



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2021 – 12:18 PM EDT

PDB ID : 6WRV
Title : Crystal structure of computationally designed protein 3DS18 in complex with the human Transferrin receptor ectodomain
Authors : Abraham, J.; Baker, D.; Sahtoe, D.D.; Coscia, A.; Clark, L.; Olal, D.
Deposited on : 2020-04-30
Resolution : 2.47 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

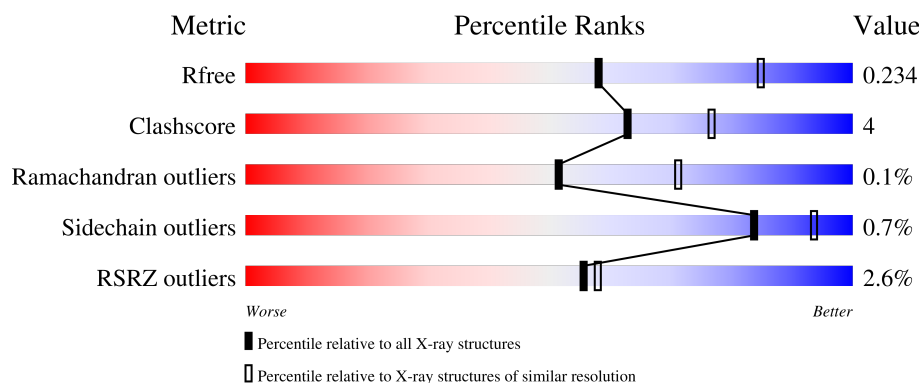
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



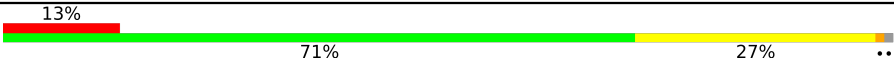
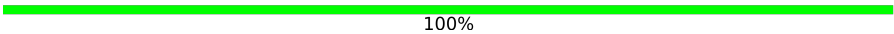
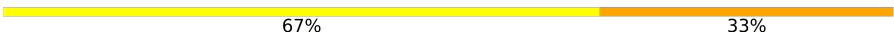
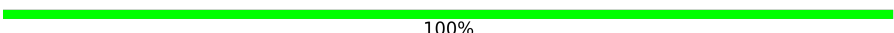
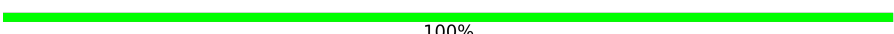
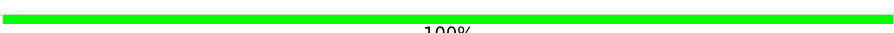
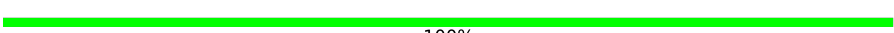



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	639	<div> <div>2%</div> <div>87%</div> <div>13%</div> </div>
1	B	639	<div> <div>2%</div> <div>90%</div> <div>10%</div> </div>
1	E	639	<div> <div>2%</div> <div>90%</div> <div>10%</div> </div>
2	C	94	<div> <div>4%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	D	94	<div> <div>9%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	94	
3	G	3	
3	H	3	
3	I	3	
3	K	3	
3	L	3	
3	M	3	
3	N	3	
3	O	3	
4	J	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	K	2	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17774 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 Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			5052	3239	850	949	14			
1	B	639	Total	C	N	O	S	0	0	0
			5048	3237	850	947	14			
1	E	637	Total	C	N	O	S	0	0	0
			5030	3227	847	942	14			

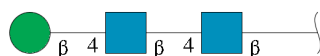
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	GLY	conflict	UNP P02786
B	142	SER	GLY	conflict	UNP P02786
E	142	SER	GLY	conflict	UNP P02786

- Molecule 2 is a protein called Computationally designed protein 3DS18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	93	Total	C	N	O	0	0	0
			767	478	137	152			
2	C	93	Total	C	N	O	0	0	0
			767	478	137	152			
2	F	93	Total	C	N	O	0	0	0
			767	478	137	152			

- 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	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	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	O	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	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

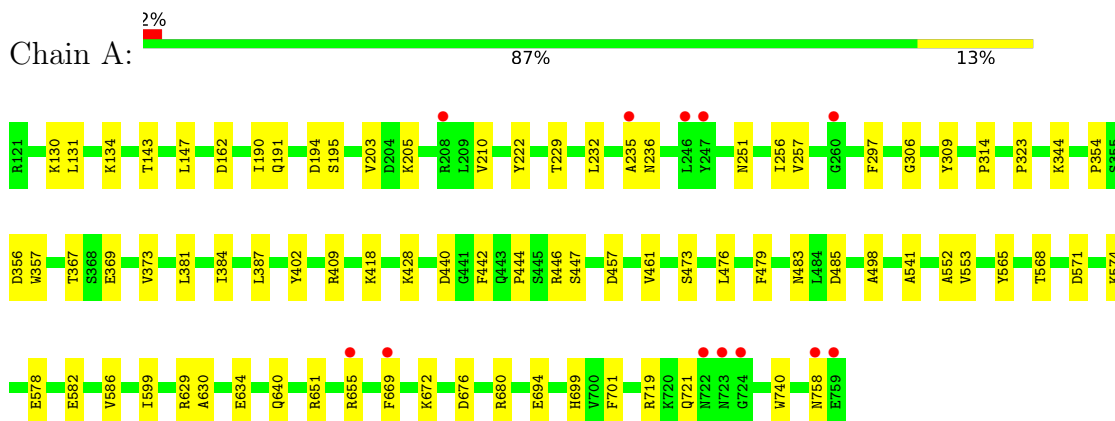
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	1	0
			1	1		
5	B	1	Total	Ca	1	0
			1	1		
5	E	1	Total	Ca	1	0
			1	1		

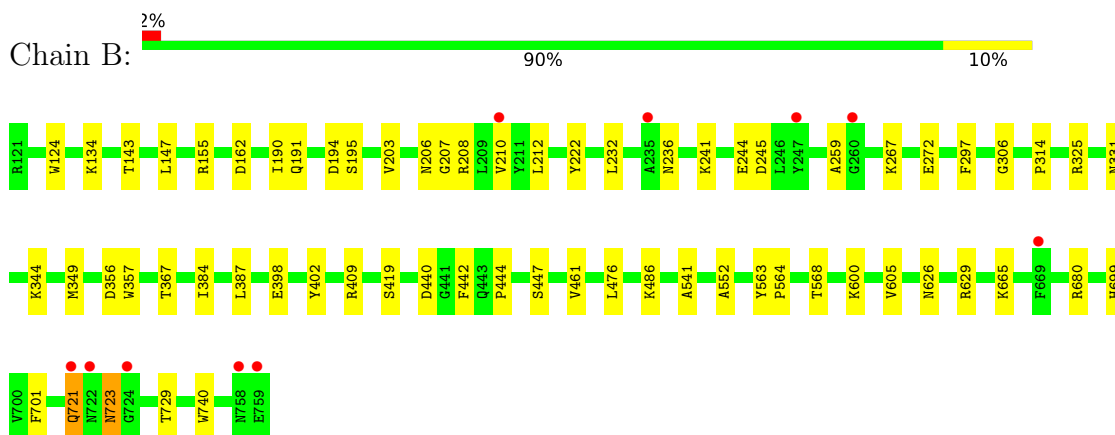
3 Residue-property plots

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.

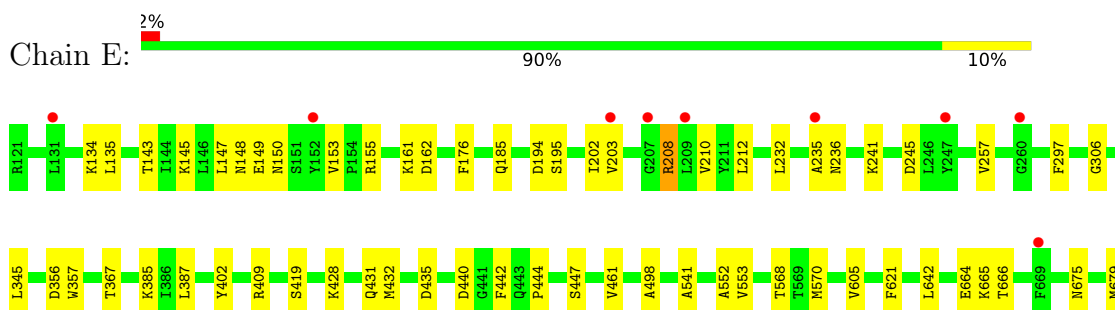
• Molecule 1: Transferrin receptor protein 1



• Molecule 1: Transferrin receptor protein 1

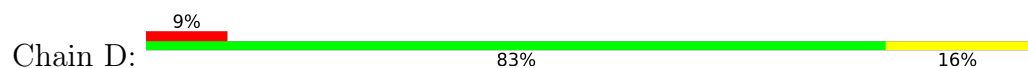


• Molecule 1: Transferrin receptor protein 1

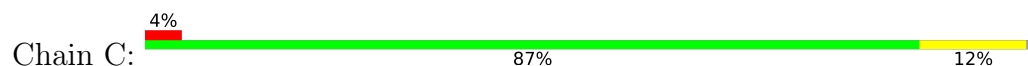




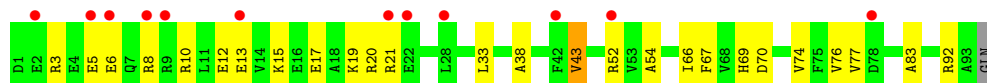
- Molecule 2: Computationally designed protein 3DS18



- Molecule 2: Computationally designed protein 3DS18



- Molecule 2: Computationally designed protein 3DS18



- 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



- 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:  100%

HA01
HA02
EM03

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

Chain L:  100%

HA01
HA02
EM03

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

Chain M:  100%

HA01
HA02
EM03

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

Chain N:  100%

HA01
HA02
EM03

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

Chain O:  100%

HA01
HA02
EM03

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

Chain J:  100%

HA01
HA02

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	256.08Å 256.08Å 128.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	128.04 – 2.47 181.08 – 2.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (128.04-2.47) 100.0 (181.08-2.47)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.221 , 0.236 0.219 , 0.234	Depositor DCC
R_{free} test set	7363 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17774	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 2.04% 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: CA, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/5172	0.43	0/7014
1	B	0.24	0/5168	0.42	0/7009
1	E	0.24	0/5149	0.41	0/6982
2	C	0.26	0/774	0.43	0/1042
2	D	0.32	0/774	0.49	0/1042
2	F	0.25	0/774	0.42	0/1042
All	All	0.25	0/17811	0.42	0/24131

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	5052	0	4982	49	0
1	B	5048	0	4979	43	0
1	E	5030	0	4960	39	0
2	C	767	0	764	8	0
2	D	767	0	764	9	0
2	F	767	0	764	18	0
3	G	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	39	0	34	2	0
3	I	39	0	34	0	0
3	K	39	0	34	0	0
3	L	39	0	34	0	0
3	M	39	0	34	0	0
3	N	39	0	34	0	0
3	O	39	0	34	0	0
4	J	28	0	25	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
All	All	17774	0	17510	152	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 4.

All (152) 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:E:241:LYS:NZ	1:E:245:ASP:OD2	1.96	0.98
1:B:241:LYS:NZ	1:B:245:ASP:OD1	2.09	0.84
1:B:206:ASN:O	1:B:208:ARG:N	2.11	0.83
2:D:81:GLU:OE2	2:D:85:ARG:NE	2.18	0.76
1:E:155:ARG:NH1	1:E:409:ARG:O	2.25	0.70
1:E:143:THR:HG21	1:E:428:LYS:HE3	1.73	0.69
1:A:323:PRO:HG2	1:B:729:THR:HG23	1.73	0.69
1:B:134:LYS:NZ	1:B:440:ASP:OD2	2.23	0.66
1:A:143:THR:HG21	1:A:428:LYS:HE3	1.78	0.66
1:B:155:ARG:NH1	1:B:409:ARG:O	2.28	0.65
2:D:2:GLU:N	2:D:2:GLU:OE1	2.29	0.64
1:B:626:ASN:O	1:B:629:ARG:HG3	1.97	0.64
1:E:306:GLY:HA2	1:E:461:VAL:HA	1.78	0.64
1:A:306:GLY:HA2	1:A:461:VAL:HA	1.80	0.63
1:B:306:GLY:HA2	1:B:461:VAL:HA	1.80	0.63
1:E:541:ALA:HB1	1:E:552:ALA:HB1	1.80	0.62
1:A:134:LYS:NZ	1:A:440:ASP:OD2	2.28	0.61
2:F:15:LYS:NZ	2:F:70:ASP:OD2	2.26	0.61
1:A:541:ALA:HB1	1:A:552:ALA:HB1	1.81	0.61
2:C:81:GLU:OE2	2:C:85:ARG:NE	2.34	0.61
1:E:203:VAL:HG12	1:E:210:VAL:HG12	1.83	0.61
1:A:162:ASP:OD1	1:A:409:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:605:VAL:HG11	1:E:665:LYS:HB3	1.84	0.59
1:A:387:LEU:O	1:A:409:ARG:NH2	2.34	0.59
1:E:402:TYR:HB3	1:E:447:SER:HB2	1.83	0.58
1:A:640:GLN:OE1	2:F:52:ARG:NE	2.35	0.58
1:A:669:PHE:HE2	1:B:398:GLU:OE2	1.87	0.57
1:B:541:ALA:HB1	1:B:552:ALA:HB1	1.85	0.57
1:E:387:LEU:O	1:E:409:ARG:NH2	2.33	0.57
2:C:2:GLU:N	2:C:2:GLU:OE1	2.38	0.57
1:E:162:ASP:OD1	1:E:409:ARG:NH1	2.39	0.56
1:B:402:TYR:HB3	1:B:447:SER:HB2	1.88	0.55
1:A:680:ARG:HH22	1:B:476:LEU:HB2	1.72	0.55
2:F:10:ARG:O	2:F:13:GLU:HG2	2.06	0.55
1:E:155:ARG:NH1	1:E:419:SER:OG	2.35	0.55
2:F:3:ARG:O	2:F:6:GLU:HG2	2.06	0.54
1:E:356:ASP:OD1	1:E:356:ASP:N	2.41	0.54
1:E:134:LYS:NZ	1:E:440:ASP:OD2	2.28	0.53
1:A:672:LYS:NZ	1:A:676:ASP:OD2	2.39	0.53
1:E:150:ASN:O	1:E:161:LYS:NZ	2.38	0.53
1:B:356:ASP:OD1	1:B:356:ASP:N	2.42	0.53
1:E:664:GLU:HG3	1:E:666:THR:H	1.74	0.52
1:B:241:LYS:HA	1:B:244:GLU:HG2	1.90	0.52
1:A:446:ARG:HD2	1:A:479:PHE:CE1	2.44	0.52
1:B:191:GLN:OE1	1:B:222:TYR:N	2.43	0.52
2:F:38:ALA:HA	2:F:76:VAL:HG22	1.92	0.52
1:E:621:PHE:HE2	1:E:642:LEU:HD21	1.74	0.52
1:A:314:PRO:HG3	1:B:740:TRP:CE2	2.44	0.51
2:D:5:GLU:OE1	2:D:8:ARG:NH2	2.25	0.51
2:F:17:GLU:O	2:F:21:ARG:NH1	2.43	0.51
1:A:297:PHE:HB3	1:A:568:THR:HG22	1.92	0.51
3:H:2:NAG:O3	3:H:3:BMA:O5	2.16	0.51
1:B:297:PHE:HB3	1:B:568:THR:HG22	1.93	0.51
1:A:442:PHE:CE2	1:A:444:PRO:HG3	2.46	0.51
1:A:721:GLN:OE1	1:A:721:GLN:N	2.41	0.51
1:B:162:ASP:OD1	1:B:409:ARG:NH1	2.45	0.50
1:B:155:ARG:NH1	1:B:419:SER:OG	2.38	0.50
2:F:15:LYS:HD2	2:F:69:HIS:HE1	1.76	0.50
1:E:185:GLN:NE2	1:E:385:LYS:HE2	2.28	0.49
1:E:297:PHE:HB3	1:E:568:THR:HG22	1.95	0.49
1:A:574:LYS:NZ	1:A:578:GLU:OE1	2.45	0.48
1:B:387:LEU:O	1:B:409:ARG:NH2	2.41	0.48
1:B:194:ASP:OD1	1:B:195:SER:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:PHE:CE2	1:B:444:PRO:HG3	2.49	0.48
1:E:232:LEU:HB3	1:E:367:THR:HG23	1.94	0.48
1:E:621:PHE:CE2	1:E:642:LEU:HD21	2.49	0.48
1:A:356:ASP:OD1	1:A:356:ASP:N	2.43	0.47
1:E:148:ASN:O	1:E:148:ASN:ND2	2.47	0.47
1:B:190:ILE:HD13	1:B:384:ILE:HD13	1.97	0.47
1:E:442:PHE:CE2	1:E:444:PRO:HG3	2.49	0.47
2:D:6:GLU:HA	2:D:9:ARG:HG2	1.97	0.47
1:A:634:GLU:OE2	1:A:719:ARG:NH1	2.33	0.47
1:A:235:ALA:HB3	1:A:257:VAL:HG12	1.97	0.47
2:F:20:ARG:HB3	2:F:21:ARG:NH1	2.29	0.47
1:A:190:ILE:HD13	1:A:384:ILE:HD13	1.97	0.46
1:A:476:LEU:HB2	1:B:680:ARG:HH22	1.80	0.46
1:E:208:ARG:HA	2:F:43:VAL:HG13	1.96	0.46
1:A:699:HIS:CE1	1:A:701:PHE:HB2	2.51	0.45
1:B:699:HIS:CE1	1:B:701:PHE:HB2	2.52	0.45
2:D:1:ASP:O	2:D:5:GLU:HG2	2.15	0.45
2:F:67:PHE:HB2	2:F:74:VAL:HB	1.97	0.45
1:B:203:VAL:HG11	2:C:26:GLN:NE2	2.32	0.45
1:B:212:LEU:HB2	2:C:33:LEU:HD21	1.98	0.45
2:F:5:GLU:OE1	2:F:8:ARG:NH2	2.49	0.45
1:A:232:LEU:HB3	1:A:367:THR:HG23	1.98	0.45
1:A:309:TYR:CZ	1:A:381:LEU:HD11	2.51	0.45
2:C:5:GLU:OE2	2:C:8:ARG:NH2	2.50	0.45
1:B:349:MET:HA	1:B:367:THR:HA	1.98	0.45
1:A:629:ARG:HG3	1:A:630:ALA:N	2.31	0.45
1:B:626:ASN:OD1	1:B:629:ARG:NH1	2.49	0.45
1:B:208:ARG:HA	2:C:43:VAL:HB	1.98	0.44
1:A:203:VAL:HG12	1:A:210:VAL:HG12	1.98	0.44
1:B:232:LEU:HB3	1:B:367:THR:HG23	1.99	0.44
1:E:642:LEU:HD12	1:E:642:LEU:HA	1.84	0.44
1:E:135:LEU:HG	1:E:432:MET:HE3	1.99	0.44
1:E:194:ASP:OD1	1:E:195:SER:N	2.50	0.44
1:A:236:ASN:HB2	1:A:357:TRP:CE2	2.52	0.44
1:B:721:GLN:NE2	1:B:723:ASN:OD1	2.51	0.44
1:A:402:TYR:HB3	1:A:447:SER:HB2	1.98	0.44
1:E:699:HIS:CE1	1:E:701:PHE:HB2	2.53	0.44
1:A:130:LYS:HE2	1:A:440:ASP:CG	2.39	0.43
2:F:54:ALA:HB1	2:F:66:ILE:HG21	2.00	0.43
1:A:418:LYS:HD3	1:A:457:ASP:OD1	2.17	0.43
1:A:629:ARG:NH2	2:F:92:ARG:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:THR:O	1:E:147:LEU:HG	2.18	0.43
1:E:149:GLU:O	1:E:153:VAL:HG22	2.19	0.43
1:E:212:LEU:HB2	2:F:33:LEU:HD21	2.00	0.43
1:A:131:LEU:HD22	1:A:599:ILE:HD12	2.00	0.43
1:A:651:ARG:O	1:A:655:ARG:HG2	2.19	0.43
1:E:498:ALA:HB2	1:E:553:VAL:HG23	2.01	0.43
1:B:236:ASN:HB2	1:B:357:TRP:CE2	2.53	0.42
1:A:191:GLN:OE1	1:A:222:TYR:N	2.52	0.42
1:A:582:GLU:O	1:A:586:VAL:HG23	2.19	0.42
2:D:54:ALA:HB1	2:D:66:ILE:HG21	2.01	0.42
2:C:5:GLU:HG2	2:C:8:ARG:HH12	1.84	0.42
1:A:314:PRO:HG3	1:B:740:TRP:NE1	2.35	0.42
1:A:143:THR:O	1:A:147:LEU:HG	2.20	0.42
1:B:143:THR:O	1:B:147:LEU:HG	2.19	0.42
1:A:483:ASN:HD21	1:A:485:ASP:HB2	1.85	0.42
1:E:675:ASN:O	1:E:679:MET:HG3	2.20	0.42
1:B:259:ALA:HA	1:B:267:LYS:HE3	2.02	0.42
1:E:176:PHE:CZ	1:E:431:GLN:HB2	2.55	0.42
2:F:20:ARG:HB3	2:F:21:ARG:HH11	1.84	0.41
1:A:354:PRO:HD2	1:A:357:TRP:CD2	2.54	0.41
1:B:486:LYS:HB2	1:B:486:LYS:HE3	1.74	0.41
1:E:747:ASN:HB3	1:E:756:ILE:HD13	2.01	0.41
2:F:33:LEU:HD12	2:F:38:ALA:HB3	2.03	0.41
1:A:740:TRP:CE2	1:B:314:PRO:HG3	2.55	0.41
1:A:194:ASP:OD1	1:A:195:SER:N	2.51	0.41
1:A:344:LYS:NZ	2:D:80:ASP:OD1	2.39	0.41
1:B:563:TYR:HA	1:B:564:PRO:HD3	1.95	0.41
1:E:235:ALA:HB3	1:E:257:VAL:HG12	2.02	0.41
1:E:236:ASN:HB2	1:E:357:TRP:CE2	2.56	0.41
1:B:272:GLU:OE2	1:B:331:ASN:HB2	2.20	0.41
1:E:202:ILE:HD11	1:E:345:LEU:HD23	2.03	0.41
1:B:605:VAL:HG21	1:B:665:LYS:HB3	2.02	0.41
1:A:498:ALA:HB2	1:A:553:VAL:HG23	2.02	0.41
2:D:67:PHE:HB2	2:D:74:VAL:HB	2.03	0.41
2:F:12:GLU:OE2	2:F:69:HIS:NE2	2.54	0.41
2:F:77:VAL:HG21	2:F:83:ALA:HB2	2.03	0.41
1:A:565:TYR:O	1:A:571:ASP:HB2	2.21	0.41
1:A:630:ALA:O	1:A:634:GLU:HG2	2.21	0.41
1:E:134:LYS:HE2	1:E:435:ASP:HB3	2.03	0.41
3:H:1:NAG:H61	3:H:2:NAG:HN2	1.86	0.41
1:A:229:THR:HA	1:A:373:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HD11	1:A:256:ILE:HB	2.03	0.40
1:B:124:TRP:CE2	1:B:600:LYS:HE3	2.56	0.40
1:B:344:LYS:HE2	2:C:80:ASP:OD1	2.21	0.40
2:D:61:VAL:HG22	2:D:85:ARG:NH1	2.35	0.40
1:B:203:VAL:HG22	1:B:210:VAL:HG12	2.03	0.40
1:E:145:LYS:HA	1:E:145:LYS:HD2	1.85	0.40
1:A:205:LYS:HE2	1:A:369:GLU:O	2.22	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	637/639 (100%)	620 (97%)	17 (3%)	0	100	100
1	B	637/639 (100%)	619 (97%)	16 (2%)	2 (0%)	41	59
1	E	633/639 (99%)	615 (97%)	18 (3%)	0	100	100
2	C	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
2	D	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
2	F	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
All	All	2180/2199 (99%)	2123 (97%)	55 (2%)	2 (0%)	51	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	GLY
1	B	721	GLN

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	547/548 (100%)	543 (99%)	4 (1%)	84	93
1	B	546/548 (100%)	544 (100%)	2 (0%)	91	96
1	E	543/548 (99%)	541 (100%)	2 (0%)	91	96
2	C	82/83 (99%)	80 (98%)	2 (2%)	49	72
2	D	82/83 (99%)	81 (99%)	1 (1%)	71	87
2	F	82/83 (99%)	80 (98%)	2 (2%)	49	72
All	All	1882/1893 (99%)	1869 (99%)	13 (1%)	84	93

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	A	473	SER
1	A	694	GLU
1	A	758	ASN
1	B	325	ARG
1	B	723	ASN
1	E	208	ARG
1	E	570	MET
2	D	15	LYS
2	C	16	GLU
2	C	20	ARG
2	F	19	LYS
2	F	43	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	ASN
1	A	527	ASN
1	E	185	GLN
1	E	197	GLN

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Mol	Chain	Res	Type
1	E	640	GLN
1	E	743	GLN
2	F	7	GLN
2	F	26	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 ⓘ

26 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	G	1	1,3	14,14,15	0.43	0	17,19,21	0.44	0
3	NAG	G	2	3	14,14,15	0.39	0	17,19,21	0.55	0
3	BMA	G	3	3	11,11,12	0.69	0	15,15,17	0.72	0
3	NAG	H	1	1,3	14,14,15	0.34	0	17,19,21	0.58	0
3	NAG	H	2	3	14,14,15	0.50	0	17,19,21	0.79	0
3	BMA	H	3	3	11,11,12	0.82	0	15,15,17	1.11	1 (6%)
3	NAG	I	1	1,3	14,14,15	0.32	0	17,19,21	0.36	0
3	NAG	I	2	3	14,14,15	0.33	0	17,19,21	0.39	0
3	BMA	I	3	3	11,11,12	0.64	0	15,15,17	0.72	0
4	NAG	J	1	1,4	14,14,15	0.48	0	17,19,21	0.46	0
4	NAG	J	2	4	14,14,15	0.47	0	17,19,21	0.40	0
3	NAG	K	1	1,3	14,14,15	0.40	0	17,19,21	0.51	0
3	NAG	K	2	3	14,14,15	0.30	0	17,19,21	0.69	0
3	BMA	K	3	3	11,11,12	0.64	0	15,15,17	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	L	1	1,3	14,14,15	0.27	0	17,19,21	0.37	0
3	NAG	L	2	3	14,14,15	0.33	0	17,19,21	0.36	0
3	BMA	L	3	3	11,11,12	0.65	0	15,15,17	0.78	0
3	NAG	M	1	1,3	14,14,15	0.42	0	17,19,21	0.44	0
3	NAG	M	2	3	14,14,15	0.42	0	17,19,21	0.72	0
3	BMA	M	3	3	11,11,12	0.52	0	15,15,17	0.89	0
3	NAG	N	1	1,3	14,14,15	0.32	0	17,19,21	0.44	0
3	NAG	N	2	3	14,14,15	0.23	0	17,19,21	0.41	0
3	BMA	N	3	3	11,11,12	0.64	0	15,15,17	0.76	0
3	NAG	O	1	1,3	14,14,15	0.42	0	17,19,21	0.42	0
3	NAG	O	2	3	14,14,15	0.35	0	17,19,21	0.48	0
3	BMA	O	3	3	11,11,12	0.63	0	15,15,17	0.80	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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	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(°)
3	H	3	BMA	C1-O5-C5	3.07	116.35	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	O	3	BMA	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C3-C2-N2-C7
3	K	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6

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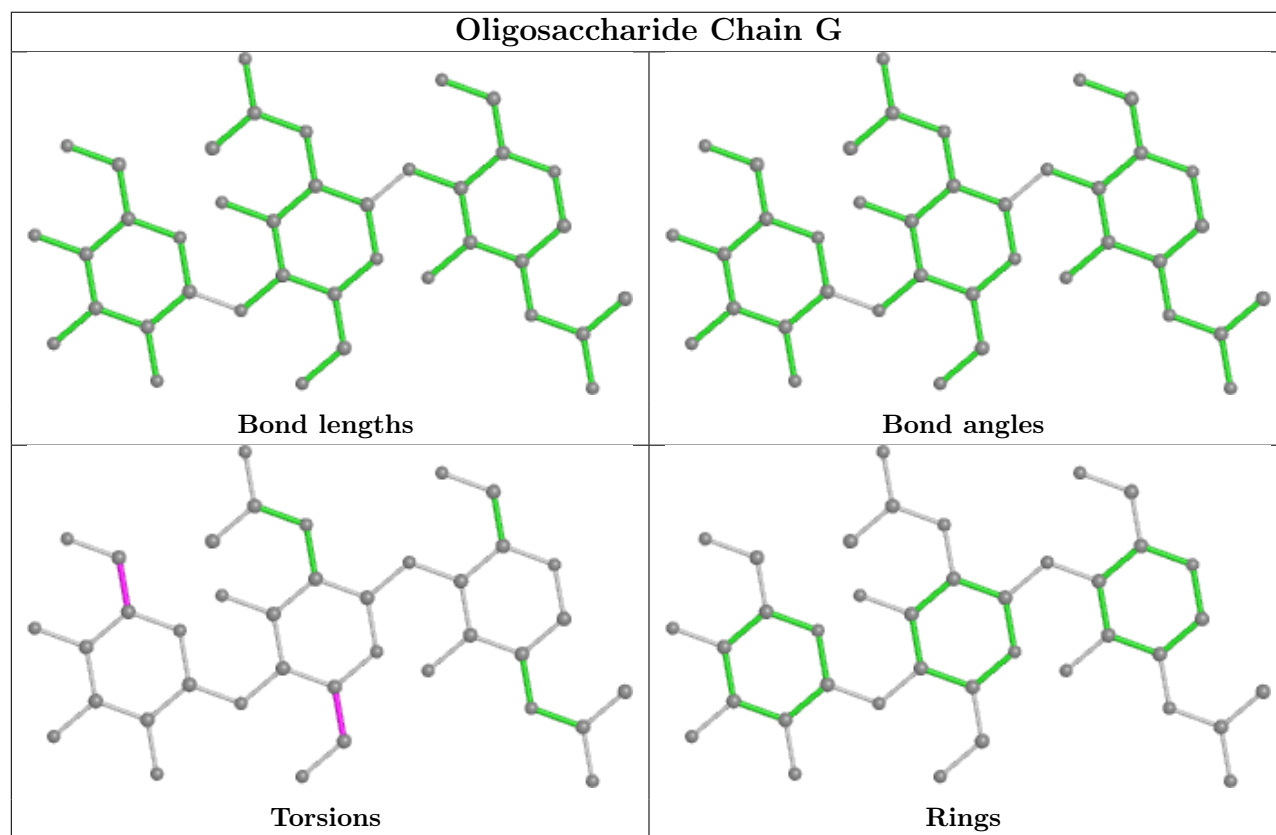
Mol	Chain	Res	Type	Atoms
3	K	3	BMA	O5-C5-C6-O6

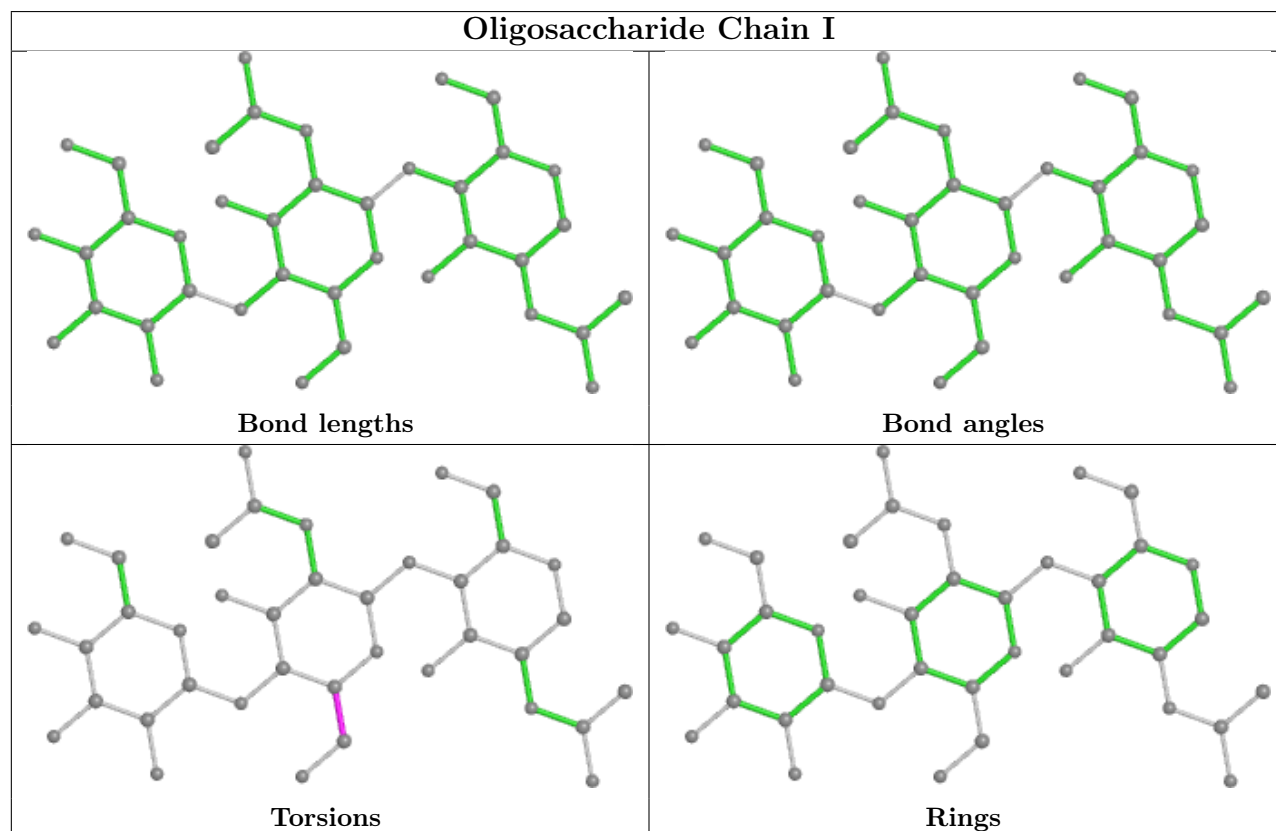
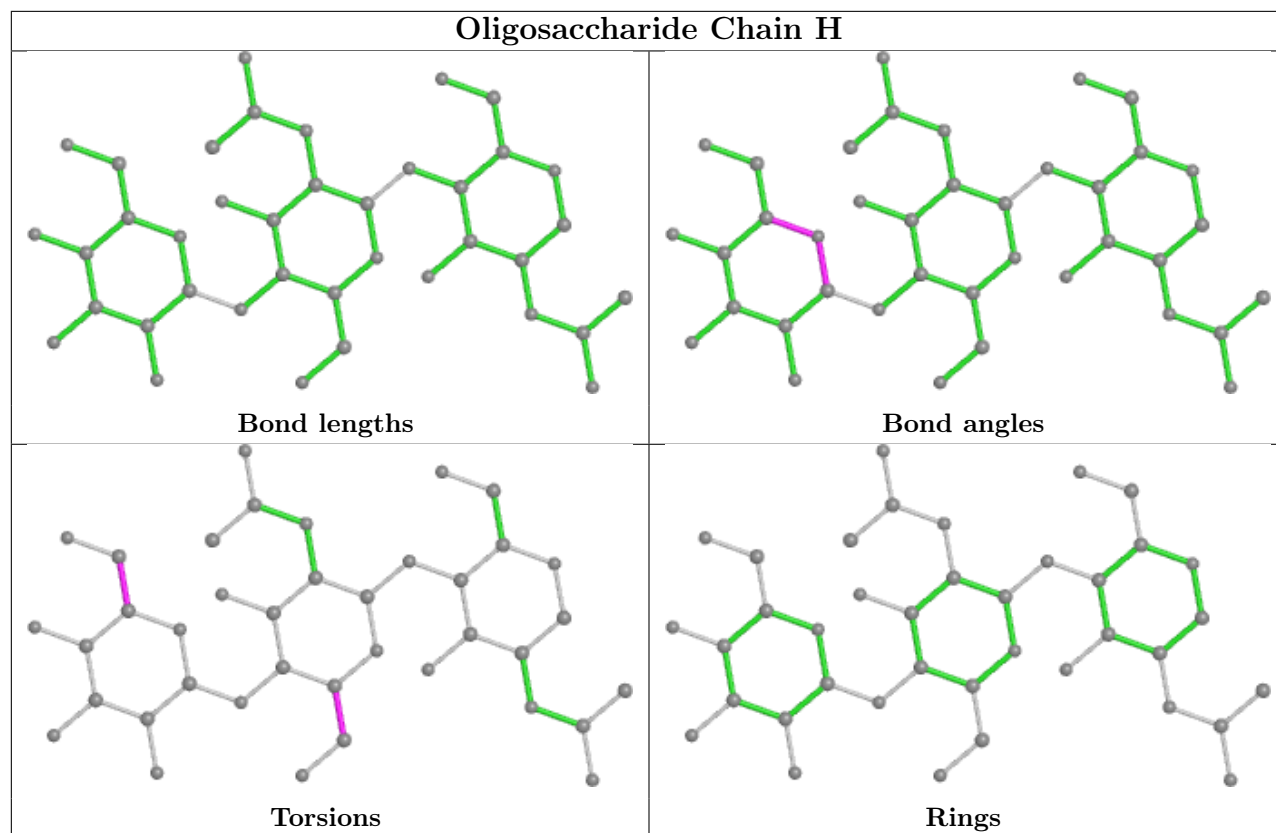
There are no ring outliers.

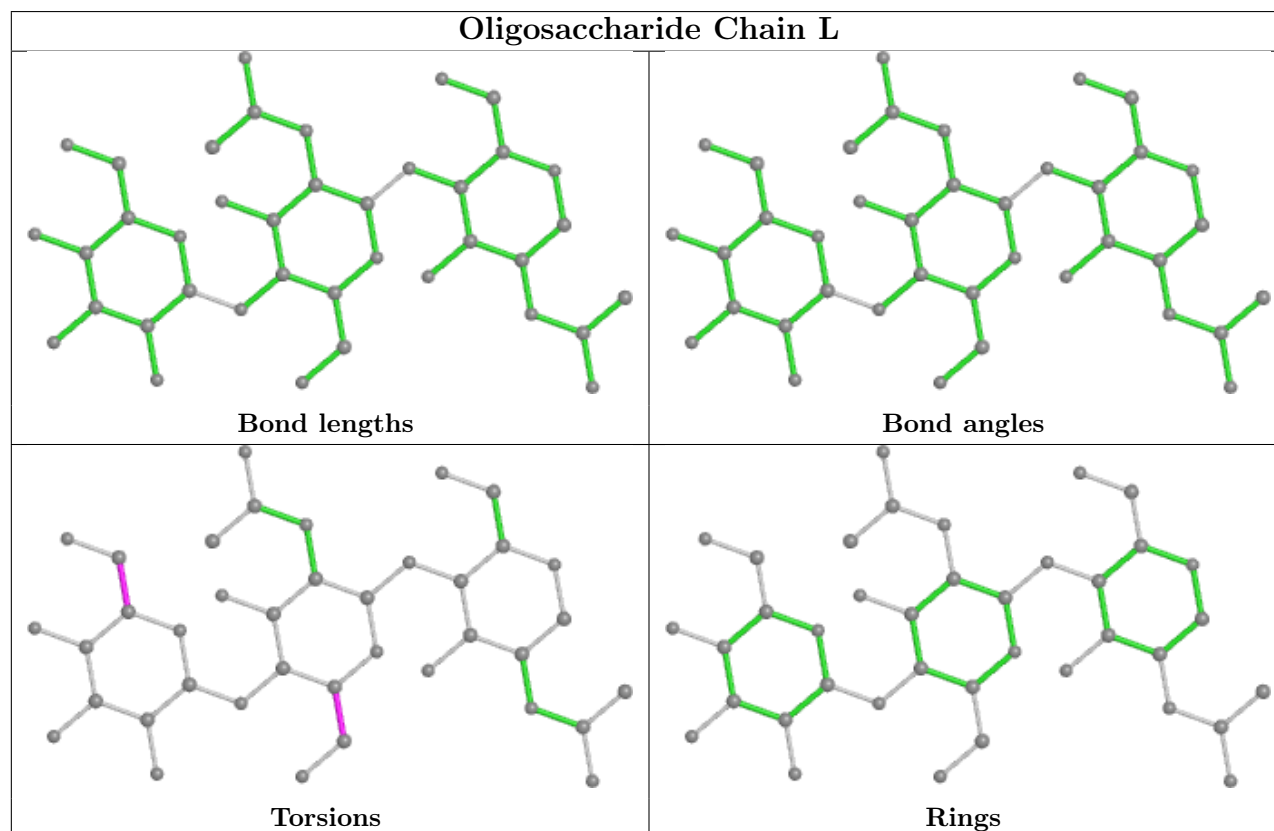
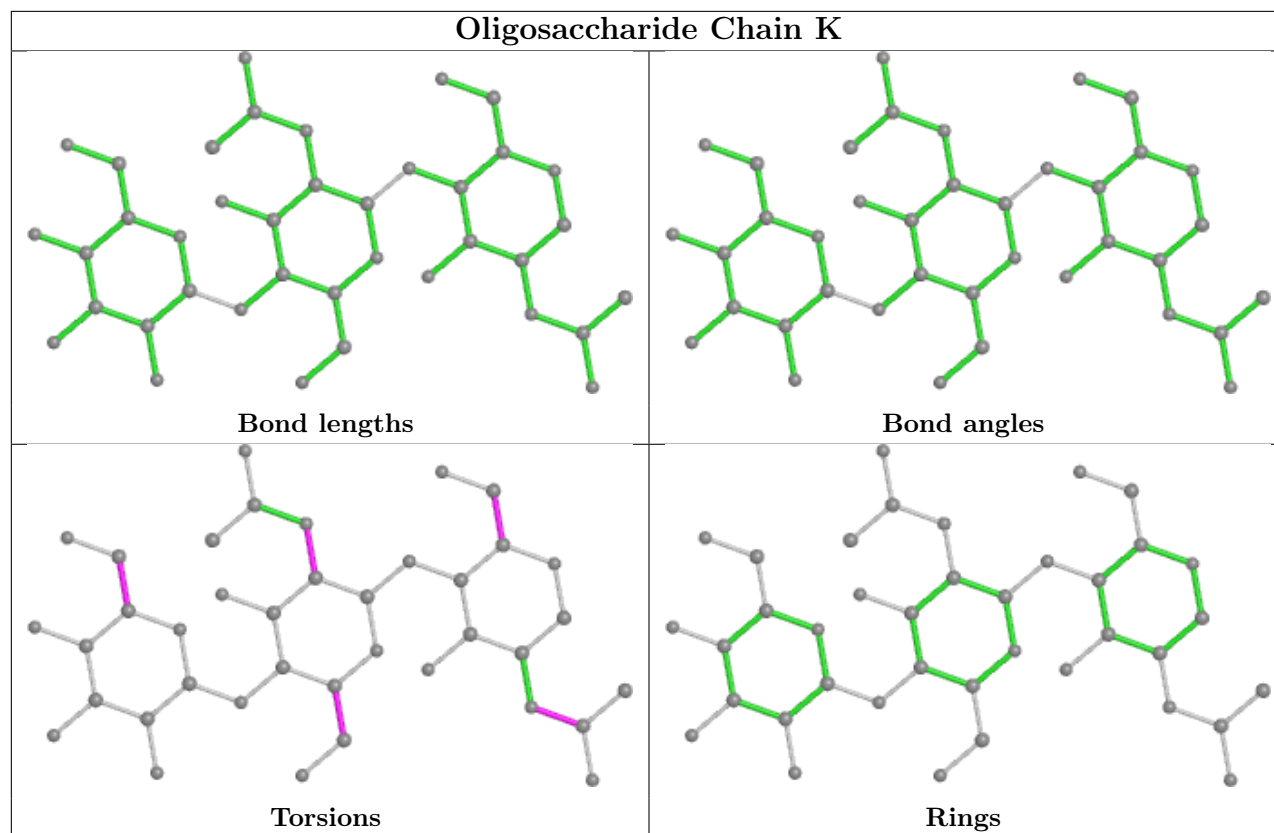
3 monomers are involved in 2 short contacts:

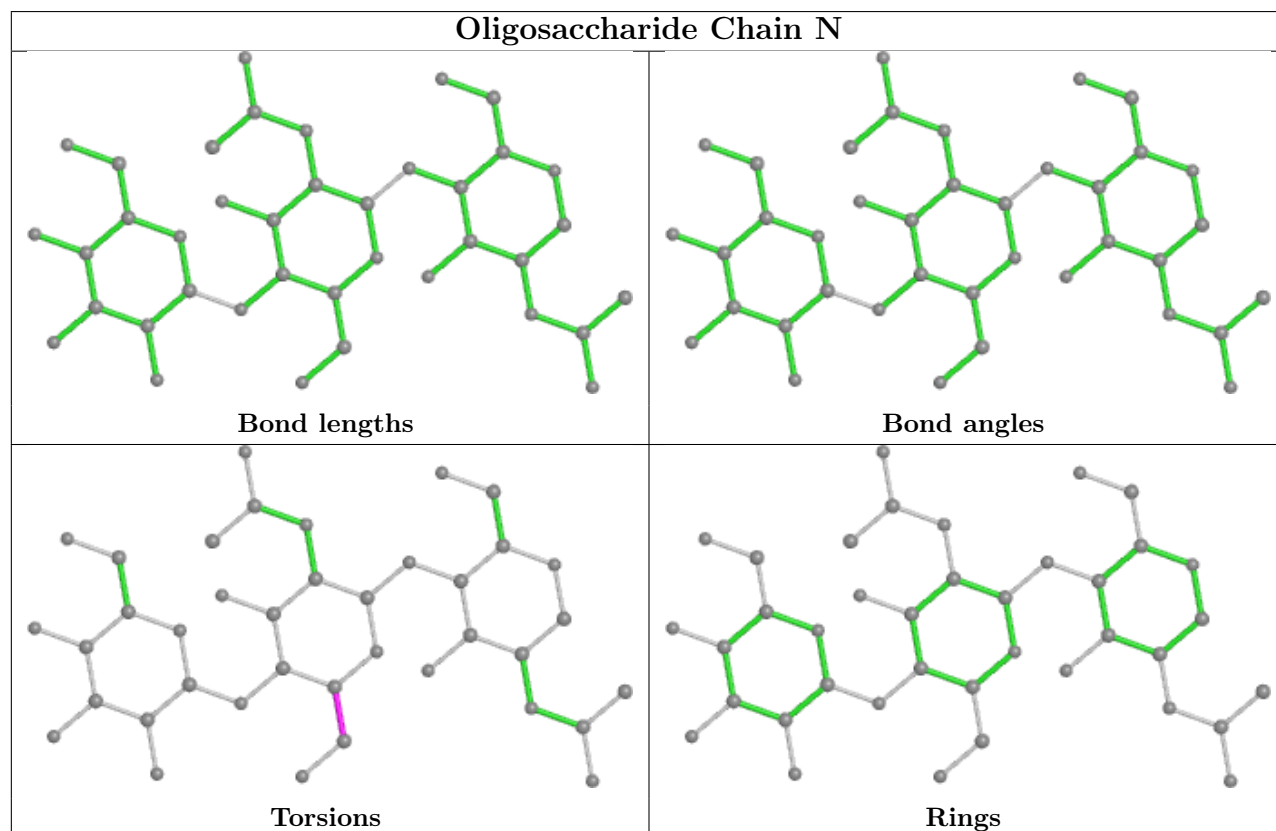
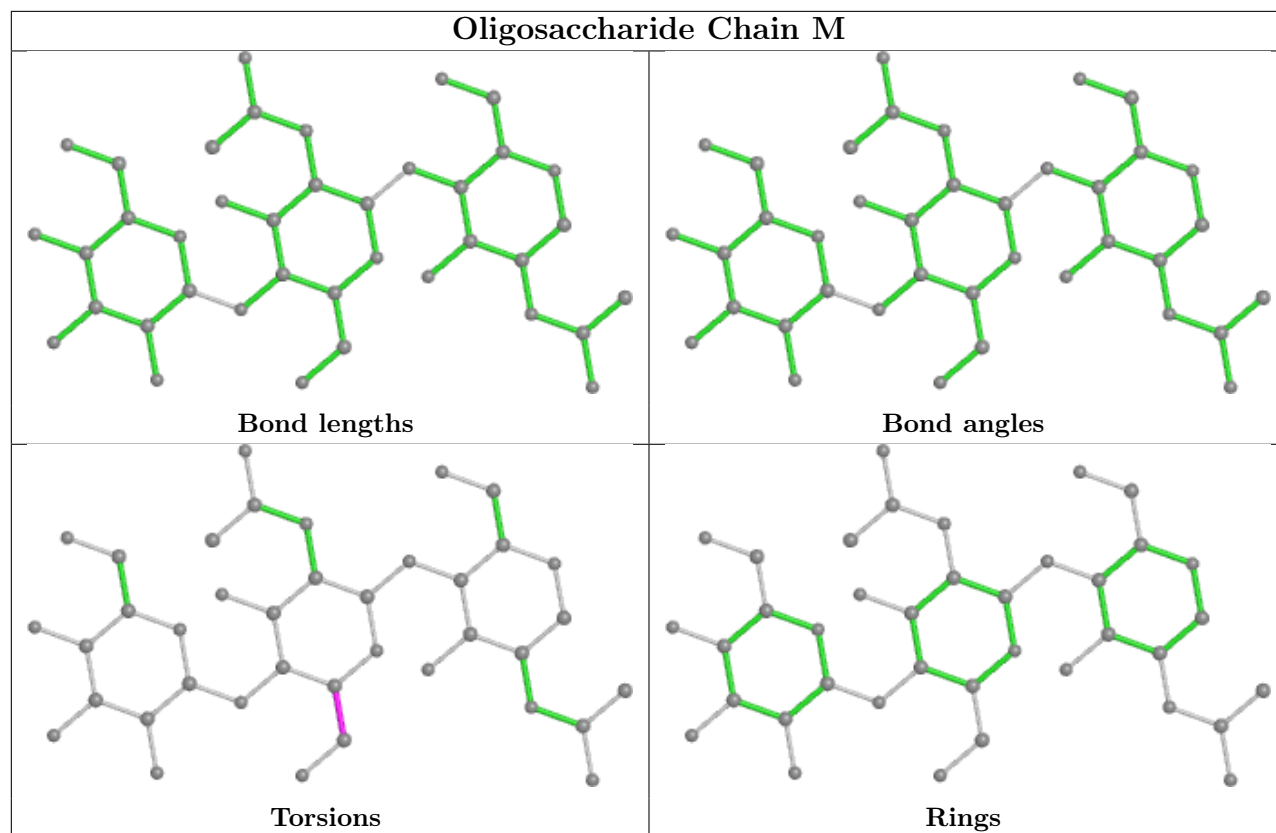
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	3	BMA	1	0
3	H	1	NAG	1	0
3	H	2	NAG	2	0

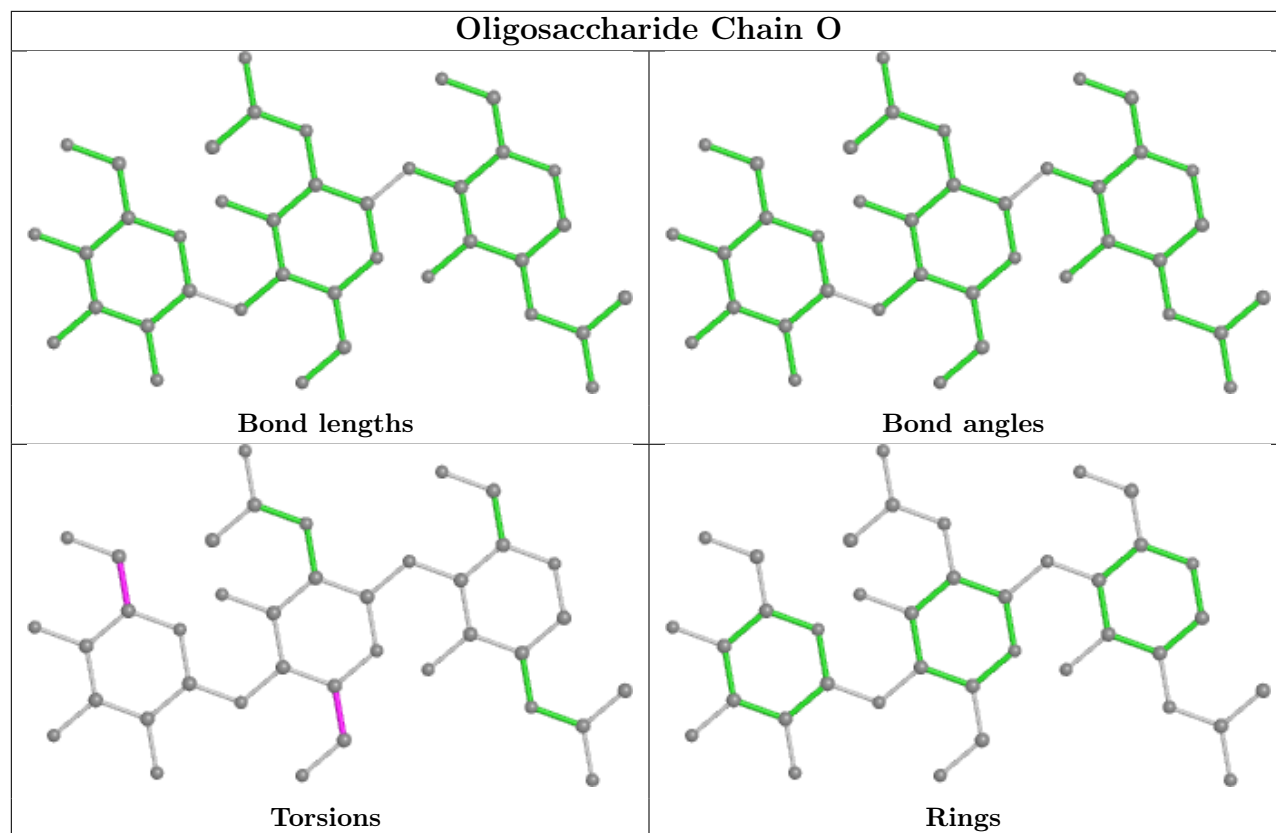
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

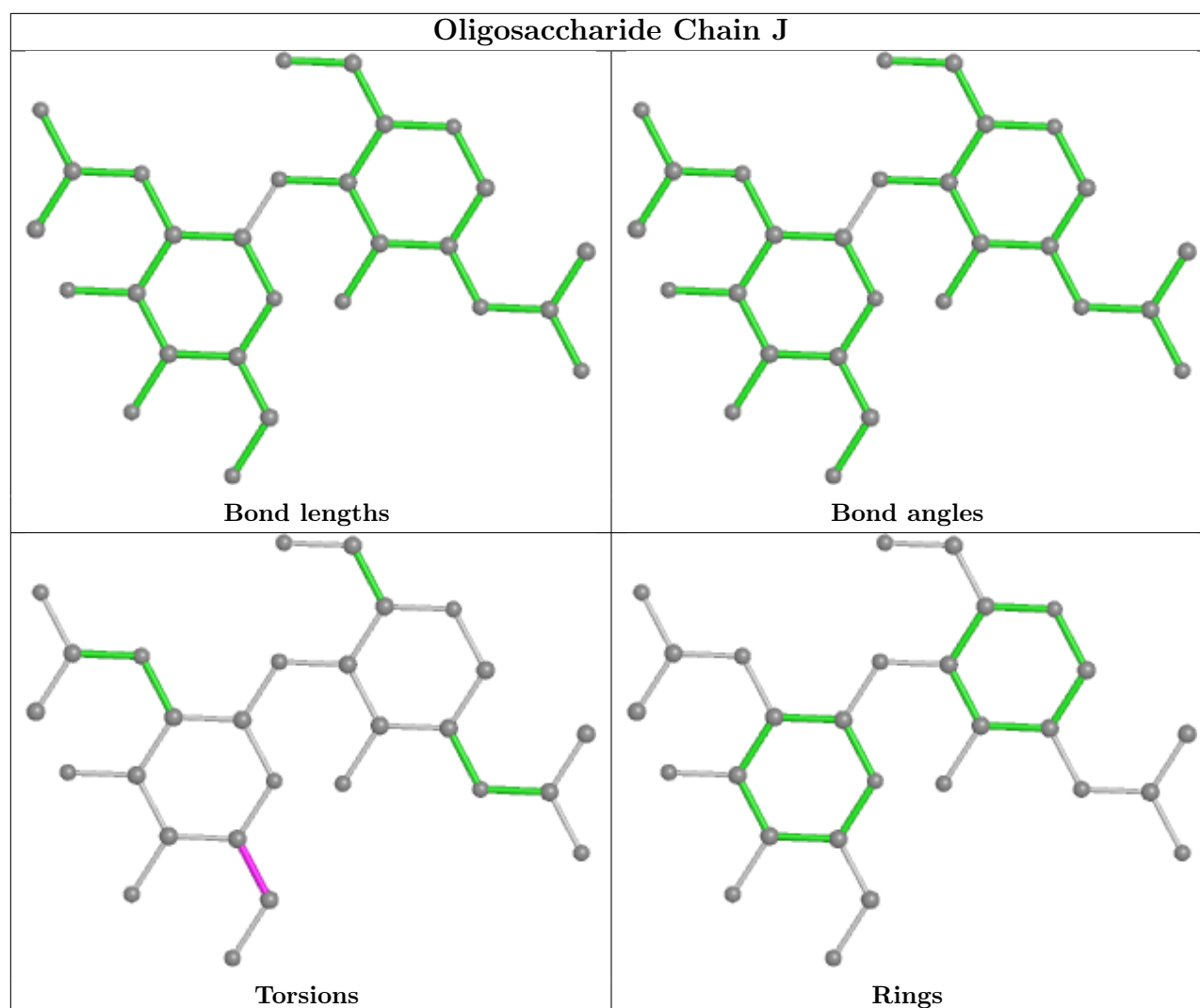












5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	639/639 (100%)	0.56	12 (1%) 66 68	46, 67, 97, 132	0
1	B	639/639 (100%)	0.61	10 (1%) 72 73	46, 64, 95, 132	0
1	E	637/639 (99%)	0.54	11 (1%) 70 71	40, 60, 92, 118	0
2	C	93/94 (98%)	0.72	4 (4%) 35 37	54, 80, 137, 151	0
2	D	93/94 (98%)	0.96	8 (8%) 10 10	62, 88, 138, 151	0
2	F	93/94 (98%)	1.01	12 (12%) 3 3	52, 75, 116, 133	0
All	All	2194/2199 (99%)	0.61	57 (2%) 56 58	40, 66, 105, 151	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	724	GLY	5.6
1	E	759	GLU	5.4
1	A	247	TYR	5.1
2	D	23	ARG	5.0
1	A	723	ASN	4.8
1	B	758	ASN	4.6
1	B	669	PHE	4.5
1	E	669	PHE	4.0
1	A	260	GLY	3.7
1	E	758	ASN	3.6
2	D	22	GLU	3.5
2	F	21	ARG	3.4
1	B	724	GLY	3.3
2	F	8	ARG	3.2
1	A	722	ASN	3.2
1	A	758	ASN	3.2
1	B	247	TYR	3.1
2	F	2	GLU	3.1
1	E	260	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	67	PHE	2.8
1	E	235	ALA	2.8
1	E	247	TYR	2.8
2	D	32	TYR	2.7
2	F	6	GLU	2.7
1	B	260	GLY	2.7
1	A	235	ALA	2.6
2	C	11	LEU	2.6
2	F	78	ASP	2.6
1	A	669	PHE	2.6
1	E	207	GLY	2.6
2	C	13	GLU	2.6
1	A	759	GLU	2.5
2	F	22	GLU	2.5
1	A	655	ARG	2.4
1	B	759	GLU	2.4
2	C	78	ASP	2.4
1	B	721	GLN	2.4
1	B	722	ASN	2.4
2	F	9	ARG	2.3
1	E	152	TYR	2.3
1	B	235	ALA	2.3
1	E	131	LEU	2.3
2	F	52	ARG	2.2
1	B	210	VAL	2.2
1	E	209	LEU	2.2
1	A	208	ARG	2.2
2	D	3	ARG	2.2
2	D	31	LEU	2.1
2	D	69	HIS	2.1
2	F	42	PHE	2.1
2	F	13	GLU	2.1
1	E	203	VAL	2.1
2	D	41	VAL	2.1
2	F	5	GLU	2.1
2	F	28	LEU	2.1
1	A	246	LEU	2.0
2	C	67	PHE	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 ⓘ

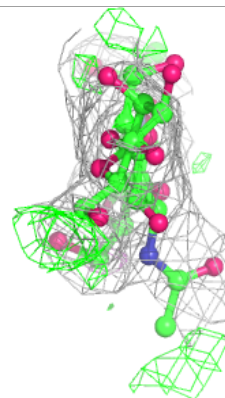
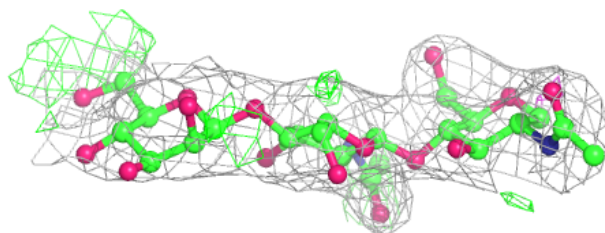
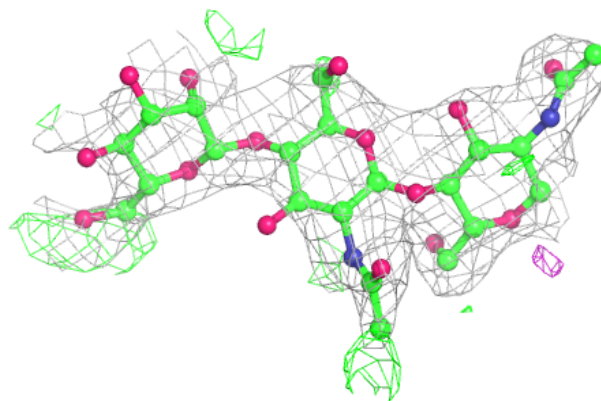
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	BMA	H	3	11/12	0.41	0.37	137,149,155,155	0
3	BMA	N	3	11/12	0.53	0.24	139,148,152,153	0
3	BMA	M	3	11/12	0.55	0.32	134,148,155,156	0
3	BMA	O	3	11/12	0.57	0.17	136,148,155,156	0
3	BMA	K	3	11/12	0.59	0.39	141,153,157,157	0
3	BMA	G	3	11/12	0.61	0.20	146,148,152,152	0
3	NAG	K	2	14/15	0.64	0.45	121,143,153,156	0
3	NAG	M	2	14/15	0.67	0.36	117,142,152,157	0
3	BMA	L	3	11/12	0.67	0.30	144,147,150,151	0
3	BMA	I	3	11/12	0.70	0.18	137,141,145,146	0
3	NAG	N	2	14/15	0.71	0.27	93,115,135,146	0
3	NAG	H	1	14/15	0.75	0.23	91,101,117,132	0
3	NAG	H	2	14/15	0.77	0.31	126,142,154,155	0
3	NAG	L	2	14/15	0.81	0.31	84,124,135,144	0
3	NAG	O	2	14/15	0.82	0.18	120,130,137,146	0
3	NAG	M	1	14/15	0.82	0.18	76,91,109,126	0
3	NAG	G	2	14/15	0.83	0.21	123,126,136,142	0
4	NAG	J	2	14/15	0.84	0.19	115,120,124,126	0
3	NAG	I	2	14/15	0.86	0.26	93,124,133,141	0
3	NAG	O	1	14/15	0.87	0.15	68,81,98,107	0
3	NAG	G	1	14/15	0.87	0.19	75,89,103,118	0
3	NAG	K	1	14/15	0.88	0.18	86,98,114,131	0
4	NAG	J	1	14/15	0.91	0.13	70,90,97,108	0
3	NAG	N	1	14/15	0.92	0.14	73,83,97,106	0
3	NAG	L	1	14/15	0.92	0.18	69,81,91,106	0
3	NAG	I	1	14/15	0.93	0.16	71,80,93,104	0

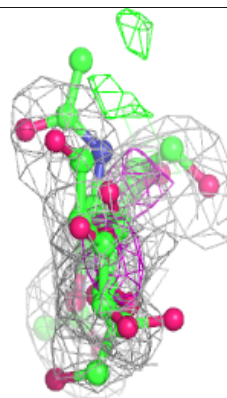
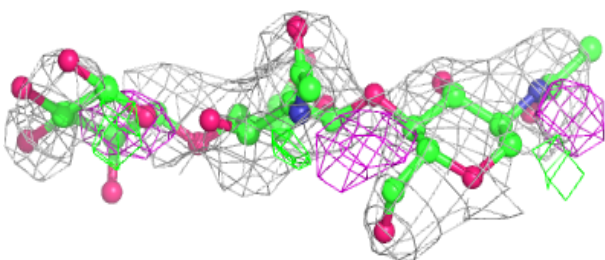
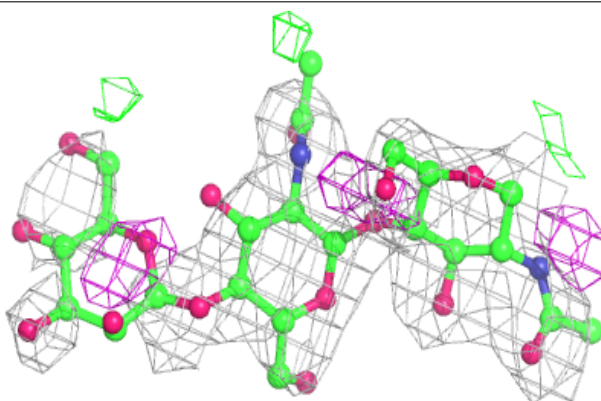
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

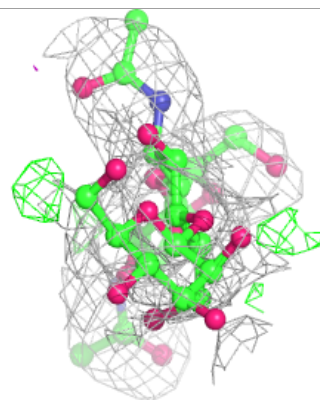
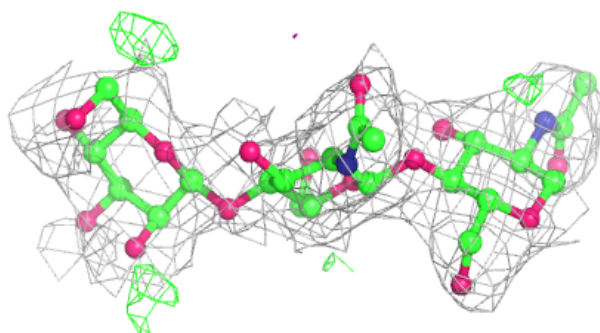
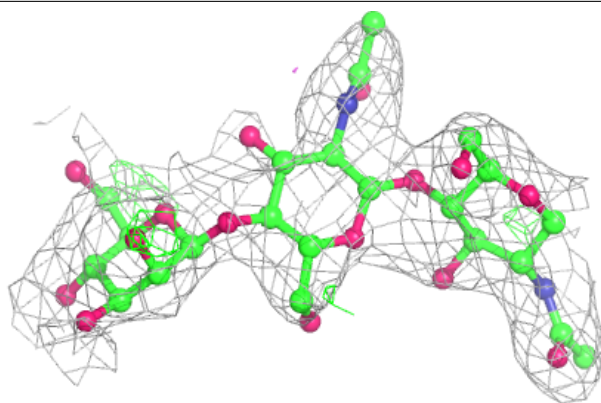
**Electron density around Chain H:**

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

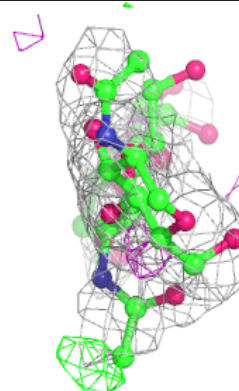
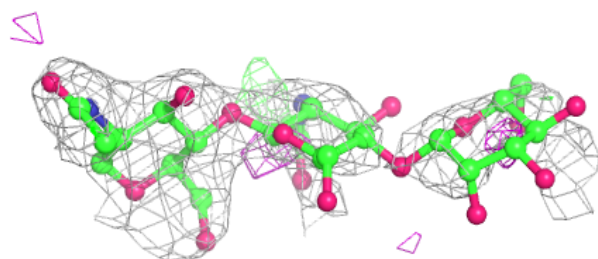
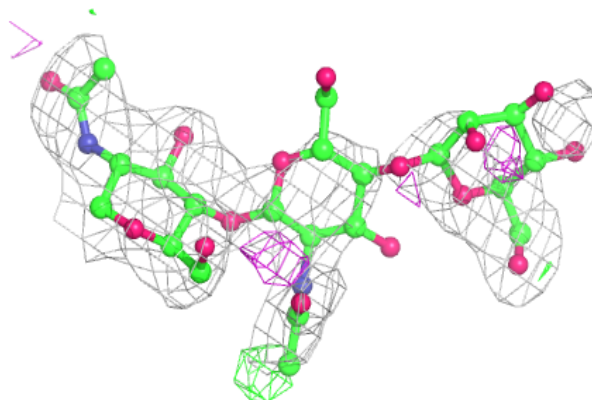


Electron density around Chain I:

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

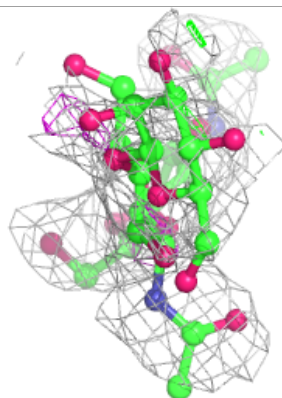
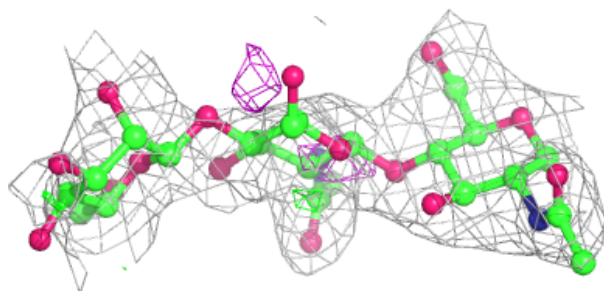
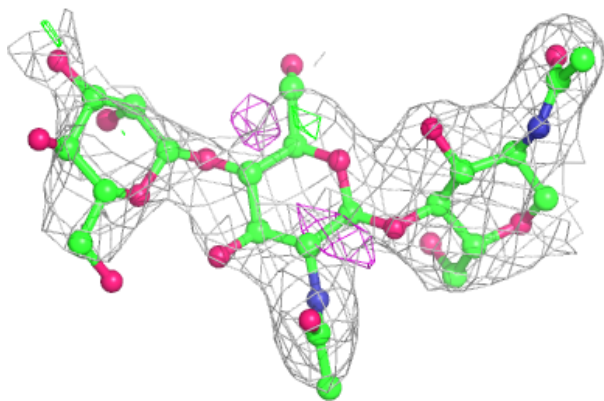
**Electron density around Chain K:**

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

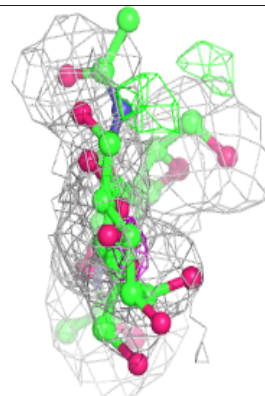
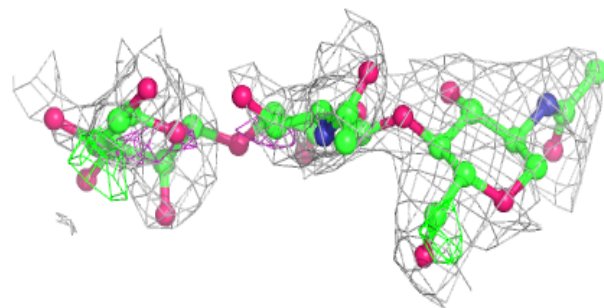
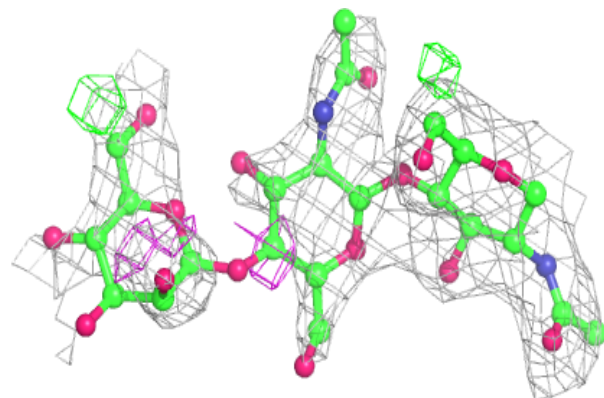


Electron density around Chain L:

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

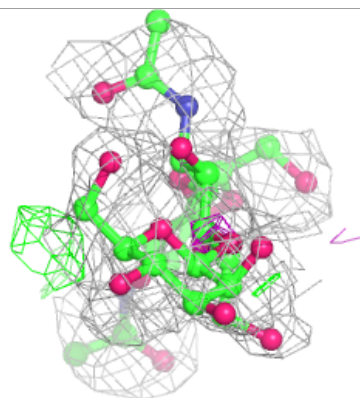
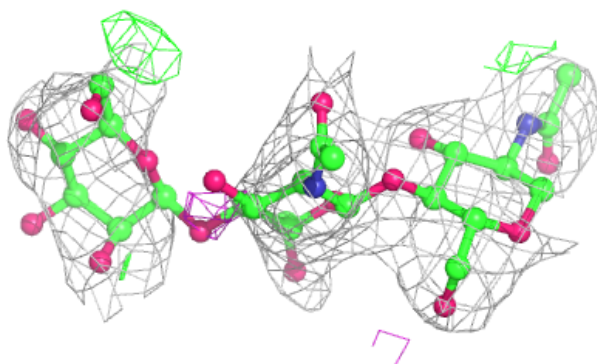
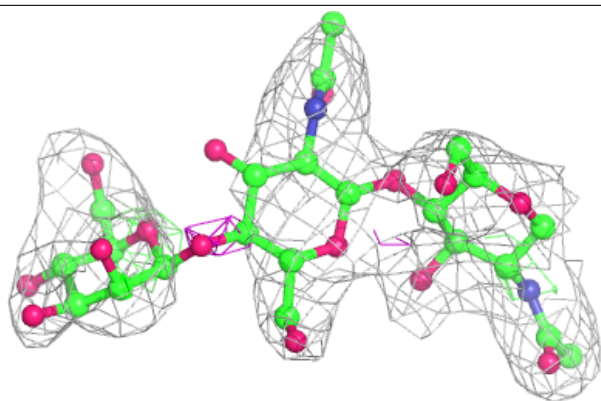
**Electron density around Chain M:**

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

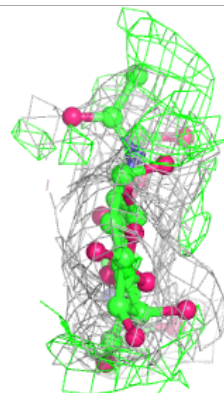
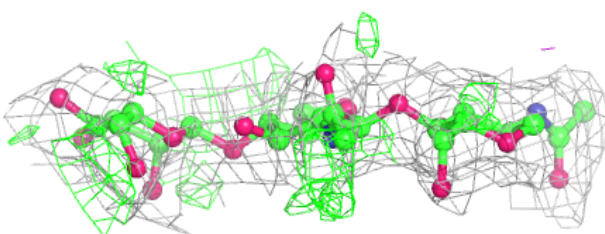
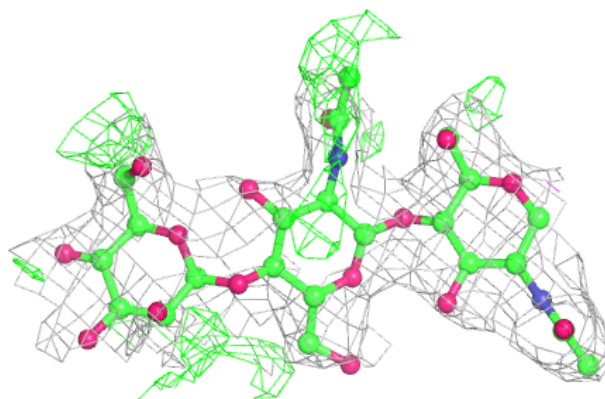


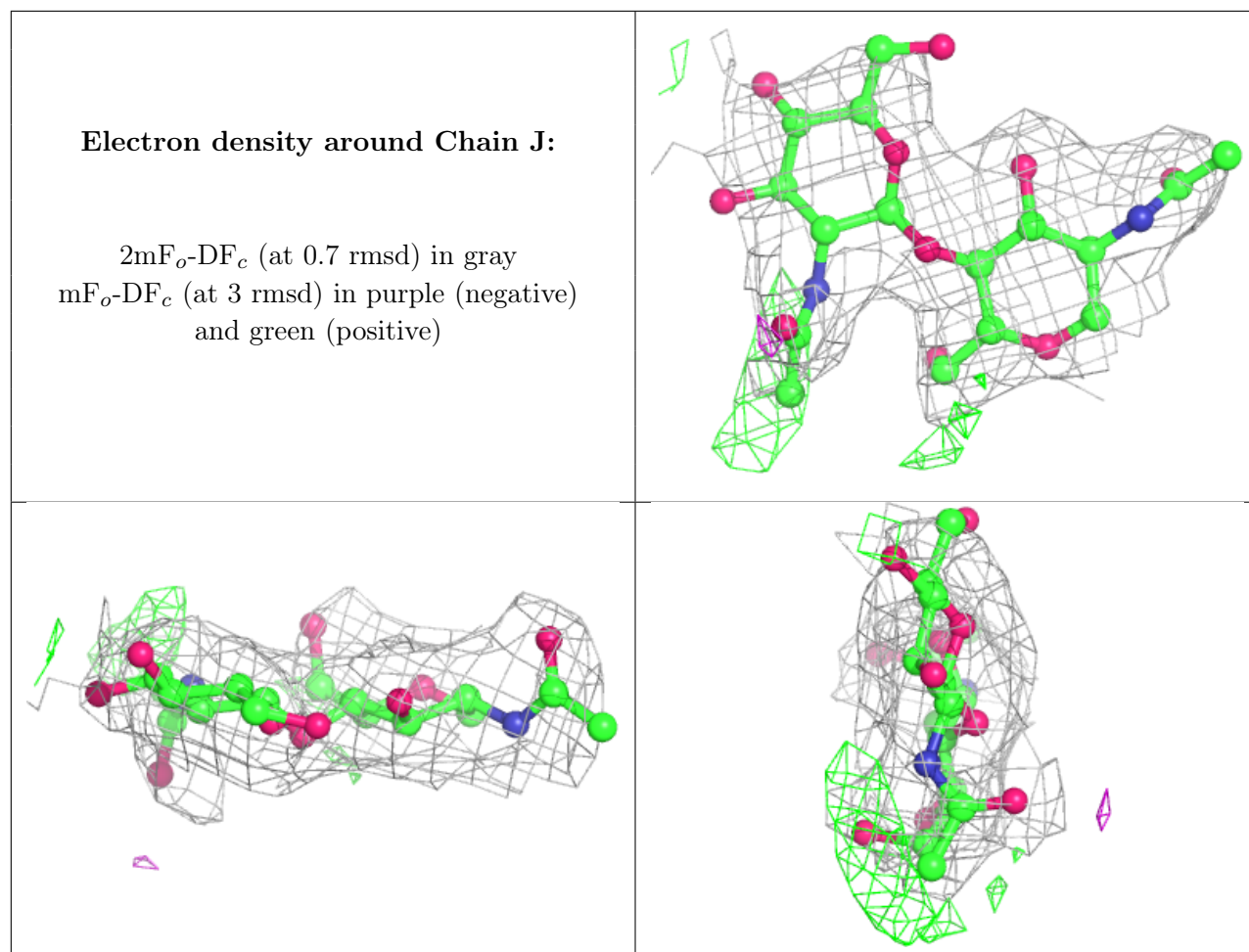
Electron density around Chain N:

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

**Electron density around Chain O:**

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





6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.