



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:49 PM UTC

PDB ID : 2X1W / pdb_00002x1w
Title : Crystal Structure of VEGF-C in Complex with Domains 2 and 3 of VEGFR2
Authors : Leppanen, V.M.; Prota, A.E.; Jeltsch, M.; Anisimov, A.; Kalkkinen, N.; Strandin, T.; Lankinen, H.; Goldman, A.; Ballmer-Hofer, K.; Alitalo, K.
Deposited on : 2010-01-08
Resolution : 2.70 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

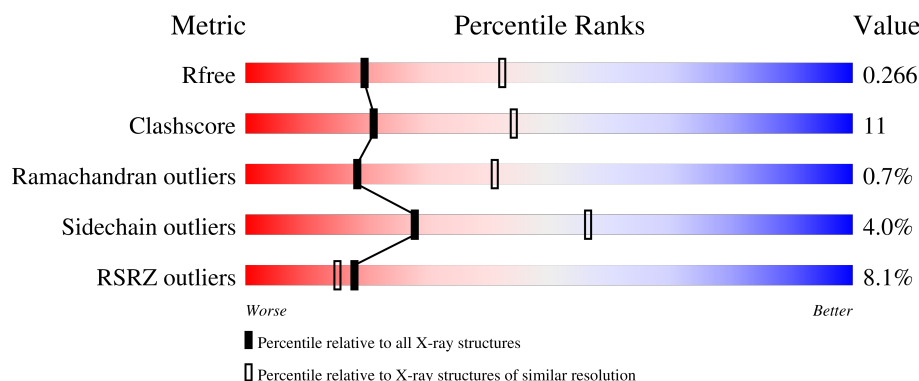
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	110	13% 65% 22% • 11%
1	B	110	6% 71% 16% • 11%
1	C	110	4% 68% 18% • 12%
1	D	110	5% 67% 19% • 10%
2	L	213	8% 69% 20% • 8%

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Mol	Chain	Length	Quality of chain
2	M	213	
2	N	213	
2	O	213	
3	E	3	
3	F	3	
3	G	3	
3	H	3	
3	I	3	
3	J	3	
3	K	3	
3	P	3	
3	S	3	
4	Q	2	
4	R	2	
4	T	2	
4	U	2	

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	S	1	X	-	-	-
6	NAG	L	2401	X	-	-	-
6	NAG	O	2001	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9720 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 VASCULAR ENDOTHELIAL GROWTH FACTOR C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			750	468	127	144	11			
1	B	98	Total	C	N	O	S	0	0	0
			752	470	128	143	11			
1	C	97	Total	C	N	O	S	0	0	0
			743	465	127	140	11			
1	D	99	Total	C	N	O	S	0	0	0
			760	476	129	144	11			

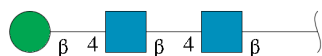
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ALA	CYS	engineered mutation	UNP P49767
B	137	ALA	CYS	engineered mutation	UNP P49767
C	137	ALA	CYS	engineered mutation	UNP P49767
D	137	ALA	CYS	engineered mutation	UNP P49767

- Molecule 2 is a protein called VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	196	Total	C	N	O	S	0	0	0
			1535	977	261	287	10			
2	M	179	Total	C	N	O	S	0	0	0
			1402	894	236	262	10			
2	N	194	Total	C	N	O	S	0	0	0
			1522	969	255	288	10			
2	O	193	Total	C	N	O	S	0	0	0
			1516	967	256	283	10			

- Molecule 3 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
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

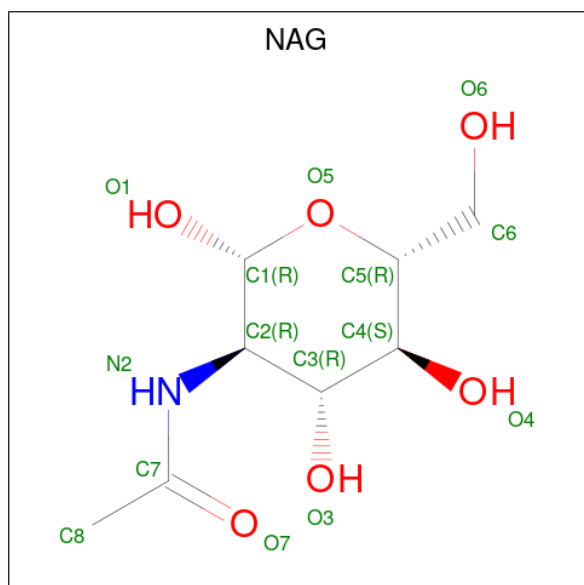


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CESIUM ION (CCD ID: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cs 1 1	0	0
5	C	1	Total Cs 1 1	0	0

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



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

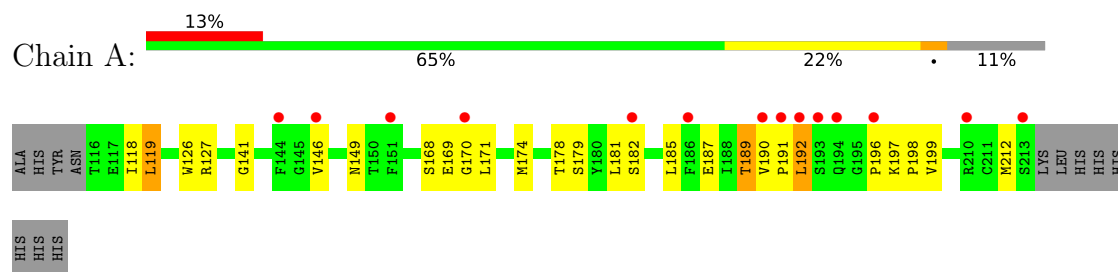
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total 14	O 14	0	0
7	B	11	Total 11	O 11	0	0
7	C	32	Total 32	O 32	0	0
7	D	19	Total 19	O 19	0	0
7	L	31	Total 31	O 31	0	0
7	M	12	Total 12	O 12	0	0
7	N	34	Total 34	O 34	0	0
7	O	24	Total 24	O 24	0	0

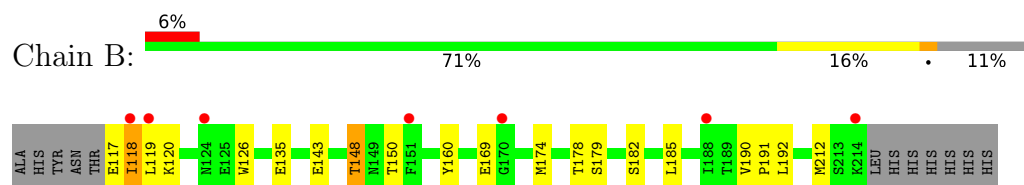
3 Residue-property plots

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.

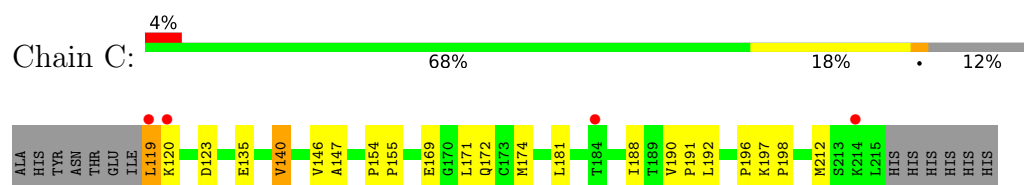
• Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C



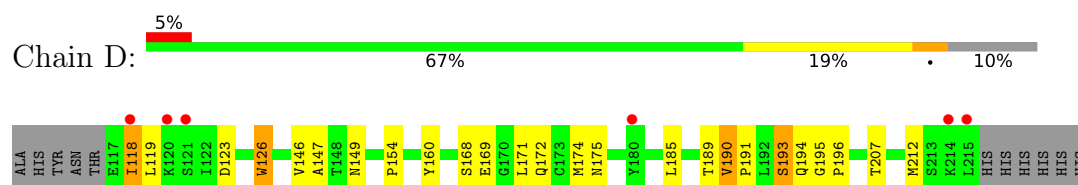
• Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C



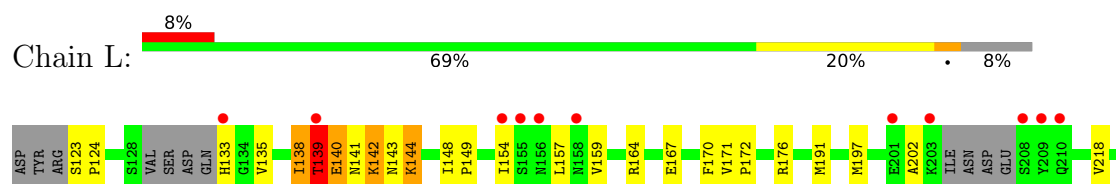
• Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C

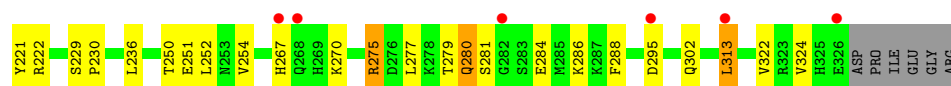


• Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C

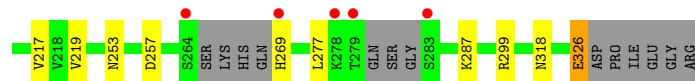
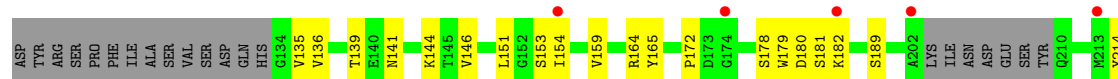


• Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2

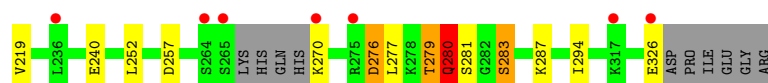
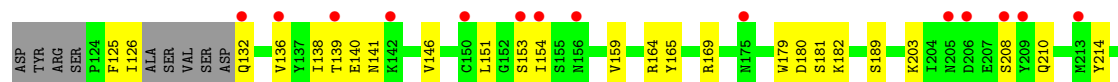
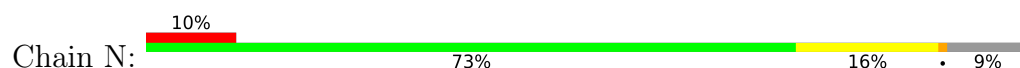




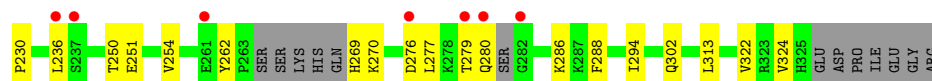
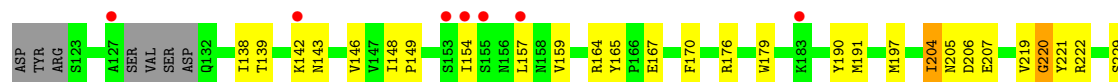
• Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2



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• Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2



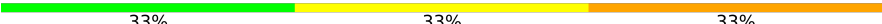
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain G:  33% 33% 33%



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

Chain H:  33% 67%



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

Chain I:  67% 33%

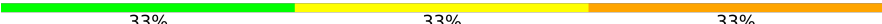


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  67% 33%



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

Chain K:  33% 33% 33%



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

Chain P:  33% 67%



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

Chain S:  33% 67%



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

Chain Q:  100%



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

Chain R:  100%



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

Chain T:  100%



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

Chain U:  50%  50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.75Å 123.83Å 211.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.96 – 2.70 52.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (52.96-2.70) 99.6 (52.96-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.227 , 0.280 (Not available) , 0.266	Depositor DCC
R_{free} test set	2747 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9720	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	0/765	0.75	0/1035
1	B	0.41	0/767	0.81	0/1036
1	C	0.43	0/758	0.76	0/1024
1	D	0.38	0/775	0.75	0/1047
2	L	0.37	0/1565	0.76	2/2113 (0.1%)
2	M	0.35	0/1426	0.74	0/1925
2	N	0.40	0/1550	0.77	0/2093
2	O	0.37	0/1544	0.78	0/2085
All	All	0.38	0/9150	0.76	2/12358 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	123	SER	CA-C-N	5.45	125.54	119.87
2	L	123	SER	C-N-CA	5.45	125.54	119.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	750	0	732	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	752	0	738	11	0
1	C	743	0	732	15	0
1	D	760	0	749	23	0
2	L	1535	0	1540	54	0
2	M	1402	0	1415	25	0
2	N	1522	0	1526	37	0
2	O	1516	0	1518	34	0
3	E	39	0	34	1	0
3	F	39	0	34	2	0
3	G	39	0	34	1	0
3	H	39	0	34	3	0
3	I	39	0	34	0	0
3	J	39	0	34	1	0
3	K	39	0	34	1	0
3	P	39	0	34	4	0
3	S	39	0	34	2	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	L	28	0	26	0	0
6	N	28	0	26	0	0
6	O	42	0	39	3	0
7	A	14	0	0	0	0
7	B	11	0	0	1	0
7	C	32	0	0	1	0
7	D	19	0	0	1	0
7	L	31	0	0	0	0
7	M	12	0	0	0	0
7	N	34	0	0	0	0
7	O	24	0	0	0	0
All	All	9720	0	9447	208	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 11.

All (208) 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)
2:N:280:GLN:HB2	2:N:281:SER:HA	1.22	1.14
2:N:280:GLN:CB	2:N:281:SER:HA	1.78	1.11
2:O:138:ILE:HG22	2:O:146:VAL:HG11	1.41	1.00
2:L:142:LYS:HG3	2:L:143:ASN:H	1.37	0.89
1:A:141:GLY:HA2	1:A:146:VAL:HG21	1.59	0.82
2:L:124:PRO:HB2	2:L:157:LEU:HD11	1.60	0.82
2:O:276:ASP:O	2:O:277:LEU:HD23	1.80	0.82
1:D:146:VAL:HG22	1:D:147:ALA:H	1.45	0.81
2:L:141:ASN:CG	2:L:142:LYS:H	1.88	0.79
1:C:140:VAL:HG12	1:C:155:PRO:O	1.82	0.79
1:A:181:LEU:HD21	3:F:1:NAG:H82	1.64	0.78
2:N:280:GLN:CB	2:N:281:SER:CA	2.59	0.78
2:O:190:TYR:CZ	6:O:2001:NAG:H5	2.21	0.76
1:D:190:VAL:HA	1:D:191:PRO:C	2.11	0.75
1:A:192:LEU:H	1:A:192:LEU:HD22	1.55	0.72
2:L:142:LYS:HG3	2:L:143:ASN:N	2.04	0.72
2:L:142:LYS:HE3	2:L:142:LYS:HA	1.72	0.71
1:D:196:PRO:HD2	2:L:135:VAL:HG21	1.71	0.71
2:N:280:GLN:HB3	2:N:281:SER:HA	1.73	0.71
2:O:164:ARG:HG2	2:O:167:GLU:HG2	1.74	0.70
1:B:148:THR:HG23	2:N:276:ASP:CG	2.18	0.69
2:O:139:THR:HA	2:O:219:VAL:O	1.93	0.68
1:D:123:ASP:HA	2:O:197:MET:HE1	1.75	0.68
2:L:142:LYS:CG	2:L:143:ASN:H	2.07	0.67
2:L:252:LEU:HG	2:L:284:GLU:HG2	1.76	0.67
2:O:204:ILE:HG23	2:O:204:ILE:O	1.93	0.66
2:N:280:GLN:HB2	2:N:281:SER:CA	2.09	0.66
2:O:204:ILE:C	2:O:206:ASP:H	2.02	0.66
2:L:164:ARG:HG2	2:L:167:GLU:HG2	1.76	0.65
1:D:207:THR:HA	3:P:1:NAG:O6	1.96	0.65
1:D:168:SER:HB2	1:D:171:LEU:HD12	1.78	0.65
2:O:190:TYR:OH	6:O:2001:NAG:H5	1.97	0.64
2:N:126:ILE:HD13	2:N:151:LEU:HB3	1.78	0.64
2:O:270:LYS:HB3	2:O:294:ILE:HG12	1.80	0.63
2:N:280:GLN:H	2:N:280:GLN:CD	2.07	0.62
2:L:221:TYR:HB2	2:L:313:LEU:HB2	1.81	0.61
2:L:140:GLU:O	2:L:140:GLU:HG3	1.99	0.61
2:L:267:HIS:HB2	2:L:270:LYS:HD2	1.83	0.61
2:O:270:LYS:CB	2:O:294:ILE:HG12	2.30	0.60
1:B:117:GLU:HA	1:B:120:LYS:HD2	1.82	0.60
2:L:279:THR:HG23	2:L:280:GLN:N	2.16	0.60
2:N:138:ILE:HG22	2:N:140:GLU:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLU:OE2	2:M:253:ASN:N	2.35	0.59
1:C:169:GLU:OE1	2:L:286:LYS:HD3	2.03	0.59
1:A:178:THR:HG22	1:A:179:SER:O	2.03	0.59
2:M:217:VAL:HG12	2:M:219:VAL:HG13	1.84	0.59
2:M:153:SER:HB2	2:M:154:ILE:HD12	1.85	0.58
1:A:196:PRO:HD3	2:M:135:VAL:HG21	1.85	0.58
2:O:221:TYR:HB2	2:O:313:LEU:HB2	1.85	0.58
1:D:118:ILE:HB	1:D:119:LEU:HD12	1.85	0.58
2:N:153:SER:HB2	2:N:154:ILE:HD12	1.86	0.58
1:C:190:VAL:HA	1:C:191:PRO:C	2.29	0.58
1:D:146:VAL:HG22	1:D:147:ALA:N	2.19	0.58
2:N:159:VAL:HG21	2:N:179:TRP:CE2	2.38	0.58
1:C:174:MET:HB2	1:C:212:MET:HE2	1.86	0.57
2:L:143:ASN:O	2:L:176:ARG:NH2	2.37	0.57
1:A:196:PRO:CD	2:M:135:VAL:HG21	2.34	0.57
1:A:170:GLY:HA3	2:N:252:LEU:CD1	2.35	0.57
2:M:159:VAL:HG21	2:M:179:TRP:CE2	2.40	0.57
2:L:141:ASN:CG	2:L:142:LYS:N	2.57	0.57
1:A:149:ASN:ND2	1:A:189:THR:HG22	2.19	0.56
1:A:119:LEU:HD23	2:N:132:GLN:HE21	1.70	0.56
1:A:170:GLY:HA3	2:N:252:LEU:HD13	1.85	0.56
1:A:127:ARG:HG3	2:N:165:TYR:CE2	2.41	0.56
2:L:252:LEU:CD1	2:L:284:GLU:HG2	2.36	0.56
2:O:204:ILE:HG22	2:O:207:GLU:H	1.69	0.56
2:N:146:VAL:HG23	2:N:189:SER:HB3	1.89	0.55
2:O:222:ARG:HB2	2:O:251:GLU:CD	2.30	0.55
1:D:174:MET:HB2	1:D:212:MET:HE2	1.88	0.55
2:L:139:THR:O	2:L:140:GLU:CB	2.54	0.55
2:L:140:GLU:O	2:L:140:GLU:CG	2.54	0.54
2:N:136:VAL:HG23	2:N:214:TYR:HB3	1.90	0.54
1:B:178:THR:HG22	1:B:179:SER:O	2.08	0.54
1:B:169:GLU:HG3	2:M:253:ASN:OD1	2.08	0.53
2:M:146:VAL:HG23	2:M:189:SER:HB3	1.90	0.53
2:L:170:PHE:CE1	2:L:191:MET:HE2	2.43	0.53
2:L:139:THR:CG2	2:L:140:GLU:N	2.71	0.53
2:N:203:LYS:HG2	2:N:208:SER:HB3	1.90	0.53
2:M:136:VAL:HG23	2:M:214:TYR:HB3	1.91	0.53
1:C:119:LEU:HD22	1:C:120:LYS:N	2.23	0.53
2:N:279:THR:HG22	2:N:280:GLN:N	2.24	0.53
1:D:118:ILE:HD12	1:D:118:ILE:H	1.73	0.52
2:L:139:THR:HG22	2:L:140:GLU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:222:ARG:HB2	2:L:251:GLU:CD	2.35	0.52
2:M:318:ASN:OD1	3:S:1:NAG:H83	2.10	0.51
1:D:193:SER:C	1:D:195:GLY:H	2.18	0.51
2:L:286:LYS:HE3	2:L:288:PHE:CZ	2.45	0.51
2:M:141:ASN:ND2	2:M:144:LYS:HB2	2.25	0.51
2:N:180:ASP:O	2:N:181:SER:HB3	2.11	0.51
2:L:252:LEU:CG	2:L:284:GLU:HG2	2.41	0.51
2:O:170:PHE:CE1	2:O:191:MET:HE2	2.45	0.51
2:M:299:ARG:HH21	2:M:326:GLU:HB3	1.76	0.51
2:L:279:THR:HG23	2:L:280:GLN:H	1.76	0.50
1:A:192:LEU:HD22	1:A:192:LEU:N	2.24	0.50
7:B:2009:HOH:O	3:H:1:NAG:H2	2.11	0.50
2:N:154:ILE:HD12	2:N:154:ILE:N	2.26	0.50
1:D:196:PRO:CD	2:L:135:VAL:HG21	2.41	0.50
2:L:236:LEU:O	2:L:324:VAL:HA	2.11	0.50
2:N:126:ILE:CD1	2:N:151:LEU:HB3	2.42	0.50
2:L:295:ASP:CG	2:N:169:ARG:HE	2.18	0.50
1:D:118:ILE:H	1:D:118:ILE:CD1	2.25	0.49
2:O:286:LYS:HE3	2:O:288:PHE:CZ	2.47	0.49
1:C:123:ASP:HA	2:L:197:MET:HE1	1.94	0.49
2:O:302:GLN:HG3	2:O:322:VAL:O	2.12	0.49
2:M:154:ILE:HD12	2:M:154:ILE:N	2.27	0.49
2:O:262:TYR:CD2	2:O:270:LYS:HD2	2.47	0.49
1:C:172:GLN:HB3	1:C:174:MET:HE3	1.95	0.49
2:M:180:ASP:O	2:M:181:SER:HB3	2.11	0.48
3:S:1:NAG:H4	3:S:2:NAG:HN2	1.78	0.48
1:D:169:GLU:CD	7:D:2011:HOH:O	2.56	0.48
2:L:159:VAL:HG22	2:L:202:ALA:HB2	1.94	0.48
1:D:149:ASN:O	1:D:189:THR:HA	2.14	0.48
2:O:236:LEU:O	2:O:324:VAL:HA	2.13	0.48
2:M:277:LEU:HD12	2:M:287:LYS:HG2	1.96	0.48
2:N:138:ILE:HG23	2:N:189:SER:HB2	1.95	0.48
1:C:135:GLU:HG2	7:C:2013:HOH:O	2.14	0.47
1:D:172:GLN:HB3	1:D:174:MET:HE3	1.96	0.47
2:N:125:PHE:HA	2:N:151:LEU:O	2.14	0.47
1:C:146:VAL:HG13	1:C:147:ALA:O	2.14	0.47
2:N:180:ASP:C	2:N:182:LYS:H	2.23	0.47
1:D:160:TYR:CG	3:P:1:NAG:H5	2.50	0.47
2:L:252:LEU:HG	2:L:284:GLU:CG	2.43	0.47
2:L:279:THR:O	2:L:281:SER:N	2.48	0.47
2:N:146:VAL:CG2	2:N:189:SER:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:277:LEU:HD12	2:N:287:LYS:HG2	1.96	0.47
1:D:154:PRO:HD2	1:D:185:LEU:HD12	1.97	0.47
1:C:181:LEU:HD21	3:J:1:NAG:H82	1.97	0.47
2:L:138:ILE:HG13	2:L:139:THR:HB	1.97	0.46
2:M:146:VAL:CG2	2:M:189:SER:HB3	2.44	0.46
2:M:180:ASP:C	2:M:182:LYS:H	2.23	0.46
1:A:190:VAL:HA	1:A:191:PRO:C	2.40	0.46
1:B:169:GLU:OE2	2:M:253:ASN:HA	2.16	0.46
2:L:144:LYS:HB2	2:L:144:LYS:NZ	2.31	0.46
2:O:229:SER:HA	2:O:230:PRO:C	2.40	0.46
1:A:181:LEU:CD2	3:F:1:NAG:H82	2.41	0.46
2:O:204:ILE:C	2:O:206:ASP:N	2.70	0.45
2:L:302:GLN:HG3	2:L:322:VAL:O	2.16	0.45
2:O:176:ARG:HG3	2:O:176:ARG:HH11	1.82	0.45
1:D:193:SER:O	1:D:194:GLN:HB2	2.17	0.45
2:L:221:TYR:HB2	2:L:313:LEU:CB	2.47	0.45
2:O:142:LYS:C	2:O:143:ASN:HD22	2.24	0.45
1:A:169:GLU:C	1:A:171:LEU:H	2.23	0.45
2:L:138:ILE:O	2:L:218:VAL:HA	2.16	0.45
1:C:154:PRO:HG3	1:D:126:TRP:CD2	2.51	0.45
1:C:188:ILE:HD11	1:C:196:PRO:HG3	1.99	0.45
2:N:280:GLN:H	2:N:280:GLN:NE2	2.14	0.45
2:L:275:ARG:HD2	2:L:277:LEU:HD23	1.98	0.45
2:M:141:ASN:ND2	2:M:144:LYS:HE3	2.32	0.45
2:L:142:LYS:HE3	2:L:142:LYS:CA	2.44	0.45
2:M:151:LEU:HD13	2:M:181:SER:O	2.17	0.45
1:A:187:GLU:OE1	1:A:199:VAL:HG11	2.17	0.44
2:L:170:PHE:CD1	2:L:191:MET:HE2	2.52	0.44
2:O:148:ILE:HA	2:O:149:PRO:HD3	1.74	0.44
2:N:139:THR:C	2:N:141:ASN:H	2.25	0.44
1:A:197:LYS:HA	1:A:198:PRO:HD3	1.87	0.44
3:H:1:NAG:H61	3:H:2:NAG:C7	2.47	0.44
1:D:146:VAL:CG2	1:D:147:ALA:H	2.23	0.43
2:L:133:HIS:ND1	2:L:133:HIS:C	2.75	0.43
2:L:138:ILE:CG1	2:L:139:THR:HB	2.48	0.43
2:N:240:GLU:OE2	2:N:240:GLU:HA	2.17	0.43
2:L:142:LYS:CE	2:L:143:ASN:H	2.31	0.43
1:B:190:VAL:HG13	1:B:191:PRO:HA	2.01	0.43
3:G:2:NAG:H83	3:G:2:NAG:H2	1.88	0.43
1:A:174:MET:HE2	1:A:212:MET:HB2	2.00	0.43
2:N:151:LEU:HD13	2:N:181:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:204:ILE:O	2:O:205:ASN:HB3	2.19	0.43
1:C:197:LYS:HA	1:C:198:PRO:HD3	1.80	0.43
1:B:174:MET:HE2	1:B:212:MET:HB2	2.01	0.42
3:H:1:NAG:H61	3:H:2:NAG:N2	2.34	0.42
1:B:118:ILE:HD12	1:B:118:ILE:H	1.84	0.42
2:N:138:ILE:HG22	2:N:140:GLU:N	2.33	0.42
2:L:229:SER:HA	2:L:230:PRO:C	2.43	0.42
2:L:140:GLU:O	2:L:141:ASN:C	2.62	0.42
2:O:154:ILE:HB	2:O:157:LEU:HG	2.02	0.42
2:O:170:PHE:CD1	2:O:191:MET:HE2	2.54	0.42
2:M:164:ARG:HD3	2:M:165:TYR:CE1	2.55	0.42
2:L:250:THR:HG21	2:L:254:VAL:HG11	2.01	0.42
1:C:171:LEU:HA	1:C:212:MET:O	2.19	0.41
2:L:142:LYS:HE2	2:L:143:ASN:H	1.84	0.41
2:N:164:ARG:HD3	2:N:165:TYR:CE1	2.55	0.41
1:A:168:SER:HB2	1:A:171:LEU:HD22	2.01	0.41
2:L:286:LYS:HE3	2:L:288:PHE:HZ	1.85	0.41
1:B:135:GLU:HG3	1:B:160:TYR:CE1	2.54	0.41
1:D:207:THR:HA	3:P:1:NAG:HO6	1.81	0.41
2:L:138:ILE:CB	2:L:139:THR:HB	2.50	0.41
2:M:172:PRO:HB3	2:M:178:SER:HA	2.02	0.41
2:M:299:ARG:HE	2:M:326:GLU:HB3	1.86	0.41
1:C:188:ILE:HG23	1:C:192:LEU:CD2	2.50	0.41
2:M:141:ASN:CG	2:M:144:LYS:HB2	2.45	0.41
2:O:164:ARG:HB3	2:O:165:TYR:CG	2.56	0.41
2:L:154:ILE:HB	2:L:157:LEU:HG	2.03	0.41
2:L:171:VAL:HG13	2:L:172:PRO:HD2	2.02	0.41
2:O:142:LYS:HD3	6:O:2001:NAG:O7	2.21	0.41
2:O:250:THR:HG21	2:O:254:VAL:HG11	2.03	0.41
2:O:286:LYS:HE3	2:O:288:PHE:HZ	1.84	0.41
1:B:148:THR:HG23	2:N:276:ASP:OD2	2.21	0.41
2:N:280:GLN:HA	2:N:283:SER:HB3	2.03	0.41
2:L:148:ILE:HA	2:L:149:PRO:HD3	1.75	0.41
2:O:221:TYR:HB2	2:O:313:LEU:CB	2.50	0.41
3:E:2:NAG:H4	3:E:3:BMA:H2	1.87	0.41
1:A:192:LEU:H	1:A:192:LEU:CD2	2.28	0.41
2:L:176:ARG:HG3	2:L:176:ARG:HH11	1.84	0.40
2:O:219:VAL:HB	2:O:220:GLY:HA3	2.04	0.40
3:P:1:NAG:H61	3:P:2:NAG:H82	2.01	0.40
1:D:175:ASN:ND2	3:K:1:NAG:O7	2.53	0.40
2:M:164:ARG:HA	2:M:165:TYR:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:159:VAL:HG21	2:O:179:TRP:CE2	2.56	0.40
2:N:270:LYS:HG2	2:N:294:ILE:HG12	2.03	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	24/110 (22%)	23 (96%)	1 (4%)	0	100	100
1	B	71/110 (64%)	70 (99%)	0	1 (1%)	9	23
1	C	95/110 (86%)	93 (98%)	2 (2%)	0	100	100
1	D	97/110 (88%)	89 (92%)	7 (7%)	1 (1%)	12	32
2	L	190/213 (89%)	175 (92%)	12 (6%)	3 (2%)	7	20
2	M	154/213 (72%)	140 (91%)	14 (9%)	0	100	100
2	N	166/213 (78%)	147 (89%)	18 (11%)	1 (1%)	21	44
2	O	168/213 (79%)	157 (94%)	10 (6%)	1 (1%)	21	44
All	All	965/1292 (75%)	894 (93%)	64 (7%)	7 (1%)	18	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	140	GLU
2	N	280	GLN
2	L	280	GLN
1	B	192	LEU
1	D	193	SER
2	L	139	THR
2	O	220	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	89/100 (89%)	82 (92%)	7 (8%)	11	28
1	B	89/100 (89%)	81 (91%)	8 (9%)	9	23
1	C	88/100 (88%)	86 (98%)	2 (2%)	44	73
1	D	90/100 (90%)	87 (97%)	3 (3%)	33	63
2	L	176/192 (92%)	170 (97%)	6 (3%)	32	62
2	M	161/192 (84%)	157 (98%)	4 (2%)	42	71
2	N	175/192 (91%)	167 (95%)	8 (5%)	24	51
2	O	173/192 (90%)	169 (98%)	4 (2%)	44	73
All	All	1041/1168 (89%)	999 (96%)	42 (4%)	28	56

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ILE
1	A	119	LEU
1	A	126	TRP
1	A	182	SER
1	A	185	LEU
1	A	189	THR
1	A	192	LEU
1	B	118	ILE
1	B	119	LEU
1	B	126	TRP
1	B	143	GLU
1	B	148	THR
1	B	150	THR
1	B	182	SER
1	B	185	LEU
1	C	119	LEU
1	C	140	VAL
1	D	118	ILE
1	D	126	TRP

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Mol	Chain	Res	Type
1	D	190	VAL
2	L	138	ILE
2	L	139	THR
2	L	142	LYS
2	L	144	LYS
2	L	275	ARG
2	L	313	LEU
2	M	139	THR
2	M	257	ASP
2	M	269	HIS
2	M	326	GLU
2	N	210	GLN
2	N	219	VAL
2	N	257	ASP
2	N	276	ASP
2	N	279	THR
2	N	280	GLN
2	N	283	SER
2	N	326	GLU
2	O	204	ILE
2	O	269	HIS
2	O	279	THR
2	O	280	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	167	ASN
2	L	268	GLN
2	M	141	ASN
2	N	132	GLN
2	N	280	GLN
2	O	253	ASN
2	O	280	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

35 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	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.66	0	17,19,21	1.21	2 (11%)
3	NAG	E	2	3	14,14,15	0.49	0	17,19,21	0.74	0
3	BMA	E	3	3	11,11,12	0.63	0	15,15,17	0.77	0
3	NAG	F	1	1,3	14,14,15	0.62	0	17,19,21	1.04	1 (5%)
3	NAG	F	2	3	14,14,15	0.52	0	17,19,21	1.04	2 (11%)
3	BMA	F	3	3	11,11,12	0.69	0	15,15,17	0.50	0
3	NAG	G	1	1,3	14,14,15	0.53	0	17,19,21	1.05	1 (5%)
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	0.83	1 (5%)
3	BMA	G	3	3	11,11,12	0.59	0	15,15,17	0.88	0
3	NAG	H	1	1,3	14,14,15	0.72	0	17,19,21	1.34	3 (17%)
3	NAG	H	2	3	14,14,15	0.59	0	17,19,21	1.03	1 (5%)
3	BMA	H	3	3	11,11,12	0.63	0	15,15,17	0.74	0
3	NAG	I	1	1,3	14,14,15	0.53	0	17,19,21	1.20	2 (11%)
3	NAG	I	2	3	14,14,15	0.54	0	17,19,21	0.81	0
3	BMA	I	3	3	11,11,12	0.62	0	15,15,17	0.88	0
3	NAG	J	1	1,3	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
3	NAG	J	2	3	14,14,15	0.64	0	17,19,21	0.65	0
3	BMA	J	3	3	11,11,12	0.67	0	15,15,17	0.82	0
3	NAG	K	1	1,3	14,14,15	0.51	0	17,19,21	1.38	1 (5%)
3	NAG	K	2	3	14,14,15	0.37	0	17,19,21	1.08	1 (5%)
3	BMA	K	3	3	11,11,12	0.59	0	15,15,17	0.74	0
3	NAG	P	1	1,3	14,14,15	0.46	0	17,19,21	1.14	3 (17%)
3	NAG	P	2	3	14,14,15	0.64	0	17,19,21	1.13	2 (11%)
3	BMA	P	3	3	11,11,12	0.68	0	15,15,17	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	Q	1	2,4	14,14,15	0.55	0	17,19,21	0.75	0
4	NAG	Q	2	4	14,14,15	0.54	0	17,19,21	0.72	0
4	NAG	R	1	2,4	14,14,15	0.52	0	17,19,21	0.82	0
4	NAG	R	2	4	14,14,15	0.53	0	17,19,21	0.74	0
3	NAG	S	1	2,3	14,14,15	0.59	0	17,19,21	1.61	3 (17%)
3	NAG	S	2	3	14,14,15	0.64	0	17,19,21	1.17	2 (11%)
3	BMA	S	3	3	11,11,12	0.59	0	15,15,17	1.04	1 (6%)
4	NAG	T	1	2,4	14,14,15	0.46	0	17,19,21	1.57	3 (17%)
4	NAG	T	2	4	14,14,15	0.47	0	17,19,21	1.20	3 (17%)
4	NAG	U	1	2,4	14,14,15	0.60	0	17,19,21	0.85	0
4	NAG	U	2	4	14,14,15	0.59	0	17,19,21	1.14	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
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	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	-	3/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	P	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
4	NAG	Q	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
3	NAG	S	1	2,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	BMA	S	3	3	-	1/2/19/22	0/1/1/1
4	NAG	T	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	1/6/23/26	0/1/1/1
4	NAG	U	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	1	NAG	C3-C4-C5	-4.00	102.97	110.23
3	K	1	NAG	C2-N2-C7	-3.54	118.15	122.90
3	J	1	NAG	O5-C1-C2	-3.49	105.89	111.29
4	T	1	NAG	C1-O5-C5	3.47	116.83	112.19
3	H	1	NAG	C4-C3-C2	3.23	115.75	111.02
3	S	1	NAG	O4-C4-C3	3.03	117.51	110.38
3	E	1	NAG	O5-C1-C2	-2.93	106.75	111.29
4	T	2	NAG	C1-O5-C5	2.88	116.05	112.19
3	E	1	NAG	C2-N2-C7	-2.85	119.08	122.90
3	I	1	NAG	C2-N2-C7	-2.81	119.14	122.90
3	S	2	NAG	C2-N2-C7	2.75	126.58	122.90
3	I	1	NAG	O5-C1-C2	-2.74	107.05	111.29
3	S	3	BMA	C3-C4-C5	2.72	115.16	110.23
3	P	3	BMA	C1-O5-C5	-2.60	108.70	112.19
3	H	1	NAG	C2-N2-C7	-2.55	119.49	122.90
4	T	1	NAG	C6-C5-C4	-2.51	106.86	113.02
3	H	2	NAG	C4-C3-C2	2.50	114.69	111.02
3	S	2	NAG	C1-O5-C5	2.50	115.53	112.19
4	U	2	NAG	C4-C3-C2	2.47	114.64	111.02
4	T	1	NAG	O5-C1-C2	-2.36	107.64	111.29
3	F	2	NAG	O5-C1-C2	-2.35	107.65	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	NAG	O5-C1-C2	-2.30	107.74	111.29
3	G	2	NAG	C1-O5-C5	2.28	115.24	112.19
4	T	2	NAG	C2-N2-C7	-2.23	119.91	122.90
3	S	1	NAG	C4-C3-C2	-2.21	107.78	111.02
3	J	1	NAG	C2-N2-C7	-2.20	119.95	122.90
4	T	2	NAG	C4-C3-C2	-2.18	107.82	111.02
3	P	1	NAG	C2-N2-C7	-2.18	119.98	122.90
3	F	2	NAG	C2-N2-C7	-2.10	120.09	122.90
3	K	2	NAG	C6-C5-C4	-2.09	107.89	113.02
3	P	1	NAG	C1-O5-C5	2.08	114.98	112.19
3	H	1	NAG	C1-O5-C5	2.06	114.95	112.19
3	G	1	NAG	C3-C4-C5	2.04	113.92	110.23
3	P	2	NAG	O5-C1-C2	2.03	114.44	111.29
3	P	2	NAG	C4-C3-C2	2.03	113.99	111.02
3	F	1	NAG	O5-C1-C2	-2.02	108.17	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	S	1	NAG	C1

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C3-C2-N2-C7
4	Q	2	NAG	O7-C7-N2-C2
4	U	2	NAG	C1-C2-N2-C7
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2

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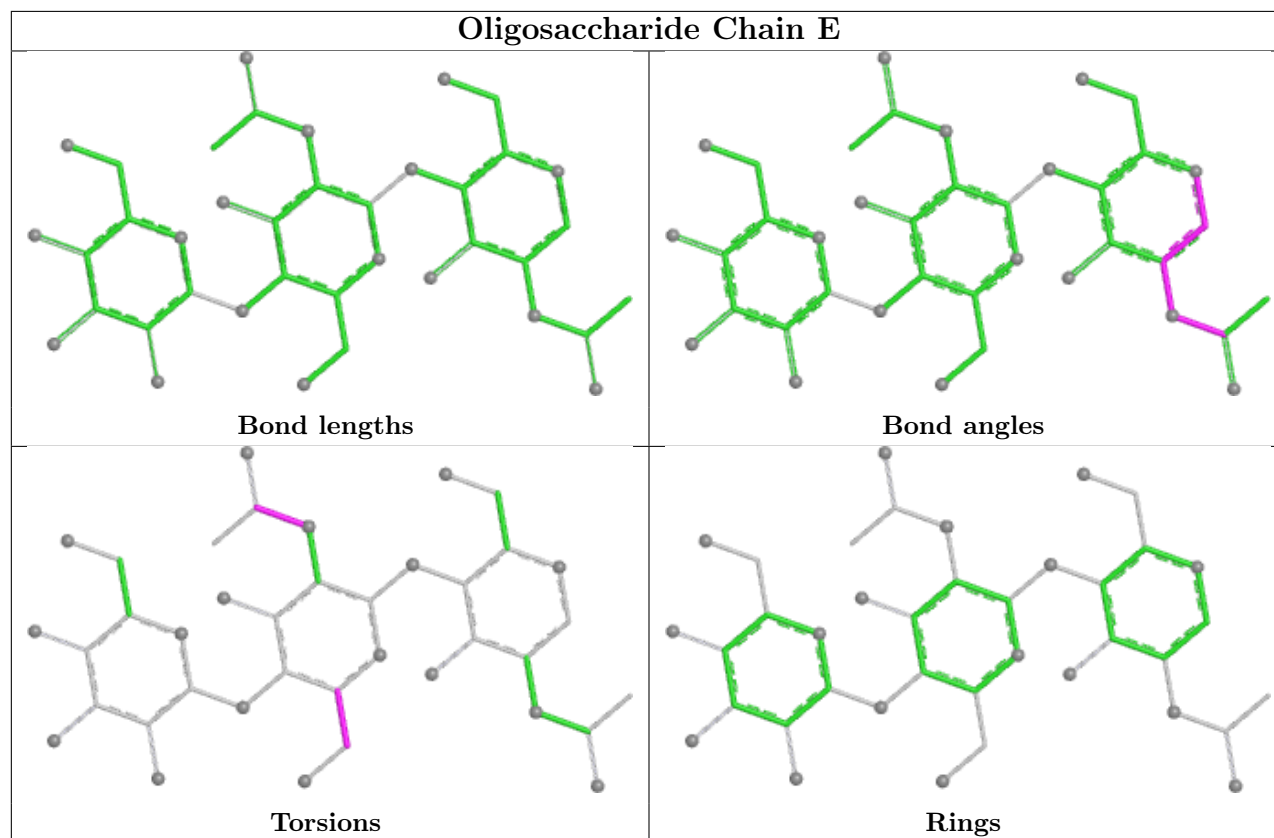
Mol	Chain	Res	Type	Atoms
3	P	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
3	P	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C8-C7-N2-C2
3	G	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
3	I	3	BMA	O5-C5-C6-O6
3	P	1	NAG	O7-C7-N2-C2
3	F	3	BMA	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
4	R	1	NAG	C8-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
4	R	1	NAG	O7-C7-N2-C2
4	Q	1	NAG	C1-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
3	J	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C8-C7-N2-C2
3	H	3	BMA	O5-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
4	U	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6

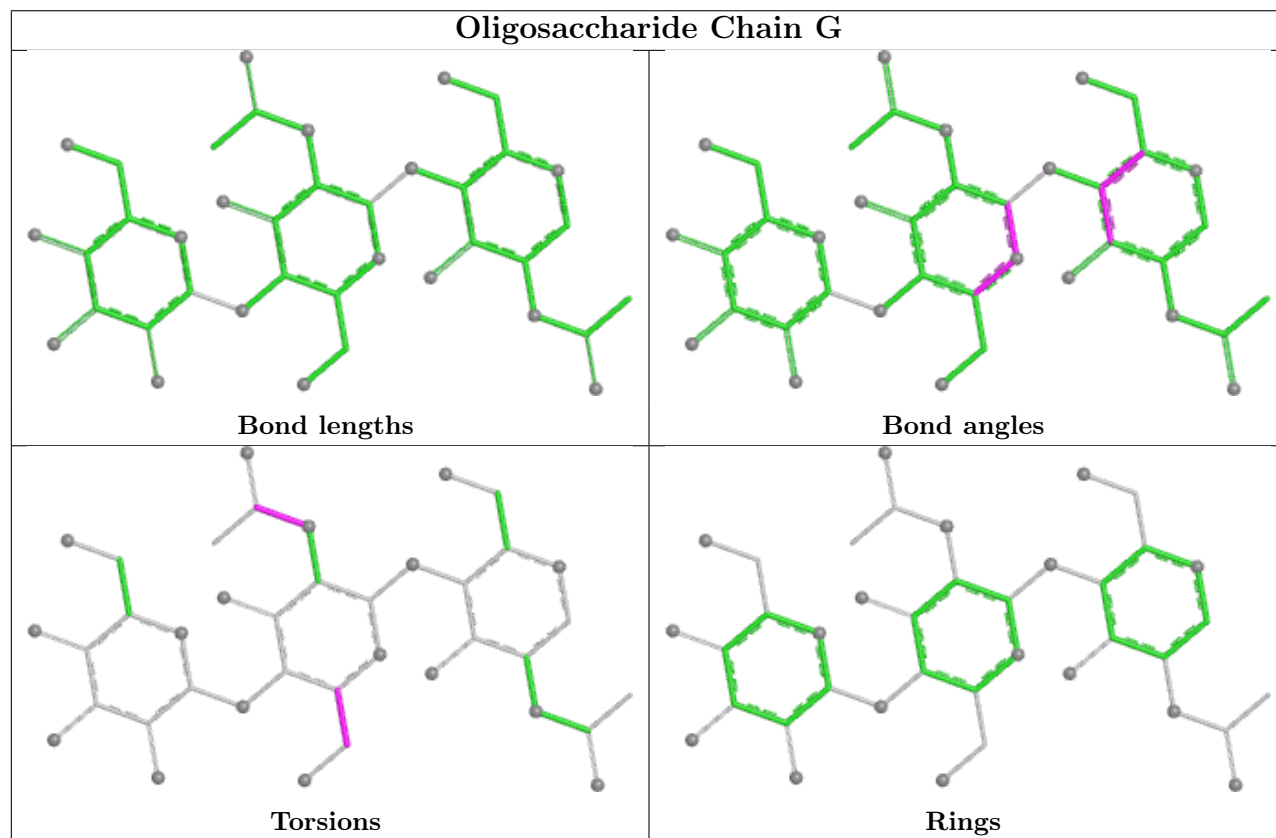
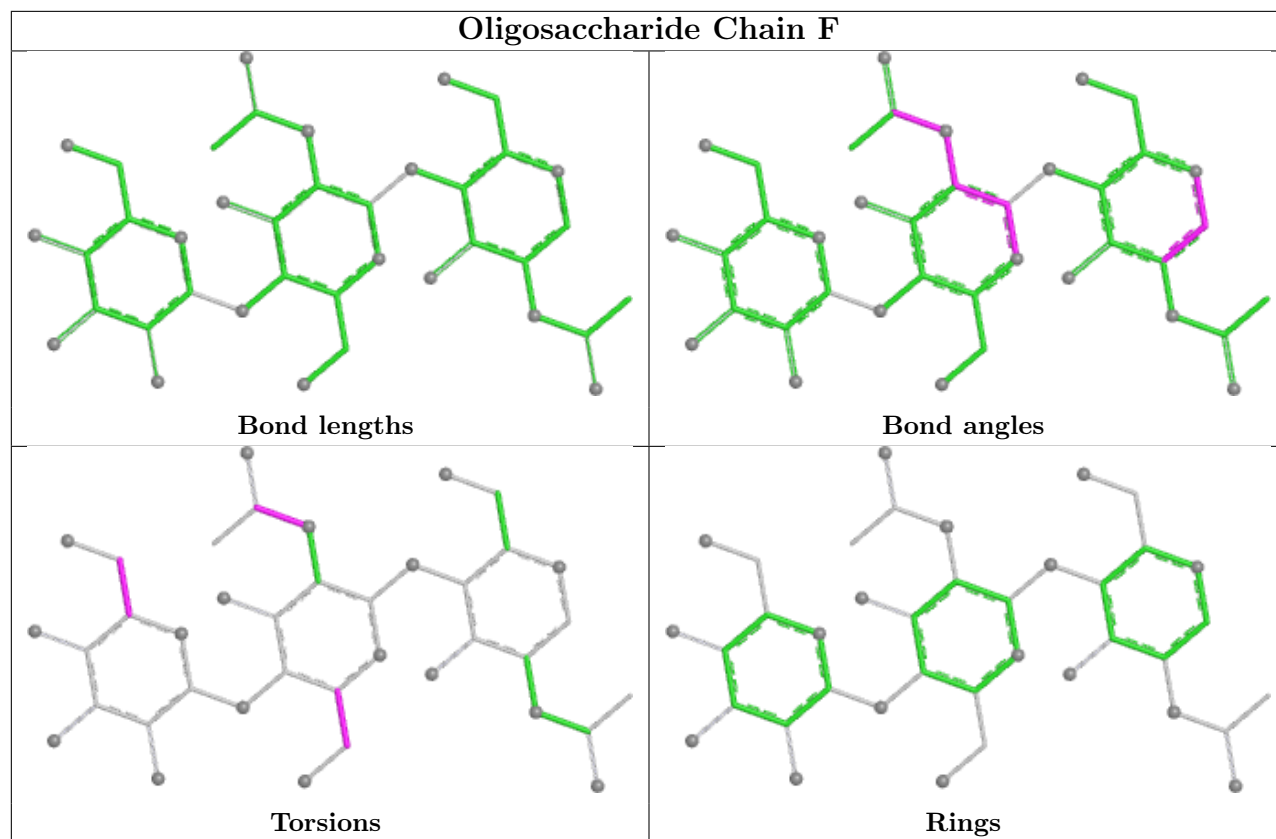
There are no ring outliers.

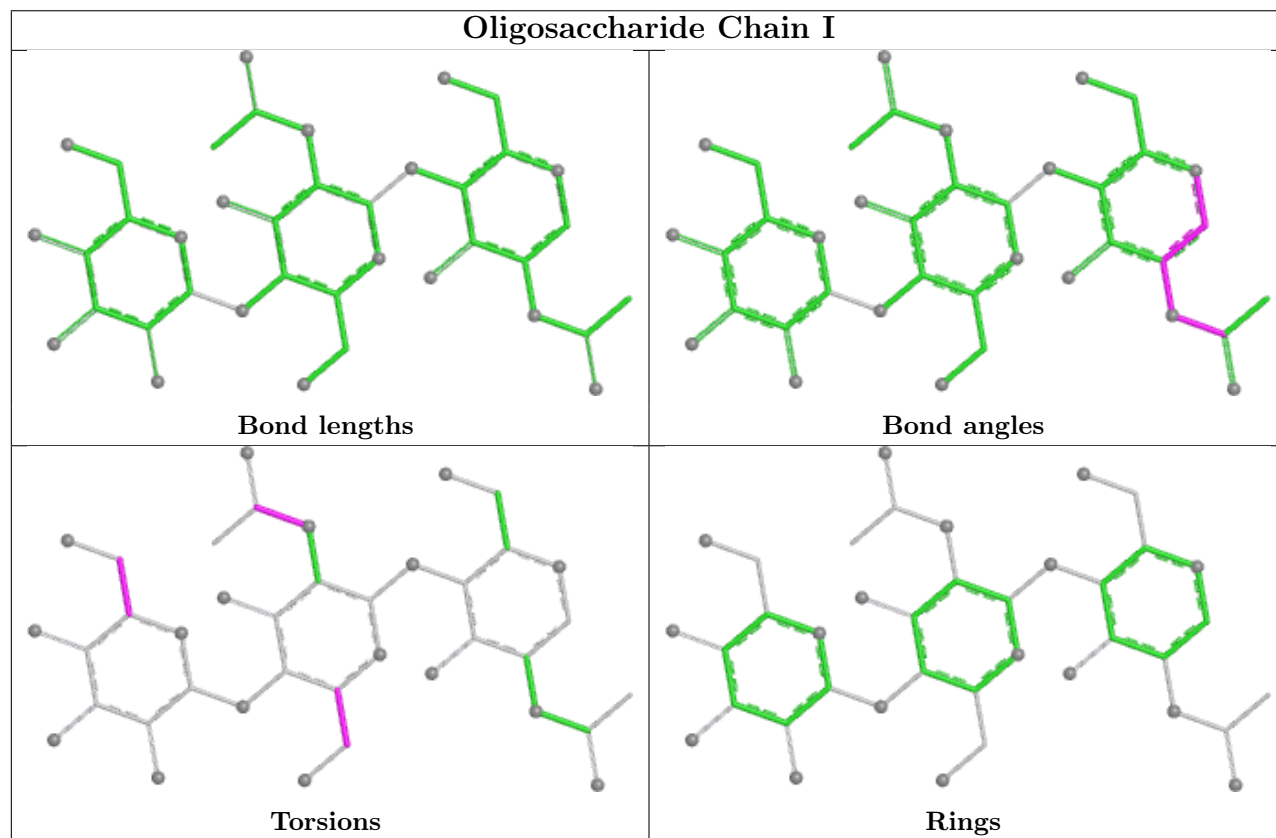
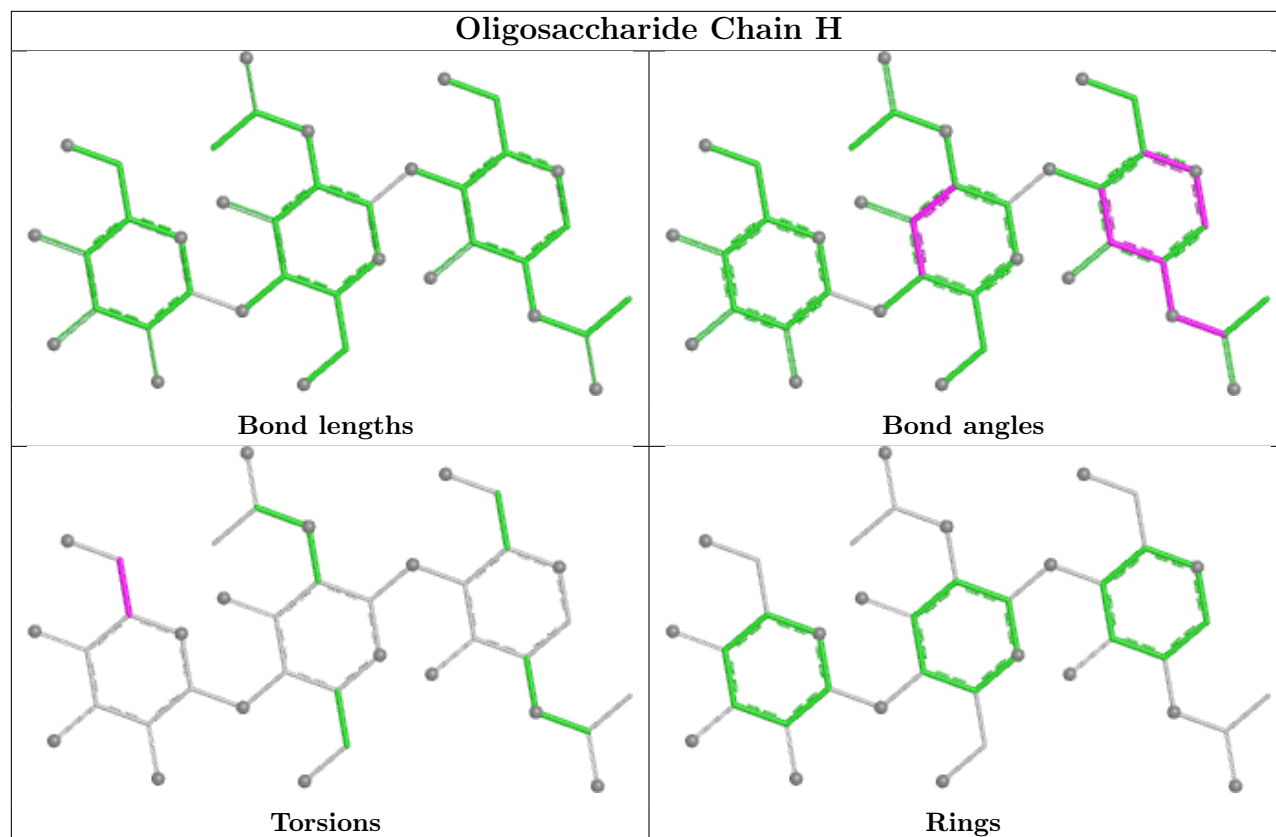
12 monomers are involved in 15 short contacts:

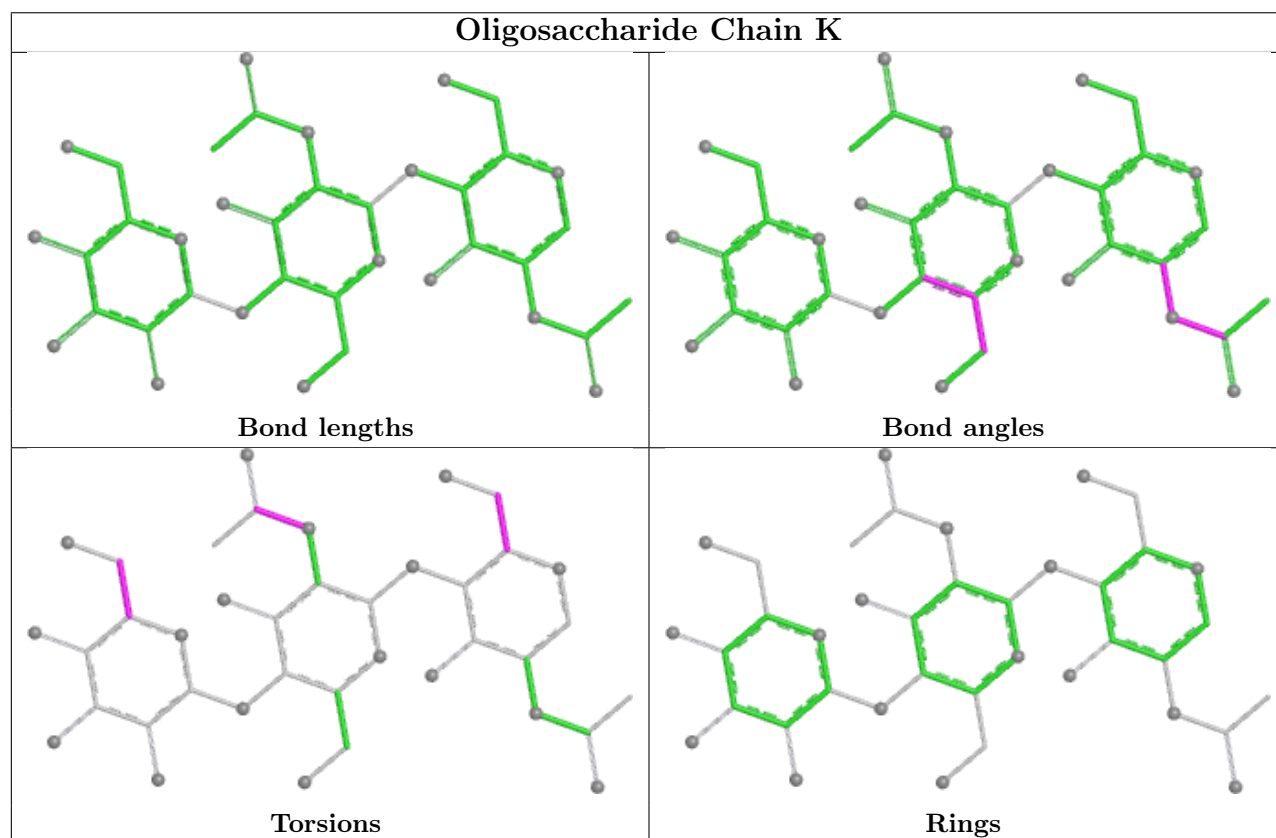
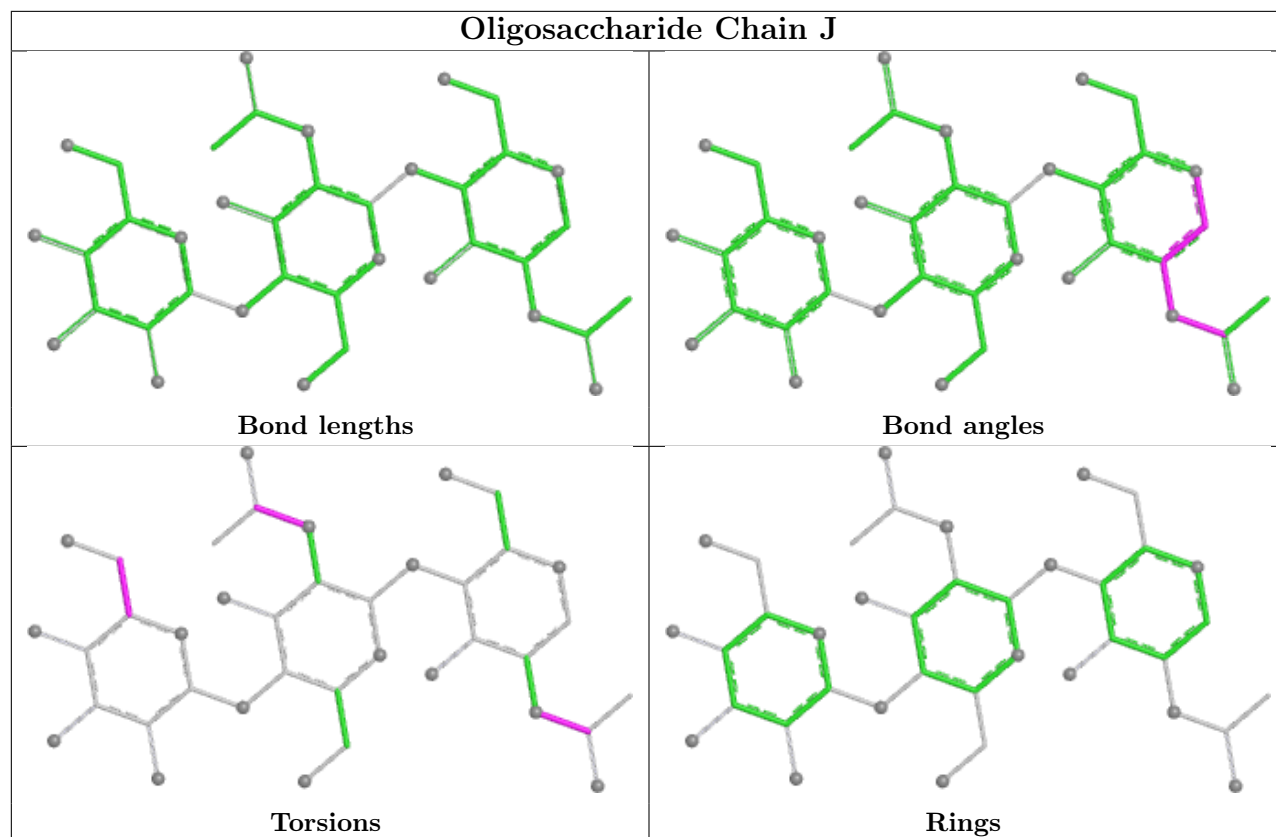
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
3	P	2	NAG	1	0
3	H	1	NAG	3	0
3	F	1	NAG	2	0
3	G	2	NAG	1	0
3	J	1	NAG	1	0
3	P	1	NAG	4	0
3	K	1	NAG	1	0
3	S	1	NAG	2	0
3	S	2	NAG	1	0
3	E	3	BMA	1	0
3	H	2	NAG	2	0

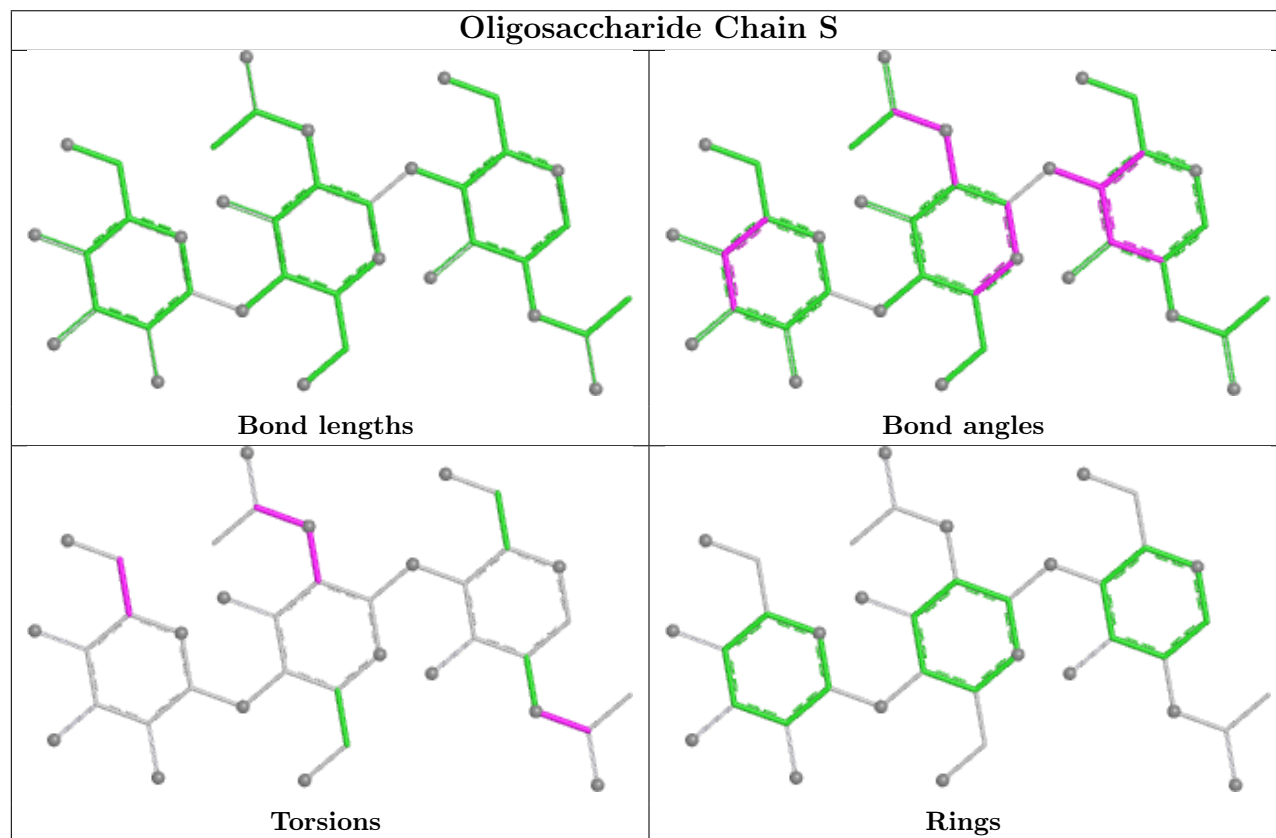
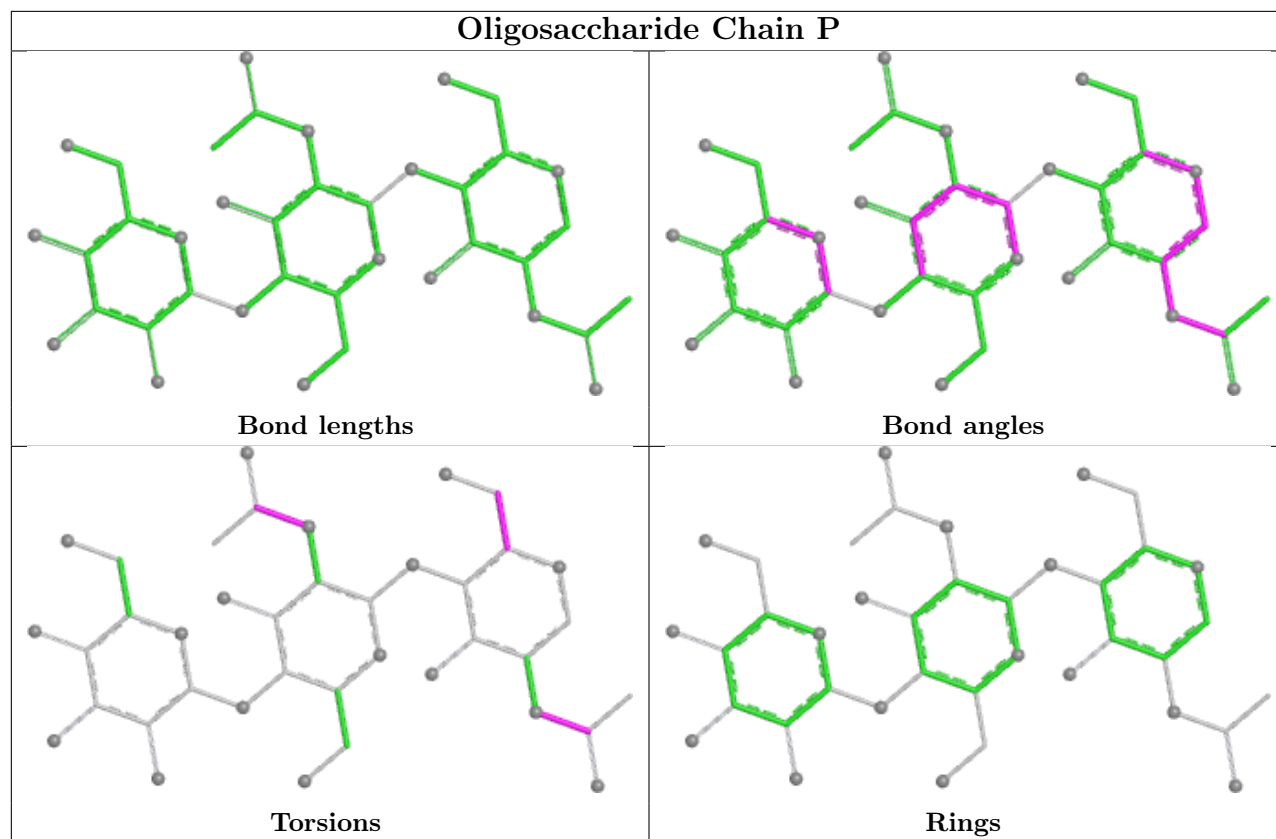
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

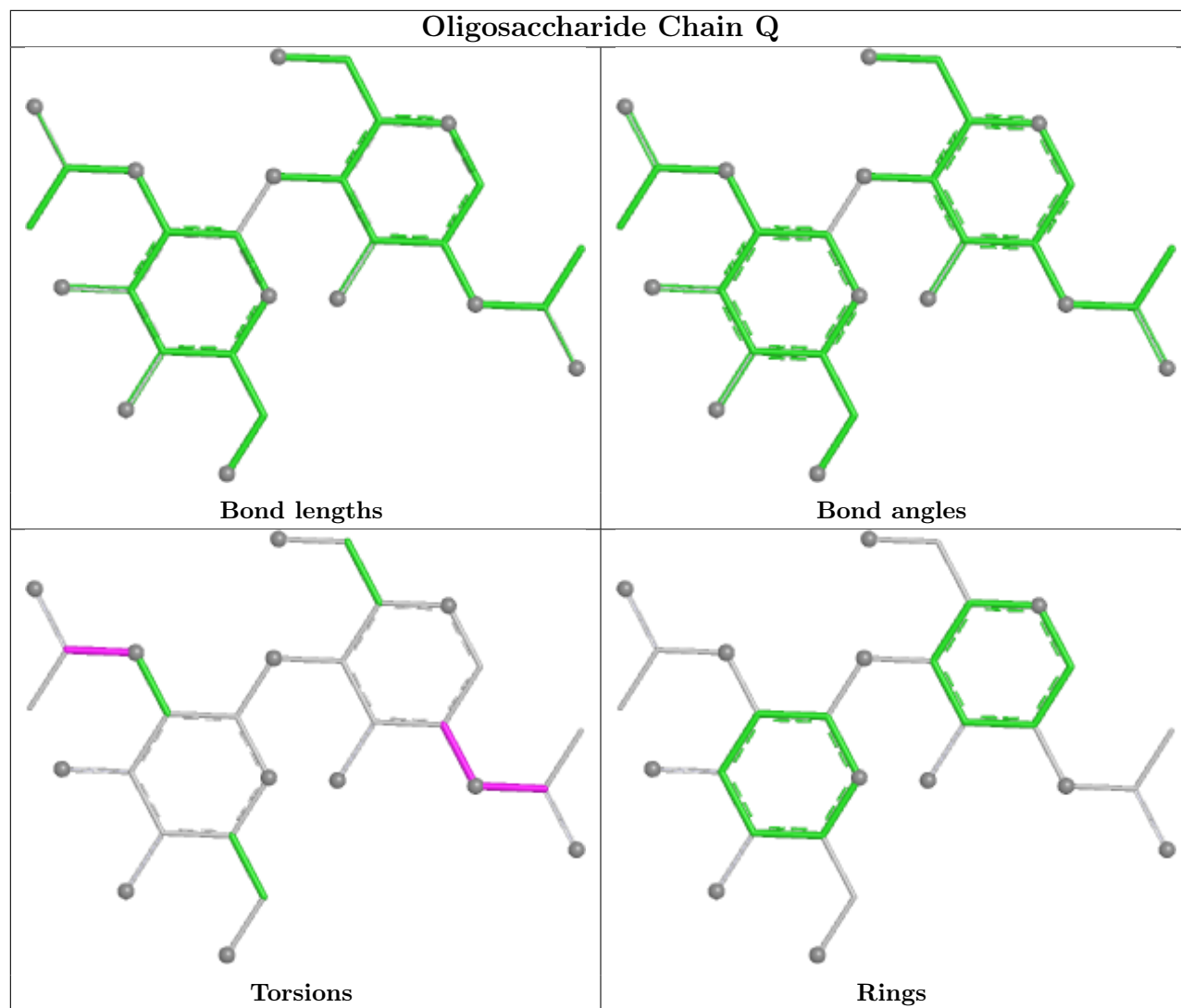


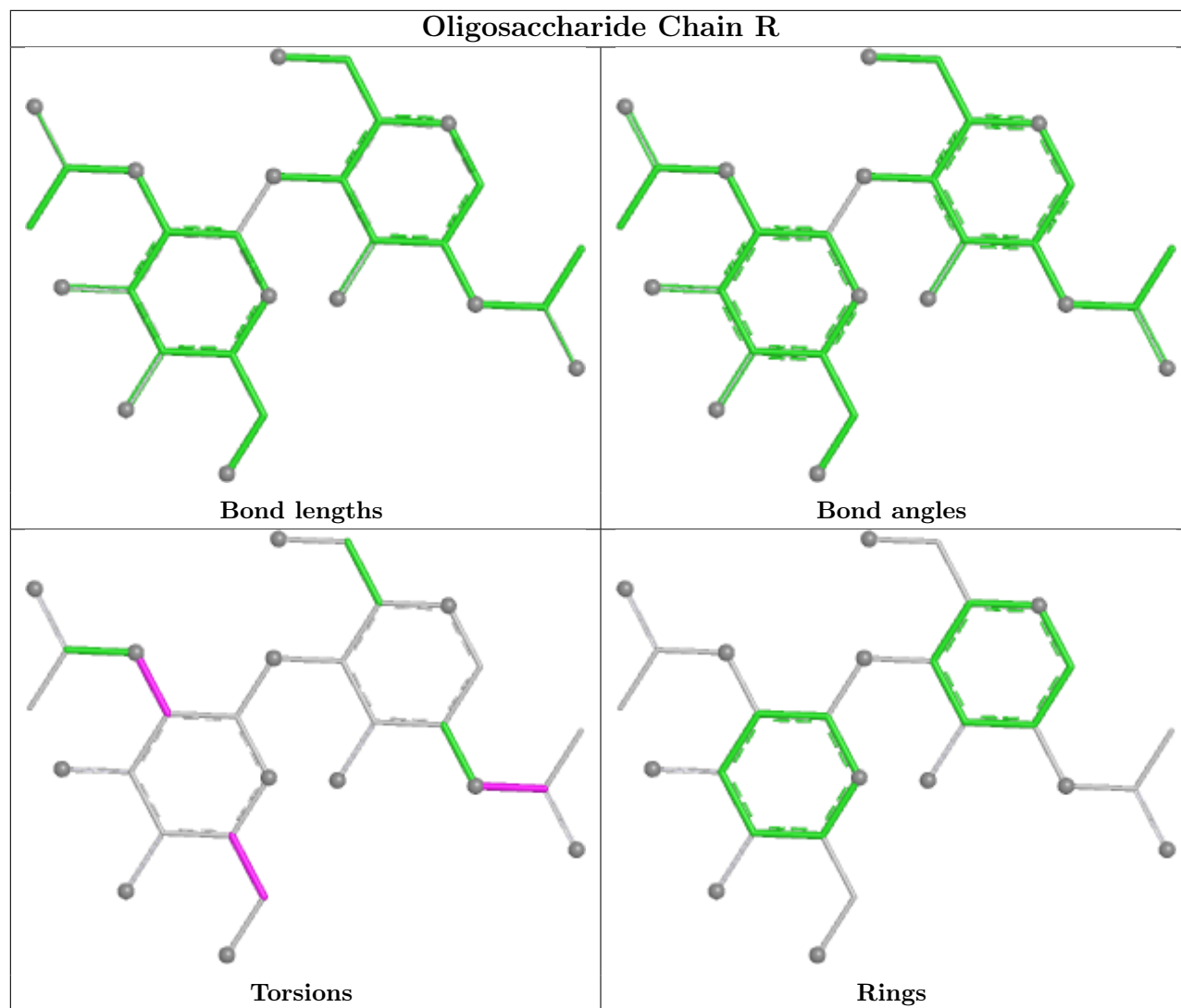


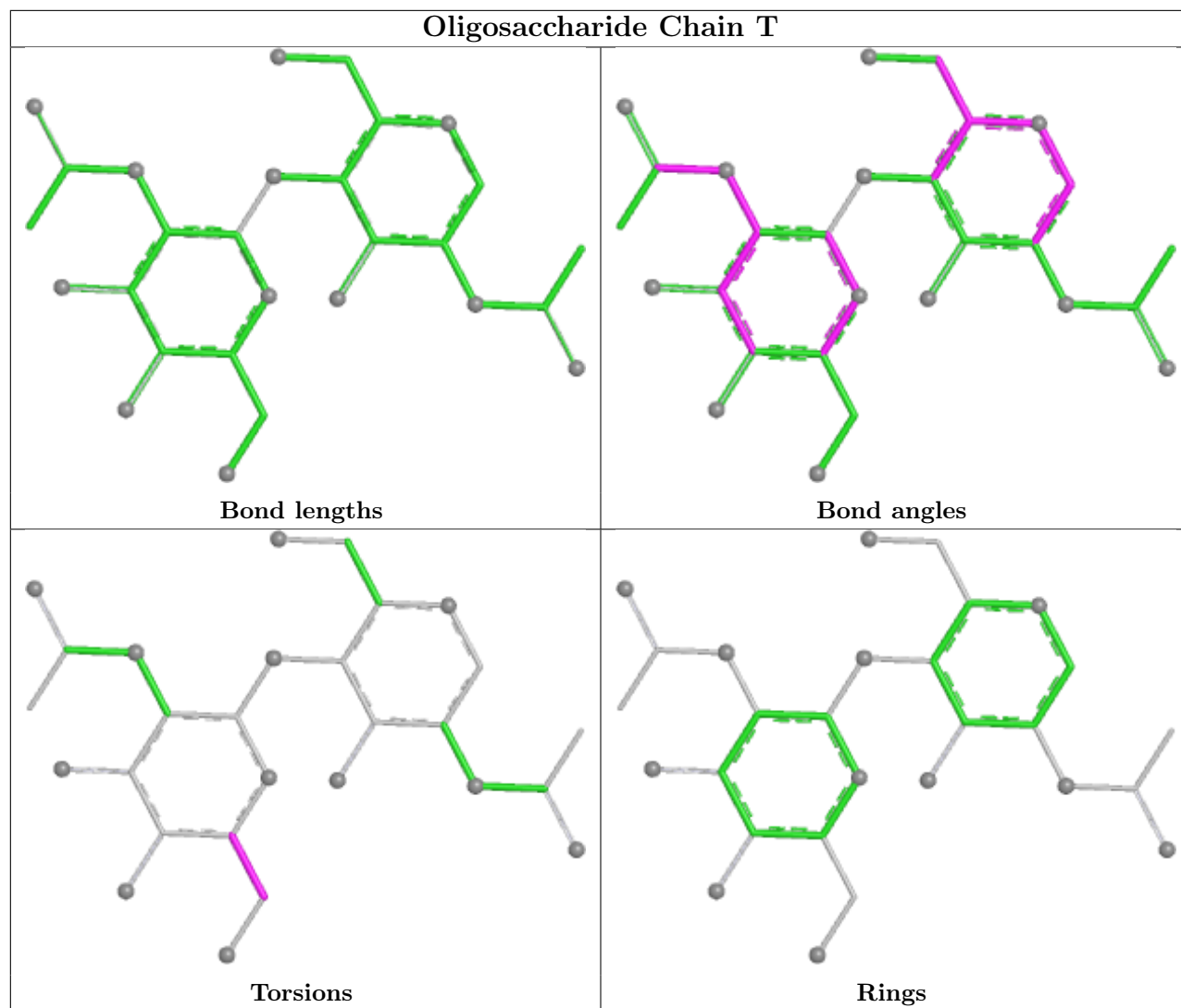


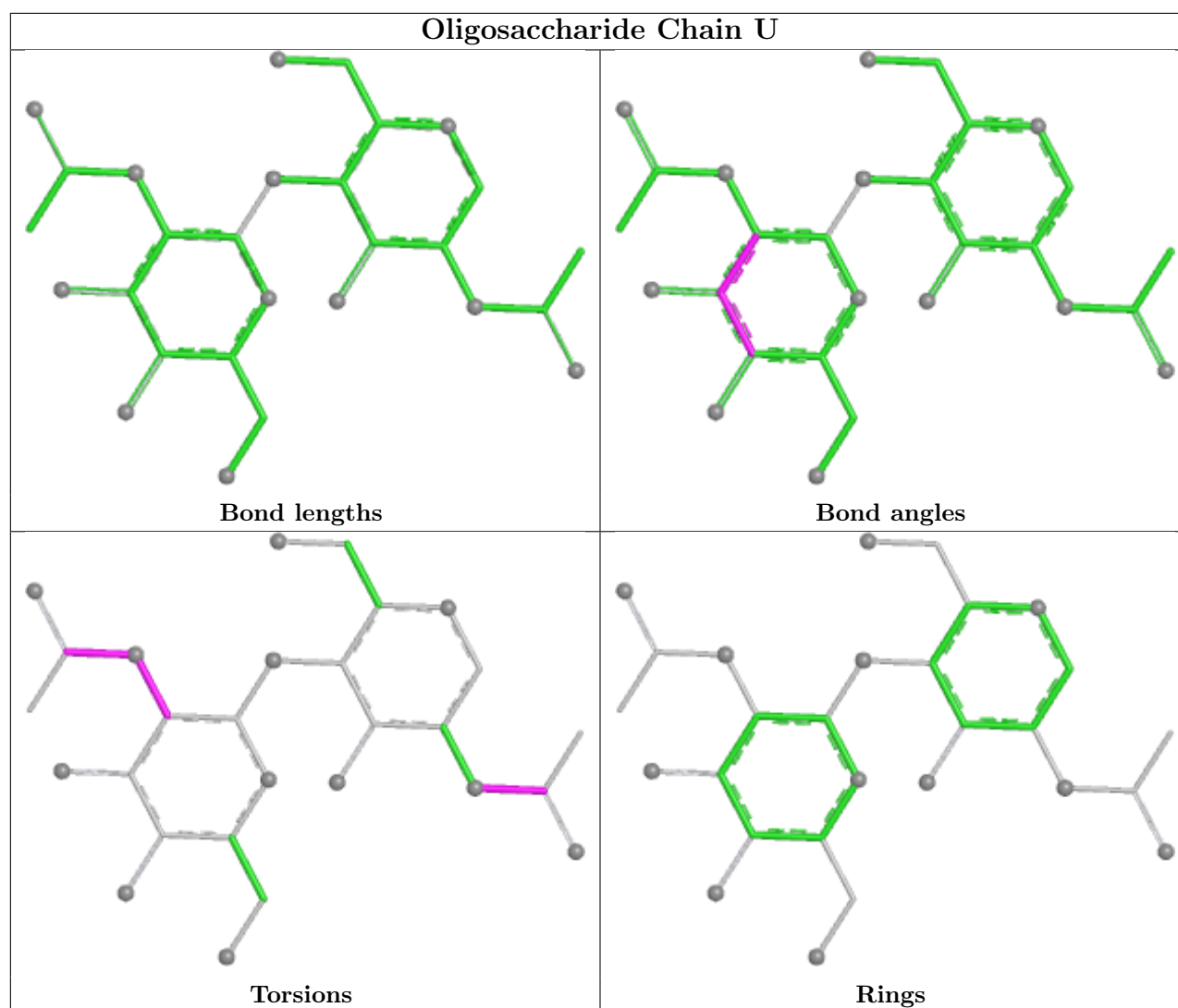












5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	O	2301	2	14,14,15	0.44	0	17,19,21	0.97	0
6	NAG	N	1401	2	14,14,15	0.61	0	17,19,21	0.90	0
6	NAG	L	2701	2	14,14,15	0.44	0	17,19,21	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	N	1601	2	14,14,15	0.49	0	17,19,21	1.21	1 (5%)
6	NAG	O	2001	2	14,14,15	0.57	0	17,19,21	1.58	4 (23%)
6	NAG	O	2101	2	14,14,15	0.44	0	17,19,21	0.97	1 (5%)
6	NAG	L	2401	2	14,14,15	0.46	0	17,19,21	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	O	2301	2	-	0/6/23/26	0/1/1/1
6	NAG	N	1401	2	-	3/6/23/26	0/1/1/1
6	NAG	L	2701	2	-	2/6/23/26	0/1/1/1
6	NAG	O	2001	2	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	N	1601	2	-	0/6/23/26	0/1/1/1
6	NAG	O	2101	2	-	3/6/23/26	0/1/1/1
6	NAG	L	2401	2	1/1/5/7	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	2001	NAG	C1-O5-C5	4.38	118.06	112.19
6	N	1601	NAG	O5-C1-C2	-3.78	105.45	111.29
6	L	2701	NAG	O5-C5-C6	3.15	113.80	107.66
6	O	2001	NAG	C3-C4-C5	-2.45	105.80	110.23
6	O	2101	NAG	C1-O5-C5	2.35	115.34	112.19
6	L	2701	NAG	C6-C5-C4	-2.27	107.44	113.02
6	O	2001	NAG	C4-C3-C2	-2.11	107.92	111.02
6	O	2001	NAG	C2-N2-C7	-2.07	120.12	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	2401	NAG	C1
6	O	2001	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	1401	NAG	C8-C7-N2-C2
6	N	1401	NAG	O7-C7-N2-C2
6	O	2001	NAG	C8-C7-N2-C2
6	L	2401	NAG	C8-C7-N2-C2
6	L	2401	NAG	O7-C7-N2-C2
6	O	2001	NAG	O7-C7-N2-C2
6	O	2101	NAG	C8-C7-N2-C2
6	O	2101	NAG	O7-C7-N2-C2
6	L	2701	NAG	O5-C5-C6-O6
6	O	2101	NAG	O5-C5-C6-O6
6	L	2701	NAG	C4-C5-C6-O6
6	N	1401	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	2001	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	98/110 (89%)	0.66	14 (14%) 6 5	43, 69, 129, 148	0
1	B	98/110 (89%)	0.44	7 (7%) 22 19	44, 65, 109, 125	0
1	C	97/110 (88%)	0.16	4 (4%) 41 37	35, 53, 93, 137	0
1	D	99/110 (90%)	0.32	6 (6%) 27 24	35, 57, 118, 142	0
2	L	196/213 (92%)	0.38	17 (8%) 16 13	40, 61, 120, 166	0
2	M	179/213 (84%)	0.48	10 (5%) 30 26	42, 68, 130, 150	0
2	N	194/213 (91%)	0.57	21 (10%) 11 9	37, 67, 125, 143	0
2	O	193/213 (90%)	0.41	14 (7%) 21 18	35, 62, 114, 159	0
All	All	1154/1292 (89%)	0.44	93 (8%) 18 15	35, 62, 121, 166	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119	LEU	5.9
2	O	153	SER	5.8
1	A	192	LEU	5.6
1	B	118	ILE	5.5
2	O	282	GLY	5.4
1	A	191	PRO	5.1
1	D	118	ILE	5.0
2	N	205	ASN	4.9
1	D	215	LEU	4.9
2	L	203	LYS	4.6
2	O	280	GLN	3.9
2	M	283	SER	3.9
2	L	268	GLN	3.8
2	L	267	HIS	3.8
1	A	144	PHE	3.8
2	M	202	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	O	127	ALA	3.7
1	B	170	GLY	3.6
2	M	264	SER	3.5
2	L	201	GLU	3.3
2	O	237	SER	3.3
2	N	154	ILE	3.3
1	C	184	THR	3.2
2	L	208	SER	3.2
2	O	154	ILE	3.2
1	A	194	GLN	3.2
1	C	214	LYS	3.0
1	A	196	PRO	3.0
2	N	206	ASP	3.0
2	N	275	ARG	2.9
2	O	236	LEU	2.9
2	L	209	TYR	2.8
2	N	132	GLN	2.8
1	A	186	PHE	2.8
1	B	214	LYS	2.7
2	N	150	CYS	2.7
1	A	170	GLY	2.6
2	O	142	LYS	2.6
2	L	210	GLN	2.6
2	N	156	ASN	2.6
2	N	213	MET	2.6
1	A	210	ARG	2.6
2	L	133	HIS	2.6
2	N	142	LYS	2.5
2	N	270	LYS	2.5
2	N	265	SER	2.5
1	B	188	ILE	2.5
1	D	120	LYS	2.5
2	L	139	THR	2.5
2	O	157	LEU	2.5
2	L	295	ASP	2.5
1	B	119	LEU	2.4
1	A	193	SER	2.4
2	O	276	ASP	2.4
2	M	182	LYS	2.4
2	O	183	LYS	2.4
2	M	279	THR	2.4
1	D	214	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	O	261	GLU	2.4
1	A	182	SER	2.3
2	N	264	SER	2.3
1	C	120	LYS	2.3
2	L	154	ILE	2.3
1	A	213	SER	2.3
2	L	282	GLY	2.3
2	L	313	LEU	2.3
2	N	209	TYR	2.3
2	O	155	SER	2.3
2	L	156	ASN	2.2
2	N	139	THR	2.2
1	A	146	VAL	2.2
2	N	236	LEU	2.2
2	L	326	GLU	2.2
2	L	158	ASN	2.1
2	L	155	SER	2.1
2	O	279	THR	2.1
2	M	278	LYS	2.1
2	M	269	HIS	2.1
1	A	190	VAL	2.1
2	N	136	VAL	2.1
1	B	151	PHE	2.1
2	N	326	GLU	2.1
2	M	154	ILE	2.1
1	A	151	PHE	2.1
1	D	121	SER	2.1
2	N	208	SER	2.1
2	M	174	GLY	2.1
2	N	153	SER	2.0
2	N	175	ASN	2.0
2	N	317	LYS	2.0
2	M	213	MET	2.0
1	B	124	ASN	2.0
1	D	180	TYR	2.0

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, 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.

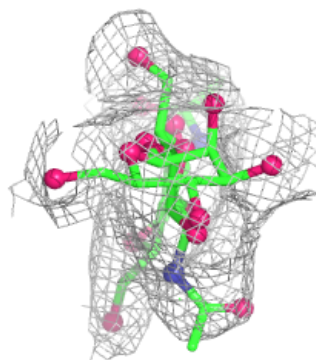
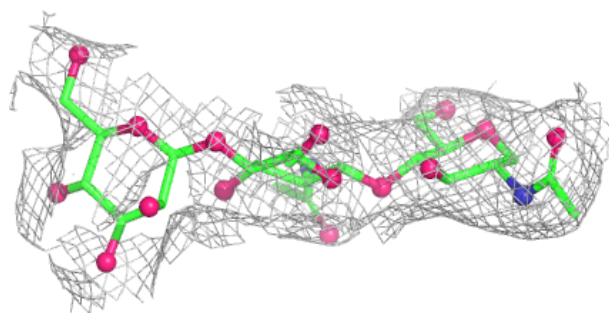
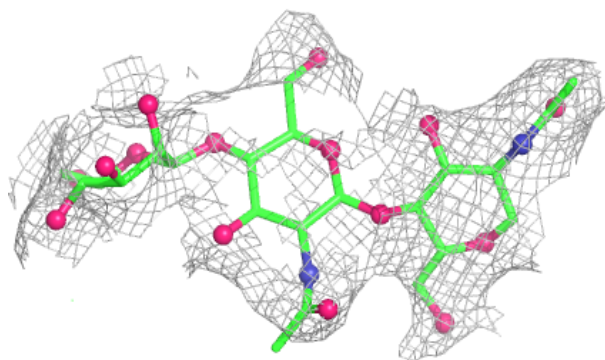
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	1	14/15	-	-	40,70,88,97	0
3	NAG	E	2	14/15	-	-	114,125,140,150	0
3	BMA	E	3	11/12	-	-	125,142,155,155	0
3	NAG	F	1	14/15	-	-	62,80,96,97	0
3	NAG	F	2	14/15	-	-	89,106,114,120	0
3	BMA	F	3	11/12	-	-	85,115,129,137	0
3	NAG	G	1	14/15	-	-	59,77,85,101	0
3	NAG	G	2	14/15	-	-	93,118,130,141	0
3	BMA	G	3	11/12	-	-	107,138,147,149	0
3	NAG	H	1	14/15	-	-	56,83,105,109	0
3	NAG	H	2	14/15	-	-	57,90,111,128	0
3	BMA	H	3	11/12	-	-	90,122,131,131	0
3	BMA	I	3	11/12	0.37	0.13	92,123,139,140	0
3	BMA	P	3	11/12	0.55	0.16	94,126,135,139	0
3	BMA	K	3	11/12	0.60	0.14	91,130,139,139	0
4	NAG	Q	2	14/15	0.60	0.15	80,124,130,132	0
3	NAG	K	2	14/15	0.61	0.12	74,105,121,133	0
3	BMA	S	3	11/12	0.65	0.11	119,134,140,141	0
3	NAG	S	2	14/15	0.67	0.15	89,121,127,140	0
4	NAG	U	2	14/15	0.67	0.16	105,122,131,132	0
3	BMA	J	3	11/12	0.72	0.14	57,81,102,112	0
3	NAG	J	2	14/15	0.72	0.14	53,64,75,81	0
3	NAG	S	1	14/15	0.74	0.16	64,89,127,133	0
3	NAG	I	2	14/15	0.76	0.11	50,60,72,83	0
4	NAG	R	2	14/15	0.78	0.10	91,110,119,119	0
4	NAG	T	2	14/15	0.81	0.11	29,98,118,119	0
3	NAG	P	2	14/15	0.82	0.14	64,89,111,123	0
3	NAG	K	1	14/15	0.88	0.11	50,72,92,103	0
4	NAG	T	1	14/15	0.89	0.12	39,52,73,81	0
3	NAG	J	1	14/15	0.91	0.11	32,55,61,75	0
4	NAG	Q	1	14/15	0.91	0.12	59,82,106,112	0
3	NAG	P	1	14/15	0.91	0.14	56,71,89,91	0
4	NAG	R	1	14/15	0.91	0.10	57,70,96,96	0
3	NAG	I	1	14/15	0.92	0.11	36,50,63,66	0
4	NAG	U	1	14/15	0.93	0.09	56,77,100,102	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

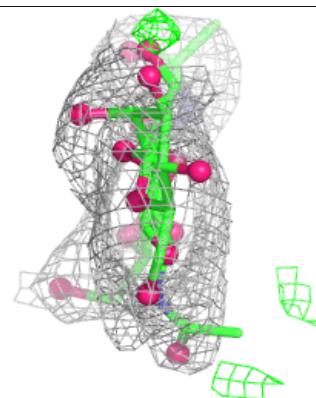
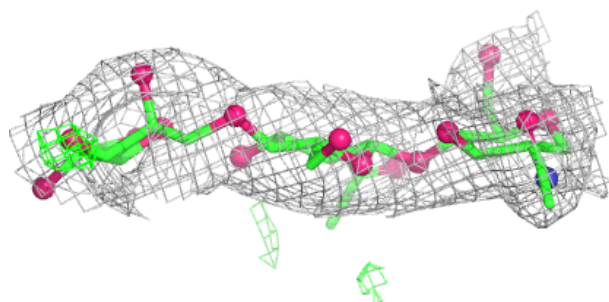
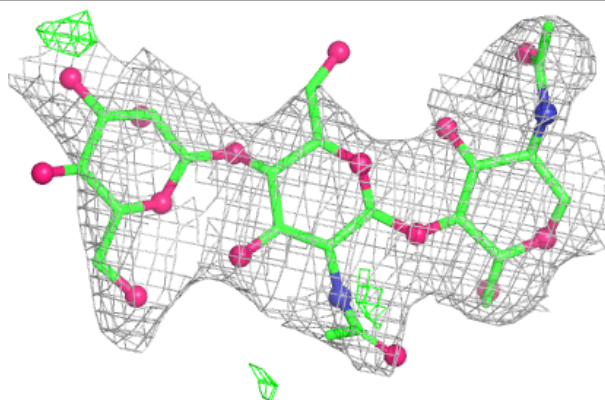
Electron density around Chain E:

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



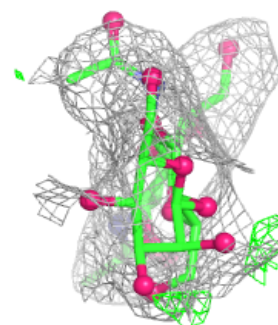
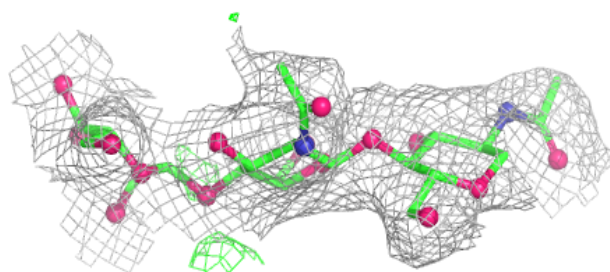
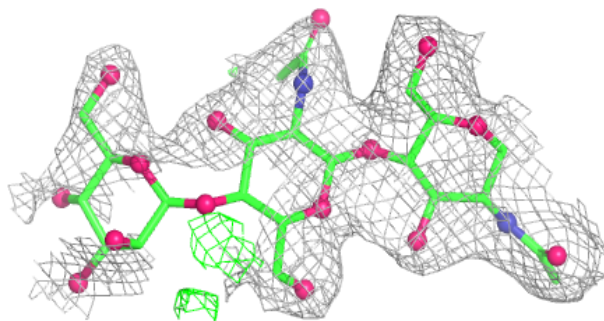
Electron density around Chain F:

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

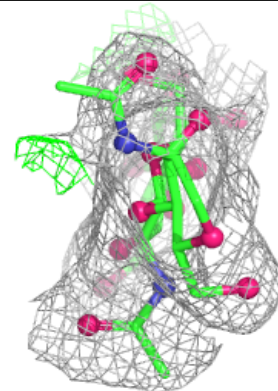
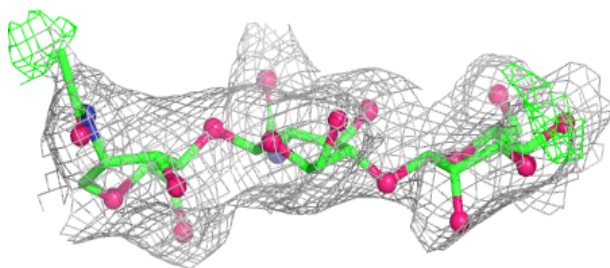
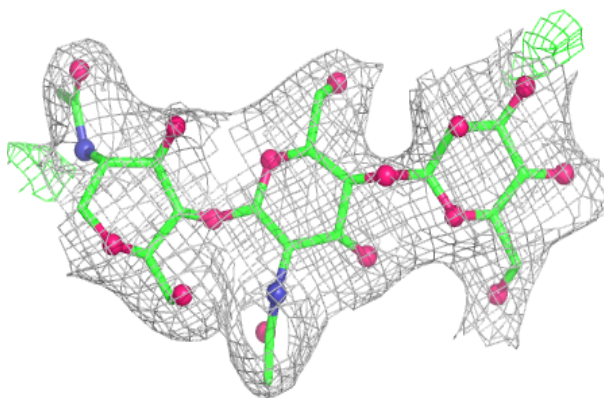


Electron density around Chain G:

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

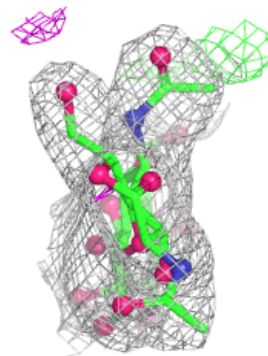
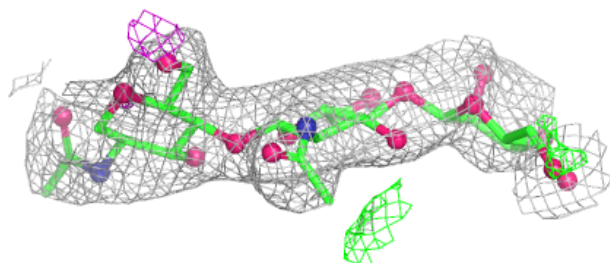
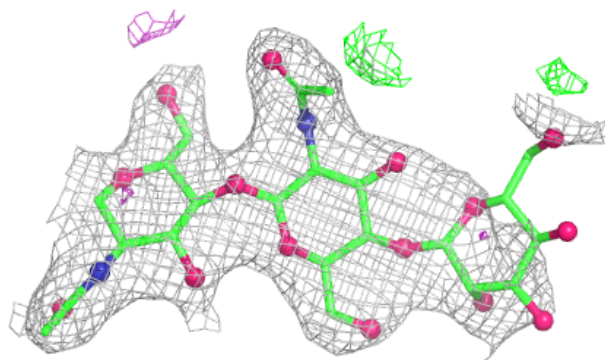
**Electron density around Chain H:**

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

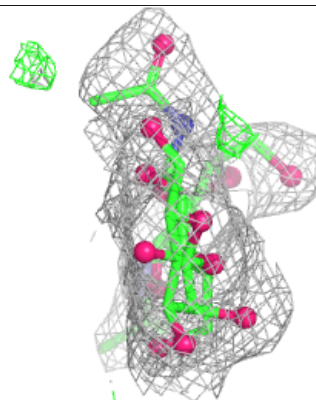
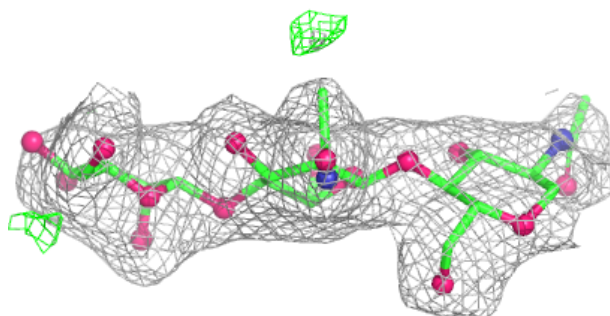
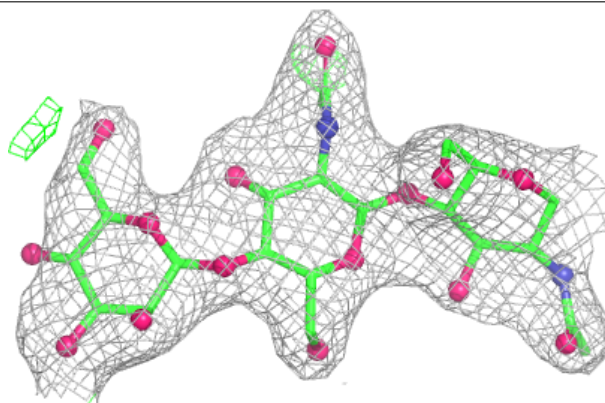


Electron density around Chain I:

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

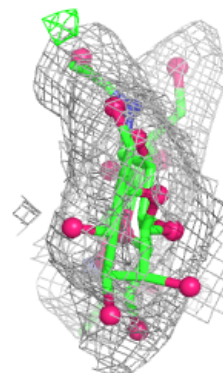
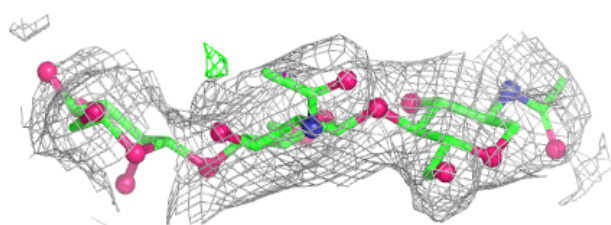
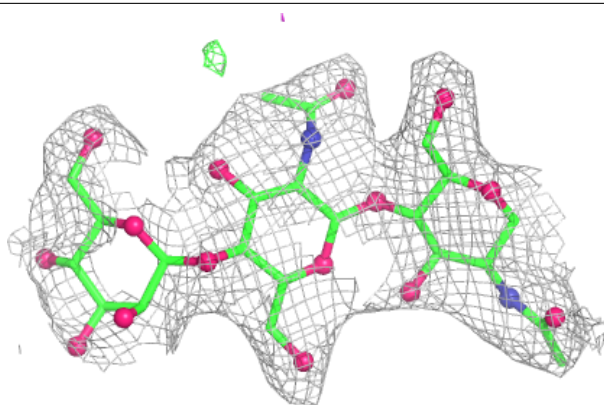
**Electron density around Chain J:**

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

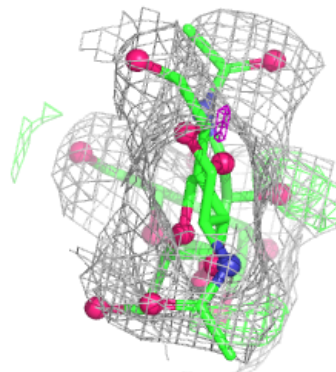
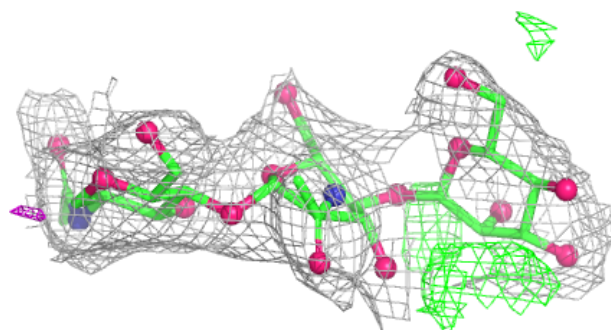
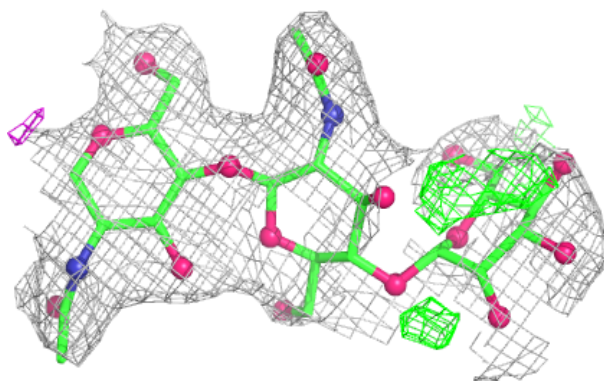


Electron density around Chain K:

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

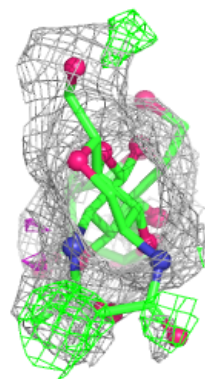
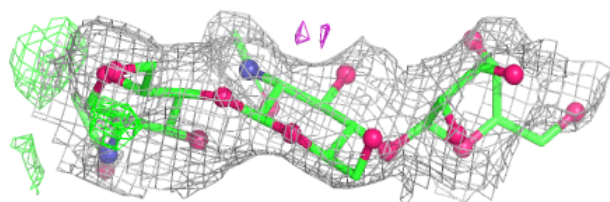
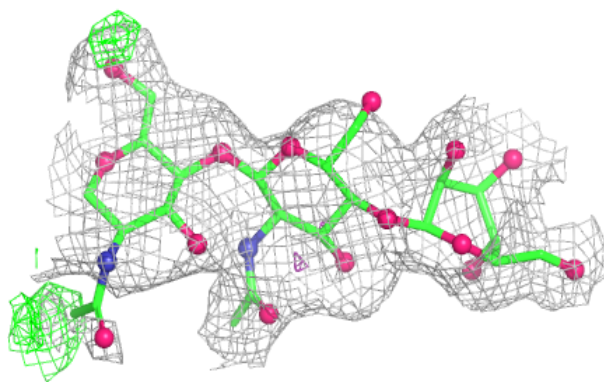
**Electron density around Chain P:**

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

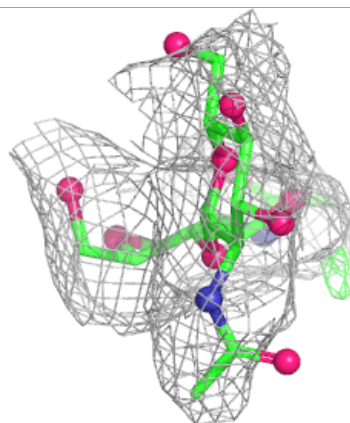
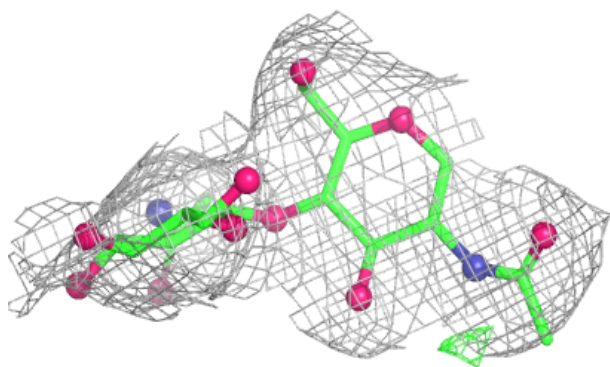
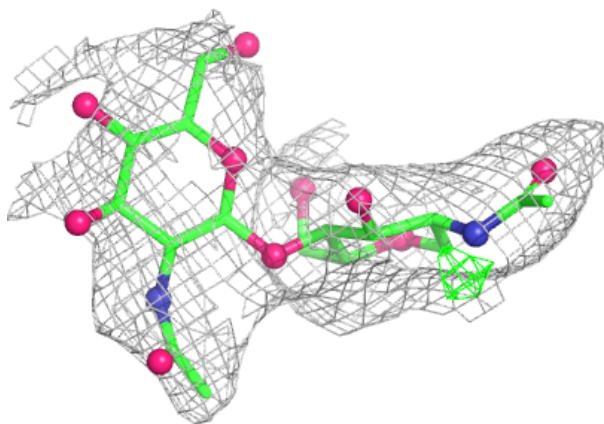


Electron density around Chain S:

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

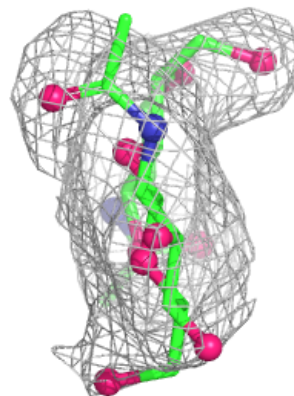
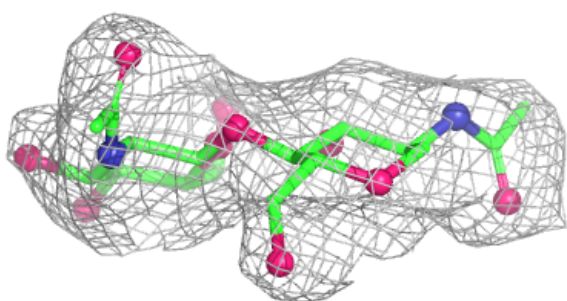
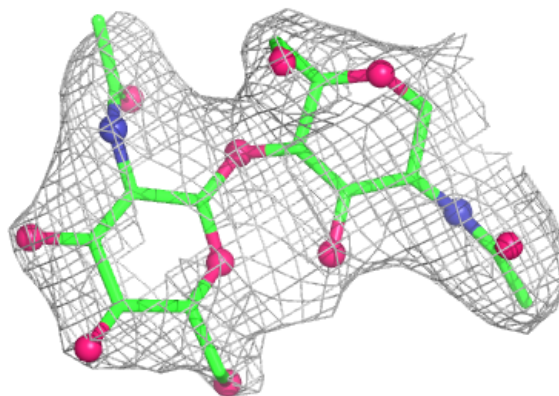
**Electron density around Chain Q:**

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



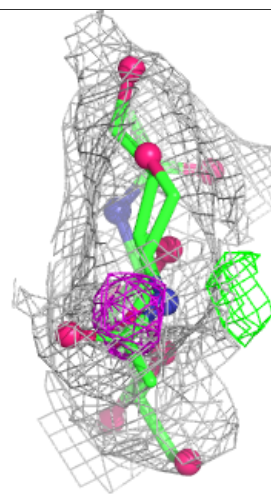
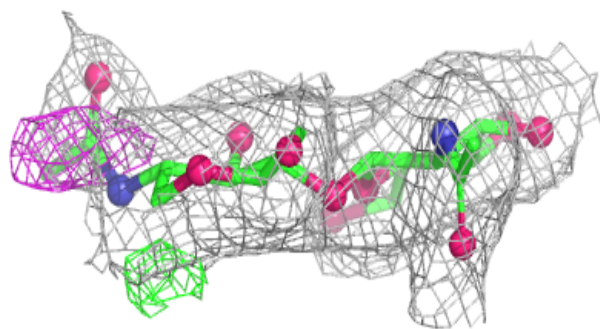
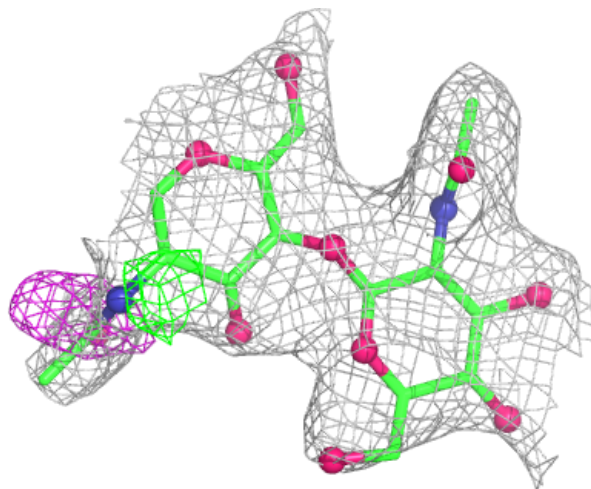
Electron density around Chain R:

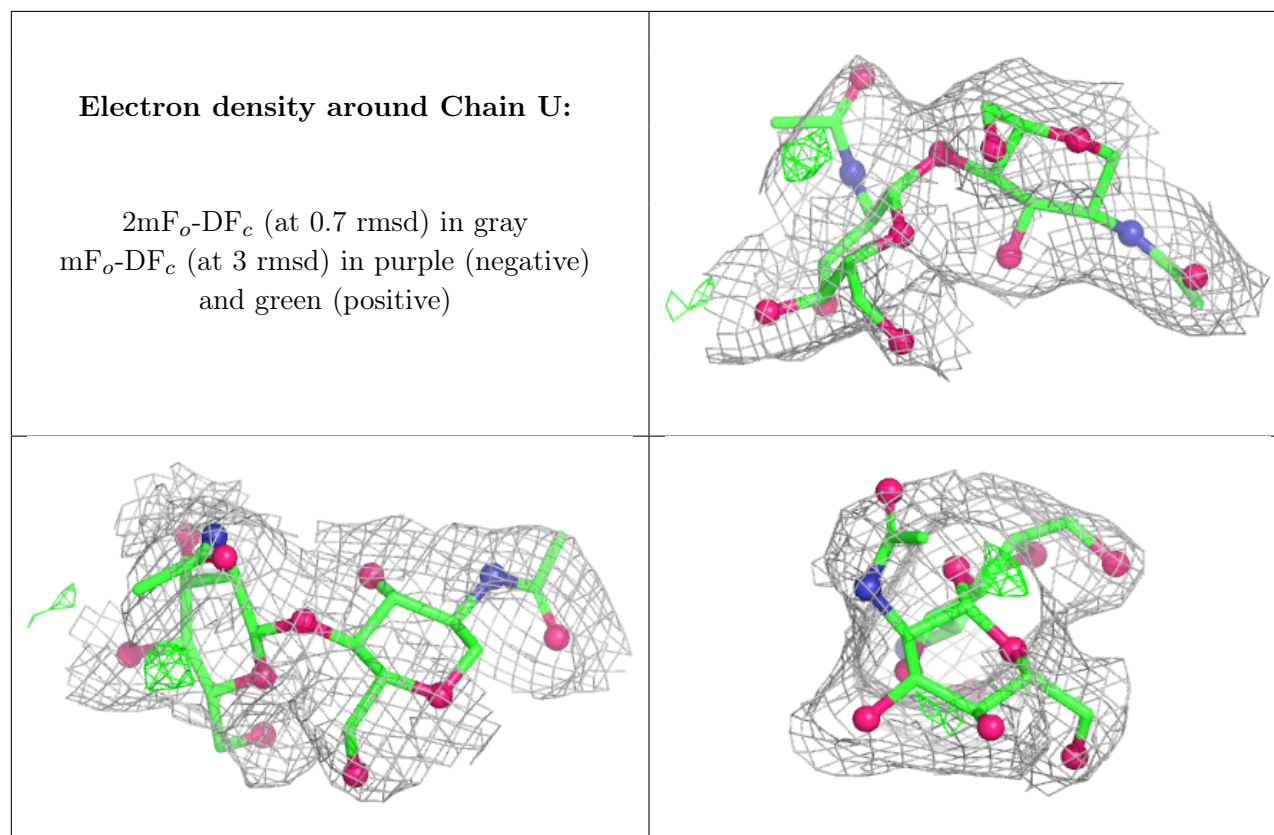
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain T:

$2mF_o-DF_c$ (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
6	NAG	L	2401	14/15	0.44	0.20	111,164,183,184	0
6	NAG	N	1401	14/15	0.53	0.13	99,119,126,128	0
6	NAG	O	2101	14/15	0.64	0.14	88,114,133,134	0
6	NAG	O	2001	14/15	0.68	0.23	72,132,193,197	0
6	NAG	L	2701	14/15	0.88	0.12	55,72,90,100	0
5	CS	C	1216	1/1	0.90	0.13	135,135,135,135	0
6	NAG	N	1601	14/15	0.90	0.10	34,61,71,78	0
6	NAG	O	2301	14/15	0.90	0.09	49,71,78,90	0
5	CS	B	1215	1/1	0.96	0.06	85,85,85,85	1

6.5 Other polymers [i](#)

There are no such residues in this entry.