



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:18 AM UTC

PDB ID : 3ZDZ / pdb_00003zdz
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 : 2.75 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

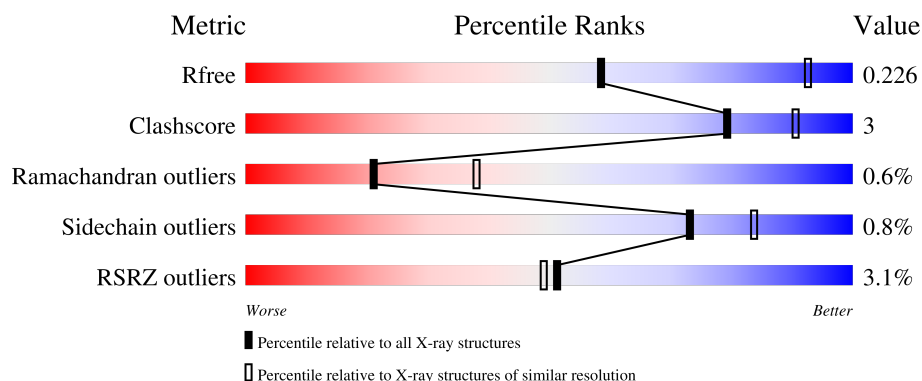
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	0% 96% .
1	C	457	2% 94% ..
2	B	472	4% 88% 9% ..
2	D	472	3% 92% 7% .
3	E	221	8% 92% 5% .

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

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 41823 atoms, of which 20224 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	455	Total	C	H	N	O	S	2	6	0
			6889	2240	3368	607	666	8			
1	C	453	Total	C	H	N	O	S	2	2	0
			6795	2214	3311	600	662	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	1	0
			7083	2233	3498	612	707	33			
2	D	469	Total	C	H	N	O	S	11	0	0
			7133	2248	3521	617	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			

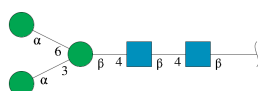
- Molecule 4 is a protein called 10E5 FAB LIGHT CHAIN.

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 a protein called RGD PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	0	0
			75	22	34	9	10			
5	J	5	Total	C	H	N	O	0	0	0
			60	17	27	8	8			

- Molecule 6 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
6	G	5	Total	C	H	N	O	0	0	0
			113	34	52	2	25			

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



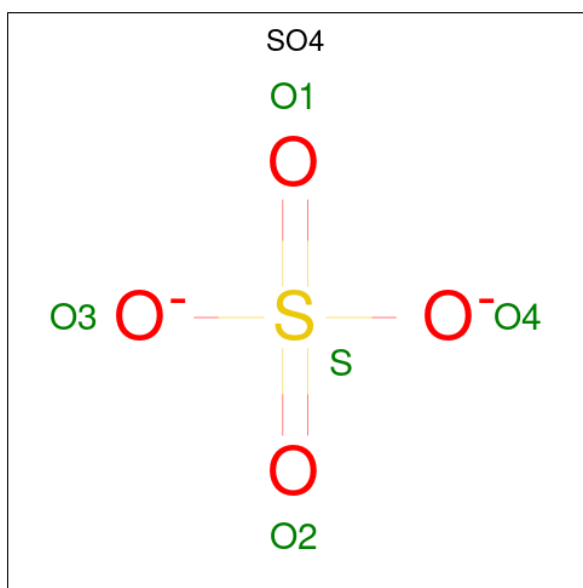
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
7	N	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 8 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
8	M	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

- 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	C	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		

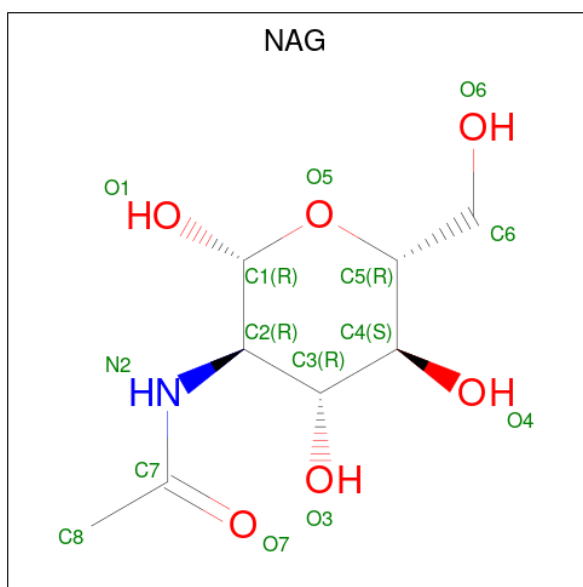
- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	Cl	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	251	Total	O	0	0
			251	251		
14	B	103	Total	O	0	0
			103	103		
14	C	92	Total	O	0	0
			92	92		
14	D	46	Total	O	0	0
			46	46		
14	E	7	Total	O	0	0
			7	7		
14	F	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	21	Total 21	O 21	0	0
14	I	1	Total 1	O 1	0	0
14	J	1	Total 1	O 1	0	0
14	L	15	Total 15	O 15	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.

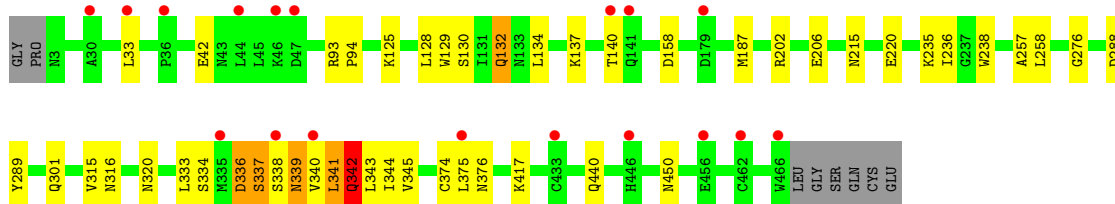
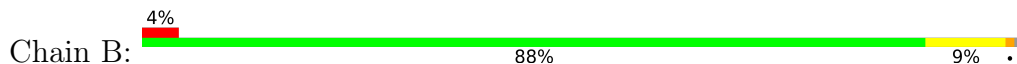
• Molecule 1: INTEGRIN ALPHA-IIB



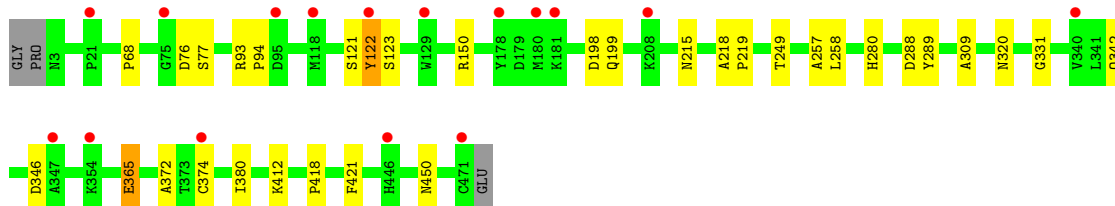
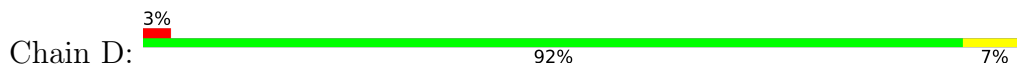
• Molecule 1: INTEGRIN ALPHA-IIB



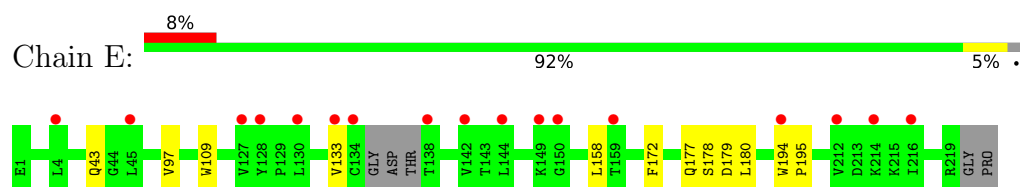
• Molecule 2: INTEGRIN BETA-3



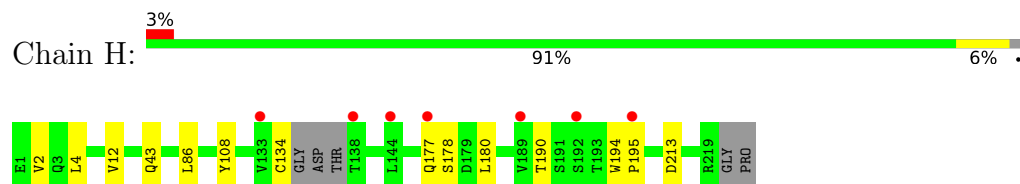
• Molecule 2: INTEGRIN BETA-3



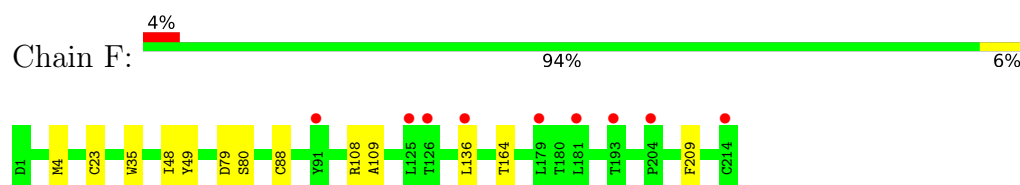
• Molecule 3: 10E5 FAB HEAVY CHAIN



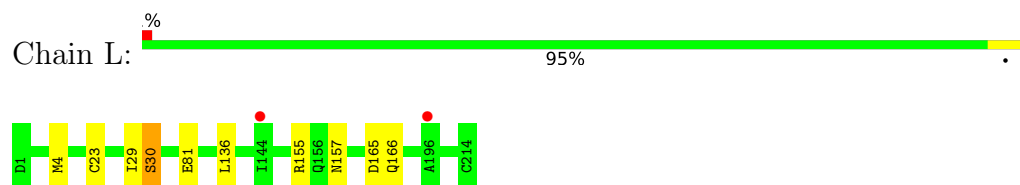
- Molecule 3: 10E5 FAB HEAVY CHAIN



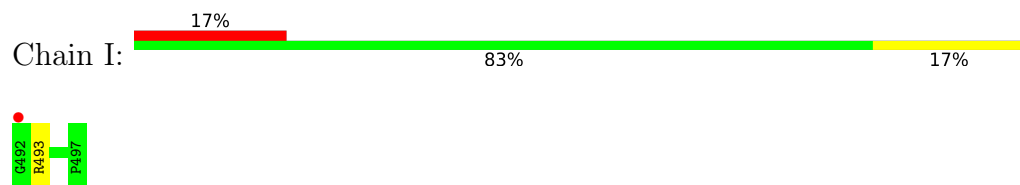
- Molecule 4: 10E5 FAB LIGHT CHAIN



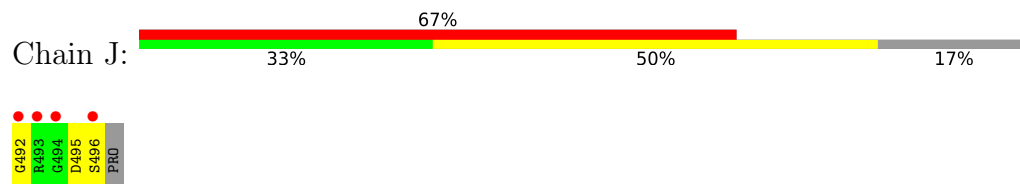
- Molecule 4: 10E5 FAB LIGHT CHAIN



- Molecule 5: RGD PEPTIDE



- Molecule 5: RGD PEPTIDE



- Molecule 6: 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



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

Chain K:  100%

NAG1
NAG2

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

Chain N:  100%

NAG1
NAG2

- Molecule 8: 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 M:  100%

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	259.62Å 144.47Å 104.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 2.75 48.28 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.28-2.75) 99.8 (48.28-2.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.184 , 0.221 0.190 , 0.226	Depositor DCC
R_{free} test set	1032 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41823	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, MN, CA, BMA, NAG, SO4, CL

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	0.28	0/3636	0.64	0/4954
1	C	0.26	0/3587	0.63	2/4888 (0.0%)
2	B	0.27	0/3654	0.66	1/4954 (0.0%)
2	D	0.25	0/3678	0.61	0/4986
3	E	0.24	0/1684	0.60	0/2305
3	H	0.24	0/1684	0.60	0/2305
4	F	0.23	0/1673	0.56	0/2269
4	L	0.24	0/1673	0.59	0/2269
5	I	0.30	0/41	0.59	0/52
5	J	0.36	0/32	0.64	0/40
All	All	0.26	0/21342	0.62	3/29022 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	342	GLN	N-CA-C	-8.33	102.90	113.23
1	C	39	ALA	CA-C-N	5.56	125.27	119.82
1	C	39	ALA	C-N-CA	5.56	125.27	119.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3521	3368	3377	10	0
1	C	3484	3311	3320	13	0
2	B	3585	3498	3504	32	0
2	D	3612	3521	3527	21	0
3	E	1642	1597	1600	7	0
3	H	1642	1597	1600	10	0
4	F	1637	1550	1553	8	0
4	L	1637	1550	1553	7	0
5	I	41	34	34	1	0
5	J	33	27	27	6	0
6	G	61	52	52	2	0
7	K	28	25	25	0	0
7	N	28	25	25	1	0
8	M	50	43	43	0	0
9	A	5	0	0	1	0
9	C	5	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	3	0	0	0	0
11	D	3	0	0	0	0
12	B	14	13	13	0	0
12	D	14	13	13	0	0
13	C	1	0	0	0	0
14	A	251	0	0	3	1
14	B	103	0	0	3	0
14	C	92	0	0	1	1
14	D	46	0	0	4	0
14	E	7	0	0	0	0
14	F	3	0	0	0	0
14	H	21	0	0	3	0
14	I	1	0	0	0	0
14	J	1	0	0	1	0
14	L	15	0	0	2	0
All	All	21599	20224	20266	111	1

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 3.

All (111) 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:B:336:ASP:O	2:B:337:SER:OG	2.07	0.71
6:G:3:BMA:H62	6:G:5:MAN:H5	1.73	0.69
3:H:134:CYS:SG	14:H:4018:HOH:O	2.51	0.68
9:A:1456:SO4:S	14:A:4225:HOH:O	2.52	0.67
2:B:301:GLN:NE2	14:B:4082:HOH:O	2.28	0.67
2:D:150:ARG:NH1	14:D:4012:HOH:O	2.27	0.66
2:D:68:PRO:O	14:D:4002:HOH:O	2.15	0.64
4:F:108:ARG:NH1	4:F:109:ALA:O	2.32	0.62
1:C:73:ARG:NH1	14:C:4023:HOH:O	2.32	0.61
2:D:331:GLY:N	14:D:4036:HOH:O	2.33	0.61
3:H:134:CYS:N	14:H:4018:HOH:O	2.33	0.61
2:D:280:HIS:O	14:D:4031:HOH:O	2.17	0.59
1:A:225:SER:O	5:I:493:ARG:NH2	2.36	0.58
1:C:122:ALA:O	1:C:123:GLU:HB2	2.04	0.57
1:A:122:ALA:O	1:A:123:GLU:HB2	2.04	0.57
6:G:3:BMA:H62	6:G:5:MAN:C5	2.35	0.57
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.38	0.57
5:J:495:ASP:O	5:J:496:SER:C	2.49	0.56
1:A:341:GLY:N	14:A:4187:HOH:O	2.39	0.55
1:C:224:ASP:OD1	1:C:225:SER:N	2.38	0.55
2:B:125:LYS:O	14:B:4012:HOH:O	2.18	0.55
3:H:177:GLN:N	3:H:180:LEU:O	2.41	0.54
2:B:257:ALA:O	2:B:258:LEU:HB2	2.08	0.54
1:A:90[A]:ARG:NH1	14:A:4055:HOH:O	2.40	0.53
2:B:235:LYS:NZ	2:B:276:GLY:O	2.42	0.52
2:B:342:GLN:O	2:B:345:VAL:N	2.42	0.52
1:A:122:ALA:O	1:A:123:GLU:CB	2.57	0.52
5:J:492:GLY:N	14:J:4001:HOH:O	2.41	0.52
2:B:450:ASN:O	2:B:450:ASN:ND2	2.43	0.52
2:B:340:VAL:O	2:B:341:LEU:CB	2.59	0.51
1:C:24:ASP:OD1	1:C:25:PHE:N	2.44	0.51
1:C:160:PHE:CD2	5:J:492:GLY:N	2.78	0.51
1:C:28:ASP:OD1	1:C:32:ARG:N	2.44	0.51
1:C:122:ALA:O	1:C:123:GLU:CB	2.59	0.51
2:D:257:ALA:O	2:D:258:LEU:HB2	2.11	0.50
2:D:76:ASP:OD1	2:D:77:SER:N	2.45	0.50
4:L:155:ARG:O	14:L:4011:HOH:O	2.19	0.49
2:B:129:TRP:CE3	2:B:130:SER:HA	2.47	0.49
3:H:194:TRP:CG	3:H:195:PRO:HA	2.48	0.49
2:B:158:ASP:HB3	2:B:187:MET:CE	2.42	0.49
2:B:340:VAL:O	2:B:341:LEU:HB2	2.11	0.49
1:C:2:ASN:N	1:C:2:ASN:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:ASN:OD1	2:B:342:GLN:N	2.46	0.49
7:N:1:NAG:O3	7:N:2:NAG:O5	2.23	0.49
2:B:340:VAL:O	2:B:341:LEU:HG	2.14	0.48
2:D:198:ASP:OD1	2:D:199:GLN:NE2	2.46	0.48
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.94	0.48
2:B:130:SER:O	2:B:341:LEU:CD1	2.61	0.48
3:E:194:TRP:CG	3:E:195:PRO:HA	2.49	0.48
3:H:213:ASP:OD1	3:H:213:ASP:N	2.47	0.48
1:A:194:LEU:HD12	1:A:194:LEU:C	2.38	0.47
4:L:4:MET:HE3	4:L:23:CYS:SG	2.55	0.47
1:A:132:LEU:HD12	1:A:132:LEU:N	2.29	0.47
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.97	0.46
2:D:342:GLN:NE2	2:D:346:ASP:OD1	2.48	0.46
2:D:121:SER:O	2:D:123:SER:N	2.49	0.46
2:B:288:ASP:OD1	2:B:289:TYR:N	2.50	0.45
4:L:157:ASN:ND2	14:L:4014:HOH:O	2.49	0.45
2:B:134:LEU:HA	2:B:137:LYS:CD	2.46	0.45
4:F:35:TRP:CZ3	4:F:88:CYS:HB3	2.52	0.45
2:D:121:SER:HB2	5:J:495:ASP:OD1	2.16	0.45
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.52	0.45
2:B:333:LEU:HA	2:B:340:VAL:HG13	1.98	0.44
2:D:450:ASN:O	2:D:450:ASN:ND2	2.51	0.44
4:F:4:MET:HE3	4:F:23:CYS:SG	2.58	0.44
2:D:288:ASP:OD1	2:D:289:TYR:N	2.46	0.44
1:A:271:ASP:OD1	1:A:271:ASP:C	2.61	0.43
4:F:136:LEU:HD12	4:F:136:LEU:N	2.33	0.43
2:D:93:ARG:HB2	2:D:94:PRO:HD2	2.00	0.43
2:B:42:GLU:OE1	2:B:42:GLU:N	2.51	0.43
4:F:48:ILE:HG22	4:F:49:TYR:N	2.34	0.43
4:F:79:ASP:OD1	4:F:80:SER:N	2.50	0.43
2:B:341:LEU:O	14:B:4095:HOH:O	2.21	0.43
1:A:285:MET:O	1:A:286:ALA:HB3	2.19	0.43
3:H:190:THR:O	14:H:4020:HOH:O	2.20	0.43
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.54	0.43
2:D:122:TYR:N	5:J:495:ASP:OD2	2.52	0.43
4:L:136:LEU:HD12	4:L:136:LEU:N	2.33	0.43
3:E:178:SER:O	3:E:179:ASP:HB2	2.19	0.43
3:H:43:GLN:OE1	3:H:43:GLN:N	2.52	0.43
2:B:220:GLU:HA	2:B:220:GLU:OE1	2.19	0.42
1:C:194:LEU:C	1:C:194:LEU:HD12	2.44	0.42
3:E:177:GLN:N	3:E:180:LEU:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:81:GLU:OE1	4:L:81:GLU:N	2.53	0.42
2:B:236:ILE:HG21	2:B:238:TRP:CE2	2.55	0.42
2:B:315:VAL:HG13	2:B:316:ASN:N	2.35	0.42
2:B:339:ASN:CG	2:B:342:GLN:HB3	2.45	0.42
3:E:43:GLN:OE1	3:E:43:GLN:N	2.51	0.42
1:A:285:MET:SD	2:B:320:ASN:HB3	2.60	0.41
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.53	0.41
2:B:129:TRP:CE3	2:B:130:SER:CA	3.03	0.41
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.50	0.41
4:F:209:PHE:CD1	4:F:209:PHE:C	2.98	0.41
4:L:165:ASP:O	4:L:166:GLN:C	2.63	0.41
2:D:249:THR:HG22	2:D:309:ALA:HB3	2.01	0.41
2:B:342:GLN:C	2:B:344:ILE:N	2.78	0.41
3:H:2:VAL:HG11	3:H:108:TYR:CD2	2.56	0.41
2:B:338:SER:O	2:B:339:ASN:HB2	2.21	0.41
2:B:374:CYS:O	2:B:376:ASN:N	2.53	0.41
1:C:285:MET:SD	2:D:320:ASN:HB3	2.60	0.41
2:D:372:ALA:O	2:D:380:ILE:N	2.52	0.41
3:E:158:LEU:HD23	3:E:158:LEU:C	2.46	0.41
3:H:4:LEU:HD12	3:H:4:LEU:N	2.36	0.41
1:C:390:LEU:HD12	1:C:390:LEU:N	2.36	0.41
2:B:341:LEU:HD23	2:B:341:LEU:HA	1.93	0.40
1:C:280:LEU:CD1	1:C:306:LEU:HD23	2.52	0.40
1:C:235:TRP:CZ2	1:C:270:LEU:HD11	2.55	0.40
3:E:97:VAL:HG22	3:E:109:TRP:CD2	2.56	0.40
2:B:334:SER:O	2:B:340:VAL:HG21	2.21	0.40
4:L:29:ILE:O	4:L:30:SER:C	2.63	0.40
2:D:123:SER:HB3	5:J:495:ASP:O	2.22	0.40

All (1) 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:4236:HOH:O	14:C:4002:HOH:O[1_554]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/457 (100%)	442 (96%)	16 (4%)	1 (0%)	43	64
1	C	453/457 (99%)	431 (95%)	21 (5%)	1 (0%)	43	64
2	B	463/472 (98%)	435 (94%)	20 (4%)	8 (2%)	7	14
2	D	467/472 (99%)	437 (94%)	28 (6%)	2 (0%)	30	50
3	E	212/221 (96%)	196 (92%)	15 (7%)	1 (0%)	24	43
3	H	212/221 (96%)	197 (93%)	14 (7%)	1 (0%)	24	43
4	F	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
4	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	43
5	I	4/6 (67%)	4 (100%)	0	0	100	100
5	J	3/6 (50%)	3 (100%)	0	0	100	100
All	All	2697/2740 (98%)	2548 (94%)	134 (5%)	15 (1%)	21	38

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	341	LEU
2	B	343	LEU
1	A	123	GLU
2	B	337	SER
2	B	339	ASN
2	B	375	LEU
2	B	440	GLN
1	C	123	GLU
3	E	133	VAL
2	B	33	LEU
2	D	122	TYR
3	H	178	SER
2	B	132	GLN
2	D	374	CYS

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Mol	Chain	Res	Type
4	L	30	SER

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	369/364 (101%)	363 (98%)	6 (2%)	55	73
1	C	363/364 (100%)	359 (99%)	4 (1%)	65	79
2	B	412/417 (99%)	405 (98%)	7 (2%)	53	71
2	D	415/417 (100%)	413 (100%)	2 (0%)	81	89
3	E	187/190 (98%)	187 (100%)	0	100	100
3	H	187/190 (98%)	187 (100%)	0	100	100
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
5	I	4/4 (100%)	4 (100%)	0	100	100
5	J	3/4 (75%)	3 (100%)	0	100	100
All	All	2316/2326 (100%)	2297 (99%)	19 (1%)	73	84

All (19) 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	267	VAL
1	A	270	LEU
1	A	288	TYR
2	B	128	LEU
2	B	132	GLN
2	B	140	THR
2	B	215	ASN
2	B	336	ASP
2	B	342	GLN

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Mol	Chain	Res	Type
2	B	417	LYS
1	C	23	LEU
1	C	166	TYR
1	C	270	LEU
1	C	288	TYR
2	D	215	ASN
2	D	365	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	197	GLN
1	A	215	HIS
1	A	338	HIS
1	A	372	ASN
2	B	272	GLN
2	B	305	ASN
1	C	158	ASN
1	C	388	GLN
2	D	199	GLN
2	D	210	GLN
2	D	301	GLN
2	D	305	ASN
2	D	450	ASN
4	F	190	ASN
3	H	170	HIS
4	L	27	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	$\# Z > 2$
6	NAG	G	1	2,6	14,14,15	0.54	0	17,19,21	0.67	0
6	NAG	G	2	6	14,14,15	0.57	0	17,19,21	0.71	0
6	BMA	G	3	6	11,11,12	0.59	0	15,15,17	0.70	0
6	MAN	G	4	6	11,11,12	0.62	0	15,15,17	0.53	0
6	MAN	G	5	6	11,11,12	0.46	0	15,15,17	1.58	1 (6%)
7	NAG	K	1	2,7	14,14,15	0.58	0	17,19,21	0.86	0
7	NAG	K	2	7	14,14,15	0.53	0	17,19,21	0.54	0
8	NAG	M	1	2,8	14,14,15	0.53	0	17,19,21	0.71	0
8	NAG	M	2	8	14,14,15	0.53	0	17,19,21	0.58	0
8	BMA	M	3	8	11,11,12	0.64	0	15,15,17	0.72	0
8	MAN	M	4	8	11,11,12	0.63	0	15,15,17	0.55	0
7	NAG	N	1	2,7	14,14,15	0.59	0	17,19,21	0.73	0
7	NAG	N	2	7	14,14,15	0.53	0	17,19,21	0.57	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	G	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	2/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	2/2/19/22	0/1/1/1
7	NAG	K	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
8	NAG	M	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
8	BMA	M	3	8	-	0/2/19/22	0/1/1/1
8	MAN	M	4	8	-	0/2/19/22	0/1/1/1
7	NAG	N	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	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($^{\circ}$)	Ideal($^{\circ}$)
6	G	5	MAN	C1-O5-C5	5.34	119.34	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

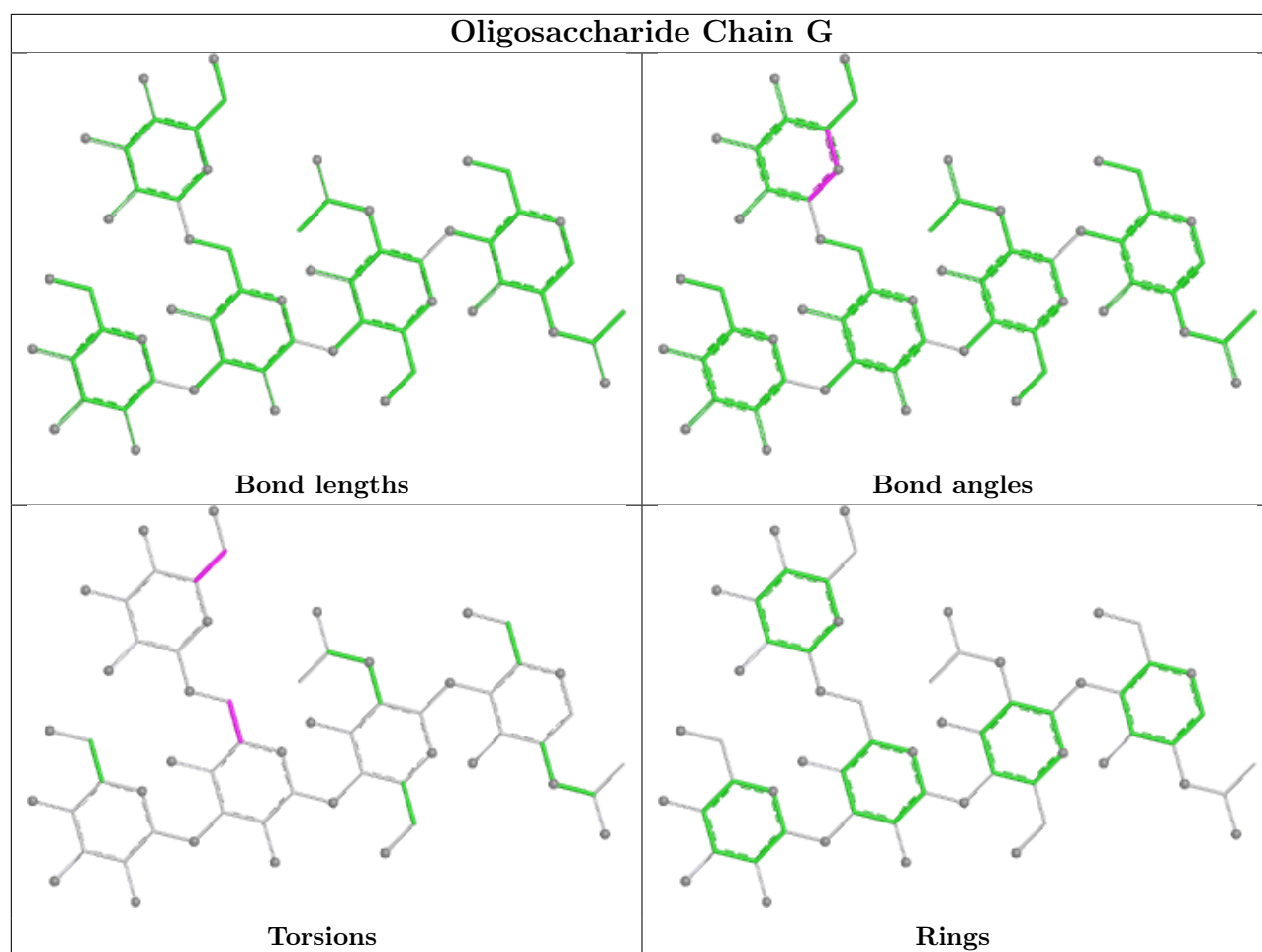
Mol	Chain	Res	Type	Atoms
7	N	2	NAG	C8-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
8	M	2	NAG	O7-C7-N2-C2
8	M	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O5-C5-C6-O6
7	N	1	NAG	C8-C7-N2-C2
6	G	5	MAN	C4-C5-C6-O6
6	G	3	BMA	C4-C5-C6-O6
7	N	1	NAG	O7-C7-N2-C2
6	G	5	MAN	O5-C5-C6-O6
6	G	3	BMA	O5-C5-C6-O6

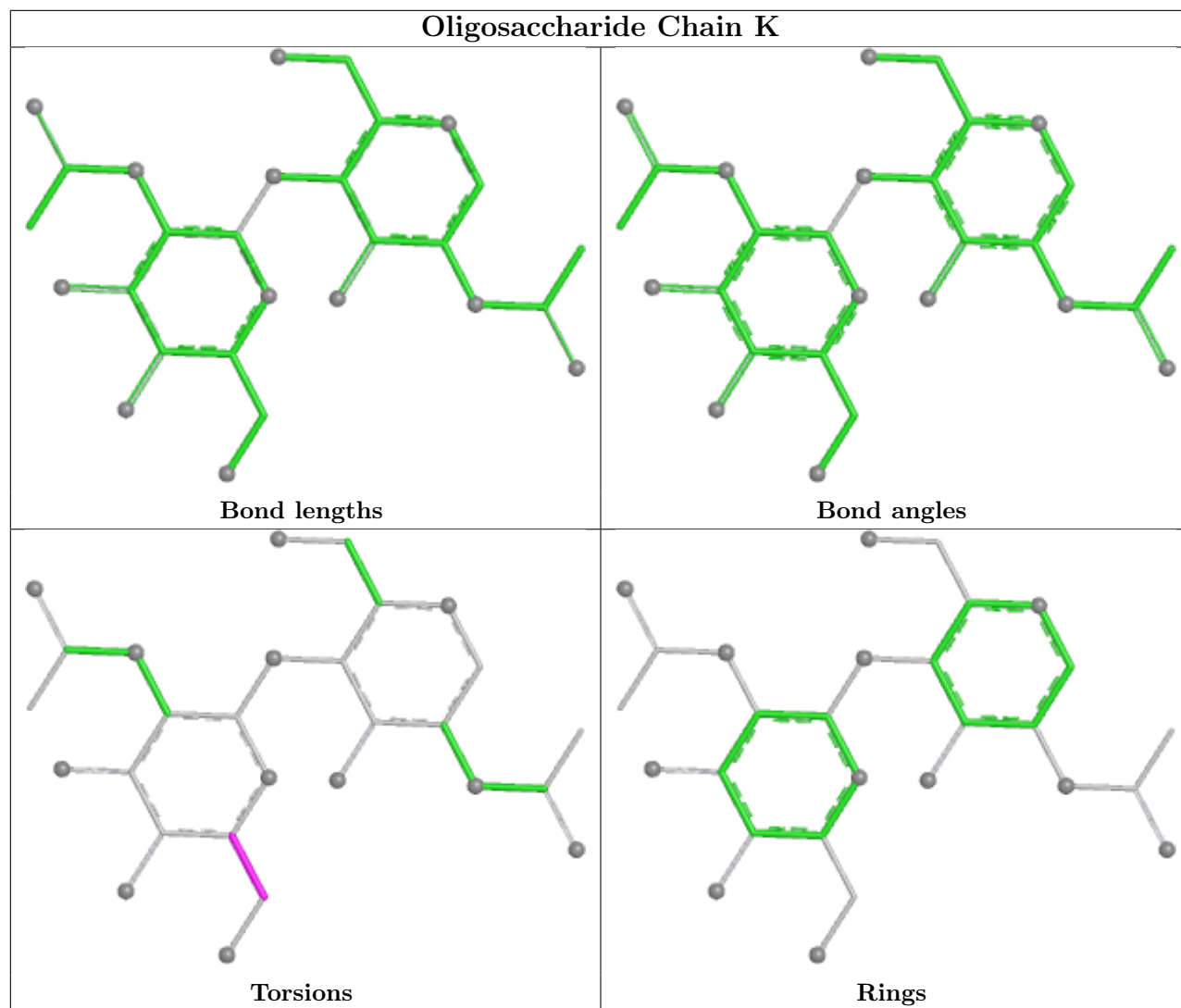
There are no ring outliers.

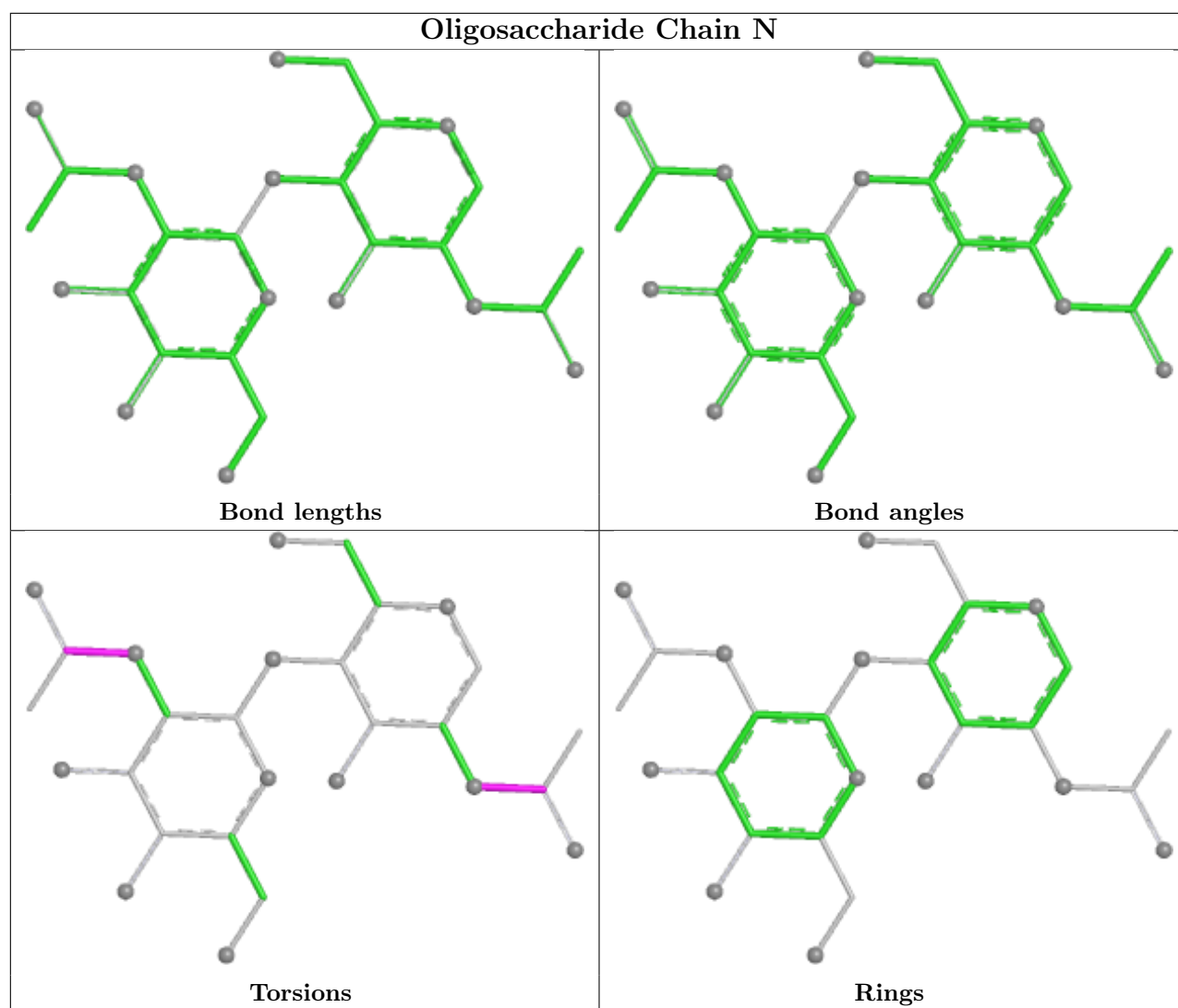
4 monomers are involved in 3 short contacts:

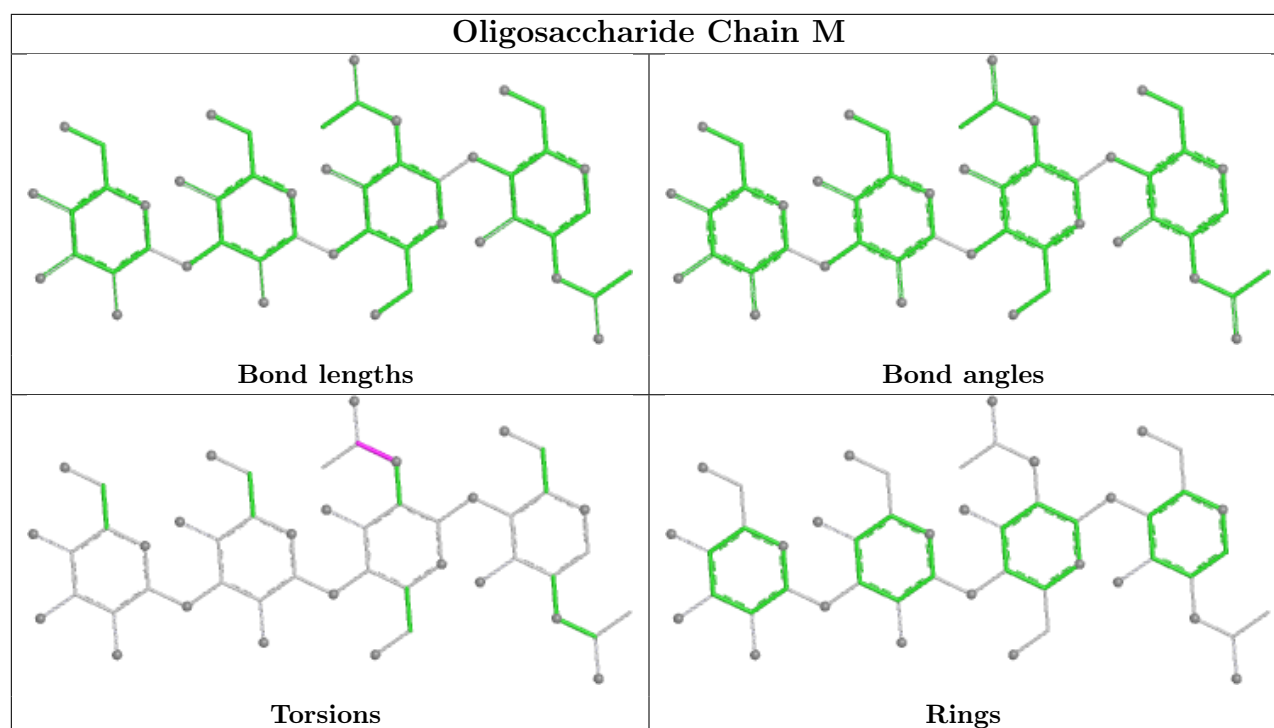
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	3	BMA	2	0
6	G	5	MAN	2	0
7	N	2	NAG	1	0
7	N	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 15 are monoatomic - leaving 5 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	$\# Z > 2$
12	NAG	D	3099	2	14,14,15	0.52	0	17,19,21	0.55	0
9	SO4	L	1215	-	4,4,4	0.23	0	6,6,6	0.08	0
12	NAG	B	3099	2	14,14,15	0.49	0	17,19,21	0.66	0
9	SO4	A	1456	-	4,4,4	0.24	0	6,6,6	0.07	0
9	SO4	C	1454	-	4,4,4	0.23	0	6,6,6	0.10	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
12	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
12	NAG	D	3099	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	3099	NAG	O5-C5-C6-O6
12	D	3099	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1456	SO4	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	455/457 (99%)	-0.53	3 (0%) 84 84	17, 39, 75, 146	9 (1%)
1	C	453/457 (99%)	-0.01	7 (1%) 72 71	31, 70, 110, 164	4 (0%)
2	B	464/472 (98%)	0.09	18 (3%) 43 40	17, 80, 176, 218	3 (0%)
2	D	469/472 (99%)	0.52	16 (3%) 48 46	48, 103, 168, 217	3 (0%)
3	E	216/221 (97%)	0.87	17 (7%) 18 19	81, 140, 193, 217	0
3	H	216/221 (97%)	0.33	7 (3%) 50 48	46, 109, 178, 211	0
4	F	214/214 (100%)	0.62	9 (4%) 40 39	83, 141, 221, 272	0
4	L	214/214 (100%)	0.15	2 (0%) 81 81	55, 92, 130, 193	0
5	I	6/6 (100%)	0.64	1 (16%) 4 4	43, 63, 89, 101	0
5	J	5/6 (83%)	5.81	4 (80%) 0 0	23, 31, 99, 115	2 (40%)
All	All	2712/2740 (98%)	0.18	84 (3%) 51 49	17, 87, 178, 272	21 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	493	ARG	11.7
5	J	492	GLY	8.3
4	F	181	LEU	5.3
1	A	455	LYS	4.2
2	B	375	LEU	4.1
5	J	496	SER	4.0
3	E	127	VAL	3.9
2	B	466	TRP	3.4
2	B	141	GLN	3.3
1	C	232	ASP	3.3
2	D	181	LYS	3.3
1	C	1	LEU	3.3
3	H	177	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	36	PRO	3.2
3	E	144	LEU	3.2
3	E	133	VAL	3.2
2	D	446	HIS	3.1
5	J	494	GLY	3.1
1	C	339	ALA	3.0
3	E	142	VAL	3.0
3	E	214	LYS	2.9
2	D	471	CYS	2.9
1	C	453	VAL	2.9
4	F	193	THR	2.9
2	B	340	VAL	2.9
2	D	75	GLY	2.8
3	E	128	TYR	2.8
1	A	454	VAL	2.7
3	H	133	VAL	2.7
3	E	45	LEU	2.7
3	H	144	LEU	2.6
3	E	138	THR	2.6
4	F	126	THR	2.6
2	B	335	MET	2.6
4	F	214	CYS	2.6
3	E	134	CYS	2.6
2	B	338	SER	2.5
1	A	337	PRO	2.5
3	E	159	THR	2.4
2	D	95	ASP	2.4
2	B	456	GLU	2.4
2	D	118	MET	2.4
1	C	45	PRO	2.4
3	E	212	VAL	2.4
3	H	138	THR	2.4
2	B	33	LEU	2.3
4	L	196	ALA	2.3
3	E	216	ILE	2.3
2	D	374	CYS	2.3
2	D	129	TRP	2.3
2	B	462	CYS	2.2
2	D	122	TYR	2.2
1	C	32	ARG	2.2
3	H	192	SER	2.2
5	I	492	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
4	L	144	ILE	2.2
4	F	204	PRO	2.2
2	B	46	LYS	2.2
3	E	149	LYS	2.2
2	B	433	CYS	2.2
2	B	44	LEU	2.2
2	D	180	MET	2.2
3	H	189	VAL	2.2
2	B	30	ALA	2.2
2	D	21	PRO	2.2
4	F	179	LEU	2.2
3	E	194	TRP	2.1
2	B	140	THR	2.1
3	E	130	LEU	2.1
3	E	150	GLY	2.1
4	F	136	LEU	2.1
2	B	446	HIS	2.1
2	D	340	VAL	2.1
2	B	47	ASP	2.1
2	B	179	ASP	2.1
2	D	354	LYS	2.1
3	H	195	PRO	2.1
3	E	4	LEU	2.1
2	D	347	ALA	2.0
2	D	208	LYS	2.0
4	F	125	LEU	2.0
1	C	338	HIS	2.0
2	D	178	TYR	2.0
4	F	91	TYR	2.0

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

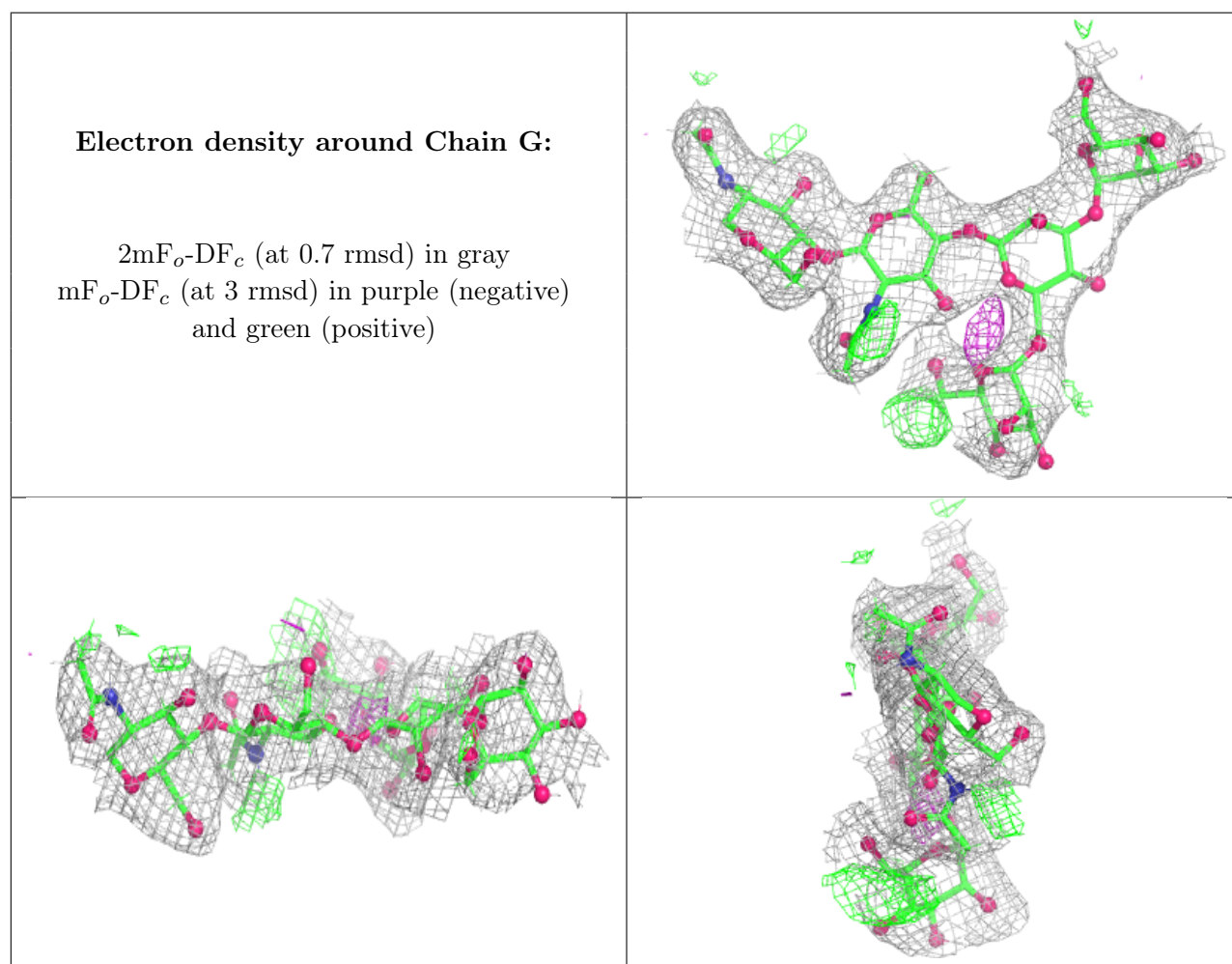
There are no non-standard protein/DNA/RNA residues in this entry.

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.

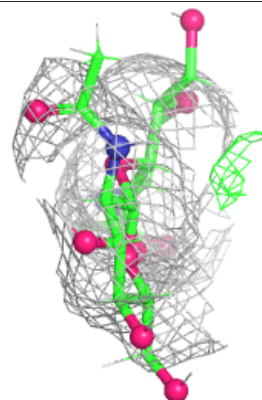
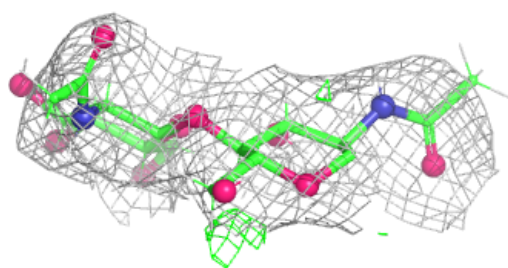
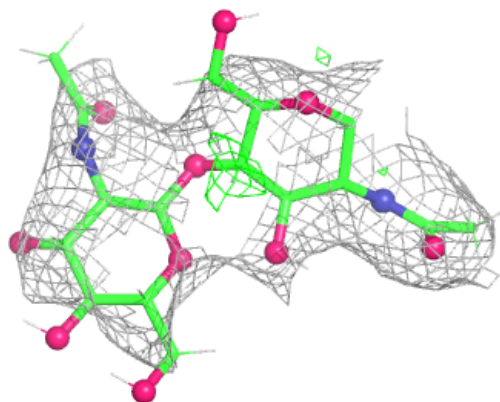
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	G	1	14/15	-	-	27,39,54,62	0
6	NAG	G	2	14/15	-	-	58,81,101,107	0
6	BMA	G	3	11/12	-	-	105,123,149,152	0
6	MAN	G	4	11/12	-	-	113,126,150,153	0
6	MAN	G	5	11/12	-	-	107,119,140,143	0
7	NAG	N	2	14/15	0.20	0.14	149,155,186,188	0
8	MAN	M	4	11/12	0.41	0.15	170,173,208,208	0
8	BMA	M	3	11/12	0.58	0.13	148,158,186,190	0
7	NAG	N	1	14/15	0.83	0.12	101,135,155,162	0
8	NAG	M	2	14/15	0.83	0.10	107,128,152,154	0
7	NAG	K	2	14/15	0.89	0.10	125,150,180,183	0
8	NAG	M	1	14/15	0.95	0.10	67,97,119,119	0
7	NAG	K	1	14/15	0.96	0.07	89,118,147,149	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.

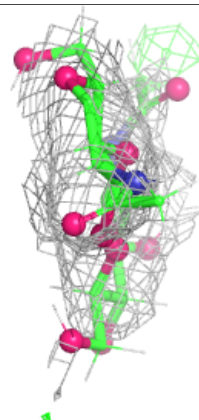
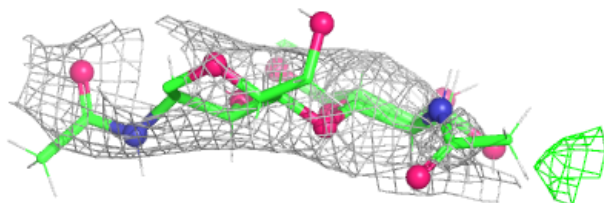
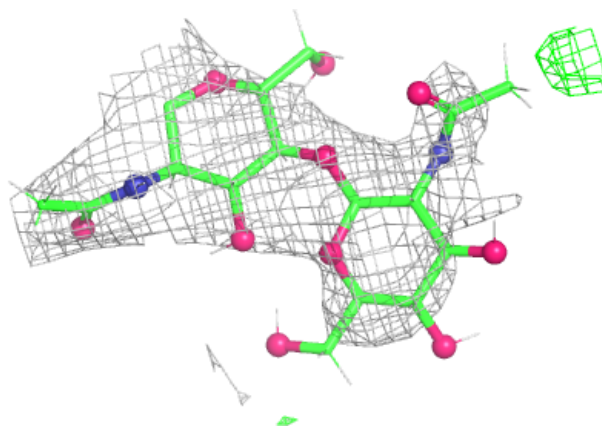


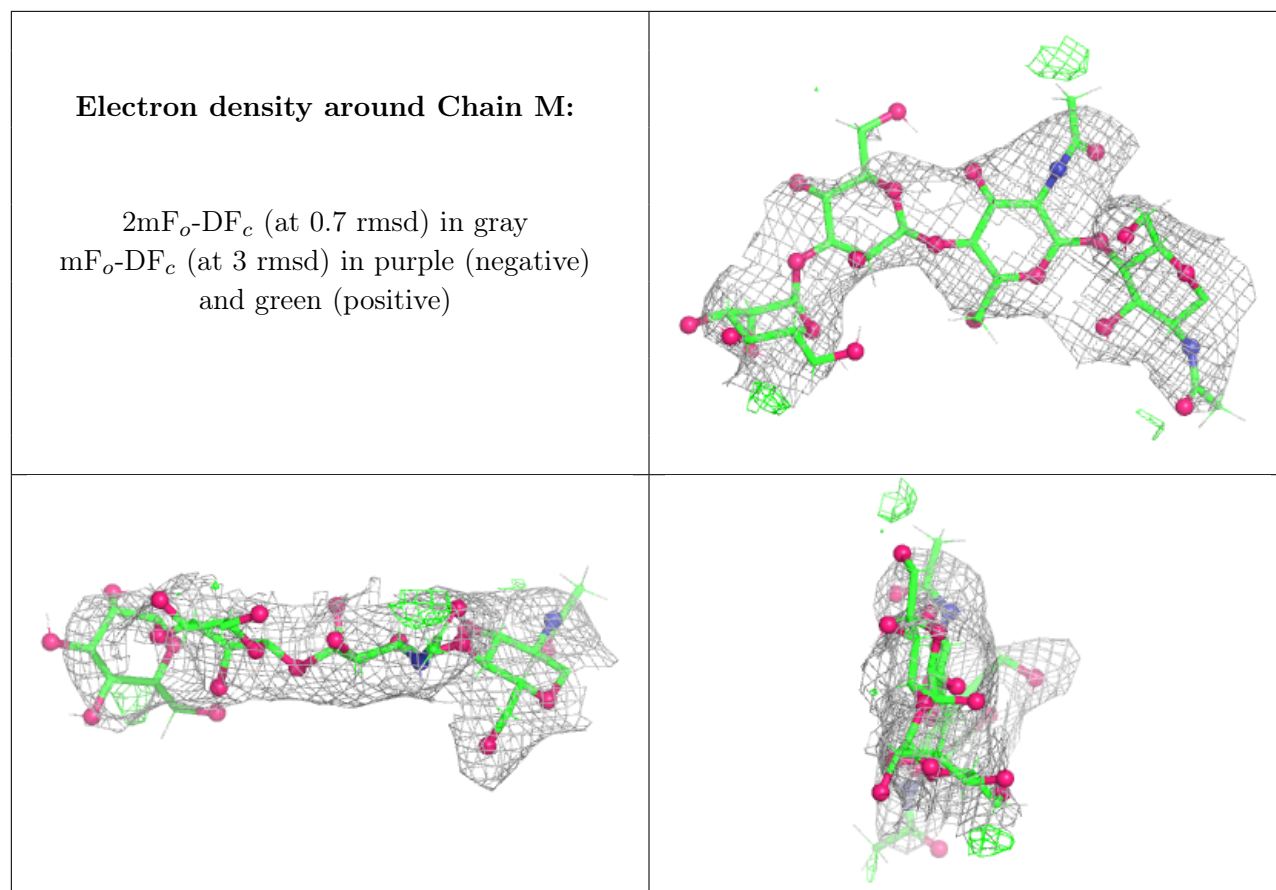
Electron density around Chain K:

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

**Electron density around Chain N:**

$2mF_o-DF_c$ (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
12	NAG	D	3099	14/15	0.55	0.16	95,125,149,149	0
12	NAG	B	3099	14/15	0.82	0.10	91,120,143,146	0
9	SO4	L	1215	5/5	0.86	0.11	130,131,132,133	0
9	SO4	C	1454	5/5	0.87	0.14	130,131,132,134	0
11	MN	D	2002	1/1	0.91	0.08	129,129,129,129	0
9	SO4	A	1456	5/5	0.96	0.09	66,73,78,90	0
13	CL	C	1455	1/1	0.97	0.16	73,73,73,73	0
10	CA	C	2004	1/1	0.98	0.04	100,100,100,100	0
10	CA	C	2007	1/1	0.99	0.04	59,59,59,59	0
11	MN	B	2002	1/1	0.99	0.03	58,58,58,58	0
11	MN	D	2001	1/1	0.99	0.04	81,81,81,81	0
10	CA	A	2005	1/1	0.99	0.04	34,34,34,34	0
11	MN	D	2003	1/1	0.99	0.05	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	CA	A	2006	1/1	0.99	0.02	33,33,33,33	0
10	CA	A	2004	1/1	0.99	0.02	40,40,40,40	0
10	CA	C	2006	1/1	0.99	0.03	62,62,62,62	0
10	CA	A	2007	1/1	1.00	0.01	30,30,30,30	0
11	MN	B	2003	1/1	1.00	0.02	45,45,45,45	0
10	CA	C	2005	1/1	1.00	0.02	78,78,78,78	0
11	MN	B	2001	1/1	1.00	0.13	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.