I	5	11/12	0.26	0.26	225,241,245,246	0
4	BMA	J	3	11/12	0.28	0.20	276,290,297,300	0
2	MAN	B	4	11/12	0.41	0.20	262,282,287,288	0
4	MAN	F	7	11/12	0.42	0.30	230,245,248,256	0
3	BMA	I	3	11/12	0.45	0.17	253,262,269,272	0
6	NAG	H	2	14/15	0.47	0.12	224,240,248,256	0
6	BMA	H	3	11/12	0.49	0.13	218,235,247,251	0
6	NAG	H	1	14/15	0.51	0.19	192,213,227,237	0
3	BMA	C	3	11/12	0.52	0.13	235,240,250,265	0
4	MAN	J	7	11/12	0.54	0.19	244,272,282,284	0
4	MAN	E	7	11/12	0.60	0.12	232,245,257,259	0
2	BMA	B	3	11/12	0.61	0.16	218,254,267,281	0
3	MAN	C	5	11/12	0.67	0.18	227,255,259,262	0
3	MAN	I	4	11/12	0.68	0.19	229,248,250,253	0
4	MAN	E	5	11/12	0.69	0.27	197,204,207,215	0
3	NAG	I	2	14/15	0.69	0.31	227,255,266,272	0
4	MAN	J	6	11/12	0.71	0.31	264,275,278,279	0
2	MAN	D	4	11/12	0.74	0.10	210,234,236,238	0
5	MAN	G	5	11/12	0.75	0.19	229,246,253,254	0
4	MAN	E	4	11/12	0.76	0.13	208,222,237,250	0
5	BMA	G	3	11/12	0.76	0.12	217,237,244,251	0
2	NAG	D	2	14/15	0.76	0.18	206,233,247,257	0
2	NAG	B	1	14/15	0.77	0.25	143,163,173,182	0
3	MAN	C	6	11/12	0.77	0.21	247,257,267,268	0
3	MAN	I	6	11/12	0.77	0.15	236,244,249,250	0
3	NAG	I	1	14/15	0.79	0.40	230,258,278,292	0
4	MAN	E	6	11/12	0.82	0.35	246,255,269,271	0
5	MAN	G	4	11/12	0.82	0.18	189,227,234,237	0
3	NAG	C	2	14/15	0.82	0.17	184,202,222,233	0
4	NAG	J	1	14/15	0.83	0.25	186,212,241,250	0
4	NAG	F	2	14/15	0.83	0.15	206,226,233,240	0
4	NAG	F	1	14/15	0.83	0.15	166,190,206,218	0

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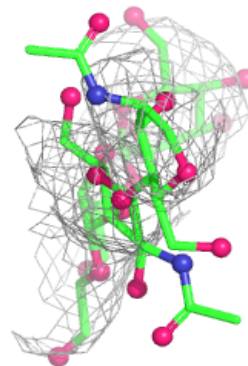
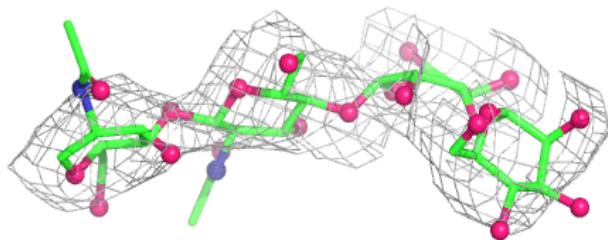
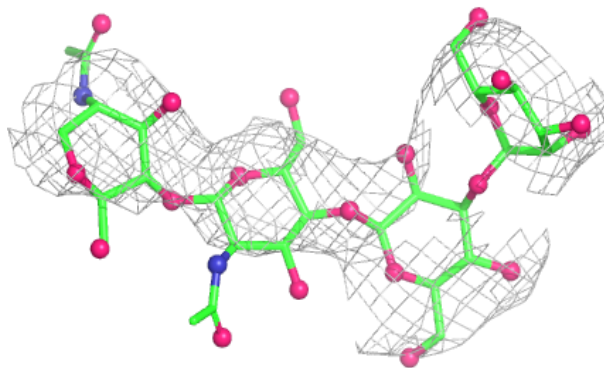
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	F	4	11/12	0.85	0.25	235,258,264,269	0
2	NAG	D	1	14/15	0.85	0.20	170,185,213,214	0
2	NAG	B	2	14/15	0.86	0.20	192,203,221,240	0
5	NAG	G	1	14/15	0.86	0.17	112,127,138,142	0
4	BMA	F	3	11/12	0.87	0.15	244,248,254,254	0
4	NAG	J	2	14/15	0.87	0.28	253,275,297,308	0
4	MAN	F	6	11/12	0.89	0.17	246,253,256,257	0
4	NAG	E	2	14/15	0.89	0.19	182,208,219,230	0
3	NAG	C	1	14/15	0.93	0.16	130,149,159,165	0
4	NAG	E	1	14/15	0.93	0.23	171,181,191,194	0
4	MAN	F	5	11/12	0.94	0.16	250,253,259,261	0
5	NAG	G	2	14/15	0.94	0.20	148,161,174,195	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.



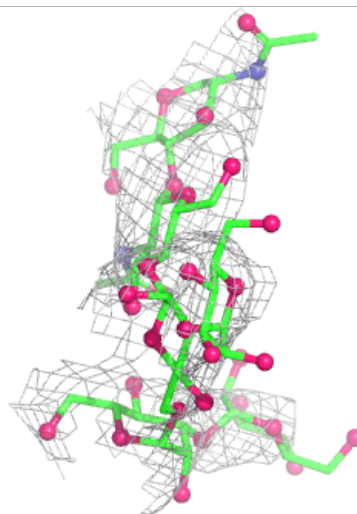
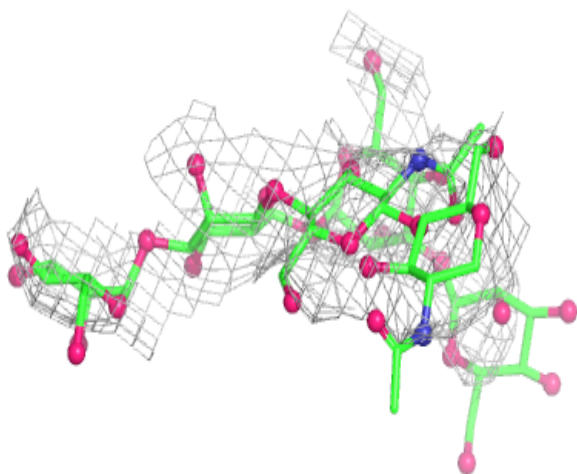
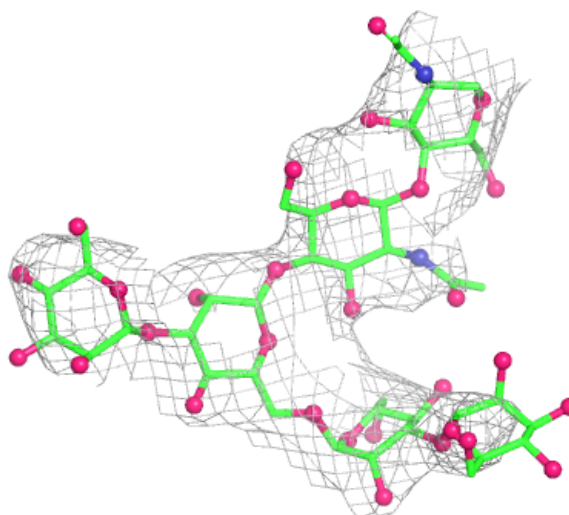
Electron density around Chain D:

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



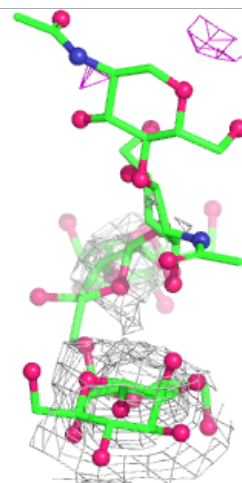
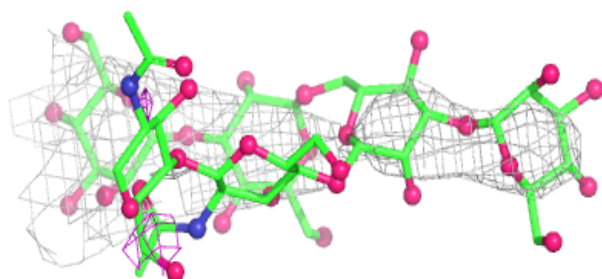
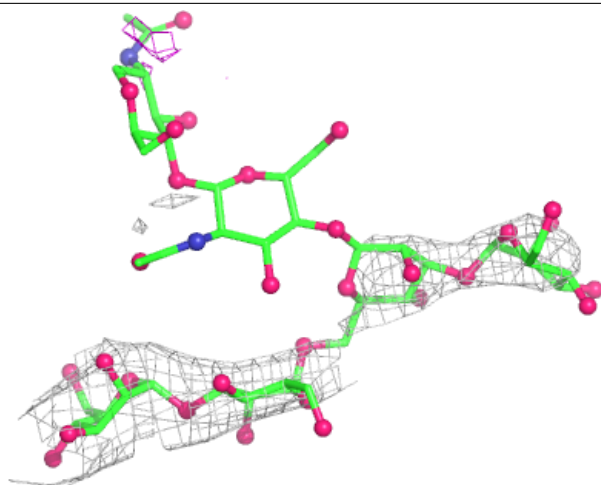
Electron density around Chain C:

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



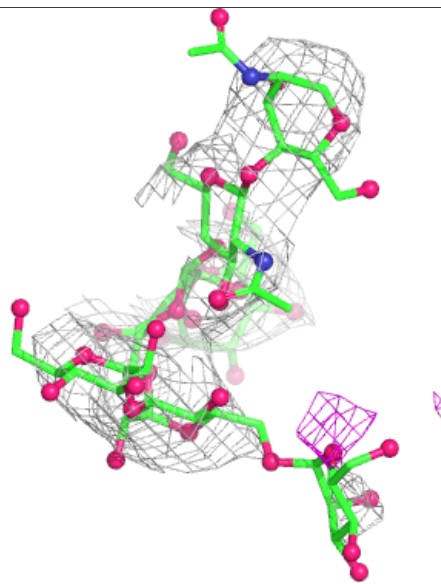
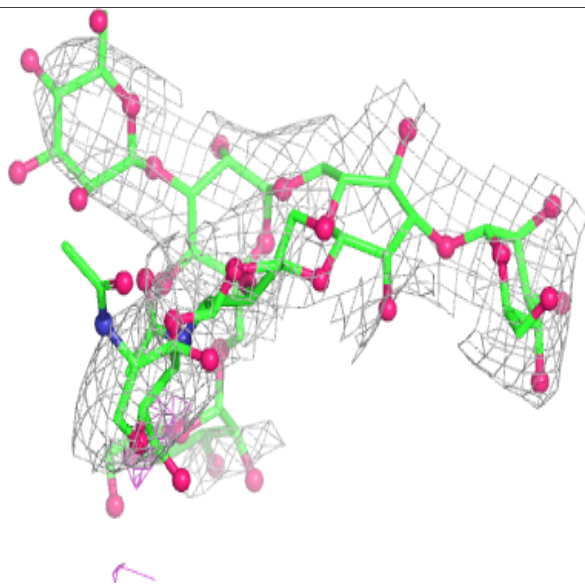
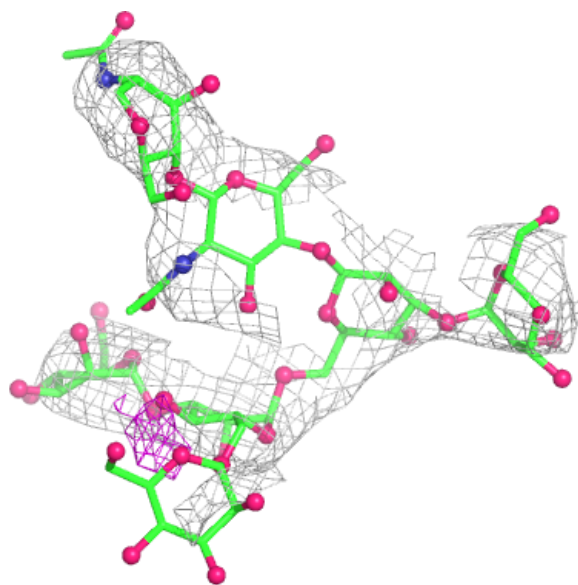
Electron density around Chain I:

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



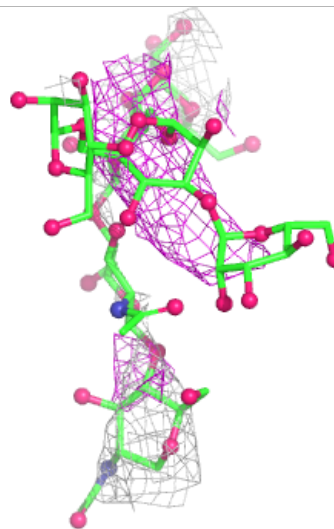
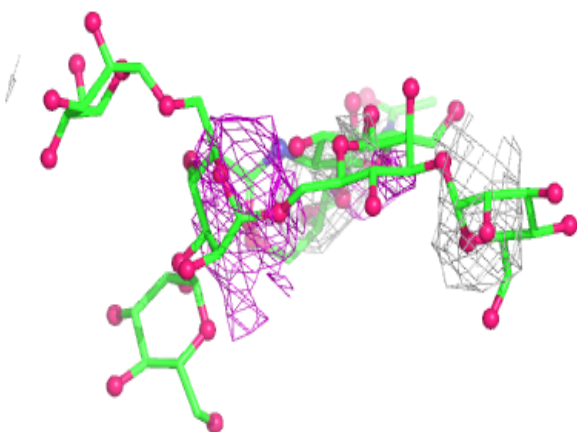
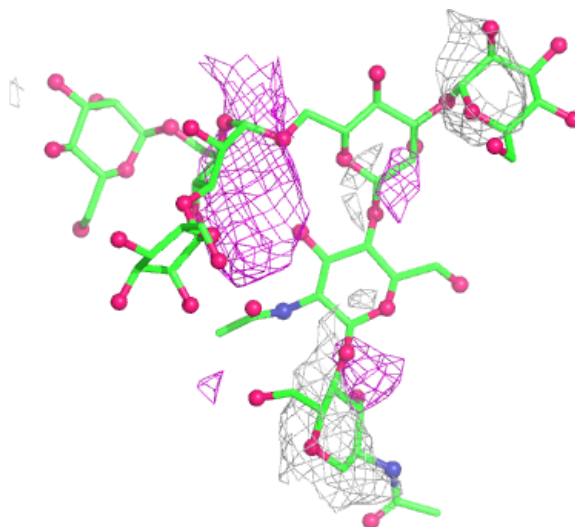
Electron density around Chain E:

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



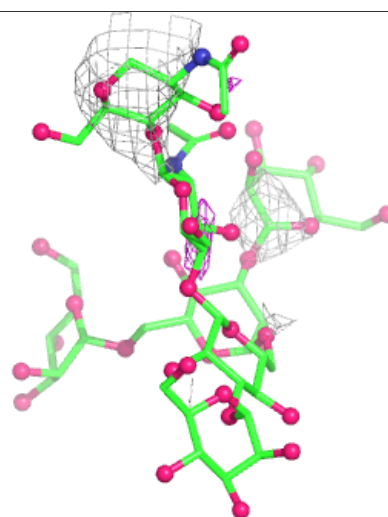
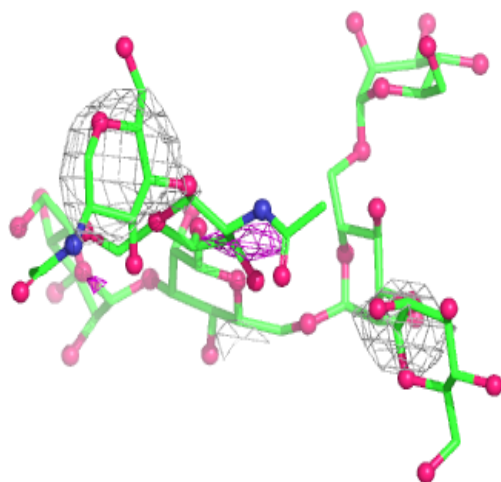
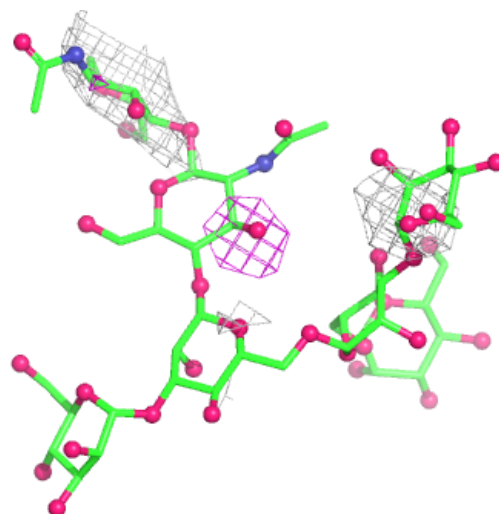
Electron density around Chain F:

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



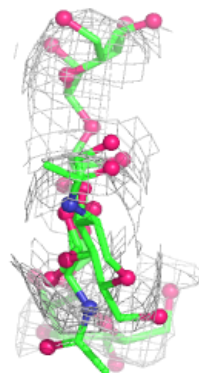
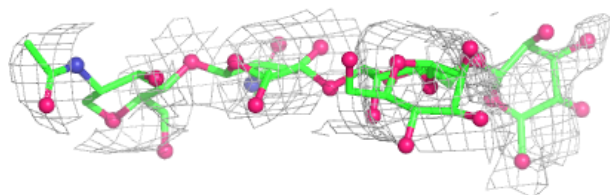
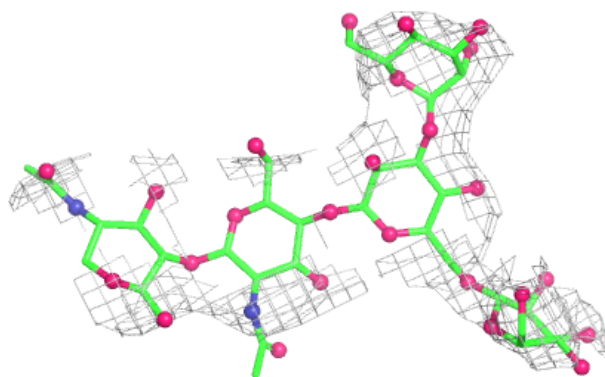
Electron density around Chain J:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

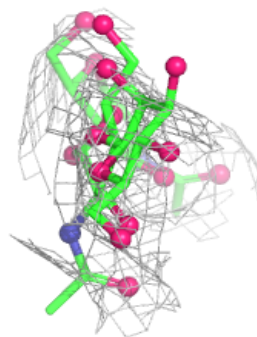
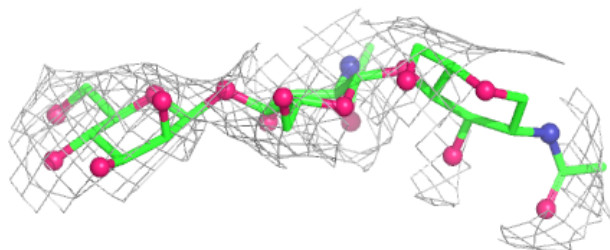
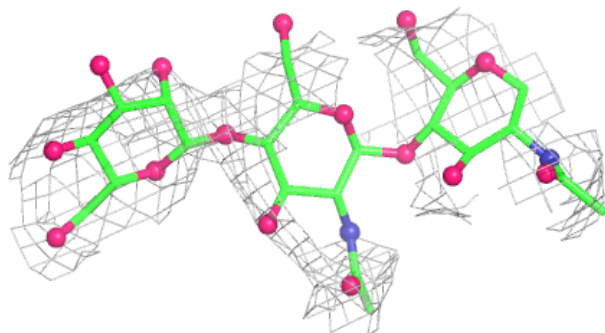


Electron density around Chain G:

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

**Electron density around Chain H:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	A	1334	14/15	0.58	0.21	203,226,240,242	0

6.5 Other polymers [i](#)

There are no such residues in this entry.