



# Full wwPDB X-ray Structure Validation Report

Dec 17, 2023 – 10:58 am GMT

PDB ID : 3ZDY  
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](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

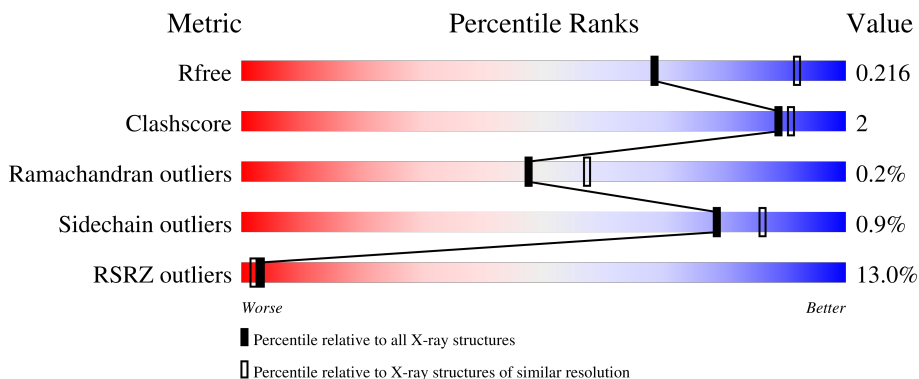
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 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	
1	C	457	
2	B	472	
2	D	472	
3	E	221	

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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	1459	-	-	-	X
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
			Total	C	H	N	O	S			
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
			Total	C	H	N	O	S			
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
			Total	C	H	N	O	S			
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
			Total	C	H	N	O	S			
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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- 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		



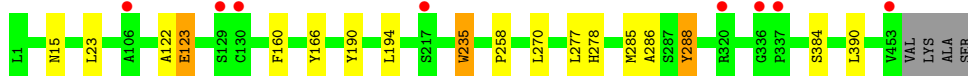
### 3 Residue-property plots [i](#)

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.

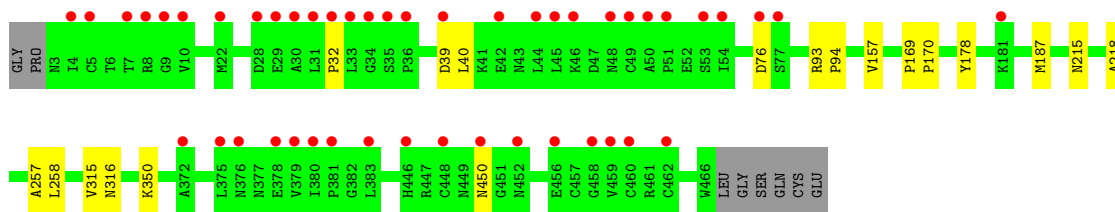
- Molecule 1: INTEGRIN ALPHA-IIB



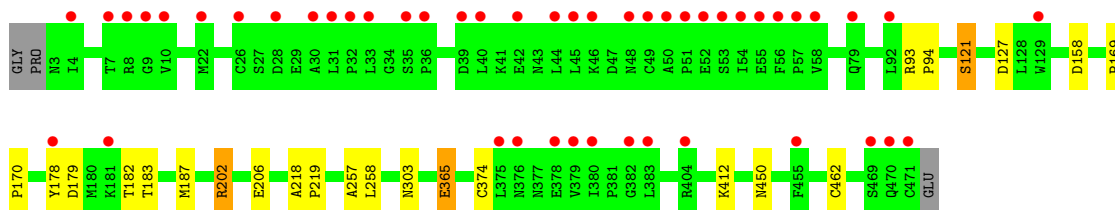
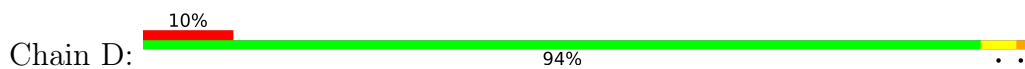
- Molecule 1: INTEGRIN ALPHA-IIB



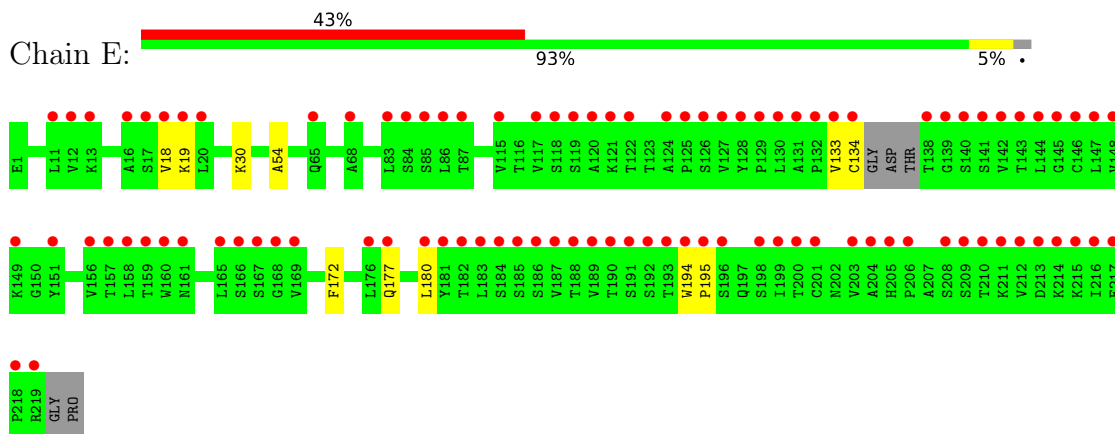
- Molecule 2: INTEGRIN BETA-3



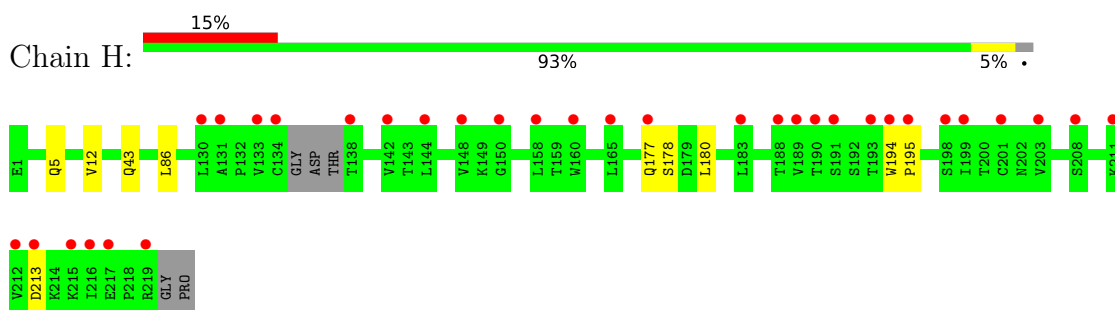
- Molecule 2: INTEGRIN BETA-3



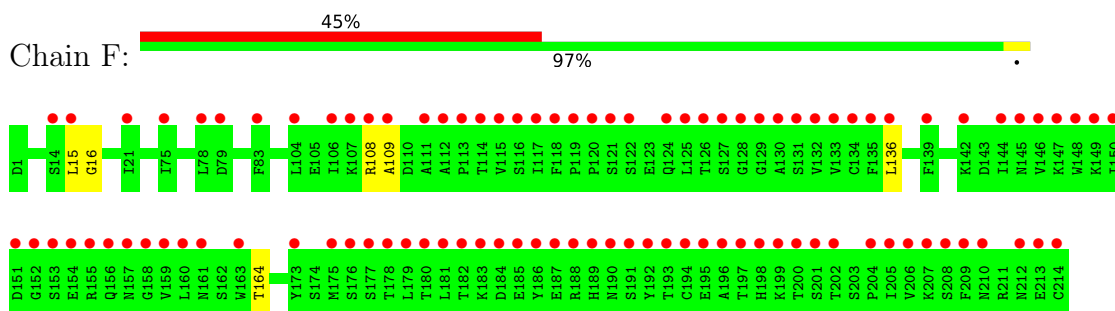
- Molecule 3: 10E5 FAB HEAVY CHAIN



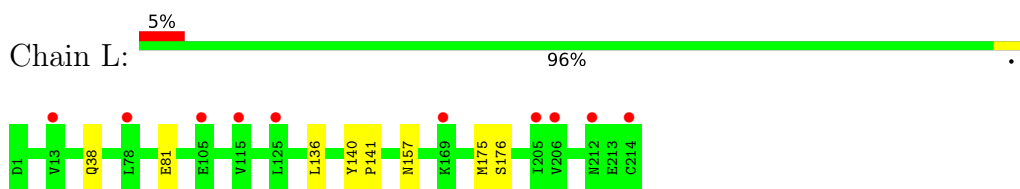
- Molecule 3: 10E5 FAB HEAVY CHAIN



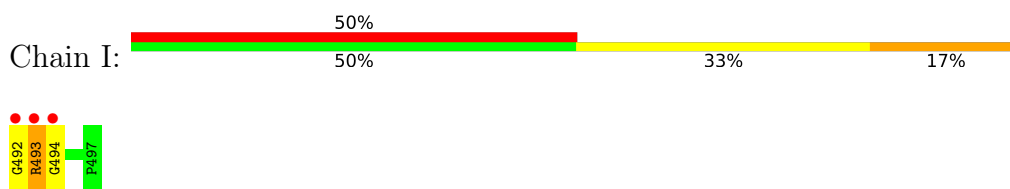
- Molecule 4: 10E5 FAB LIGHT CHAIN



- Molecule 4: 10E5 FAB LIGHT CHAIN



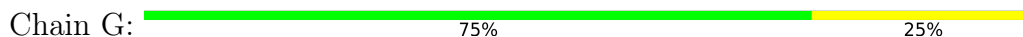
- Molecule 5: RGD PEPTIDE



- Molecule 5: RGD PEPTIDE



- Molecule 6: alpha-D-mannopyranose-(1-3)-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



- Molecule 7: 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.182 , 0.216 0.181 , 0.216	Depositor DCC
$R_{free}$ test set	1015 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtrriage
Anisotropy	0.365	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 64.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	42366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, MAN, MG, BMA, CA, 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	0.22	0/3628	0.40	0/4945
1	C	0.22	0/3596	0.39	0/4900
2	B	0.21	0/3684	0.38	0/4994
2	D	0.21	0/3694	0.37	0/5009
3	E	0.20	0/1684	0.38	0/2305
3	H	0.21	0/1684	0.38	0/2305
4	F	0.21	0/1673	0.36	0/2269
4	L	0.21	0/1673	0.37	0/2269
5	I	0.20	0/60	0.43	0/76
5	J	0.21	0/51	0.37	0/64
All	All	0.21	0/21427	0.38	0/29136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	16	0
1	C	3490	3319	3328	10	0
2	B	3606	3525	3530	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3623	3531	3537	12	0
3	E	1642	1597	1600	6	0
3	H	1642	1597	1600	6	0
4	F	1637	1550	1553	4	0
4	L	1637	1550	1553	6	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	17	1
12	B	157	0	0	1	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	79	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 (79) 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:413:THR:OG1	12:A:3331:HOH:O	2.15	0.63
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
2:D:257:ALA:O	2:D:258:LEU:HB2	2.10	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: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
4:L:81:GLU:N	4:L:81:GLU:OE1	2.44	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
2:B:350:LYS:NZ	12:B:3135:HOH:O	2.48	0.46
1:C:122:ALA:O	1:C:123:GLU:CB	2.64	0.46
1:C:194:LEU:C	1:C:194:LEU:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.99	0.45
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
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
1:A:194:LEU:HD12	1:A:194:LEU:C	2.36	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
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: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%)	47 57
1	C	454/457 (99%)	440 (97%)	13 (3%)	1 (0%)	47 57
2	B	467/472 (99%)	445 (95%)	20 (4%)	2 (0%)	34 41
2	D	468/472 (99%)	449 (96%)	18 (4%)	1 (0%)	47 57
3	E	212/221 (96%)	197 (93%)	15 (7%)	0	100 100
3	H	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	29 34
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%)	47 57

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 [i](#)

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%)	67	77
1	C	364/364 (100%)	358 (98%)	6 (2%)	62	74
2	B	416/417 (100%)	414 (100%)	2 (0%)	88	93
2	D	416/417 (100%)	410 (99%)	6 (1%)	67	77
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%)	2301 (99%)	23 (1%)	78	84

All (23) 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	190	TYR
1	A	288	TYR
2	B	178	TYR
2	B	215	ASN
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	235	TRP
1	C	288	TYR
2	D	121	SER
2	D	127	ASP
2	D	202	ARG

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Mol	Chain	Res	Type
2	D	303	ASN
2	D	365	GLU
2	D	462	CYS
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3	ASN
2	D	3	ASN
2	D	82	GLN
3	E	202	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	0.52	0	17,19,21	0.63	0
6	NAG	G	2	6	14,14,15	0.59	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BMA	G	3	6	11,11,12	0.65	0	15,15,17	0.87	1 (6%)
6	MAN	G	4	6	11,11,12	0.63	0	15,15,17	0.71	0
7	NAG	K	1	7,2	14,14,15	0.56	0	17,19,21	0.73	0
7	NAG	K	2	7	14,14,15	0.51	0	17,19,21	0.60	0
6	NAG	M	1	6,2	14,14,15	0.53	0	17,19,21	0.71	0
6	NAG	M	2	6	14,14,15	0.56	0	17,19,21	0.73	1 (5%)
6	BMA	M	3	6	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
6	MAN	M	4	6	11,11,12	0.64	0	15,15,17	0.67	0
7	NAG	N	1	7,2	14,14,15	0.57	0	17,19,21	0.70	0
7	NAG	N	2	7	14,14,15	0.52	0	17,19,21	0.66	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	7,2	-	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	7,2	-	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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	3	BMA	C1-C2-C3	2.86	113.18	109.67
6	G	3	BMA	C1-C2-C3	2.15	112.31	109.67
6	M	2	NAG	O5-C5-C6	2.10	110.49	107.20

There are no chirality outliers.

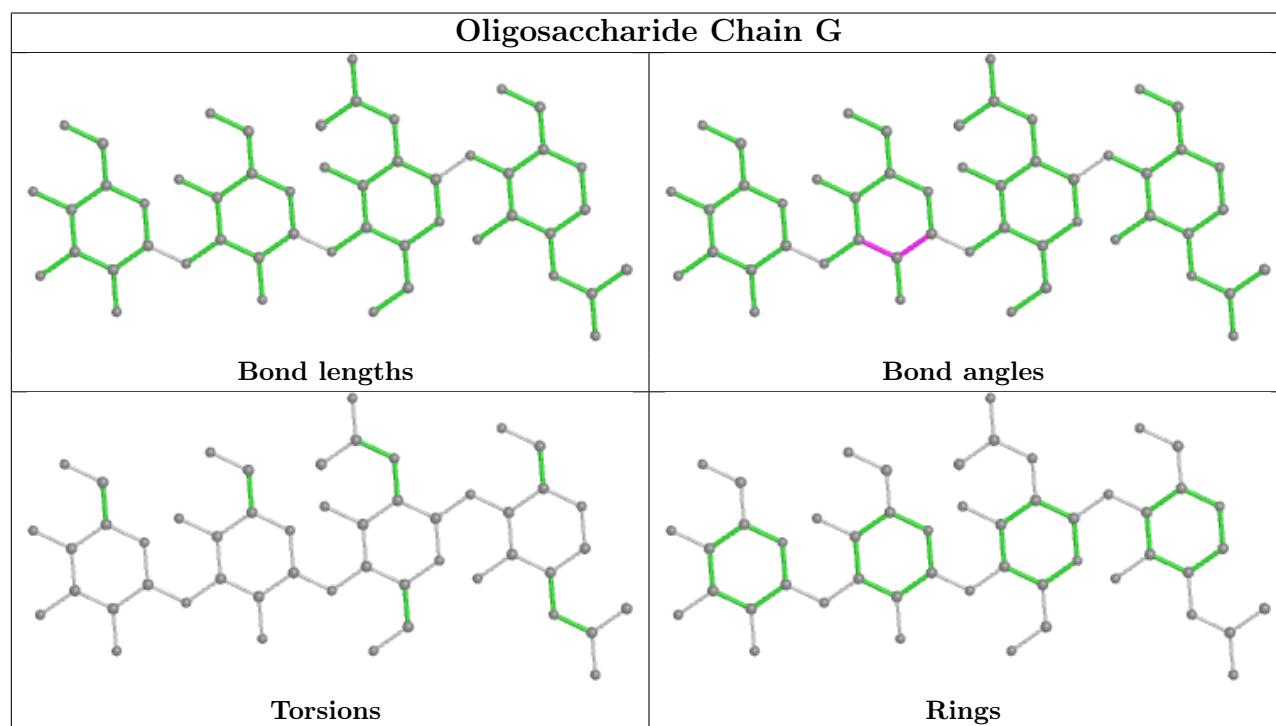
All (7) torsion outliers are listed below:

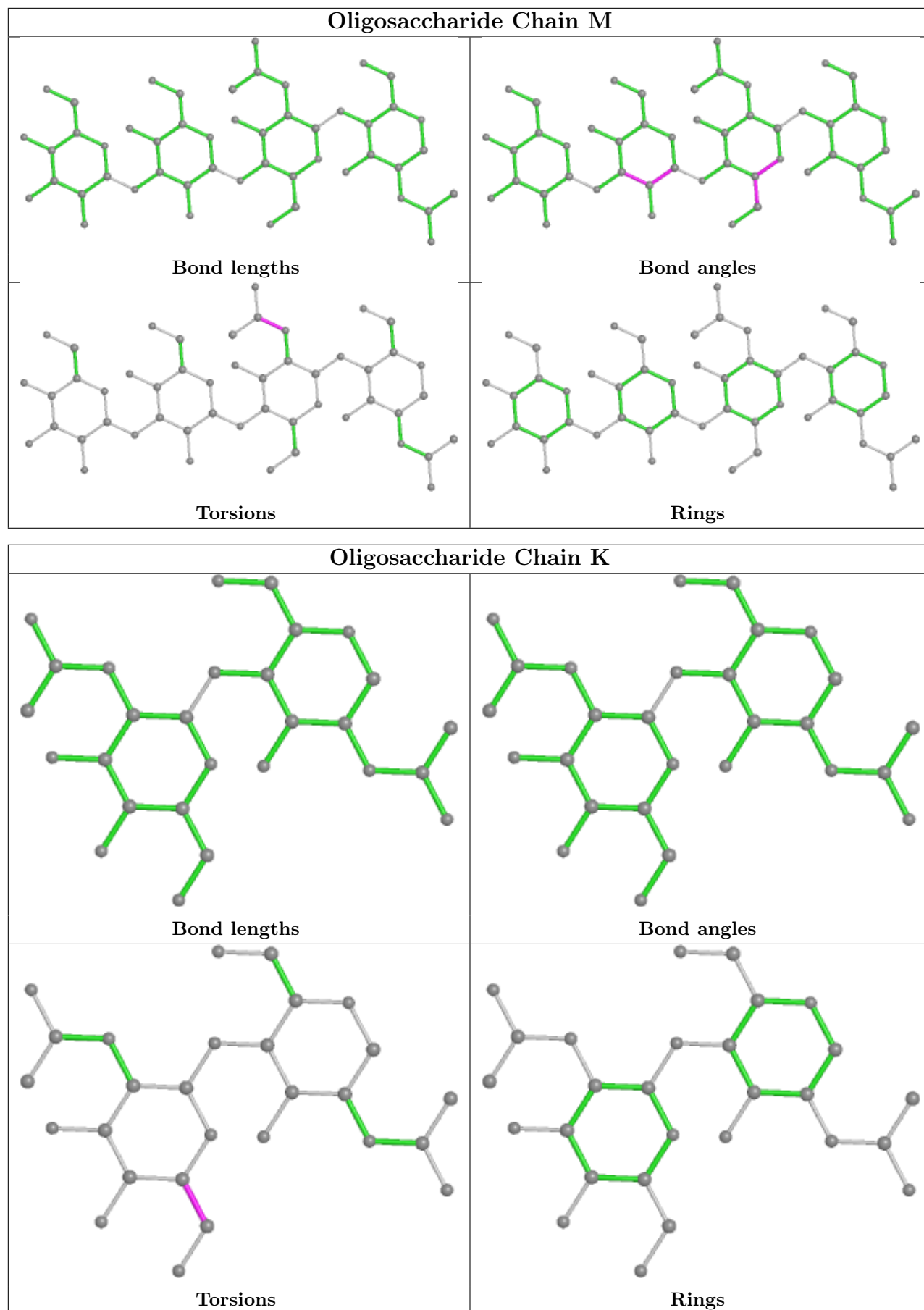
Mol	Chain	Res	Type	Atoms
7	N	2	NAG	C8-C7-N2-C2
7	N	1	NAG	C8-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
7	K	2	NAG	O5-C5-C6-O6
6	M	2	NAG	O7-C7-N2-C2

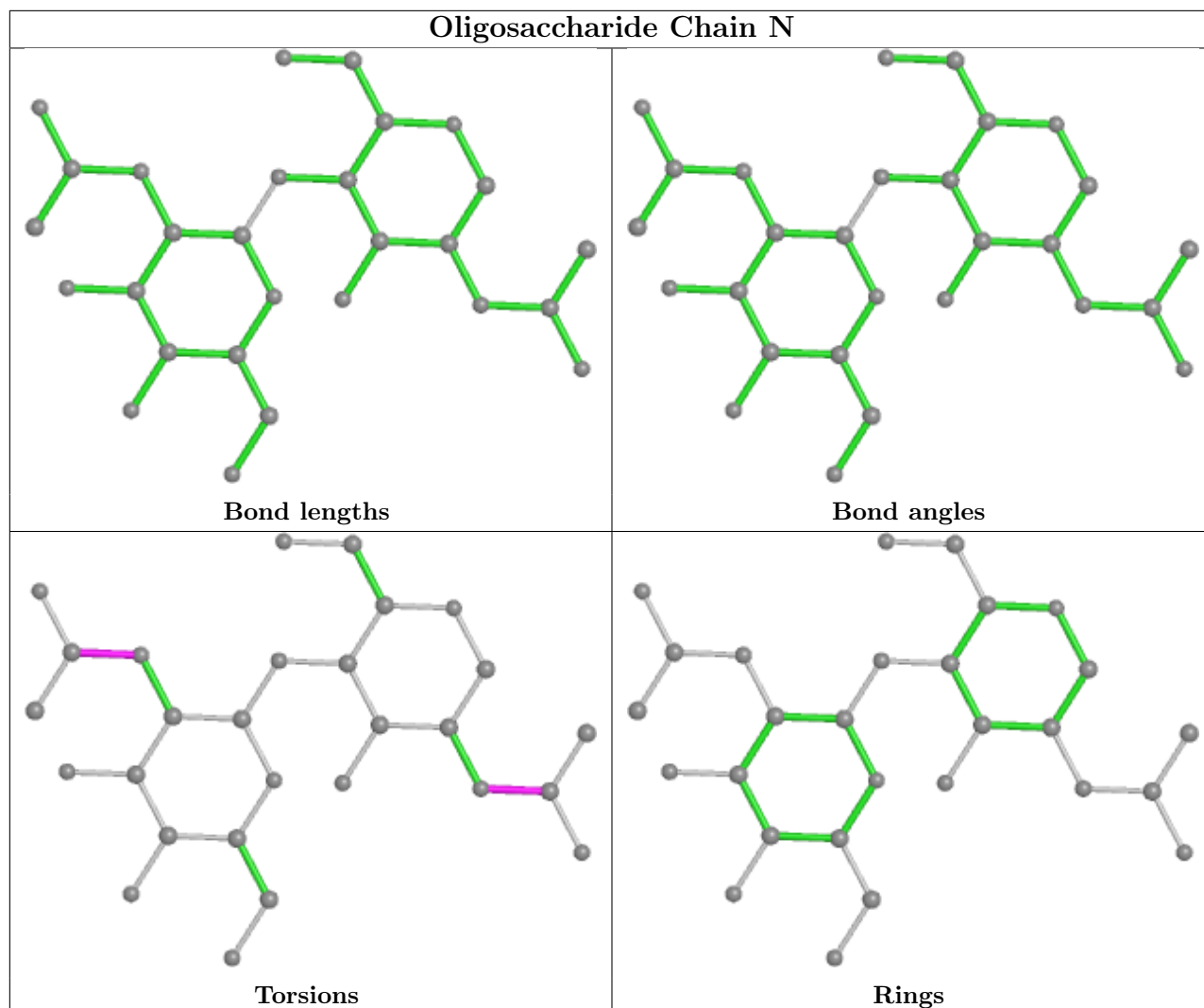
There are no ring outliers.

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	1455	-	4,4,4	0.15	0	6,6,6	0.05	0
8	SO4	A	1456	-	4,4,4	0.14	0	6,6,6	0.04	0
8	SO4	B	1469	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	D	1472	-	4,4,4	0.14	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	A	1458	-	4,4,4	0.14	0	6,6,6	0.04	0
8	SO4	A	1460	-	4,4,4	0.14	0	6,6,6	0.06	0
8	SO4	C	1455	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	L	1215	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	C	1458	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	1461	-	4,4,4	0.15	0	6,6,6	0.06	0
8	SO4	C	1457	-	4,4,4	0.14	0	6,6,6	0.04	0
8	SO4	L	1216	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	1459	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	B	1468	-	4,4,4	0.15	0	6,6,6	0.05	0
8	SO4	A	1457	-	4,4,4	0.14	0	6,6,6	0.04	0
8	SO4	A	1463	-	4,4,4	0.15	0	6,6,6	0.05	0
8	SO4	A	1462	-	4,4,4	0.14	0	6,6,6	0.06	0
8	SO4	C	1456	-	4,4,4	0.14	0	6,6,6	0.05	0
11	NAG	B	3319	2	14,14,15	0.52	0	17,19,21	0.71	0
11	NAG	D	3319	2	14,14,15	0.51	0	17,19,21	0.59	0
8	SO4	C	1454	-	4,4,4	0.15	0	6,6,6	0.05	0
8	SO4	B	1467	-	4,4,4	0.15	0	6,6,6	0.04	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	B	3319	2	-	0/6/23/26	0/1/1/1
11	NAG	D	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	C	1458	SO4	1	0
8	A	1462	SO4	4	2



## 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 i

### 6.1 Protein, DNA and RNA chains i

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	454/457 (99%)	0.49	8 (1%) 68 65	18, 32, 62, 132	2 (0%)
1	C	453/457 (99%)	0.33	8 (1%) 68 65	27, 46, 80, 121	1 (0%)
2	B	464/472 (98%)	0.72	47 (10%) 7 4	20, 56, 137, 181	2 (0%)
2	D	469/472 (99%)	0.53	48 (10%) 6 4	30, 60, 128, 179	3 (0%)
3	E	216/221 (97%)	2.65	96 (44%) 0 0	56, 116, 214, 250	0
3	H	216/221 (97%)	0.72	33 (15%) 2 1	38, 90, 145, 182	0
4	F	214/214 (100%)	2.62	97 (45%) 0 0	57, 123, 220, 256	1 (0%)
4	L	214/214 (100%)	0.44	10 (4%) 31 29	38, 75, 110, 212	0
5	I	6/6 (100%)	1.83	3 (50%) 0 0	75, 80, 91, 97	0
5	J	5/6 (83%)	2.53	3 (60%) 0 0	83, 90, 105, 121	0
All	All	2711/2740 (98%)	0.87	353 (13%) 3 2	18, 61, 157, 256	9 (0%)

All (353) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	133	VAL	18.0
4	F	181	LEU	16.2
4	F	179	LEU	14.6
3	E	199	ILE	14.4
4	F	214	CYS	14.2
3	E	142	VAL	13.3
3	E	216	ILE	13.0
3	E	131	ALA	12.3
3	E	194	TRP	12.3
3	E	200	THR	11.3
3	E	134	CYS	11.1
4	F	193	THR	10.9
4	F	205	ILE	10.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	130	LEU	10.4
4	F	148	TRP	10.4
3	E	212	VAL	10.2
3	E	201	CYS	10.1
3	E	132	PRO	10.0
4	F	130	ALA	9.7
3	E	144	LEU	9.6
3	E	196	SER	9.4
4	F	194	CYS	9.3
3	E	219	ARG	9.0
4	F	206	VAL	9.0
4	F	159	VAL	8.9
4	F	119	PRO	8.8
4	F	120	PRO	8.6
3	E	129	PRO	8.6
3	E	145	GLY	8.5
2	B	33	LEU	8.5
4	F	125	LEU	8.5
4	F	115	VAL	8.3
4	F	180	THR	8.0
2	B	36	PRO	7.9
3	E	139	GLY	7.9
4	F	186	TYR	7.8
4	F	133	VAL	7.8
4	F	134	CYS	7.7
3	E	148	VAL	7.6
3	E	128	TYR	7.5
4	F	209	PHE	7.5
3	E	189	VAL	7.4
4	F	126	THR	7.4
4	F	117	ILE	7.3
3	H	216	ILE	7.3
4	L	214	CYS	7.2
3	E	217	GLU	7.0
4	F	129	GLY	6.9
3	E	147	LEU	6.9
4	F	195	GLU	6.7
3	E	195	PRO	6.7
3	E	165	LEU	6.6
3	E	141	SER	6.5
4	F	147	LYS	6.5
3	E	188	THR	6.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	198	SER	6.5
4	F	212	ASN	6.4
4	F	201	SER	6.4
3	E	210	THR	6.3
4	F	177	SER	6.3
2	D	44	LEU	6.1
2	B	10	VAL	6.1
4	F	204	PRO	6.1
3	E	218	PRO	6.0
4	F	210	ASN	5.9
4	F	150	ILE	5.9
2	D	33	LEU	5.9
3	E	166	SER	5.8
4	F	122	SER	5.8
4	L	125	LEU	5.8
4	F	136	LEU	5.8
3	E	215	LYS	5.8
3	E	183	LEU	5.7
4	F	182	THR	5.7
3	E	203	VAL	5.6
4	F	158	GLY	5.6
4	F	132	VAL	5.5
3	E	176	LEU	5.5
4	F	155	ARG	5.5
3	E	127	VAL	5.5
3	E	146	CYS	5.5
4	F	157	ASN	5.4
2	B	31	LEU	5.4
3	E	177	GLN	5.4
2	B	32	PRO	5.4
2	D	469	SER	5.4
3	E	160	TRP	5.3
2	D	380	ILE	5.3
4	F	208	SER	5.3
3	E	190	THR	5.3
2	B	34	GLY	5.2
2	B	4	ILE	5.2
2	B	54	ILE	5.2
3	E	16	ALA	5.2
2	B	44	LEU	5.2
4	F	118	PHE	5.2
4	F	178	THR	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	131	SER	5.1
2	B	383	LEU	5.1
3	H	217	GLU	5.1
3	E	187	VAL	5.1
2	D	54	ILE	5.0
4	F	213	GLU	5.0
2	B	35	SER	5.0
2	D	375	LEU	5.0
2	B	28	ASP	4.9
3	H	134	CYS	4.9
3	E	86	LEU	4.9
2	B	8	ARG	4.9
3	H	133	VAL	4.8
3	E	192	SER	4.8
4	F	135	PHE	4.8
3	E	138	THR	4.7
3	E	143	THR	4.7
4	F	106	ILE	4.7
3	E	193	THR	4.6
2	D	470	GLN	4.6
2	B	9	GLY	4.6
4	F	144	ILE	4.6
1	A	454	VAL	4.5
2	D	181	LYS	4.5
3	H	203	VAL	4.5
2	B	46	LYS	4.5
2	B	51	PRO	4.4
4	F	114	THR	4.4
4	F	207	LYS	4.4
3	H	160	TRP	4.3
2	B	459	VAL	4.2
4	F	154	GLU	4.2
2	B	50	ALA	4.2
2	B	49	CYS	4.2
2	D	9	GLY	4.1
4	L	212	ASN	4.1
2	D	48	ASN	4.1
2	D	46	LYS	4.1
2	B	30	ALA	4.1
4	F	192	TYR	4.1
2	D	51	PRO	4.0
4	F	160	LEU	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	168	GLY	4.0
3	H	130	LEU	4.0
3	E	126	SER	4.0
4	F	116	SER	4.0
5	J	496	SER	4.0
4	F	151	ASP	4.0
3	E	158	LEU	4.0
3	E	149	LYS	3.9
4	F	107	LYS	3.9
1	A	336	GLY	3.9
2	B	375	LEU	3.9
2	B	45	LEU	3.9
2	D	4	ILE	3.9
3	E	157	THR	3.9
3	E	17	SER	3.9
4	L	206	VAL	3.8
4	F	146	VAL	3.8
4	F	190	ASN	3.8
2	B	77	SER	3.8
4	F	149	LYS	3.7
5	J	492[A]	GLY	3.7
2	D	50	ALA	3.7
4	F	83	PHE	3.7
4	L	205	ILE	3.7
5	I	493[A]	ARG	3.6
3	H	189	VAL	3.6
3	H	215	LYS	3.6
3	H	213	ASP	3.6
2	B	48	ASN	3.6
4	F	185	GLU	3.6
3	H	201	CYS	3.6
3	E	12	VAL	3.6
3	E	191	SER	3.5
4	F	121	SER	3.5
3	H	144	LEU	3.5
4	F	196	ALA	3.5
3	E	211	LYS	3.5
3	E	140	SER	3.5
3	E	83	LEU	3.5
4	F	15	LEU	3.4
4	F	156	GLN	3.4
4	F	108	ARG	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	H	219	ARG	3.4
3	H	158	LEU	3.4
4	F	128	GLY	3.4
4	F	197	THR	3.4
1	A	337	PRO	3.4
3	E	156	VAL	3.4
2	B	379	VAL	3.3
3	H	212	VAL	3.3
2	D	35	SER	3.3
3	H	138	THR	3.3
3	E	214	LYS	3.3
3	E	181	TYR	3.3
2	D	26	CYS	3.3
2	D	56	PHE	3.3
3	E	65	GLN	3.3
4	F	124	GLN	3.3
2	B	22	MET	3.3
2	D	42	GLU	3.3
4	F	145	ASN	3.3
3	E	115	VAL	3.3
3	E	204	ALA	3.2
1	C	337	PRO	3.2
3	H	191	SER	3.2
3	E	182	THR	3.2
2	B	5	CYS	3.2
2	D	40	LEU	3.2
4	F	175	MET	3.1
4	F	199	LYS	3.1
4	F	188	ARG	3.1
3	E	180	LEU	3.1
2	B	181	LYS	3.1
3	H	177	GLN	3.1
3	E	185	SER	3.1
2	D	57	PRO	3.1
4	F	202	THR	3.1
3	H	208	SER	3.1
5	J	493[A]	ARG	3.1
3	H	188	THR	3.1
2	D	30	ALA	3.0
4	F	109	ALA	3.0
2	B	42	GLU	3.0
3	E	184	SER	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	H	131	ALA	3.0
2	D	39	ASP	3.0
2	D	7	THR	3.0
3	E	20	LEU	3.0
3	E	84	SER	3.0
2	B	7	THR	3.0
2	B	458	GLY	3.0
4	F	104	LEU	3.0
4	F	189	HIS	2.9
2	D	129[A]	TRP	2.9
2	D	31	LEU	2.9
2	D	404	ARG	2.9
2	D	55	GLU	2.9
2	B	39	ASP	2.9
2	D	36	PRO	2.9
3	E	121	LYS	2.9
2	D	53	SER	2.9
2	D	58	VAL	2.9
2	D	379	VAL	2.9
2	B	380	ILE	2.9
3	E	120	ALA	2.9
3	E	205	HIS	2.8
3	E	213	ASP	2.8
3	E	11	LEU	2.8
1	A	338	HIS	2.8
3	E	151	TYR	2.8
2	D	8	ARG	2.8
2	D	10	VAL	2.8
3	H	194	TRP	2.7
1	A	339	ALA	2.7
4	L	78	LEU	2.7
2	B	376	ASN	2.7
4	F	187	GLU	2.7
2	D	471	CYS	2.7
2	B	53	SER	2.7
4	F	161	ASN	2.7
3	E	119	SER	2.6
3	E	209	SER	2.6
4	F	78	LEU	2.6
1	C	336	GLY	2.6
3	E	13	LYS	2.6
3	H	211	LYS	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	H	199	ILE	2.6
4	F	113	PRO	2.6
2	B	372	ALA	2.6
4	F	183	LYS	2.6
2	D	22	MET	2.6
4	F	14	SER	2.6
3	E	122	THR	2.6
2	B	450	ASN	2.6
4	F	176	SER	2.6
4	F	200	THR	2.6
4	F	163	TRP	2.6
3	E	85	SER	2.6
3	E	186	SER	2.6
2	D	383	LEU	2.5
1	C	130	CYS	2.5
4	F	198	HIS	2.5
4	F	191	SER	2.5
3	H	193	THR	2.5
3	H	150	GLY	2.5
4	F	153	SER	2.5
3	E	87	THR	2.5
1	C	453	VAL	2.5
4	L	105	GLU	2.5
3	E	68	ALA	2.5
4	F	127	SER	2.5
3	H	142	VAL	2.4
2	D	52	GLU	2.4
4	F	111	ALA	2.4
3	E	167	SER	2.4
2	D	376	ASN	2.4
3	E	206	PRO	2.4
2	B	460	CYS	2.4
3	H	190	THR	2.4
4	L	115	VAL	2.4
4	L	13	VAL	2.4
4	L	169	LYS	2.4
3	E	125	PRO	2.3
2	D	92	LEU	2.3
2	B	448	CYS	2.3
3	H	195	PRO	2.3
3	H	165	LEU	2.3
4	F	142	LYS	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	139	PHE	2.3
3	E	118	SER	2.3
3	H	183	LEU	2.3
2	D	28	ASP	2.3
2	B	446	HIS	2.3
2	B	378	GLU	2.3
2	B	456	GLU	2.3
2	D	378	GLU	2.3
3	E	169	VAL	2.2
2	D	45	LEU	2.2
4	F	173	TYR	2.2
3	E	161	ASN	2.2
1	C	217	SER	2.2
3	E	208	SER	2.2
2	B	381	PRO	2.2
2	D	382	GLY	2.2
2	D	49	CYS	2.2
4	F	152	GLY	2.2
3	E	124	ALA	2.2
4	F	184	ASP	2.2
2	D	79	GLN	2.1
1	A	130	CYS	2.1
4	F	79	ASP	2.1
3	E	19	LYS	2.1
2	B	76	ASP	2.1
2	B	462	CYS	2.1
2	D	455	PHE	2.1
3	H	198	SER	2.1
2	B	452	ASN	2.1
2	B	29	GLU	2.1
4	F	75	ILE	2.1
1	C	320	ARG	2.1
1	C	106	ALA	2.0
3	E	117	VAL	2.0
3	H	148	VAL	2.0
1	C	129	SER	2.0
2	D	178	TYR	2.0
4	F	21	ILE	2.0
1	A	171	PHE	2.0
2	D	32	PRO	2.0
3	E	18	VAL	2.0
5	I	492[A]	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	112	ALA	2.0
3	E	159	THR	2.0
5	I	494[A]	GLY	2.0
1	A	118	LYS	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](#)

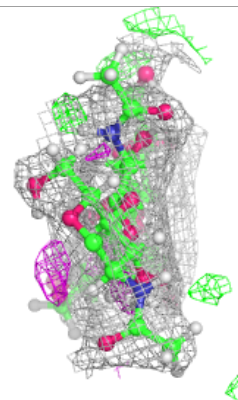
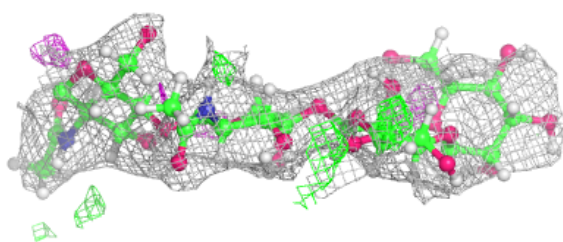
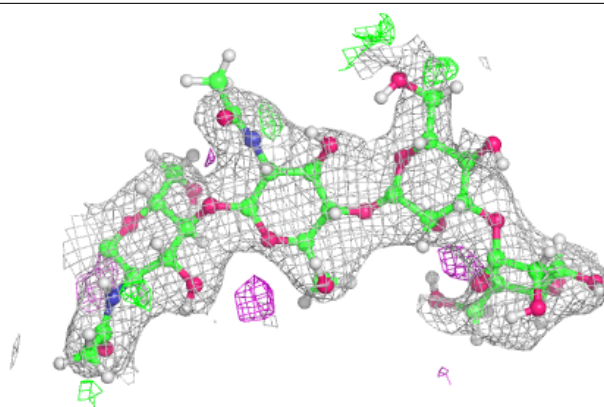
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MAN	M	4	11/12	0.75	0.30	124,133,158,159	0
6	MAN	G	4	11/12	0.77	0.28	136,140,166,168	0
6	BMA	G	3	11/12	0.77	0.22	120,135,160,162	0
7	NAG	N	1	14/15	0.83	0.27	86,108,128,132	0
6	BMA	M	3	11/12	0.84	0.38	134,142,170,170	0
7	NAG	N	2	14/15	0.86	0.36	114,138,165,167	0
6	NAG	M	2	14/15	0.89	0.32	92,115,141,144	0
7	NAG	K	1	14/15	0.90	0.26	87,104,120,125	0
6	NAG	G	2	14/15	0.92	0.15	76,93,106,112	0
7	NAG	K	2	14/15	0.92	0.34	106,129,155,157	0
6	NAG	M	1	14/15	0.93	0.15	48,64,89,91	0
6	NAG	G	1	14/15	0.95	0.14	26,53,72,78	0

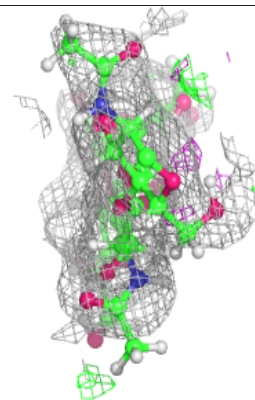
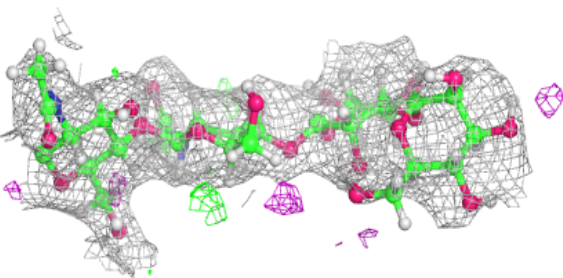
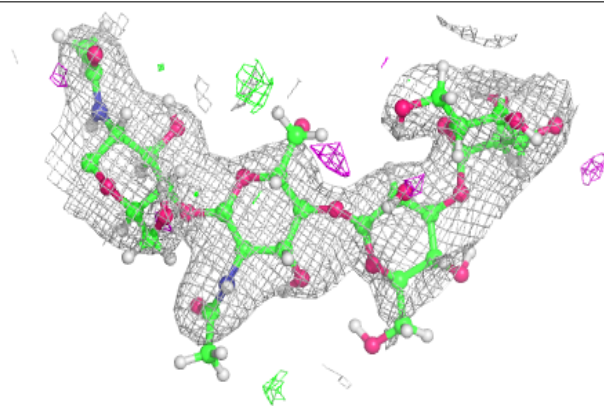
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain G:**

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

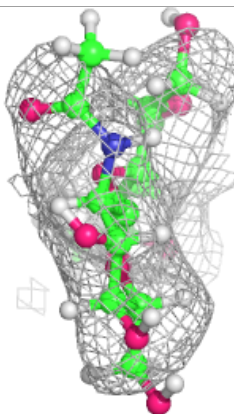
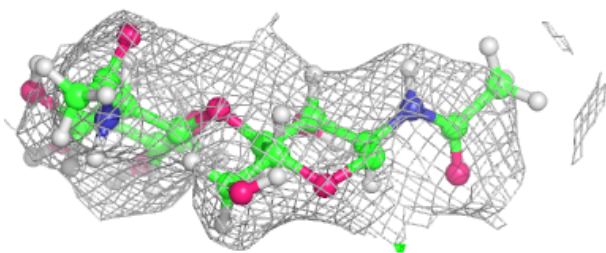
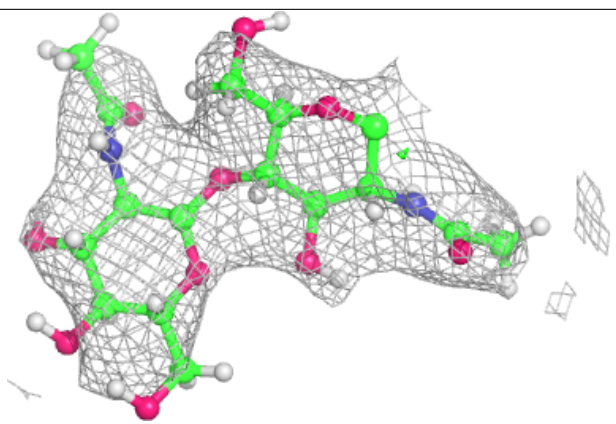
**Electron density around Chain M:**

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

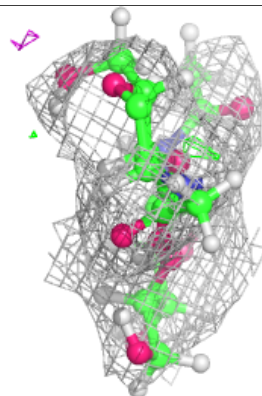
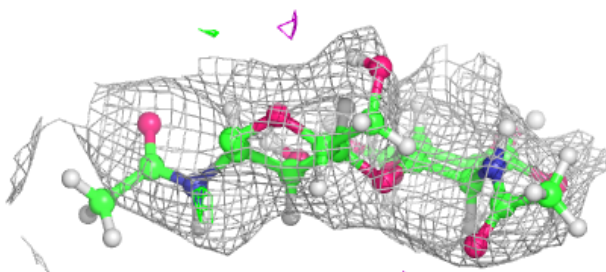
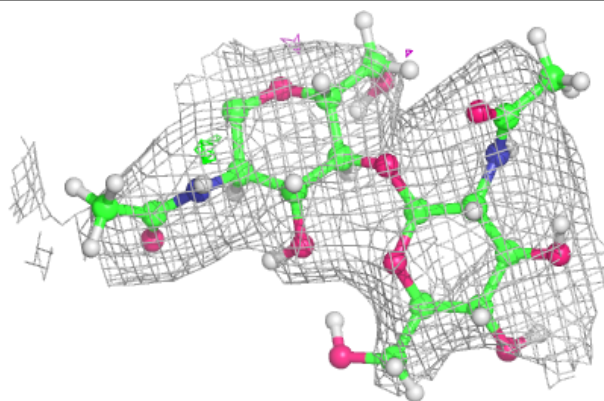


**Electron density around Chain K:**

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

**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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	SO4	B	1467	5/5	0.72	0.32	141,142,143,145	0
8	SO4	A	1459	5/5	0.77	0.49	161,161,162,162	0
8	SO4	L	1216	5/5	0.77	0.26	140,140,143,144	0
8	SO4	B	1468	5/5	0.80	0.31	153,154,154,154	0
8	SO4	C	1454	5/5	0.81	0.24	133,134,135,137	0
8	SO4	C	1456	5/5	0.82	0.17	134,135,137,138	0
8	SO4	B	1469	5/5	0.82	0.29	163,163,164,164	0
11	NAG	B	3319	14/15	0.83	0.36	104,123,147,151	0
11	NAG	D	3319	14/15	0.85	0.30	82,102,122,126	0
8	SO4	D	1472	5/5	0.86	0.20	128,130,131,133	0
8	SO4	C	1457	5/5	0.86	0.34	150,151,152,152	0
8	SO4	A	1456	5/5	0.88	0.19	117,121,123,124	0
8	SO4	A	1455	5/5	0.88	0.30	123,125,126,128	0
8	SO4	A	1457	5/5	0.90	0.22	125,125,127,128	0
8	SO4	A	1461	5/5	0.91	0.21	91,91,97,101	0
9	CA	B	2002	1/1	0.91	0.09	67,67,67,67	0
8	SO4	A	1463	5/5	0.91	0.27	116,119,120,122	0
8	SO4	A	1458	5/5	0.91	0.20	94,107,109,112	0
8	SO4	L	1215	5/5	0.92	0.23	115,116,116,118	0
9	CA	C	2004	1/1	0.92	0.04	66,66,66,66	0
8	SO4	C	1458	5/5	0.93	0.24	133,135,135,137	0
8	SO4	C	1455	5/5	0.93	0.10	104,106,106,107	0
10	MG	D	2001	1/1	0.95	0.10	50,50,50,50	0
9	CA	D	2002	1/1	0.96	0.15	53,53,53,53	0
9	CA	C	2007	1/1	0.96	0.15	39,39,39,39	0
9	CA	C	2006	1/1	0.97	0.15	49,49,49,49	0
8	SO4	A	1462	5/5	0.97	0.19	83,92,97,100	0
8	SO4	A	1460	5/5	0.98	0.16	76,76,80,83	0
9	CA	A	2004	1/1	0.98	0.08	43,43,43,43	0
9	CA	A	2005	1/1	0.98	0.15	32,32,32,32	0
9	CA	A	2006	1/1	0.98	0.21	25,25,25,25	0
10	MG	B	2001	1/1	0.99	0.20	33,33,33,33	0
9	CA	B	2003	1/1	0.99	0.26	28,28,28,28	0
9	CA	A	2007	1/1	0.99	0.21	26,26,26,26	0
9	CA	C	2005	1/1	0.99	0.04	55,55,55,55	0
9	CA	D	2003	1/1	1.00	0.23	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.