



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:09 AM UTC

PDB ID : 3ZDY / pdb_00003zdy
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:

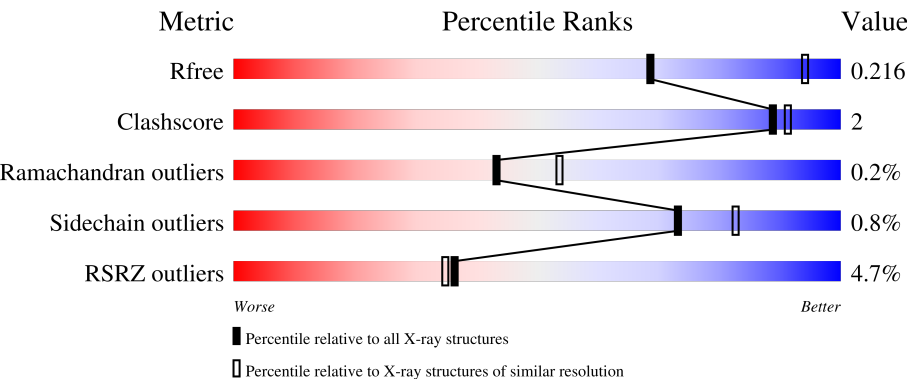
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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	% 95% ..
1	C	457	% 96% ..
2	B	472	3% 94% ..
2	D	472	2% 94% ..
3	E	221	22% 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	4	
6	M	4	
7	K	2	
7	N	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
8	SO4	A	1462	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 42366 atoms, of which 20280 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	454	Total	C	H	N	O	S	1	7	0
			6862	2233	3352	602	667	8			
1	C	453	Total	C	H	N	O	S	1	3	0
			6809	2218	3319	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	7	5	0
			7131	2246	3525	615	711	34			
2	D	469	Total	C	H	N	O	S	11	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 a protein called RGD PEPTIDE.

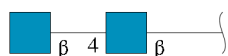
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	3	0
			112	32	52	15	13			
5	J	5	Total	C	H	N	O	0	3	0
			97	27	45	14	11			

- Molecule 6 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
6	G	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			
6	M	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	4	Total Ca 4 4	0	0
9	B	2	Total Ca 2 2	0	0
9	C	4	Total Ca 4 4	0	0
9	D	2	Total Ca 2 2	0	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Mg 1 1	0	0
10	D	1	Total Mg 1 1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 12 is water.

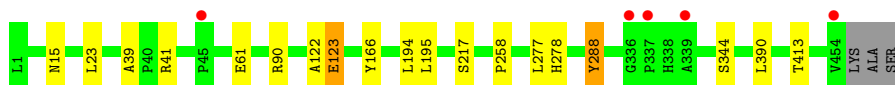
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	357	Total	O	0	2
			359	359		
12	B	157	Total	O	0	0
			157	157		
12	C	192	Total	O	0	0
			192	192		
12	D	109	Total	O	0	0
			109	109		
12	E	10	Total	O	0	0
			10	10		
12	F	9	Total	O	0	0
			9	9		
12	H	25	Total	O	0	0
			25	25		
12	I	6	Total	O	0	0
			6	6		
12	J	1	Total	O	0	0
			1	1		
12	L	21	Total	O	0	0
			21	21		

3 Residue-property plots [i](#)

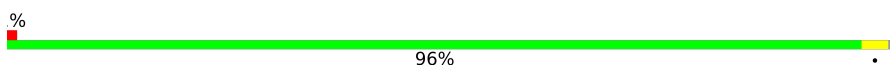
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

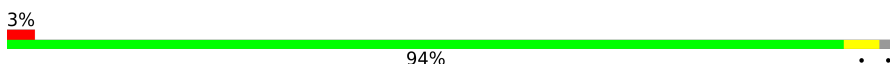


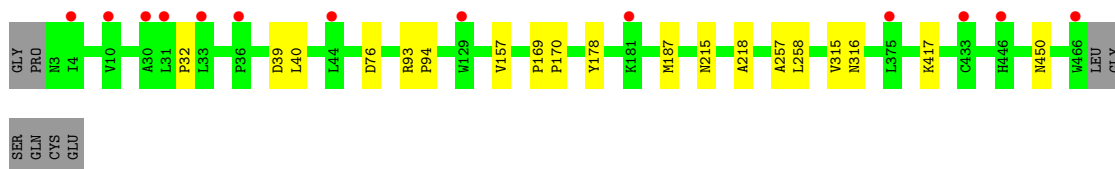
- Molecule 1: INTEGRIN ALPHA-IIB

Chain C: 

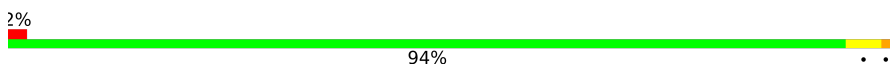


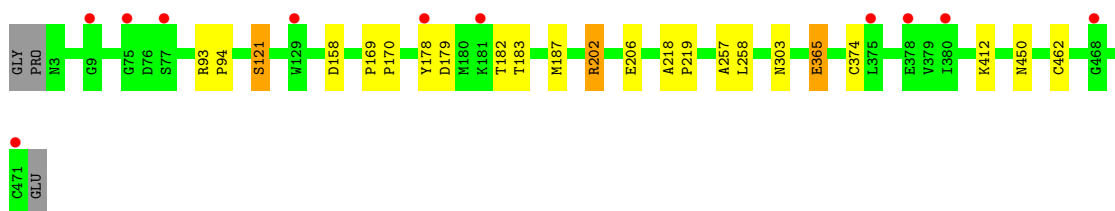
- Molecule 2: INTEGRIN BETA-3

Chain B: 

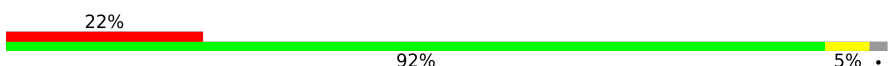


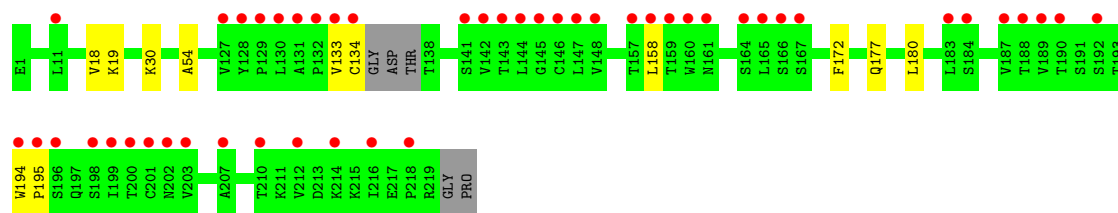
- Molecule 2: INTEGRIN BETA-3

Chain D: 

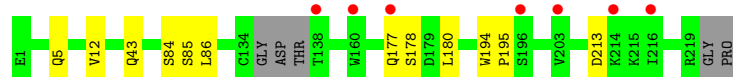


- Molecule 3: 10E5 FAB HEAVY CHAIN

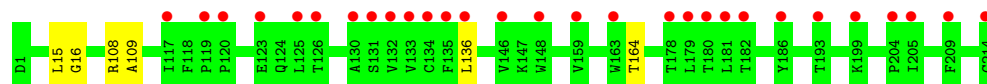
Chain E: 



• Molecule 3: 10E5 FAB HEAVY CHAIN



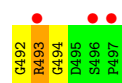
• Molecule 4: 10E5 FAB LIGHT CHAIN



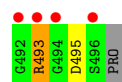
• Molecule 4: 10E5 FAB LIGHT CHAIN



• Molecule 5: RGD PEPTIDE



• Molecule 5: RGD PEPTIDE



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



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

Chain M:  75% 25%


MAG1
MAG2
BMA3
MAN4

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

Chain K:  100%


MAG1
MAG2

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

Chain N:  100%


MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	257.76Å 145.25Å 106.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.45 49.15 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-2.45) 99.8 (49.15-2.45)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.182 , 0.216 0.183 , 0.216	Depositor DCC
R_{free} test set	1015 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42366	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: CA, MG, MAN, SO4, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/3628	0.63	2/4945 (0.0%)
1	C	0.26	0/3596	0.63	0/4900
2	B	0.26	0/3684	0.63	0/4994
2	D	0.26	0/3694	0.60	0/5009
3	E	0.25	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	0.18	0/60	0.59	0/76
5	J	0.16	0/51	0.42	0/64
All	All	0.26	0/21427	0.61	2/29136 (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	A	39	ALA	CA-C-N	5.12	124.78	119.56
1	A	39	ALA	C-N-CA	5.12	124.78	119.56

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	3510	3352	3361	15	0
1	C	3490	3319	3328	10	0
2	B	3606	3525	3530	8	0
2	D	3623	3531	3537	12	0
3	E	1642	1597	1600	7	0
3	H	1642	1597	1600	7	0
4	F	1637	1550	1553	4	0
4	L	1637	1550	1553	7	0
5	I	60	52	51	5	0
5	J	52	45	44	5	0
6	G	50	43	43	0	0
6	M	50	43	43	0	0
7	K	28	25	25	0	0
7	N	28	25	25	0	0
8	A	45	0	0	4	2
8	B	15	0	0	0	0
8	C	25	0	0	1	0
8	D	5	0	0	0	0
8	L	10	0	0	0	0
9	A	4	0	0	0	0
9	B	2	0	0	0	0
9	C	4	0	0	0	0
9	D	2	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	14	13	13	0	0
11	D	14	13	13	0	0
12	A	359	0	0	16	1
12	B	157	0	0	0	0
12	C	192	0	0	3	3
12	D	109	0	0	0	0
12	E	10	0	0	0	0
12	F	9	0	0	0	0
12	H	25	0	0	1	0
12	I	6	0	0	1	0
12	J	1	0	0	0	0
12	L	21	0	0	1	0
All	All	22086	20280	20319	80	3

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 (80) 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)
12:A:3159:HOH:O	5:I:492[B]:GLY:N	1.99	0.95
12:A:3155:HOH:O	5:I:493[A]:ARG:NH1	2.09	0.84
8:A:1462:SO4:S	12:A:3332:HOH:O	2.36	0.83
12:A:3155:HOH:O	5:I:493[B]:ARG:NH2	2.13	0.81
8:A:1462:SO4:O4	12:A:3331:HOH:O	2.06	0.72
8:A:1462:SO4:O4	12:A:3332:HOH:O	2.08	0.70
1:A:278[B]:HIS:NE2	12:A:3228:HOH:O	2.25	0.68
1:A:344:SER:OG	12:A:3265:HOH:O	2.15	0.64
8:C:1458:SO4:O1	12:C:3191:HOH:O	2.15	0.64
4:F:108:ARG:NH1	4:F:109:ALA:O	2.31	0.64
1:A:41:ARG:NH2	12:A:3021:HOH:O	2.34	0.60
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.34	0.60
3:H:5:GLN:N	3:H:5:GLN:OE1	2.35	0.58
1:A:122:ALA:O	1:A:123:GLU:HB2	2.05	0.57
12:H:3008:HOH:O	4:L:38:GLN:OE1	2.18	0.56
1:C:384:SER:OG	12:C:3159:HOH:O	2.18	0.56
8:A:1462:SO4:O1	12:A:3332:HOH:O	2.17	0.55
3:H:177:GLN:N	3:H:180:LEU:O	2.40	0.55
2:B:257:ALA:O	2:B:258:LEU:HB2	2.06	0.55
1:A:413:THR:N	12:A:3331:HOH:O	2.39	0.54
5:I:492[A]:GLY:O	12:I:3001:HOH:O	2.18	0.54
1:A:277:LEU:O	1:A:278[B]:HIS:ND1	2.41	0.54
1:C:122:ALA:O	1:C:123:GLU:HB2	2.08	0.53
1:A:15[B]:ASN:ND2	12:A:3015:HOH:O	2.42	0.51
4:L:157:ASN:ND2	12:L:3018:HOH:O	2.43	0.51
1:A:15[B]:ASN:ND2	12:A:3016:HOH:O	2.44	0.51
1:C:194:LEU:C	1:C:194:LEU:HD12	2.37	0.50
1:A:122:ALA:O	1:A:123:GLU:CB	2.60	0.50
2:D:202:ARG:NH1	2:D:206:GLU:OE2	2.45	0.49
1:A:194:LEU:HD12	1:A:194:LEU:C	2.36	0.49
4:L:81:GLU:N	4:L:81:GLU:OE1	2.44	0.49
2:D:257:ALA:O	2:D:258:LEU:HB2	2.10	0.49
3:H:213:ASP:OD1	3:H:213:ASP:N	2.44	0.48
1:C:258:PRO:HB3	1:C:288:TYR:CD2	2.49	0.48
1:C:277:LEU:O	1:C:278[B]:HIS:ND1	2.48	0.47
3:H:194:TRP:CG	3:H:195:PRO:HA	2.49	0.47
2:B:39:ASP:OD1	2:B:40:LEU:N	2.47	0.47
3:E:133:VAL:O	3:E:134:CYS:SG	2.73	0.47
5:J:493[A]:ARG:HG2	5:J:493[A]:ARG:O	2.13	0.47
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.96	0.47
1:C:122:ALA:O	1:C:123:GLU:CB	2.64	0.46
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.98	0.45
1:C:235:TRP:CZ2	1:C:270:LEU:HD11	2.52	0.45
1:A:15[A]:ASN:ND2	12:A:3014:HOH:O	2.50	0.45
4:L:4:MET:HE3	4:L:23:CYS:SG	2.57	0.45
1:A:90:ARG:NH2	12:A:3042:HOH:O	2.49	0.45
2:B:450:ASN:O	2:B:450:ASN:ND2	2.51	0.44
1:A:217:SER:N	12:A:3174:HOH:O	2.49	0.44
3:E:194:TRP:CG	3:E:195:PRO:HA	2.52	0.44
2:D:450:ASN:O	2:D:450:ASN:ND2	2.51	0.43
2:D:121:SER:HB2	5:J:495:ASP:OD1	2.16	0.43
4:F:136:LEU:HD12	4:F:136:LEU:N	2.33	0.43
2:B:218:ALA:N	5:I:494[A]:GLY:HA2	2.33	0.43
2:B:169:PRO:HB2	2:B:170:PRO:HD2	1.99	0.43
1:C:390:LEU:HD12	1:C:390:LEU:N	2.34	0.43
2:D:218:ALA:HB2	5:J:493[A]:ARG:O	2.18	0.43
1:C:160:PHE:HB2	5:J:493[B]:ARG:HD2	2.01	0.43
3:H:43:GLN:OE1	3:H:43:GLN:N	2.52	0.43
1:A:390:LEU:HD12	1:A:390:LEU:N	2.34	0.42
2:B:315:VAL:HG13	2:B:316:ASN:N	2.34	0.42
3:H:84:SER:O	3:H:85:SER:C	2.61	0.42
1:C:285:MET:O	1:C:286:ALA:HB3	2.19	0.42
2:D:178:TYR:CG	2:D:179:ASP:N	2.87	0.42
3:E:18:VAL:HG12	3:E:19:LYS:N	2.35	0.42
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.50	0.42
12:C:3078:HOH:O	5:J:493[B]:ARG:NH1	2.48	0.42
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.55	0.42
4:L:136:LEU:HD12	4:L:136:LEU:N	2.35	0.42
4:L:140:TYR:CG	4:L:141:PRO:HA	2.55	0.41
2:D:169:PRO:CB	2:D:170:PRO:CD	2.99	0.41
4:F:15:LEU:HD23	4:F:16:GLY:N	2.35	0.41
3:E:158:LEU:HD23	3:E:158:LEU:C	2.45	0.41
3:E:177:GLN:N	3:E:180:LEU:O	2.52	0.41
4:L:175:MET:HG2	4:L:176:SER:N	2.36	0.41
1:A:258:PRO:HB2	1:A:288:TYR:CD2	2.56	0.40
2:B:157:VAL:HG11	2:B:187[B]:MET:SD	2.61	0.40
2:D:158:ASP:HB3	2:D:187:MET:CE	2.51	0.40
3:E:30:LYS:HG3	3:E:54:ALA:HA	2.03	0.40
2:D:182:THR:OG1	2:D:183:THR:N	2.55	0.40

All (3) 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)
8:A:1462:SO4:O2	12:C:3163:HOH:O[1_554]	2.04	0.16
8:A:1462:SO4:O2	12:C:3175:HOH:O[1_554]	2.06	0.14
12:A:3352:HOH:O	12:C:3174:HOH:O[1_554]	2.12	0.08

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	459/457 (100%)	440 (96%)	18 (4%)	1 (0%)	43	54
1	C	454/457 (99%)	440 (97%)	13 (3%)	1 (0%)	43	54
2	B	467/472 (99%)	445 (95%)	20 (4%)	2 (0%)	30	37
2	D	468/472 (99%)	449 (96%)	18 (4%)	1 (0%)	43	54
3	E	212/221 (96%)	197 (93%)	15 (7%)	0	100	100
3	H	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	24	32
4	F	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
4	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
5	I	6/6 (100%)	3 (50%)	3 (50%)	0	100	100
5	J	5/6 (83%)	3 (60%)	2 (40%)	0	100	100
All	All	2707/2740 (99%)	2579 (95%)	122 (4%)	6 (0%)	43	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	76	ASP
1	C	123	GLU
3	H	178	SER
2	B	32	PRO
2	D	374	CYS

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%)	364 (99%)	5 (1%)	59	72
1	C	364/364 (100%)	361 (99%)	3 (1%)	73	83
2	B	416/417 (100%)	413 (99%)	3 (1%)	76	84
2	D	416/417 (100%)	411 (99%)	5 (1%)	63	74
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	5/4 (125%)	3 (60%)	2 (40%)	0	0
5	J	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	2324/2326 (100%)	2304 (99%)	20 (1%)	73	81

All (20) 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	288	TYR
2	B	178	TYR
2	B	215	ASN
2	B	417	LYS
1	C	15	ASN
1	C	166	TYR
1	C	288	TYR
2	D	121	SER
2	D	202	ARG
2	D	303	ASN
2	D	365	GLU
2	D	462	CYS

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Mol	Chain	Res	Type
5	I	493[A]	ARG
5	I	493[B]	ARG
5	J	493[A]	ARG
5	J	493[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	215	HIS
1	A	444	GLN
2	B	141	GLN
2	B	444	ASN
2	B	450	ASN
1	C	134	GLN
1	C	158	ASN
2	D	82	GLN
2	D	210	GLN
2	D	301	GLN
2	D	319	GLN
3	E	170	HIS
4	F	27	GLN
4	F	138	ASN
4	L	24	HIS
4	L	27	GLN
4	L	161	ASN
4	L	189	HIS
4	L	190	ASN

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 ⓘ

12 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	6,2	14,14,15	0.51	0	17,19,21	0.58	0
6	NAG	G	2	6	14,14,15	0.58	0	17,19,21	0.69	0
6	BMA	G	3	6	11,11,12	0.63	0	15,15,17	0.74	0
6	MAN	G	4	6	11,11,12	0.62	0	15,15,17	0.57	0
7	NAG	K	1	2,7	14,14,15	0.55	0	17,19,21	0.68	0
7	NAG	K	2	7	14,14,15	0.50	0	17,19,21	0.55	0
6	NAG	M	1	6,2	14,14,15	0.51	0	17,19,21	0.67	0
6	NAG	M	2	6	14,14,15	0.55	0	17,19,21	0.64	0
6	BMA	M	3	6	11,11,12	0.65	0	15,15,17	0.83	1 (6%)
6	MAN	M	4	6	11,11,12	0.62	0	15,15,17	0.54	0
7	NAG	N	1	2,7	14,14,15	0.56	0	17,19,21	0.64	0
7	NAG	N	2	7	14,14,15	0.51	0	17,19,21	0.61	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	6,2	-	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	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	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
6	NAG	M	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	BMA	M	3	6	-	0/2/19/22	0/1/1/1
6	MAN	M	4	6	-	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(°)	Ideal(°)
6	M	3	BMA	C1-C2-C3	2.43	113.18	109.64

There are no chirality outliers.

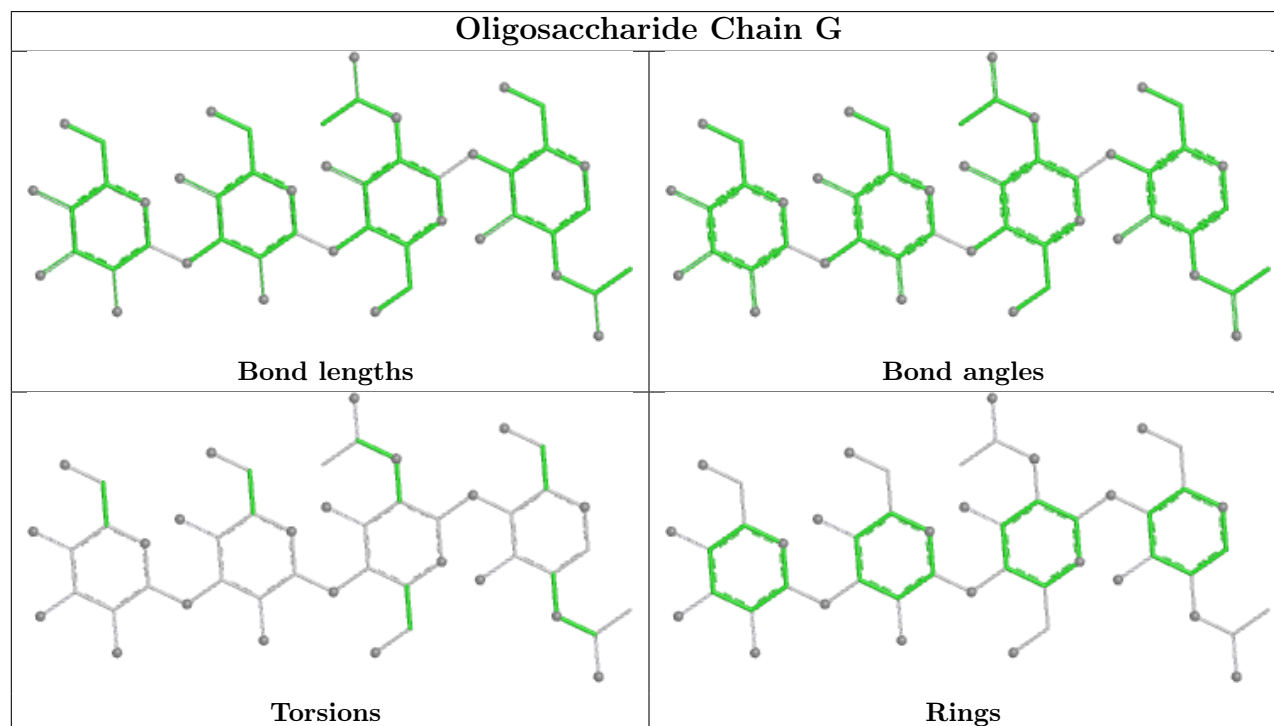
All (7) torsion outliers are listed below:

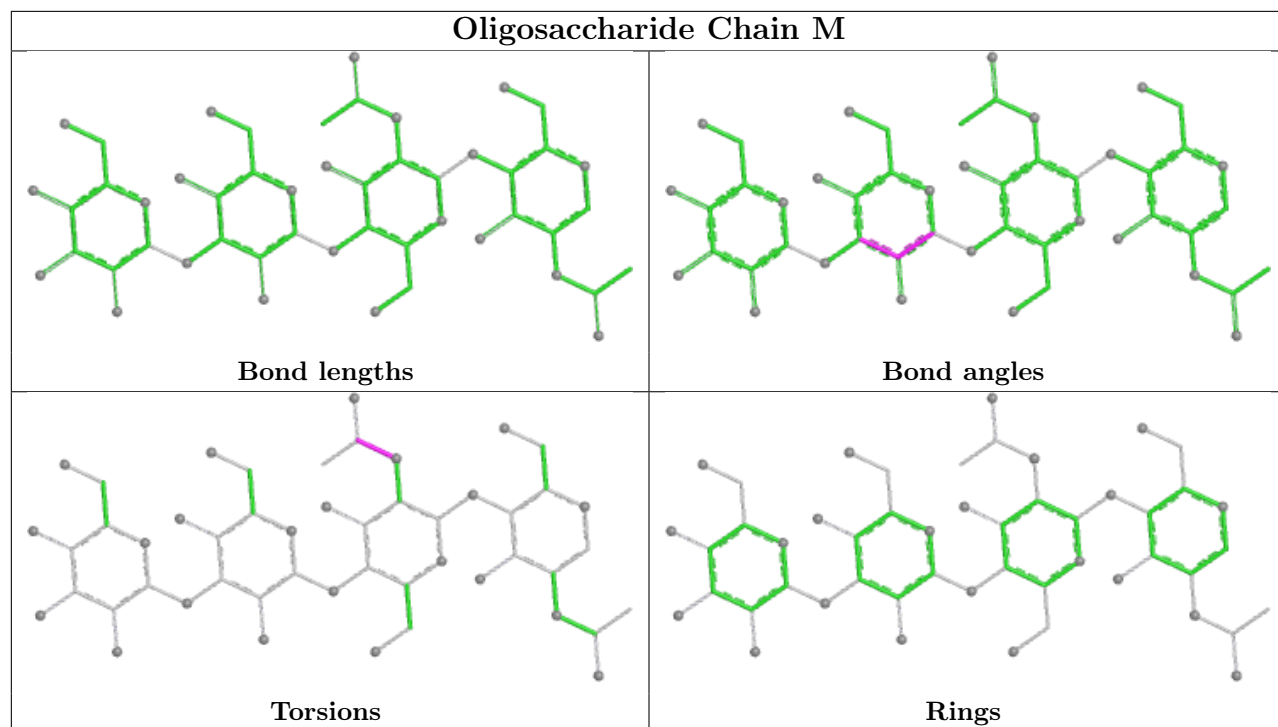
Mol	Chain	Res	Type	Atoms
7	N	2	NAG	C8-C7-N2-C2
7	N	1	NAG	C8-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
7	K	2	NAG	O5-C5-C6-O6
6	M	2	NAG	O7-C7-N2-C2

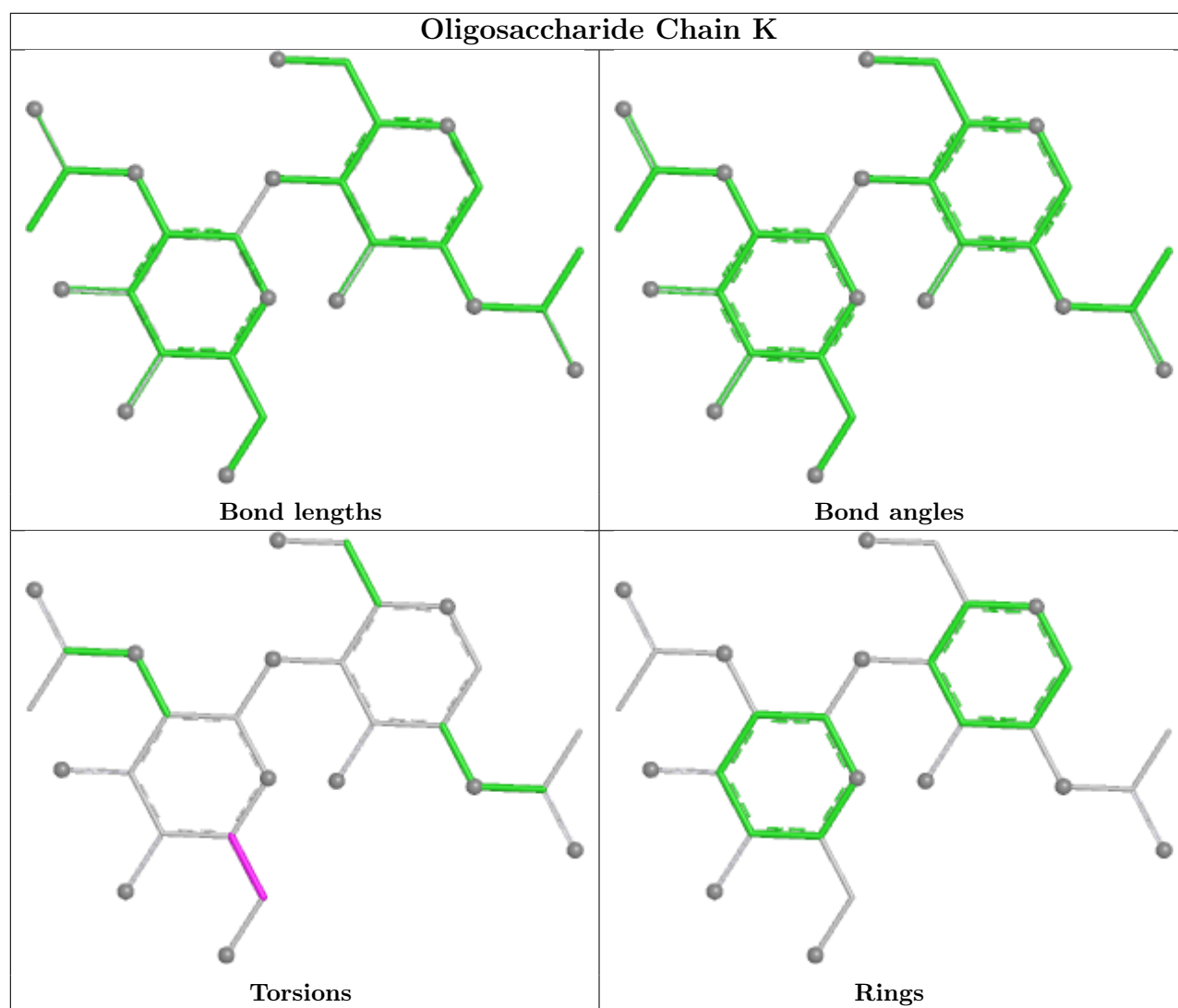
There are no ring outliers.

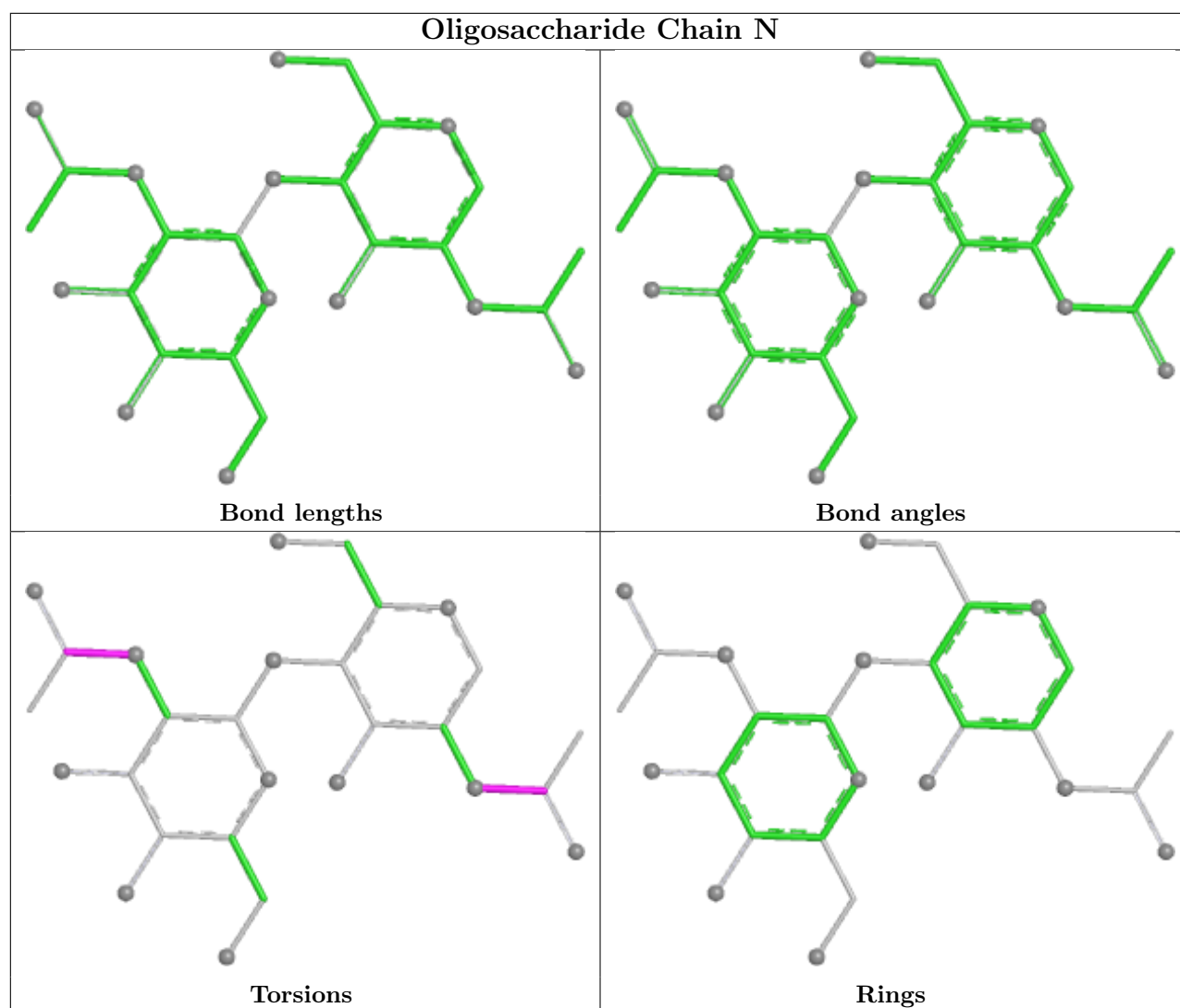
No monomer is involved in short contacts.

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 36 ligands modelled in this entry, 14 are monoatomic - leaving 22 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	$\# Z > 2$
8	SO4	A	1457	-	4,4,4	0.24	0	6,6,6	0.06	0
8	SO4	A	1458	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	L	1216	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	A	1460	-	4,4,4	0.23	0	6,6,6	0.09	0
8	SO4	A	1462	-	4,4,4	0.24	0	6,6,6	0.09	0
8	SO4	A	1459	-	4,4,4	0.23	0	6,6,6	0.07	0
8	SO4	L	1215	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	B	1468	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	D	1472	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	A	1455	-	4,4,4	0.25	0	6,6,6	0.08	0
11	NAG	D	3319	2	14,14,15	0.50	0	17,19,21	0.55	0
11	NAG	B	3319	2	14,14,15	0.52	0	17,19,21	0.67	0
8	SO4	A	1461	-	4,4,4	0.24	0	6,6,6	0.09	0
8	SO4	C	1454	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	C	1456	-	4,4,4	0.24	0	6,6,6	0.06	0
8	SO4	A	1456	-	4,4,4	0.23	0	6,6,6	0.07	0
8	SO4	C	1455	-	4,4,4	0.23	0	6,6,6	0.08	0
8	SO4	C	1457	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	C	1458	-	4,4,4	0.23	0	6,6,6	0.08	0
8	SO4	A	1463	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	B	1469	-	4,4,4	0.23	0	6,6,6	0.08	0
8	SO4	B	1467	-	4,4,4	0.25	0	6,6,6	0.07	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
11	NAG	D	3319	2	-	0/6/23/26	0/1/1/1
11	NAG	B	3319	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.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1462	SO4	4	2
8	C	1458	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	454/457 (99%)	-0.61	5 (1%) 78 79	15, 34, 69, 149	9 (1%)
1	C	453/457 (99%)	-0.37	3 (0%) 84 86	25, 50, 88, 137	4 (0%)
2	B	464/472 (98%)	-0.04	13 (2%) 55 56	16, 61, 149, 197	7 (1%)
2	D	469/472 (99%)	-0.02	11 (2%) 61 63	26, 66, 140, 202	4 (0%)
3	E	216/221 (97%)	1.15	48 (22%) 2 2	60, 128, 235, 267	0
3	H	216/221 (97%)	0.47	7 (3%) 50 51	40, 98, 158, 200	0
4	F	214/214 (100%)	0.99	29 (13%) 7 5	62, 133, 240, 274	1 (0%)
4	L	214/214 (100%)	0.13	4 (1%) 66 67	42, 81, 119, 221	0
5	I	6/6 (100%)	2.40	3 (50%) 0 0	41, 50, 94, 99	3 (50%)
5	J	5/6 (83%)	3.99	4 (80%) 0 0	45, 55, 98, 130	3 (60%)
All	All	2711/2740 (98%)	0.06	127 (4%) 36 35	15, 66, 174, 274	31 (1%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	VAL	7.6
5	J	493[A]	ARG	6.6
3	E	199	ILE	4.8
3	E	133	VAL	4.7
5	J	492[A]	GLY	4.7
3	E	130	LEU	4.6
5	I	493[A]	ARG	4.5
3	E	194	TRP	4.5
3	E	201	CYS	4.4
3	E	144	LEU	4.2
5	J	496	SER	4.1
3	E	142	VAL	4.1
4	F	181	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	205	ILE	4.0
4	F	179	LEU	4.0
3	E	203	VAL	3.9
3	H	177	GLN	3.9
4	F	119	PRO	3.9
3	E	145	GLY	3.8
2	D	375	LEU	3.6
4	F	186	TYR	3.6
3	E	212	VAL	3.6
1	A	339	ALA	3.5
3	E	189	VAL	3.5
3	E	165	LEU	3.5
3	E	216	ILE	3.5
2	B	33	LEU	3.5
3	E	131	ALA	3.4
3	E	128	TYR	3.4
3	E	164	SER	3.2
3	E	200	THR	3.2
4	F	126	THR	3.2
3	E	198	SER	3.1
4	F	209	PHE	3.1
2	B	36	PRO	3.1
2	D	471	CYS	3.0
3	E	129	PRO	3.0
3	E	196	SER	3.0
2	D	178	TYR	3.0
3	E	134	CYS	3.0
3	E	146	CYS	3.0
3	E	160	TRP	2.9
1	C	1	LEU	2.9
5	J	494[A]	GLY	2.9
2	D	181	LYS	2.9
3	E	147	LEU	2.9
5	I	497	PRO	2.9
2	B	375	LEU	2.9
4	F	180	THR	2.8
3	E	11	LEU	2.8
2	B	466	TRP	2.8
3	E	143	THR	2.8
4	L	125	LEU	2.8
4	F	135	PHE	2.8
4	F	136	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	120	PRO	2.7
2	B	129	TRP	2.7
5	I	496	SER	2.7
4	F	214	CYS	2.7
2	B	10	VAL	2.7
3	E	192	SER	2.7
3	E	132	PRO	2.6
3	E	141	SER	2.6
3	H	138	THR	2.6
2	B	446	HIS	2.6
4	F	199	LYS	2.6
3	E	195	PRO	2.6
4	F	125	LEU	2.6
4	F	131	SER	2.6
4	F	132	VAL	2.6
2	D	75	GLY	2.5
3	E	214	LYS	2.5
4	L	214	CYS	2.5
1	A	45	PRO	2.5
4	F	182	THR	2.5
3	E	161	ASN	2.5
1	C	339	ALA	2.5
4	F	178	THR	2.5
3	E	188	THR	2.4
2	D	9	GLY	2.4
3	E	148	VAL	2.4
3	H	160	TRP	2.4
4	F	163	TRP	2.4
3	E	218	PRO	2.4
4	L	129	GLY	2.4
3	H	216	ILE	2.4
4	F	193	THR	2.4
3	E	158	LEU	2.4
4	F	133	VAL	2.4
4	F	130	ALA	2.4
2	D	129[A]	TRP	2.4
4	F	148	TRP	2.4
4	F	134	CYS	2.3
4	F	123	GLU	2.3
4	L	121	SER	2.3
3	E	207	ALA	2.3
3	E	187	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	44	LEU	2.3
2	B	181	LYS	2.3
3	H	203	VAL	2.3
3	E	184	SER	2.2
1	C	453	VAL	2.2
3	E	159	THR	2.2
2	D	77	SER	2.2
4	F	117	ILE	2.2
2	D	380	ILE	2.2
2	B	31	LEU	2.2
3	E	166	SER	2.2
1	A	337	PRO	2.2
3	E	127	VAL	2.1
3	E	202	ASN	2.1
3	E	210	THR	2.1
3	H	196	SER	2.1
3	H	214	LYS	2.1
4	F	146	VAL	2.1
1	A	336	GLY	2.1
3	E	157	THR	2.1
2	B	4	ILE	2.1
4	F	204	PRO	2.1
2	B	30	ALA	2.1
3	E	183	LEU	2.1
2	B	433	CYS	2.1
4	F	159	VAL	2.0
2	D	468	GLY	2.0
2	D	378	GLU	2.0
3	E	190	THR	2.0
3	E	167	SER	2.0

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

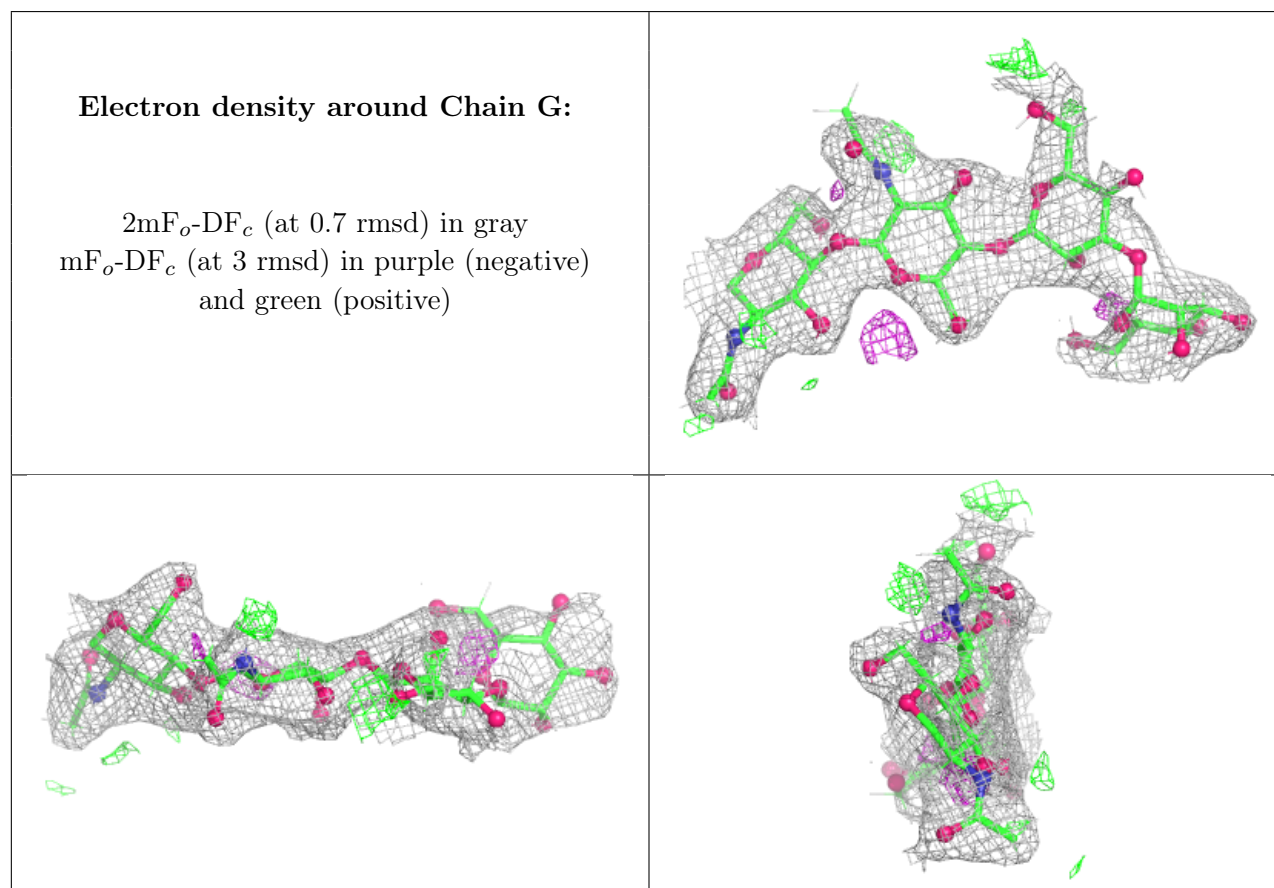
There are no non-standard protein/DNA/RNA residues in this entry.

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.

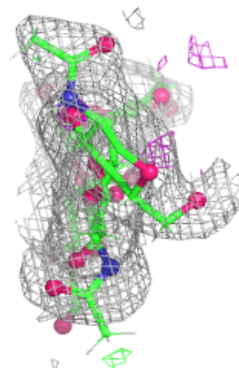
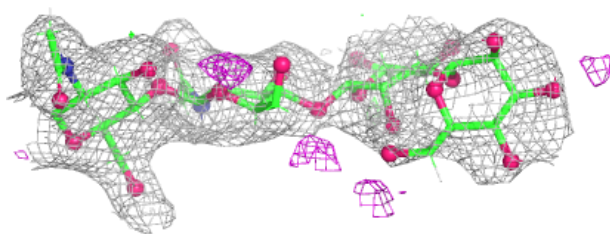
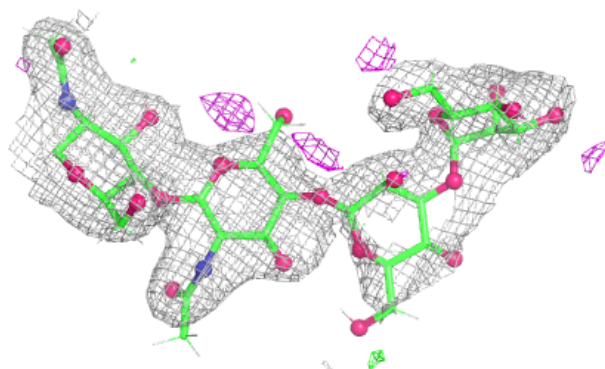
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	G	1	14/15	-	-	26,53,72,78	0
6	NAG	G	2	14/15	-	-	76,93,106,112	0
6	BMA	G	3	11/12	-	-	120,135,160,162	0
6	MAN	G	4	11/12	-	-	136,140,166,168	0
6	BMA	M	3	11/12	0.38	0.14	134,142,170,170	0
7	NAG	N	2	14/15	0.60	0.13	114,138,165,167	0
6	MAN	M	4	11/12	0.68	0.13	124,133,158,159	0
6	NAG	M	2	14/15	0.84	0.14	92,115,141,144	0
7	NAG	K	2	14/15	0.88	0.12	106,129,155,157	0
7	NAG	N	1	14/15	0.89	0.11	86,108,128,132	0
6	NAG	M	1	14/15	0.94	0.09	48,64,89,91	0
7	NAG	K	1	14/15	0.96	0.07	87,104,120,125	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.

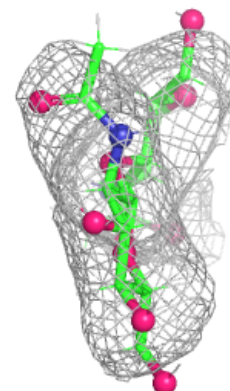
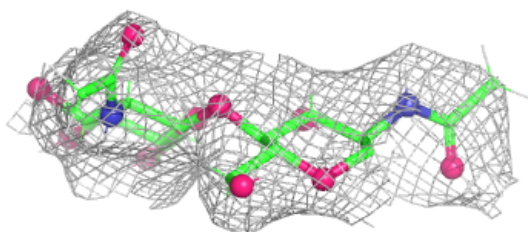
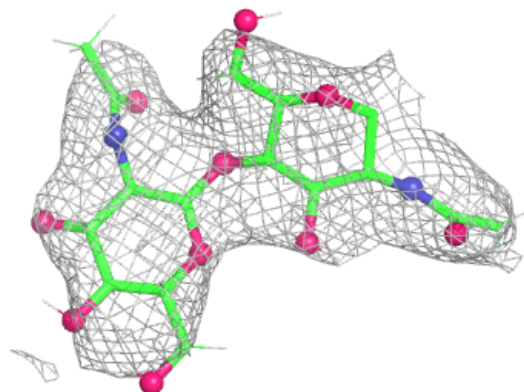


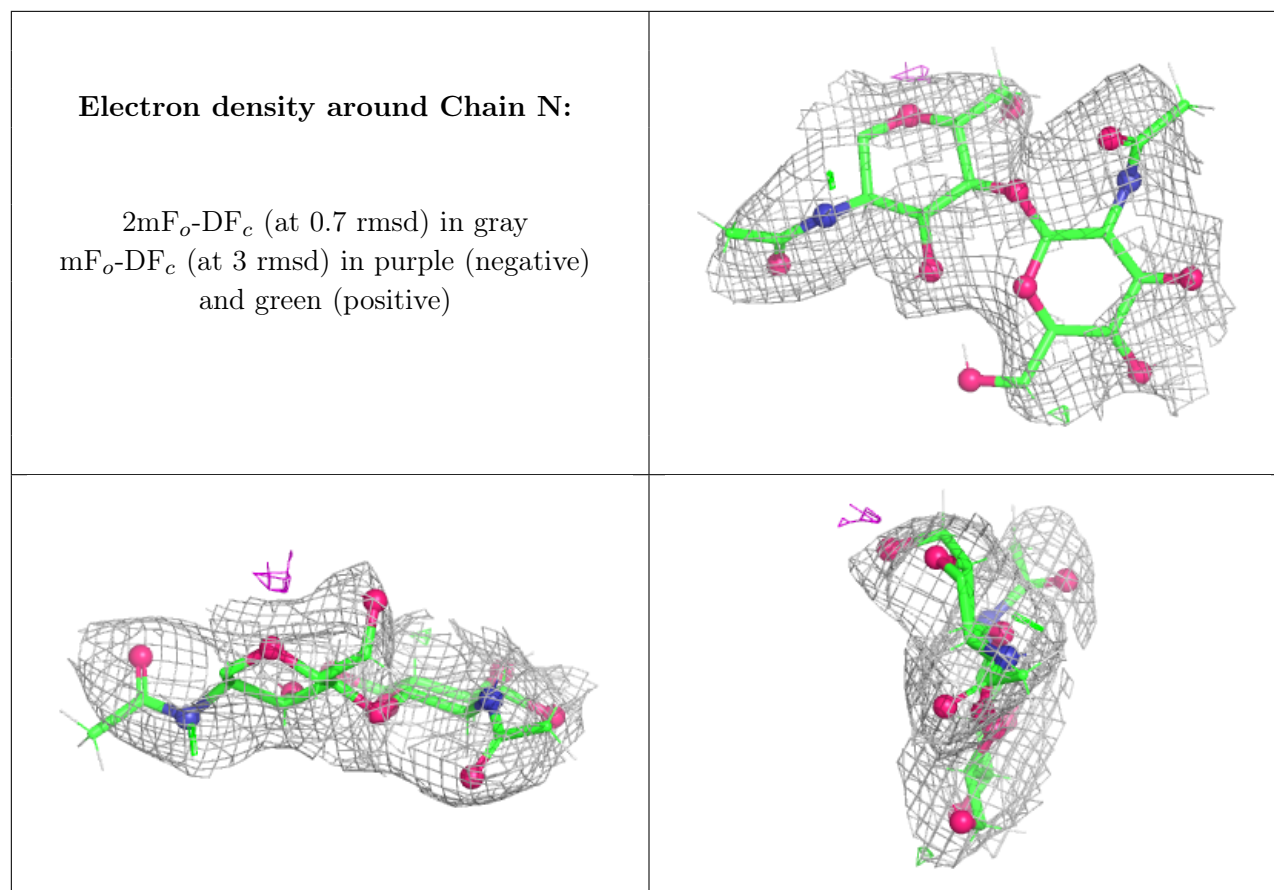
Electron density around Chain M:

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

**Electron density around Chain 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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	B	1468	5/5	0.66	0.12	153,154,154,154	0
11	NAG	B	3319	14/15	0.66	0.15	104,123,147,151	0
11	NAG	D	3319	14/15	0.75	0.14	82,102,122,126	0
8	SO4	A	1458	5/5	0.80	0.18	94,107,109,112	0
8	SO4	C	1456	5/5	0.84	0.16	134,135,137,138	0
8	SO4	L	1215	5/5	0.84	0.13	115,116,116,118	0
8	SO4	C	1458	5/5	0.86	0.19	133,135,135,137	0
8	SO4	A	1463	5/5	0.87	0.13	116,119,120,122	0
8	SO4	C	1457	5/5	0.87	0.23	150,151,152,152	0
8	SO4	L	1216	5/5	0.88	0.20	140,140,143,144	0
8	SO4	B	1467	5/5	0.88	0.20	141,142,143,145	0
8	SO4	B	1469	5/5	0.88	0.20	163,163,164,164	0
8	SO4	C	1454	5/5	0.89	0.17	133,134,135,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	A	1461	5/5	0.89	0.14	91,91,97,101	0
8	SO4	A	1457	5/5	0.90	0.17	125,125,127,128	0
8	SO4	D	1472	5/5	0.90	0.17	128,130,131,133	0
8	SO4	A	1456	5/5	0.90	0.12	117,121,123,124	0
8	SO4	A	1459	5/5	0.91	0.18	161,161,162,162	0
8	SO4	A	1455	5/5	0.92	0.18	123,125,126,128	0
8	SO4	A	1462	5/5	0.93	0.11	83,92,97,100	0
8	SO4	C	1455	5/5	0.94	0.06	104,106,106,107	0
8	SO4	A	1460	5/5	0.95	0.09	76,76,80,83	0
9	CA	B	2002	1/1	0.98	0.06	67,67,67,67	0
9	CA	C	2004	1/1	0.98	0.04	66,66,66,66	0
9	CA	C	2007	1/1	0.98	0.03	39,39,39,39	0
10	MG	D	2001	1/1	0.98	0.05	50,50,50,50	0
9	CA	A	2006	1/1	0.98	0.04	25,25,25,25	0
9	CA	A	2007	1/1	0.98	0.03	26,26,26,26	0
9	CA	A	2004	1/1	0.99	0.03	43,43,43,43	0
9	CA	D	2002	1/1	0.99	0.03	53,53,53,53	0
9	CA	D	2003	1/1	0.99	0.05	37,37,37,37	0
10	MG	B	2001	1/1	0.99	0.03	33,33,33,33	0
9	CA	A	2005	1/1	0.99	0.04	32,32,32,32	0
9	CA	C	2005	1/1	0.99	0.03	55,55,55,55	0
9	CA	C	2006	1/1	0.99	0.04	49,49,49,49	0
9	CA	B	2003	1/1	1.00	0.04	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.