



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:56 PM UTC

PDB ID : 3ZDX / pdb_00003zdx
Title : Integrin alphaIIB beta3 headpiece and RGD peptide complex
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on : 2012-12-03
Resolution : 2.45 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

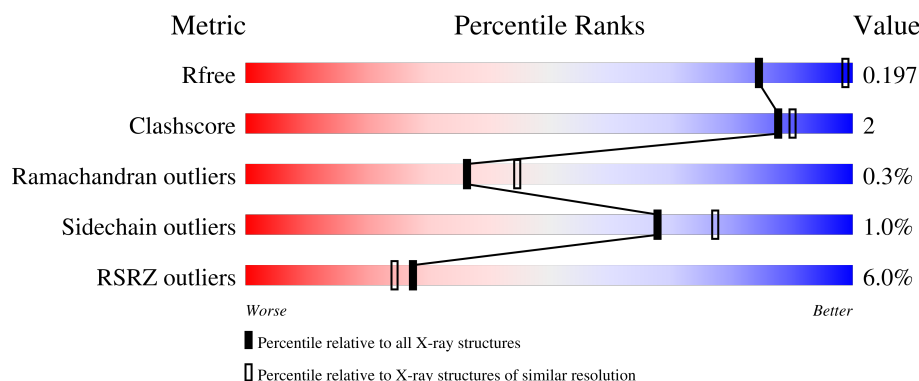
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	457	2% 96% .
1	C	457	% 93% 6% .
2	B	472	6% 92% 6% .
2	D	472	3% 94% 6% .
3	E	221	27% 90% 7% .

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Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	5	
6	I	2	
6	K	2	
7	J	4	

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
11	CL	B	1468	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 42688 atoms, of which 20255 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 INTEGRIN ALPHA-IIB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	457	Total	C	H	N	O	S	0	9	0
			6904	2248	3369	606	673	8			
1	C	453	Total	C	H	N	O	S	0	3	0
			6807	2218	3317	601	663	8			

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	464	Total	C	H	N	O	S	6	5	0
			7132	2248	3525	615	710	34			
2	D	469	Total	C	H	N	O	S	10	1	0
			7154	2258	3531	618	713	34			

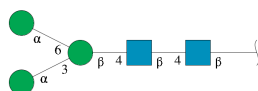
- Molecule 3 is a protein called 10E5 FAB, HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			

- Molecule 4 is a protein called 10E5 FAB, LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	5	Total	C	H	N	O	0	0	0
			113	34	52	2	25			

- Molecule 6 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
6	I	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
6	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



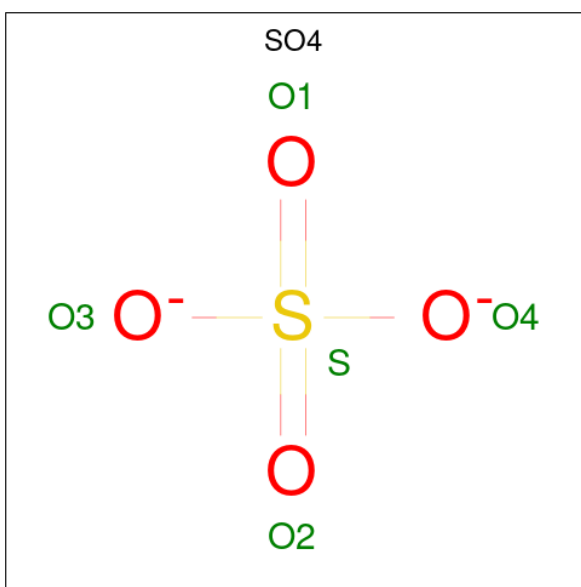
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	B	1	Total	C	H	O	0	0
			14	3	8	3		
8	C	1	Total	C	H	O	0	0
			14	3	8	3		
8	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	Ca	0	0
			4	4		
10	C	4	Total	Ca	0	0
			4	4		

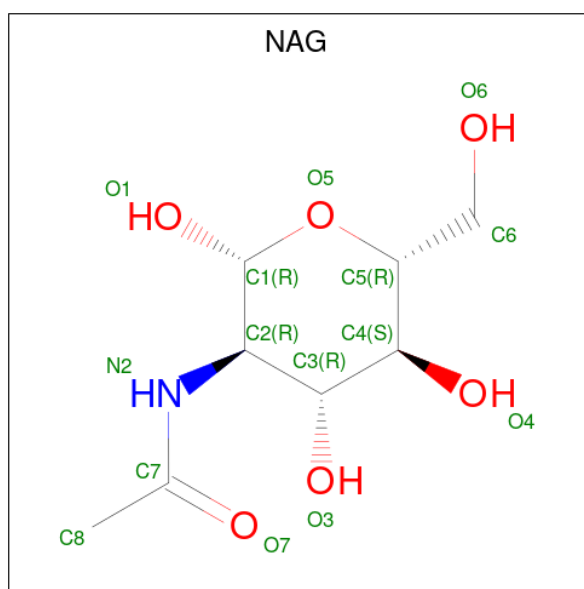
- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Cl	0	0
			1	1		

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	3	Total	Mn	0	0
			3	3		
12	D	3	Total	Mn	0	0
			3	3		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
13	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	527	Total	O	0	0
			527	527		

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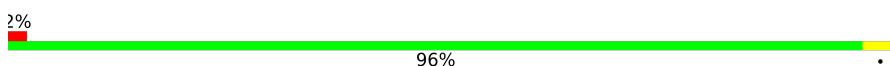
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	221	Total 221	O 221	0	0
14	C	307	Total 307	O 307	0	0
14	D	177	Total 177	O 177	0	0
14	E	11	Total 11	O 11	0	0
14	F	8	Total 8	O 8	0	0
14	H	39	Total 39	O 39	0	0
14	L	34	Total 34	O 34	0	0

3 Residue-property plots [i](#)

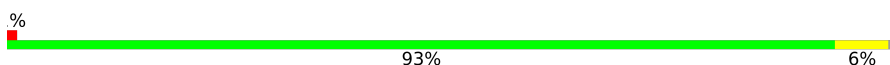
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: INTEGRIN ALPHA-IIB

Chain A: 



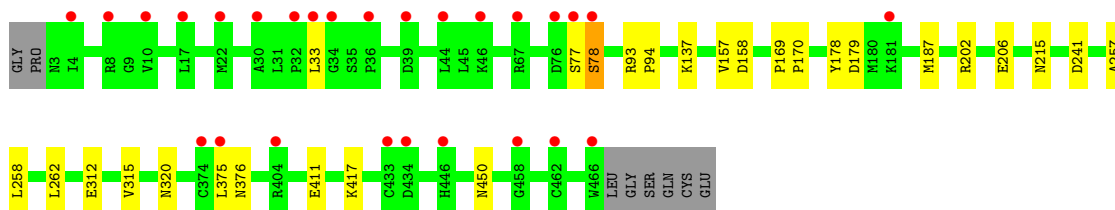
• Molecule 1: INTEGRIN ALPHA-IIB

Chain C: 

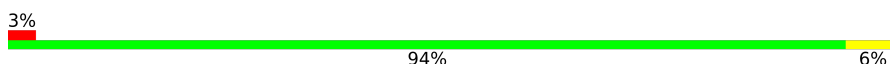


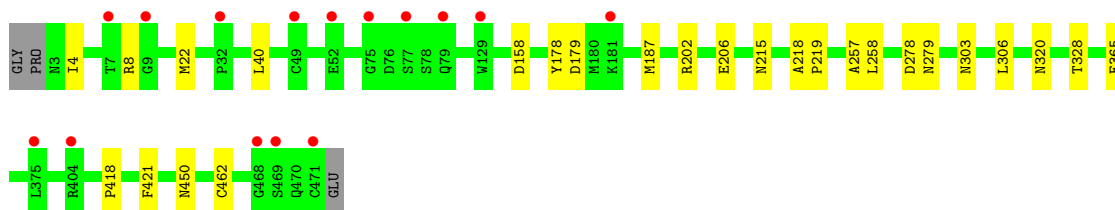
• Molecule 2: INTEGRIN BETA-3

Chain B: 

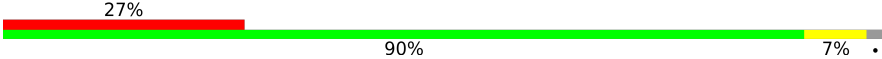


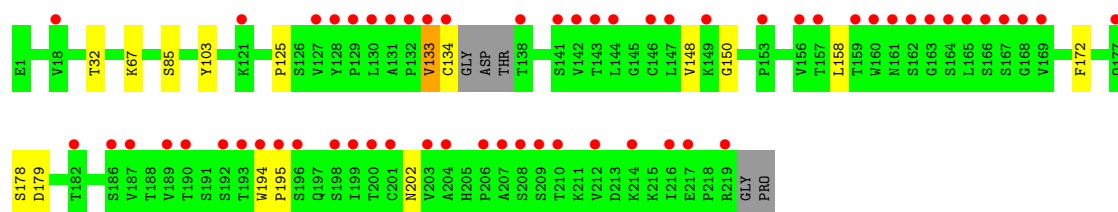
• Molecule 2: INTEGRIN BETA-3

Chain D: 

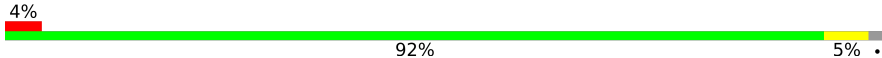


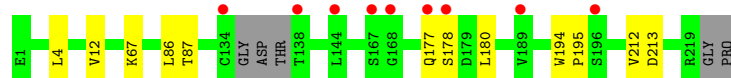
• Molecule 3: 10E5 FAB, HEAVY CHAIN

Chain E: 

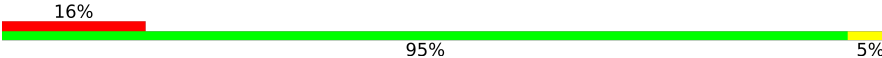


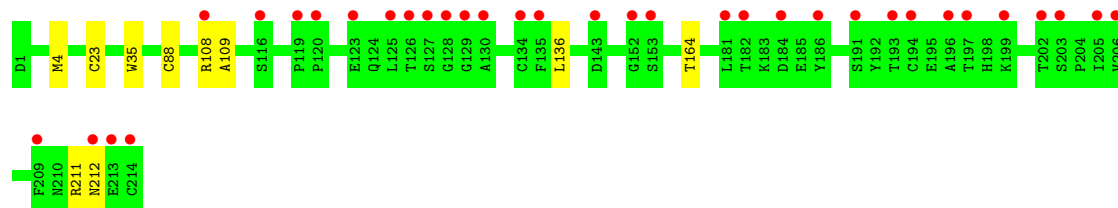
- Molecule 3: 10E5 FAB, HEAVY CHAIN

Chain H: 



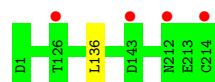
- Molecule 4: 10E5 FAB, LIGHT CHAIN

Chain F: 



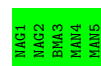
- Molecule 4: 10E5 FAB, LIGHT CHAIN

Chain L: 

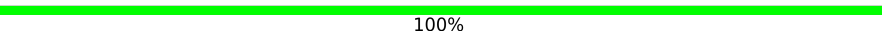


- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 



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

Chain I: 



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

Chain K:  100%

NAG1
NAG2

- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  75% 25%

NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	259.71 Å 144.96 Å 104.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.45 48.36 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.36-2.45) 99.9 (48.36-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.45 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.197 0.157 , 0.197	Depositor DCC
R_{free} test set	1008 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.8	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	0.95	EDS
Total number of atoms	42688	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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, BMA, MAN, NAG, GOL, CL, MN, SO4

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	0.31	0/3659	0.65	0/4987
1	C	0.28	0/3596	0.64	2/4900 (0.0%)
2	B	0.28	0/3685	0.64	0/4996
2	D	0.28	0/3694	0.62	0/5009
3	E	0.25	0/1684	0.60	0/2305
3	H	0.25	0/1684	0.59	0/2305
4	F	0.24	0/1673	0.58	0/2269
4	L	0.25	0/1673	0.59	0/2269
All	All	0.28	0/21348	0.62	2/29040 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	ALA	CA-C-N	5.02	124.74	119.82
1	C	39	ALA	C-N-CA	5.02	124.74	119.82

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	3535	3369	3386	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3490	3317	3328	19	1
2	B	3607	3525	3534	16	0
2	D	3623	3531	3537	12	0
3	E	1642	1597	1600	9	0
3	H	1642	1597	1600	6	0
4	F	1637	1550	1553	6	0
4	L	1637	1550	1553	1	0
5	G	61	52	52	0	0
6	I	28	25	25	0	0
6	K	28	25	25	0	0
7	J	50	43	43	0	0
8	A	18	24	24	0	0
8	B	6	8	8	0	0
8	C	12	16	16	1	0
9	A	10	0	0	0	0
9	C	25	0	0	0	0
9	D	10	0	0	0	0
9	L	5	0	0	0	0
10	A	4	0	0	0	0
10	C	4	0	0	0	0
11	B	1	0	0	3	0
12	B	3	0	0	0	0
12	D	3	0	0	0	0
13	B	14	13	13	0	0
13	D	14	13	13	0	0
14	A	527	0	0	5	4
14	B	221	0	0	4	0
14	C	307	0	0	4	3
14	D	177	0	0	0	0
14	E	11	0	0	0	0
14	F	8	0	0	0	0
14	H	39	0	0	0	0
14	L	34	0	0	0	0
All	All	22433	20255	20310	81	4

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 2.

All (81) 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)
11:B:1468:CL:CL	14:B:4039:HOH:O	2.25	0.92
11:B:1468:CL:CL	14:B:4040:HOH:O	2.29	0.86
11:B:1468:CL:CL	14:B:4124:HOH:O	2.32	0.83
1:A:41:ARG:NH2	14:A:4043:HOH:O	2.23	0.71
1:C:395:GLN:OE1	14:C:4265:HOH:O	2.11	0.69
1:C:338:HIS:O	14:C:4178:HOH:O	2.13	0.67
1:A:15[A]:ASN:ND2	14:A:4033:HOH:O	2.29	0.66
1:A:338:HIS:O	14:A:4402:HOH:O	2.12	0.66
2:D:202:ARG:NH2	2:D:206:GLU:OE2	2.30	0.64
1:C:384:SER:OG	14:C:4254:HOH:O	2.17	0.58
3:H:177:GLN:N	3:H:180:LEU:O	2.38	0.57
1:A:122:ALA:O	1:A:123:GLU:HB2	2.05	0.56
2:B:77:SER:O	2:B:78:SER:HB3	2.04	0.56
1:C:122:ALA:O	1:C:123:GLU:HB2	2.05	0.56
3:H:213:ASP:OD1	3:H:213:ASP:N	2.38	0.55
2:D:257:ALA:O	2:D:258:LEU:HB2	2.07	0.55
2:B:137:LYS:NZ	14:B:4060:HOH:O	2.40	0.54
3:H:194:TRP:CG	3:H:195:PRO:HA	2.43	0.54
1:A:351:GLN:OE1	14:A:4418:HOH:O	2.19	0.53
3:E:67:LYS:NZ	3:E:85:SER:O	2.42	0.53
2:B:169:PRO:HD2	2:B:178:TYR:CZ	2.46	0.50
1:C:194:LEU:C	1:C:194:LEU:HD12	2.38	0.49
1:A:194:LEU:HD12	1:A:194:LEU:C	2.37	0.49
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.46	0.48
1:C:122:ALA:O	1:C:123:GLU:CB	2.61	0.48
8:C:1454:GOL:O3	8:C:1454:GOL:O1	2.30	0.48
2:D:158:ASP:HB3	2:D:187:MET:CE	2.43	0.48
2:B:312:GLU:HA	2:B:315:VAL:HG23	1.95	0.48
2:B:257:ALA:O	2:B:258:LEU:HB2	2.14	0.47
2:D:450:ASN:O	2:D:450:ASN:ND2	2.47	0.47
1:A:122:ALA:O	1:A:123:GLU:CB	2.63	0.47
2:B:450:ASN:O	2:B:450:ASN:ND2	2.47	0.47
1:C:46:SER:O	1:C:47:GLN:HB2	2.15	0.47
4:F:136:LEU:HD12	4:F:136:LEU:N	2.30	0.46
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.97	0.46
3:E:133:VAL:O	3:E:134:CYS:SG	2.73	0.46
2:B:158:ASP:HB3	2:B:187[A]:MET:CE	2.45	0.46
1:C:285:MET:SD	2:D:320:ASN:HB3	2.56	0.46
2:B:169:PRO:HB2	2:B:170:PRO:HD2	1.98	0.45
1:C:215:HIS:CE1	3:E:103:TYR:CE1	3.04	0.45
2:D:178:TYR:CG	2:D:179:ASP:N	2.84	0.45
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.47	0.45
4:L:136:LEU:HD12	4:L:136:LEU:N	2.32	0.45
3:E:158:LEU:HD23	3:E:158:LEU:C	2.42	0.45
1:C:258:PRO:HB2	1:C:288:TYR:CD2	2.52	0.45
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.52	0.44
3:E:194:TRP:CG	3:E:195:PRO:HA	2.52	0.44
2:B:376:ASN:ND2	2:B:376:ASN:O	2.51	0.44
1:C:432:TYR:CZ	1:C:452:PRO:HA	2.52	0.44
1:C:278[A]:HIS:CE1	1:C:340:LEU:O	2.71	0.43
4:F:4:MET:HE3	4:F:23:CYS:SG	2.59	0.43
3:H:212:VAL:HG12	3:H:213:ASP:N	2.34	0.43
2:B:77:SER:O	2:B:78:SER:CB	2.65	0.42
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.53	0.42
3:E:178:SER:O	3:E:179:ASP:HB2	2.20	0.42
1:C:351:GLN:OE1	14:C:4228:HOH:O	2.22	0.42
2:D:4:ILE:O	2:D:8:ARG:HG2	2.19	0.42
2:D:306:LEU:HB3	2:D:328:THR:HG22	2.01	0.42
4:F:211:ARG:O	4:F:212:ASN:HB2	2.20	0.42
1:C:278[A]:HIS:CD2	1:C:339:ALA:HB1	2.55	0.42
2:B:178:TYR:CG	2:B:179:ASP:N	2.87	0.42
1:A:258:PRO:HA	1:A:289:PHE:O	2.20	0.41
1:A:285:MET:O	1:A:286:ALA:HB3	2.20	0.41
1:C:280:LEU:CD1	1:C:306:LEU:HD23	2.51	0.41
2:B:78:SER:OG	2:B:241:ASP:CG	2.64	0.41
1:C:132:LEU:N	1:C:132:LEU:HD12	2.36	0.41
4:F:35:TRP:CZ3	4:F:88:CYS:HB3	2.56	0.41
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.55	0.41
1:C:285:MET:O	1:C:286:ALA:HB3	2.20	0.41
1:A:285:MET:SD	2:B:320:ASN:HB3	2.61	0.41
1:A:390:LEU:HD12	1:A:390:LEU:N	2.35	0.41
1:A:394:GLY:HA2	1:A:399:LEU:HD23	2.03	0.41
2:B:157:VAL:HG11	2:B:187[B]:MET:SD	2.60	0.41
2:D:22:MET:HG2	2:D:40:LEU:CD2	2.51	0.41
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.03	0.41
4:F:108:ARG:HG2	4:F:109:ALA:N	2.36	0.40
3:H:4:LEU:HD12	3:H:4:LEU:N	2.37	0.40
1:A:41:ARG:NH1	14:A:4070:HOH:O	2.54	0.40
2:D:278:ASP:O	2:D:279:ASN:HB2	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4459:HOH:O	14:C:4260:HOH:O[1_554]	1.92	0.28
14:A:4459:HOH:O	14:C:4282:HOH:O[1_554]	1.99	0.21
14:A:4480:HOH:O	14:C:4279:HOH:O[1_554]	2.09	0.11
1:C:386:ARG:NH1	14:A:4485:HOH:O[1_556]	2.16	0.04

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	464/457 (102%)	446 (96%)	17 (4%)	1 (0%)	43	54
1	C	454/457 (99%)	441 (97%)	12 (3%)	1 (0%)	43	54
2	B	467/472 (99%)	444 (95%)	20 (4%)	3 (1%)	21	27
2	D	468/472 (99%)	451 (96%)	17 (4%)	0	100	100
3	E	212/221 (96%)	200 (94%)	10 (5%)	2 (1%)	14	17
3	H	212/221 (96%)	200 (94%)	11 (5%)	1 (0%)	24	32
4	F	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
All	All	2701/2728 (99%)	2589 (96%)	104 (4%)	8 (0%)	36	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	33	LEU
2	B	78	SER
2	B	375	LEU
3	E	133	VAL
1	C	123	GLU
3	H	178	SER
3	E	150	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	372/364 (102%)	366 (98%)	6 (2%)	55	69
1	C	364/364 (100%)	359 (99%)	5 (1%)	59	72
2	B	416/417 (100%)	412 (99%)	4 (1%)	68	77
2	D	416/417 (100%)	412 (99%)	4 (1%)	68	77
3	E	187/190 (98%)	186 (100%)	1 (0%)	81	87
3	H	187/190 (98%)	185 (99%)	2 (1%)	65	76
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2318/2318 (100%)	2296 (99%)	22 (1%)	68	81

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	195	LEU
1	A	270	LEU
1	A	288	TYR
2	B	215	ASN
2	B	262	LEU
2	B	411	GLU
2	B	417	LYS
1	C	23	LEU
1	C	61	GLU
1	C	166	TYR
1	C	270	LEU
1	C	288	TYR
2	D	215	ASN
2	D	303	ASN
2	D	365	GLU
2	D	462	CYS

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Mol	Chain	Res	Type
3	E	202	ASN
3	H	67	LYS
3	H	87	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	372	ASN
2	B	305	ASN
2	B	444	ASN
2	B	450	ASN
1	C	158	ASN
2	D	204	ASN
2	D	319	GLN
2	D	444	ASN
2	D	450	ASN
3	E	202	ASN
4	F	190	ASN
3	H	39	GLN
3	H	170	HIS
4	L	27	GLN
4	L	38	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 ⓘ

13 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	1	5,2	14,14,15	0.55	0	17,19,21	0.65	0
5	NAG	G	2	5	14,14,15	0.58	0	17,19,21	0.65	0
5	BMA	G	3	5	11,11,12	0.62	0	15,15,17	0.84	0
5	MAN	G	4	5	11,11,12	0.57	0	15,15,17	0.75	0
5	MAN	G	5	5	11,11,12	0.59	0	15,15,17	0.52	0
6	NAG	I	1	6,2	14,14,15	0.56	0	17,19,21	0.65	0
6	NAG	I	2	6	14,14,15	0.54	0	17,19,21	0.58	0
7	NAG	J	1	7,2	14,14,15	0.51	0	17,19,21	0.61	0
7	NAG	J	2	7	14,14,15	0.59	0	17,19,21	0.72	0
7	BMA	J	3	7	11,11,12	0.65	0	15,15,17	0.79	1 (6%)
7	MAN	J	4	7	11,11,12	0.63	0	15,15,17	0.58	0
6	NAG	K	1	6,2	14,14,15	0.62	0	17,19,21	0.84	0
6	NAG	K	2	6	14,14,15	0.53	0	17,19,21	0.55	0

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	3	BMA	C1-C2-C3	2.21	112.86	109.64

There are no chirality outliers.

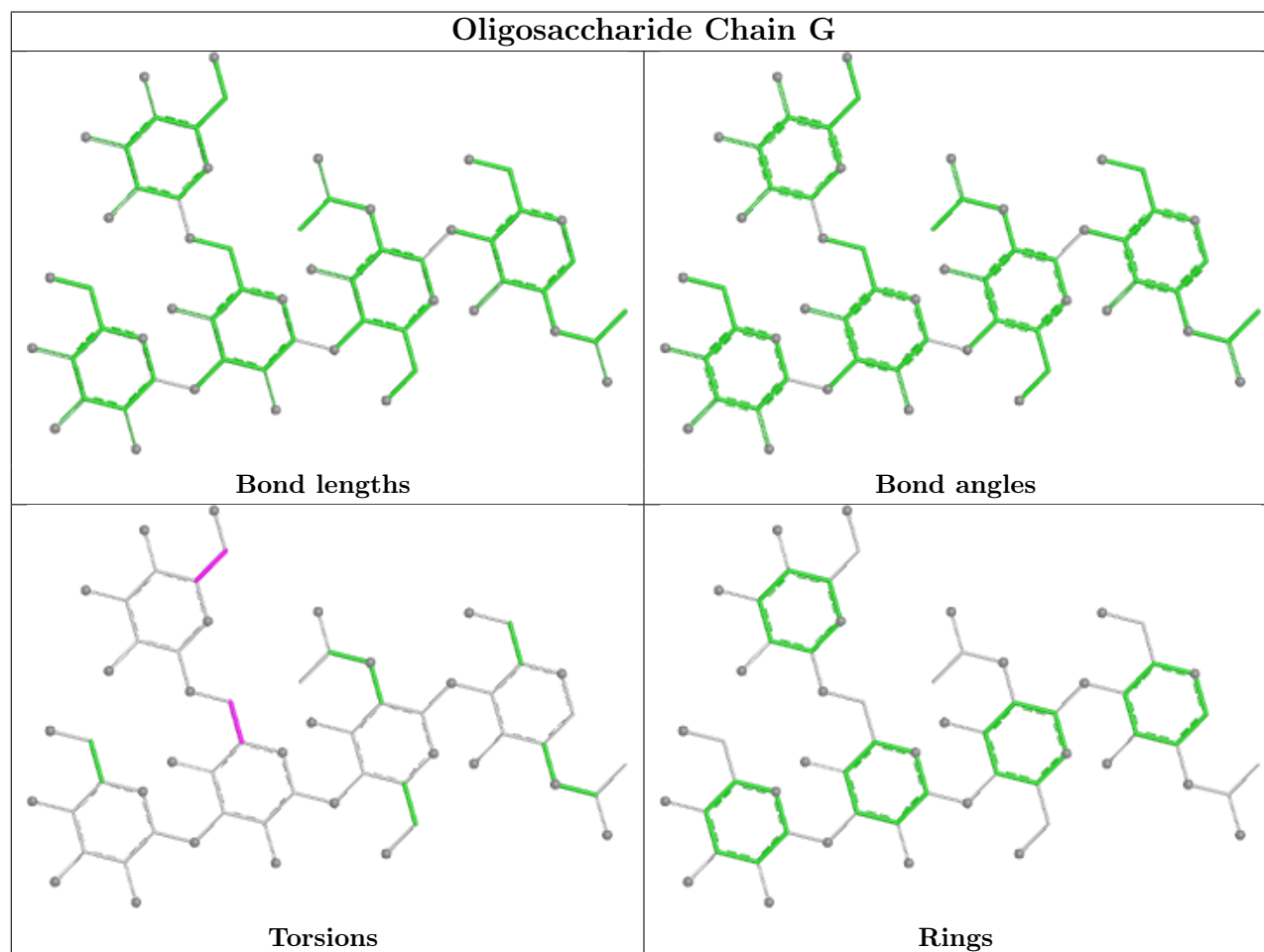
All (6) torsion outliers are listed below:

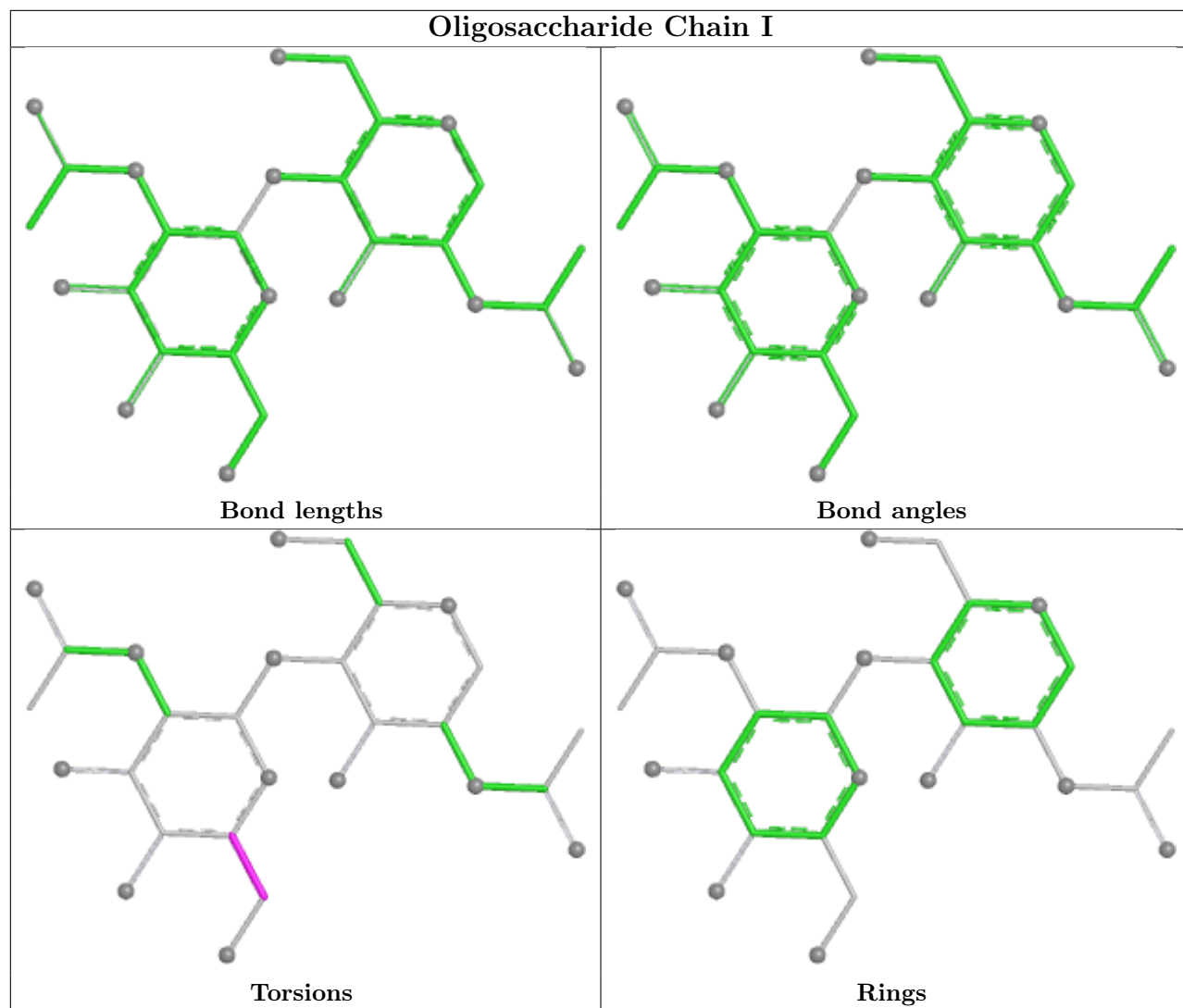
Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
6	K	2	NAG	C8-C7-N2-C2
5	G	5	MAN	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	K	2	NAG	O7-C7-N2-C2
5	G	3	BMA	C4-C5-C6-O6

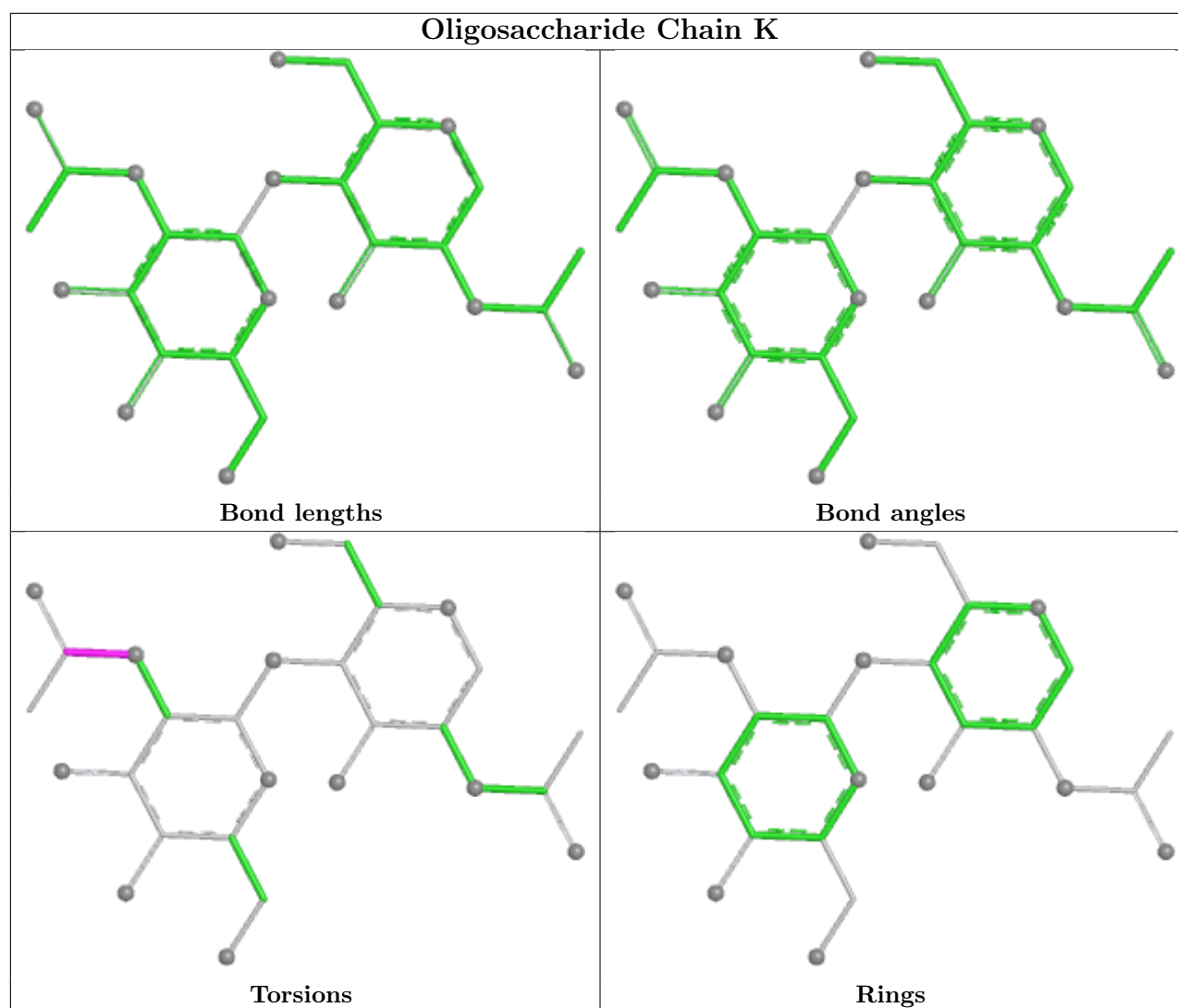
There are no ring outliers.

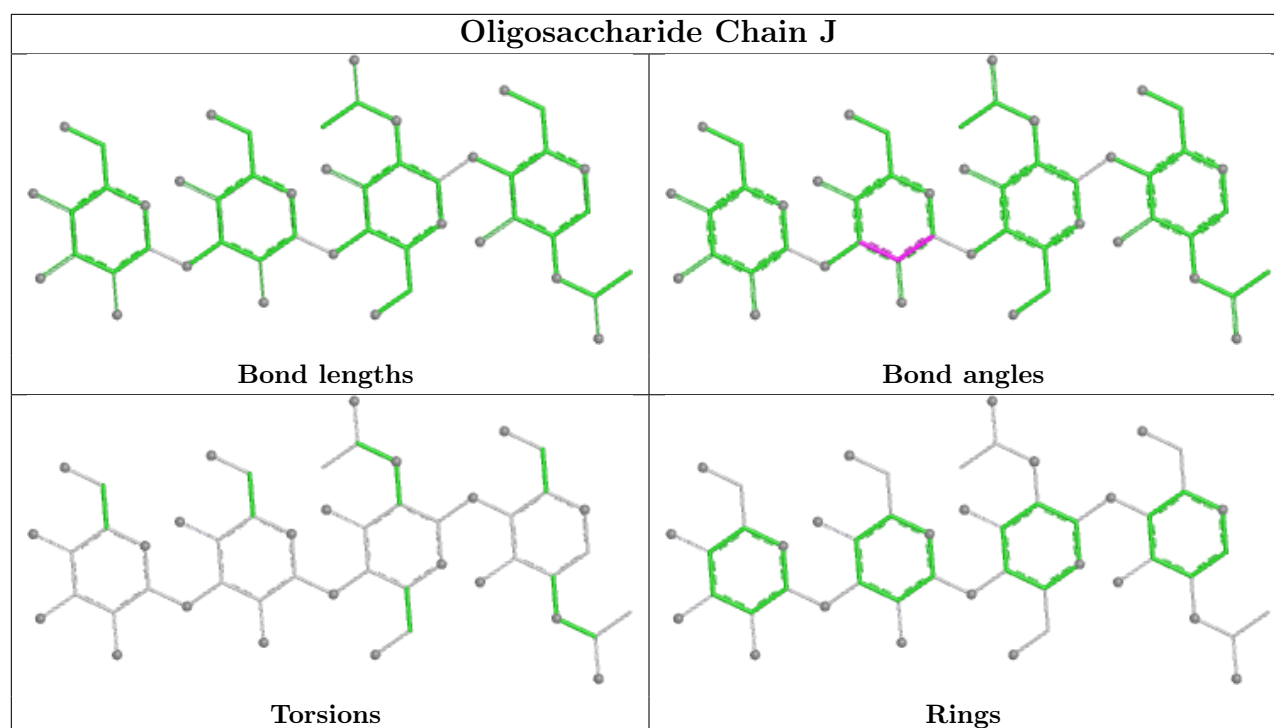
No monomer is involved in short contacts.

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 33 ligands modelled in this entry, 15 are monoatomic - leaving 18 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	$\# Z > 2$
9	SO4	D	1473	12	4,4,4	0.24	0	6,6,6	0.10	0
9	SO4	C	1456	-	4,4,4	0.25	0	6,6,6	0.08	0
9	SO4	C	1457	-	4,4,4	0.23	0	6,6,6	0.08	0
9	SO4	L	1215	-	4,4,4	0.24	0	6,6,6	0.07	0
8	GOL	B	1467	-	5,5,5	0.38	0	5,5,5	0.26	0
8	GOL	A	1458	-	5,5,5	0.38	0	5,5,5	0.28	0
9	SO4	C	1460	-	4,4,4	0.24	0	6,6,6	0.08	0
8	GOL	A	1459	-	5,5,5	0.37	0	5,5,5	0.26	0
13	NAG	D	3099	2	14,14,15	0.50	0	17,19,21	0.55	0
9	SO4	C	1459	-	4,4,4	0.23	0	6,6,6	0.06	0
8	GOL	C	1454	-	5,5,5	0.36	0	5,5,5	0.32	0
8	GOL	C	1455	-	5,5,5	0.37	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	A	1462	-	4,4,4	0.23	0	6,6,6	0.08	0
9	SO4	D	1472	-	4,4,4	0.23	0	6,6,6	0.09	0
9	SO4	A	1461	-	4,4,4	0.24	0	6,6,6	0.10	0
8	GOL	A	1460	-	5,5,5	0.38	0	5,5,5	0.18	0
13	NAG	B	3099	2	14,14,15	0.51	0	17,19,21	0.68	0
9	SO4	C	1458	-	4,4,4	0.23	0	6,6,6	0.09	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
8	GOL	B	1467	-	-	2/4/4/4	-
8	GOL	A	1458	-	-	2/4/4/4	-
8	GOL	A	1459	-	-	0/4/4/4	-
13	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
8	GOL	C	1454	-	-	2/4/4/4	-
8	GOL	C	1455	-	-	2/4/4/4	-
8	GOL	A	1460	-	-	2/4/4/4	-
13	NAG	B	3099	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1458	GOL	O1-C1-C2-O2
8	A	1458	GOL	O1-C1-C2-C3
8	A	1460	GOL	O1-C1-C2-C3
8	B	1467	GOL	O1-C1-C2-C3
8	C	1454	GOL	O1-C1-C2-C3
8	A	1460	GOL	O1-C1-C2-O2
8	C	1454	GOL	O1-C1-C2-O2
8	C	1455	GOL	O1-C1-C2-C3
8	B	1467	GOL	O1-C1-C2-O2
8	C	1455	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1454	GOL	1	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	457/457 (100%)	-0.72	7 (1%) 72 74	10, 21, 57, 138	10 (2%)
1	C	453/457 (99%)	-0.49	6 (1%) 75 77	14, 36, 74, 123	3 (0%)
2	B	464/472 (98%)	-0.00	27 (5%) 29 26	11, 50, 137, 200	7 (1%)
2	D	469/472 (99%)	-0.11	15 (3%) 50 51	17, 49, 118, 179	3 (0%)
3	E	216/221 (97%)	1.30	59 (27%) 1 1	42, 112, 195, 221	0
3	H	216/221 (97%)	0.35	9 (4%) 40 40	27, 76, 135, 156	0
4	F	214/214 (100%)	0.85	34 (15%) 5 3	41, 101, 184, 252	0
4	L	214/214 (100%)	0.01	4 (1%) 66 67	30, 60, 97, 182	0
All	All	2703/2728 (99%)	-0.02	161 (5%) 27 24	10, 49, 146, 252	23 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	36	PRO	5.9
3	E	199	ILE	5.6
3	E	165	LEU	5.3
3	E	216	ILE	5.2
3	E	160	TRP	5.1
3	E	201	CYS	4.8
3	E	134	CYS	4.6
4	F	126	THR	4.6
1	A	457	SER	4.5
2	B	33	LEU	4.5
3	E	212	VAL	4.4
3	E	194	TRP	4.4
2	B	78	SER	4.3
2	D	471	CYS	4.2
2	D	77	SER	4.1
2	D	129[A]	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
3	E	142	VAL	4.0
4	L	214	CYS	3.9
3	E	131	ALA	3.8
3	E	163	GLY	3.8
4	L	212	ASN	3.8
3	E	144	LEU	3.8
4	F	181	LEU	3.8
2	D	181	LYS	3.7
3	E	203	VAL	3.7
4	F	202	THR	3.6
4	F	130	ALA	3.6
2	B	466	TRP	3.6
2	D	375	LEU	3.5
2	B	4	ILE	3.5
3	E	138	THR	3.5
2	B	44	LEU	3.5
3	E	156	VAL	3.4
2	B	375	LEU	3.4
3	E	147	LEU	3.4
1	A	337	PRO	3.4
3	E	127	VAL	3.3
3	E	217	GLU	3.3
1	C	339	ALA	3.3
3	E	132	PRO	3.3
3	H	168	GLY	3.3
2	B	32	PRO	3.2
3	E	164	SER	3.2
3	E	198	SER	3.2
2	B	10	VAL	3.2
3	E	133	VAL	3.1
3	E	219	ARG	3.1
4	F	205	ILE	3.1
3	H	177	GLN	3.1
4	F	214	CYS	3.1
3	E	214	LYS	3.1
4	F	134	CYS	3.0
3	E	192	SER	3.0
1	C	453	VAL	3.0
3	E	167	SER	3.0
3	E	196	SER	3.0
4	F	153	SER	2.9
2	D	9	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	181	LYS	2.9
2	B	34	GLY	2.9
3	E	159	THR	2.9
4	F	125	LEU	2.9
3	E	190	THR	2.9
3	H	138	THR	2.9
3	E	195	PRO	2.8
4	F	209	PHE	2.8
4	F	194	CYS	2.8
4	F	143	ASP	2.8
4	F	119	PRO	2.7
3	E	182	THR	2.7
3	E	130	LEU	2.7
3	E	210	THR	2.7
2	B	404	ARG	2.7
4	F	123	GLU	2.6
3	E	128	TYR	2.6
4	F	186	TYR	2.6
2	D	75	GLY	2.6
4	F	120	PRO	2.6
1	A	338	HIS	2.6
2	D	468	GLY	2.6
4	F	129	GLY	2.5
3	E	200	THR	2.5
2	B	434	ASP	2.5
3	E	162	SER	2.5
3	E	186	SER	2.5
2	B	67	ARG	2.5
2	B	76	ASP	2.5
2	D	7	THR	2.5
4	F	193	THR	2.5
3	H	134	CYS	2.4
2	B	446	HIS	2.4
3	E	129	PRO	2.4
2	B	374	CYS	2.4
4	F	184	ASP	2.4
4	F	135	PHE	2.4
2	D	52	GLU	2.4
3	E	189	VAL	2.4
1	A	456	ALA	2.4
2	B	30	ALA	2.4
3	E	168	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	187	VAL	2.3
3	E	206	PRO	2.3
4	F	182	THR	2.3
2	D	404	ARG	2.3
3	E	141	SER	2.3
3	E	166	SER	2.3
3	H	196	SER	2.3
2	B	39	ASP	2.3
3	H	189	VAL	2.3
1	A	45	PRO	2.3
3	E	153	PRO	2.3
3	E	204	ALA	2.3
4	F	197	THR	2.3
2	B	77	SER	2.3
3	H	167	SER	2.3
2	B	17	LEU	2.3
2	B	46	LYS	2.3
2	B	462	CYS	2.3
3	E	161	ASN	2.3
4	F	212	ASN	2.3
4	F	199	LYS	2.3
3	E	169	VAL	2.3
2	D	49	CYS	2.3
4	F	108	ARG	2.3
1	A	339	ALA	2.2
2	D	79	GLN	2.2
1	A	455	LYS	2.2
1	C	46	SER	2.2
3	E	208	SER	2.2
3	E	209	SER	2.2
2	B	22	MET	2.2
3	E	207	ALA	2.2
2	B	433	CYS	2.2
3	E	177	GLN	2.2
2	B	8	ARG	2.2
2	B	458	GLY	2.2
2	D	469	SER	2.2
1	C	45	PRO	2.2
2	D	32	PRO	2.2
3	E	143	THR	2.1
3	H	178	SER	2.1
3	E	18	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	196	ALA	2.1
4	F	128	GLY	2.1
4	F	203	SER	2.1
1	C	47	GLN	2.1
3	E	193	THR	2.1
4	L	126	THR	2.1
4	F	213	GLU	2.1
3	E	149	LYS	2.1
3	E	146	CYS	2.1
1	C	338	HIS	2.1
4	F	206	VAL	2.1
3	E	157	THR	2.1
4	F	191	SER	2.1
3	H	144	LEU	2.0
4	F	152	GLY	2.0
3	E	121	LYS	2.0
4	L	143	ASP	2.0
4	F	116	SER	2.0
4	F	127	SER	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

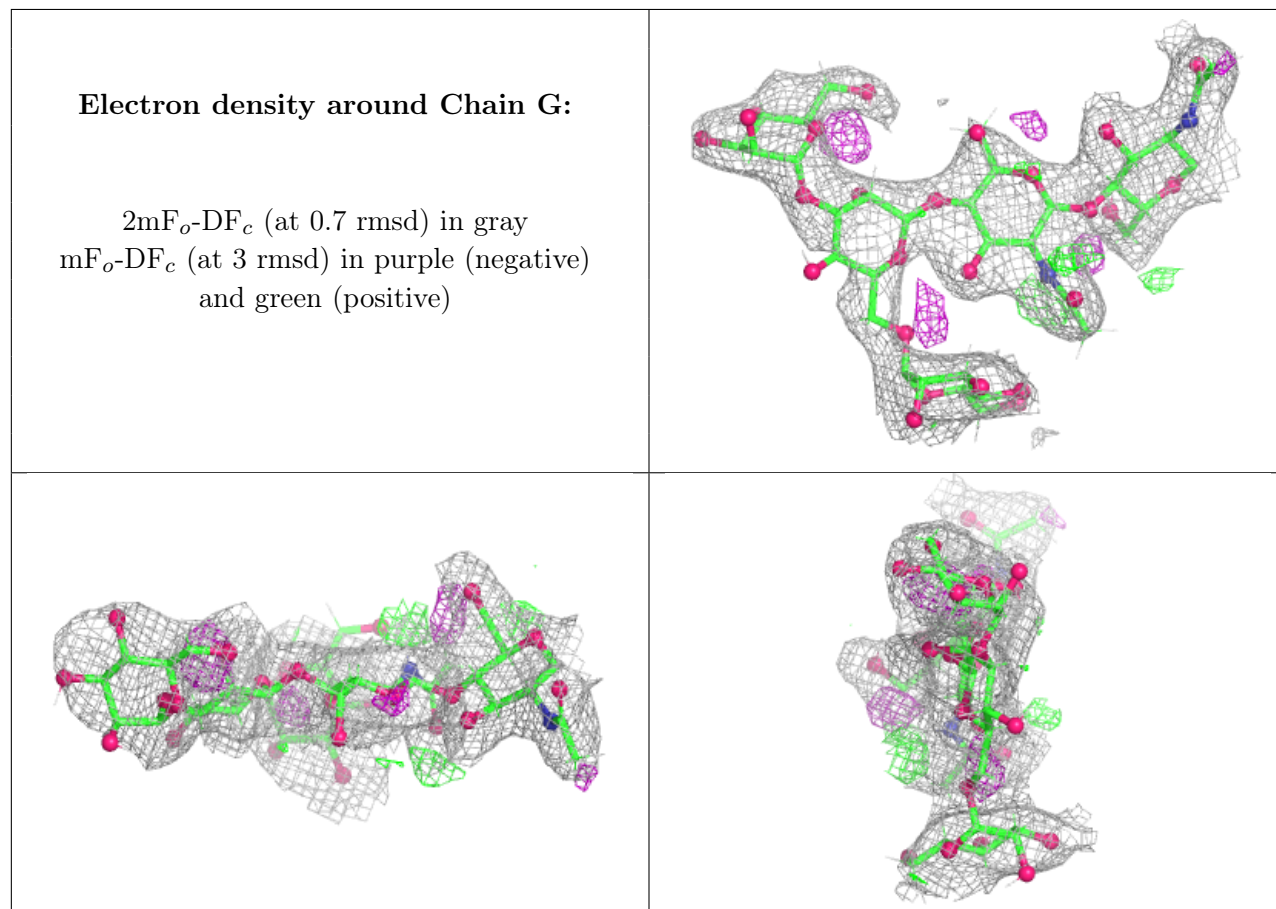
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	1	14/15	-	-	13,28,46,53	0
5	NAG	G	2	14/15	-	-	47,65,96,99	0
5	BMA	G	3	11/12	-	-	81,124,152,153	0
5	MAN	G	4	11/12	-	-	54,111,133,145	0
5	MAN	G	5	11/12	-	-	108,127,148,152	0
7	NAG	J	2	14/15	0.80	0.14	48,77,102,108	0
7	NAG	J	1	14/15	0.87	0.11	21,44,61,70	0
6	NAG	I	2	14/15	0.91	0.12	93,126,151,153	0
6	NAG	K	2	14/15	0.91	0.14	116,148,185,192	0

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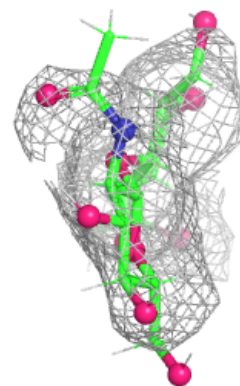
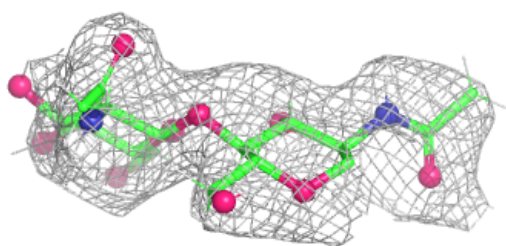
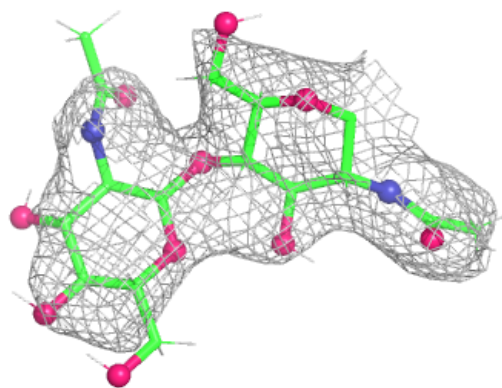
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	K	1	14/15	0.95	0.08	55,95,127,136	0
6	NAG	I	1	14/15	0.96	0.07	66,98,121,123	0
7	BMA	J	3	11/12	-	-	93,132,158,161	0
7	MAN	J	4	11/12	-	-	104,129,153,155	0

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.

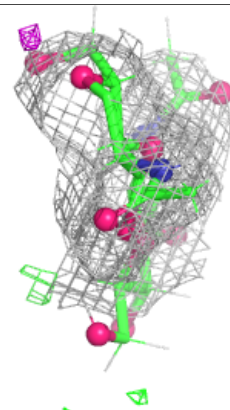
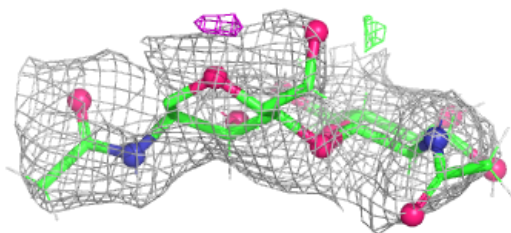
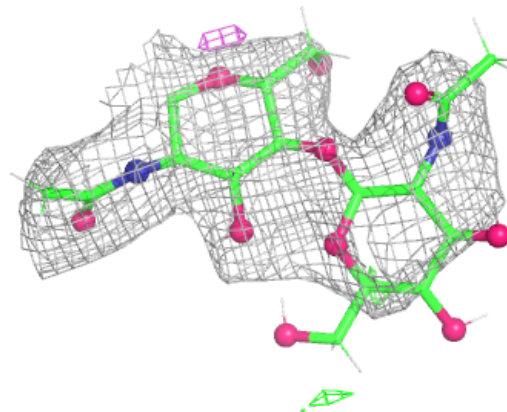


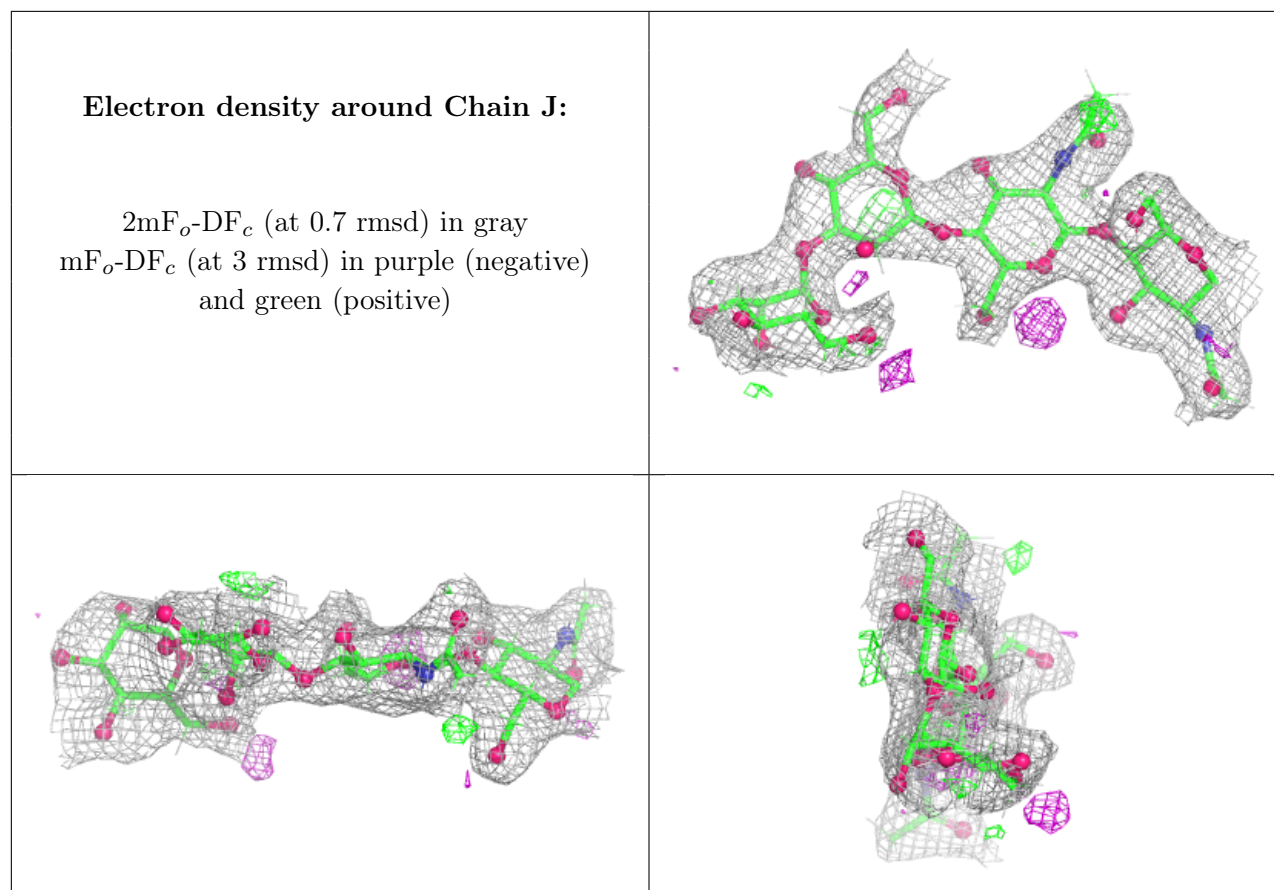
Electron density around Chain I:

$2mF_o-DF_c$ (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)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
13	NAG	B	3099	14/15	0.76	0.14	95,127,149,154	0
13	NAG	D	3099	14/15	0.79	0.14	78,100,120,127	0
9	SO4	L	1215	5/5	0.83	0.16	100,105,109,119	0
9	SO4	C	1458	5/5	0.83	0.14	59,107,112,117	0
9	SO4	C	1459	5/5	0.83	0.16	132,135,136,141	0
9	SO4	C	1457	5/5	0.86	0.10	88,112,116,117	0
9	SO4	C	1460	5/5	0.88	0.20	105,113,126,134	0
9	SO4	D	1472	5/5	0.90	0.15	62,114,118,118	0
8	GOL	A	1459	6/6	0.90	0.17	47,71,81,86	0
8	GOL	C	1455	6/6	0.91	0.14	55,86,104,124	0
8	GOL	B	1467	6/6	0.92	0.14	62,87,101,104	0
8	GOL	A	1460	6/6	0.92	0.12	50,67,81,89	0
9	SO4	A	1462	5/5	0.92	0.14	94,110,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SO4	C	1456	5/5	0.92	0.14	56,99,110,117	0
8	GOL	C	1454	6/6	0.94	0.12	46,71,85,85	0
8	GOL	A	1458	6/6	0.94	0.13	42,62,82,82	0
9	SO4	A	1461	5/5	0.95	0.17	48,71,91,109	0
10	CA	A	2007	1/1	0.98	0.02	14,14,14,14	0
10	CA	C	2004	1/1	0.98	0.04	47,47,47,47	0
12	MN	B	2002	1/1	0.98	0.04	41,41,41,41	0
9	SO4	D	1473	5/5	0.98	0.07	19,55,61,81	0
10	CA	A	2004	1/1	0.98	0.02	28,28,28,28	0
10	CA	C	2007	1/1	0.99	0.03	38,38,38,38	0
11	CL	B	1468	1/1	0.99	0.04	26,26,26,26	0
10	CA	A	2005	1/1	0.99	0.02	15,15,15,15	0
12	MN	D	2001	1/1	0.99	0.02	31,31,31,31	0
12	MN	D	2002	1/1	0.99	0.04	43,43,43,43	0
10	CA	C	2005	1/1	0.99	0.02	38,38,38,38	0
10	CA	C	2006	1/1	0.99	0.04	33,33,33,33	0
10	CA	A	2006	1/1	1.00	0.03	14,14,14,14	0
12	MN	D	2003	1/1	1.00	0.03	34,34,34,34	0
12	MN	B	2003	1/1	1.00	0.02	25,25,25,25	0
12	MN	B	2001	1/1	1.00	0.03	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.