



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 06:13 PM EDT

PDB ID : 7L8P  
Title : Integrin alphaIIb beta3 in complex with sibrifiban  
Authors : Lin, F.-Y.; Springer, T.A.  
Deposited on : 2020-12-31  
Resolution : 2.35 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)

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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

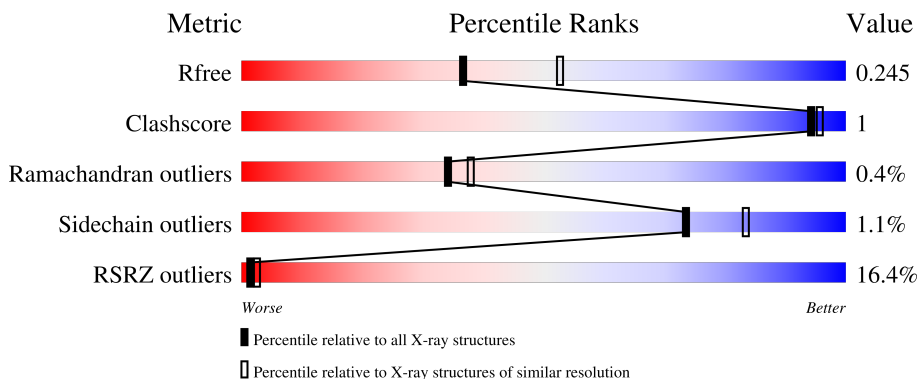
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	 7% 96%
1	C	457	 9% 95%
2	B	472	 15% 93% 6%
2	D	472	 14% 96%
3	E	221	 48% 94%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL	C	504	-	-	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 42834 atoms, of which 20392 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 Isoform 3 of 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	0	10	0
			6919	2245	3387	611	668	8			
1	C	453	Total	C	H	N	O	S	0	6	0
			6840	2224	3338	604	666	8			

- Molecule 2 is a protein called Isoform Beta-3C of Integrin beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	466	Total	C	H	N	O	S	6	10	0
			7202	2264	3568	621	715	34			
2	D	471	Total	C	H	N	O	S	10	3	0
			7206	2271	3561	622	717	35			

- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	214	Total	C	H	N	O	S	0	0	0
			3221	1035	1590	264	326	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			

- Molecule 4 is a protein called Monoclonal antibody 10E5 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
			3190	1019	1553	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	268	341	9			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	G	5	118	34	57	2	25	0	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
6	I	2	55	16	27	2	10	0	0	0
6	K	2	55	16	27	2	10	0	0	0

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



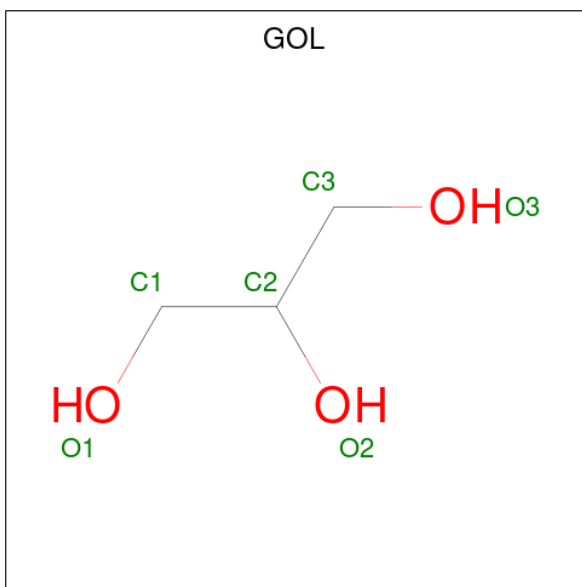
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
7	J	4	97	28	47	2	20	0	0	0

- 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	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	L	1	Total O S 5 4 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

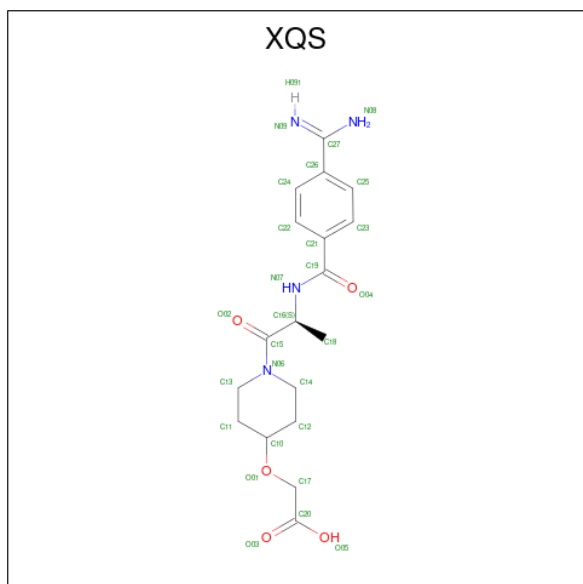
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
11	B	1	1	1	0	0
11	D	1	1	1	0	0

- Molecule 12 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	
12	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
12	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 13 is sibrifiban (active form) (three-letter code: XQS) (formula:  $C_{18}H_{24}N_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
13	B	1	Total	C	H	N	O	0	0
			51	18	24	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	H	N	O	0	0
			51	18	24	4	5		

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	2	Total	Cl	0	0
			2	2		

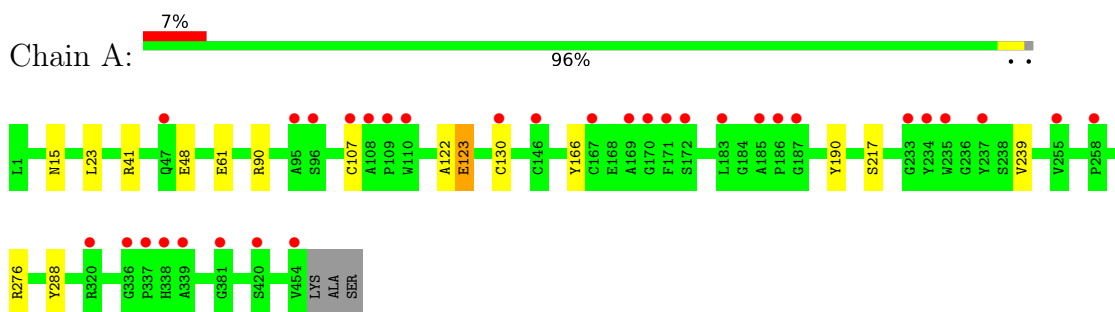
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	474	Total	O	0	0
			474	474		
15	B	245	Total	O	0	0
			245	245		
15	C	265	Total	O	0	0
			265	265		
15	D	193	Total	O	0	0
			193	193		
15	E	13	Total	O	0	0
			13	13		
15	F	11	Total	O	0	0
			11	11		
15	H	35	Total	O	0	0
			35	35		
15	L	40	Total	O	0	0
			40	40		

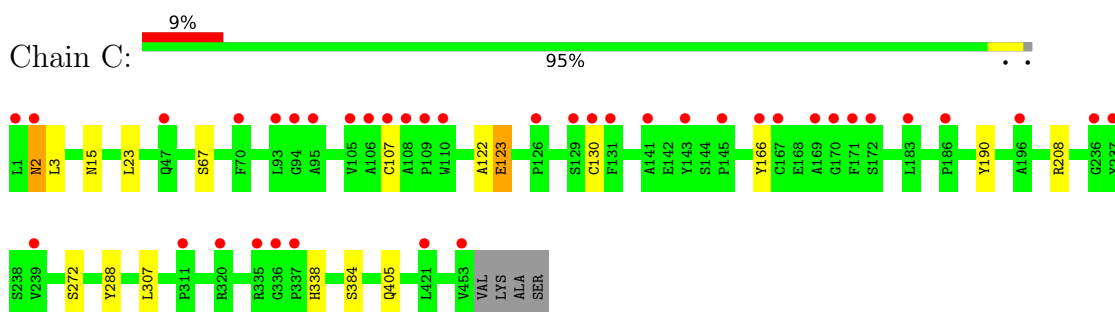
### 3 Residue-property plots [i](#)

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.

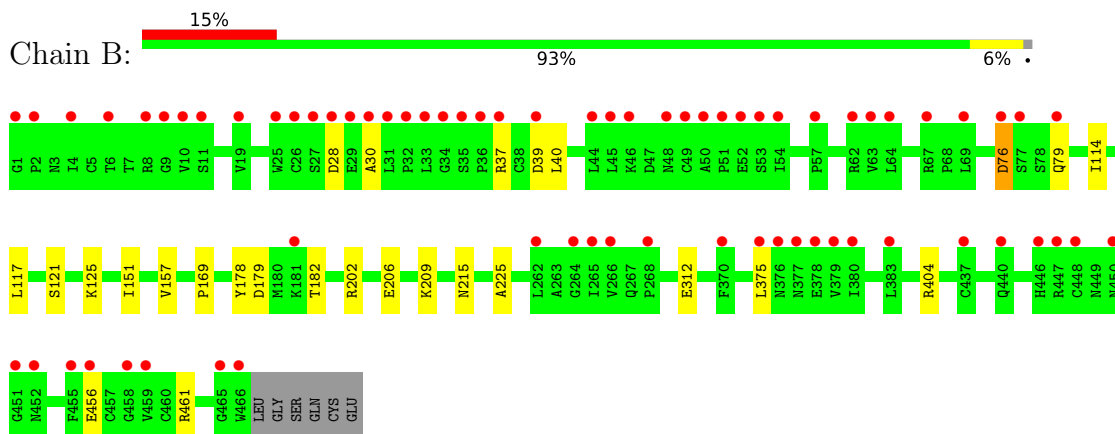
- Molecule 1: Isoform 3 of Integrin alpha-IIb



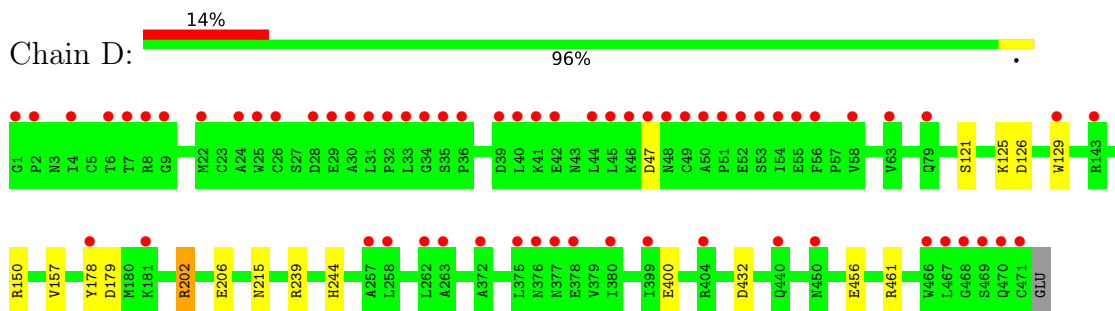
- Molecule 1: Isoform 3 of Integrin alpha-IIb



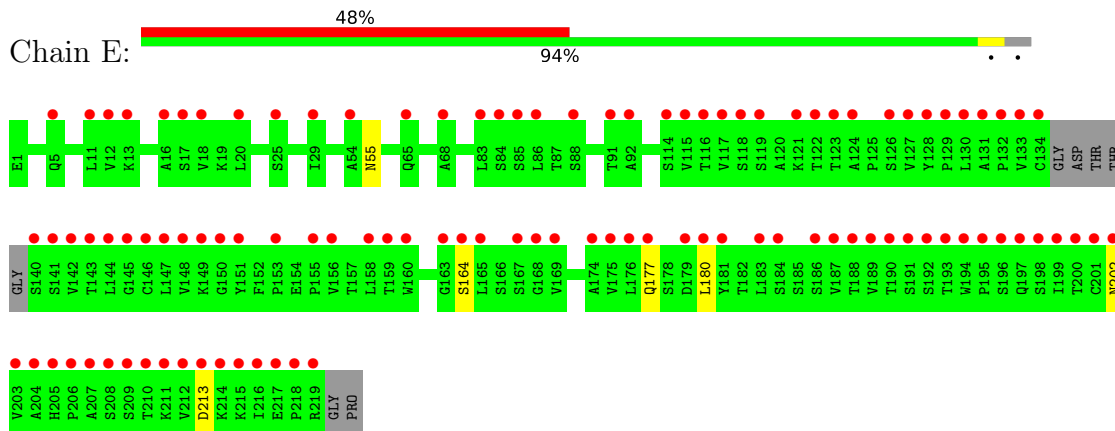
- Molecule 2: Isoform Beta-3C of Integrin beta-3



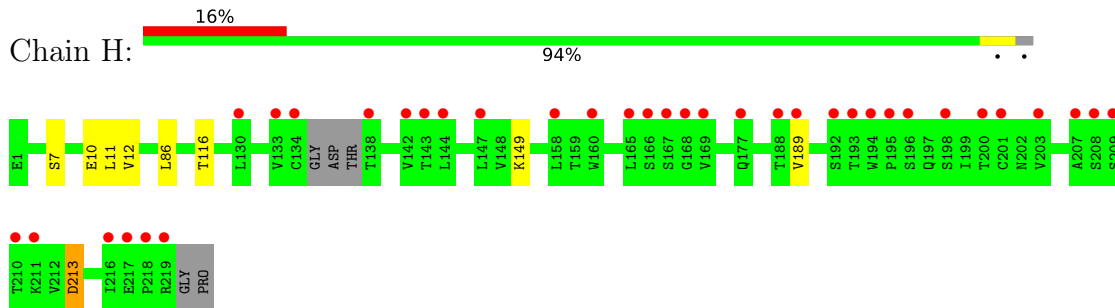
- Molecule 2: Isoform Beta-3C of Integrin beta-3



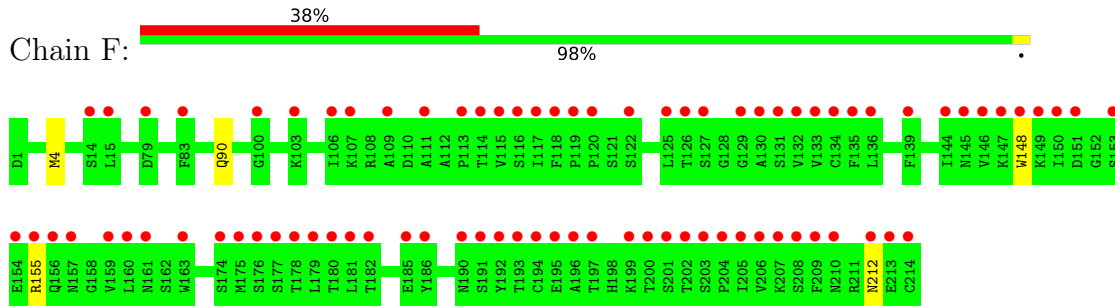
- Molecule 3: Monoclonal antibody 10E5 heavy chain



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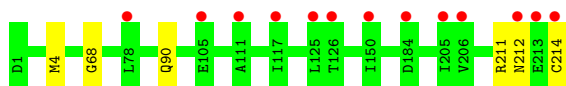


- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 4: Monoclonal antibody 10E5 light chain





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

Chain G: 60% 40%



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

Chain I: 100%



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

Chain K: 50% 50%



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

Chain J: 25% 75%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	257.50Å 144.68Å 104.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 2.35 49.22 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.22-2.35) 98.9 (49.22-2.35)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575, PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.204 , 0.245 0.203 , 0.245	Depositor DCC
$R_{free}$ test set	1992 reflections (1.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtrriage
Anisotropy	0.224	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	42834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, CA, XQS, SO4, BMA, CL, MAN, 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	0.30	0/3659	0.52	2/4986 (0.0%)
1	C	0.28	0/3618	0.48	0/4930
2	B	0.26	0/3743	0.46	0/5074
2	D	0.27	0/3726	0.46	0/5052
3	E	0.25	0/1673	0.44	0/2290
3	H	0.27	0/1684	0.46	0/2305
4	F	0.25	0/1673	0.43	0/2269
4	L	0.26	0/1673	0.46	0/2269
All	All	0.27	0/21449	0.47	2/29175 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	239[A]	VAL	CG1-CB-CG2	7.21	122.43	110.90
1	A	239[B]	VAL	CG1-CB-CG2	7.21	122.43	110.90

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3532	3387	3371	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3502	3338	3320	6	0
2	B	3634	3568	3531	14	0
2	D	3645	3561	3549	13	0
3	E	1631	1590	1590	3	0
3	H	1642	1600	1600	5	0
4	F	1637	1553	1553	2	0
4	L	1637	1553	1553	3	0
5	G	61	57	52	0	0
6	I	28	27	25	0	0
6	K	28	27	25	1	0
7	J	50	47	43	0	0
8	A	15	0	0	0	0
8	C	15	0	0	0	0
8	L	5	0	0	0	0
9	A	6	8	8	0	0
10	A	4	0	0	0	0
10	B	2	0	0	0	0
10	C	4	0	0	0	0
10	D	2	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
12	B	14	14	13	0	0
12	D	14	14	13	0	0
13	B	27	24	0	1	0
13	C	27	24	0	1	0
14	C	2	0	0	0	0
15	A	474	0	0	5	0
15	B	245	0	0	3	0
15	C	265	0	0	2	0
15	D	193	0	0	3	0
15	E	13	0	0	0	0
15	F	11	0	0	0	0
15	H	35	0	0	3	0
15	L	40	0	0	0	0
All	All	22442	20392	20246	54	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (54) 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)
15:H:324:HOH:O	4:L:214:CYS:SG	2.30	0.89
1:A:15[B]:ASN:ND2	15:A:601:HOH:O	2.21	0.69
1:C:208:ARG:O	15:C:602:HOH:O	2.13	0.67
1:C:384:SER:OG	15:C:601:HOH:O	2.12	0.65
3:H:149:LYS:NZ	15:H:302:HOH:O	2.33	0.61
3:H:10:GLU:O	15:H:301:HOH:O	2.16	0.60
1:A:48:GLU:OE2	1:A:90[B]:ARG:NH1	2.36	0.57
2:B:209:LYS:NZ	15:B:2105:HOH:O	2.37	0.57
1:A:122:ALA:O	1:A:123:GLU:HB2	2.05	0.57
1:A:90[A]:ARG:NH2	15:A:616:HOH:O	2.38	0.56
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.87	0.56
2:B:39:ASP:OD1	2:B:40:LEU:N	2.38	0.56
3:E:177:GLN:N	3:E:180:LEU:O	2.38	0.54
2:D:129[A]:TRP:NE1	15:D:2104:HOH:O	2.34	0.52
1:C:122:ALA:O	1:C:123:GLU:HB2	2.11	0.50
1:A:15[A]:ASN:ND2	15:A:622:HOH:O	2.44	0.49
2:B:28:ASP:OD1	2:B:30:ALA:N	2.45	0.49
2:B:125:LYS:NZ	15:B:2108:HOH:O	2.44	0.49
2:D:456:GLU:OE2	2:D:461:ARG:NH1	2.46	0.49
2:D:400:GLU:HB2	6:K:1:NAG:H83	1.95	0.49
1:C:2:ASN:N	1:C:2:ASN:OD1	2.47	0.48
2:B:404:ARG:NH1	15:B:2110:HOH:O	2.45	0.48
1:A:41:ARG:NH1	15:A:612:HOH:O	2.37	0.48
1:C:3:LEU:O	1:C:405:GLN:NE2	2.42	0.48
4:F:4:MET:HE2	4:F:90:GLN:HB3	1.95	0.48
3:E:202:ASN:HA	3:E:213:ASP:HB3	1.96	0.47
2:D:126:ASP:OD1	2:D:126:ASP:N	2.48	0.47
2:D:239:ARG:O	2:D:244:HIS:NE2	2.44	0.46
2:D:125:LYS:NZ	15:D:2105:HOH:O	2.37	0.46
2:D:178:TYR:CG	2:D:179:ASP:N	2.83	0.46
1:A:276:ARG:NH1	15:A:630:HOH:O	2.49	0.46
1:C:107:CYS:HA	1:C:130:CYS:HA	1.99	0.45
3:E:213:ASP:OD1	3:E:213:ASP:N	2.50	0.45
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.99	0.45
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.50	0.45
2:D:150:ARG:NH1	15:D:2113:HOH:O	2.50	0.44
13:C:510:XQS:O03	2:D:121:SER:HB2	2.17	0.43
1:A:122:ALA:O	1:A:123:GLU:CB	2.67	0.43
2:B:121:SER:HB2	13:B:2005:XQS:O03	2.18	0.43
2:B:76:ASP:HB3	2:B:79:GLN:H	1.84	0.42
2:B:178:TYR:CG	2:B:179:ASP:N	2.87	0.42
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:ARG:HE	2:D:239:ARG:HD3	1.84	0.42
3:H:213:ASP:OD1	3:H:213:ASP:N	2.53	0.42
4:L:211:ARG:O	4:L:212:ASN:HB2	2.20	0.41
2:D:126:ASP:HA	2:D:129[A]:TRP:CE3	2.56	0.41
2:B:312:GLU:CD	2:D:125:LYS:HE2	2.41	0.41
2:B:117:LEU:HD11	2:B:225:ALA:HB1	2.03	0.41
4:F:148:TRP:O	4:F:155:ARG:N	2.53	0.41
2:B:114:ILE:O	2:B:151:ILE:HA	2.21	0.41
2:B:169:PRO:HD3	2:B:178:TYR:OH	2.20	0.41
2:D:202:ARG:NH2	2:D:206:GLU:OE2	2.50	0.41
1:A:107:CYS:HA	1:A:130:CYS:HA	2.02	0.40
3:H:11:LEU:HD12	3:H:116:THR:HB	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/457 (101%)	445 (96%)	16 (4%)	1 (0%)	47	55
1	C	457/457 (100%)	443 (97%)	13 (3%)	1 (0%)	47	55
2	B	474/472 (100%)	453 (96%)	18 (4%)	3 (1%)	25	26
2	D	472/472 (100%)	447 (95%)	24 (5%)	1 (0%)	47	55
3	E	210/221 (95%)	190 (90%)	18 (9%)	2 (1%)	15	14
3	H	212/221 (96%)	199 (94%)	12 (6%)	1 (0%)	29	31
4	F	212/214 (99%)	194 (92%)	17 (8%)	1 (0%)	29	31
4	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	31
All	All	2711/2728 (99%)	2574 (95%)	126 (5%)	11 (0%)	34	38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
3	E	55	ASN
1	C	123	GLU
3	E	164	SER
2	B	76	ASP
2	B	375	LEU
4	F	212	ASN
4	L	68	GLY
3	H	189	VAL
2	B	157	VAL
2	D	157	VAL

### 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	371/364 (102%)	365 (98%)	6 (2%)	62	74
1	C	366/364 (100%)	356 (97%)	10 (3%)	44	55
2	B	422/417 (101%)	419 (99%)	3 (1%)	84	90
2	D	419/417 (100%)	415 (99%)	4 (1%)	76	85
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	185 (99%)	2 (1%)	73	83
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2327/2318 (100%)	2302 (99%)	25 (1%)	73	83

All (25) 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	217	SER

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Mol	Chain	Res	Type
1	A	288	TYR
2	B	37	ARG
2	B	182	THR
2	B	215	ASN
1	C	2	ASN
1	C	15	ASN
1	C	23	LEU
1	C	67	SER
1	C	166	TYR
1	C	190	TYR
1	C	272	SER
1	C	288	TYR
1	C	307	LEU
1	C	338	HIS
2	D	47	ASP
2	D	202	ARG
2	D	215	ASN
2	D	432	ASP
3	H	7	SER
3	H	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

13 monosaccharides are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	NAG	G	1	2,5	14,14,15	0.39	0	17,19,21	0.48	0
5	NAG	G	2	5	14,14,15	0.43	0	17,19,21	0.59	0
5	BMA	G	3	5	11,11,12	0.88	0	15,15,17	0.79	0
5	MAN	G	4	5	11,11,12	0.61	0	15,15,17	1.19	2 (13%)
5	MAN	G	5	5	11,11,12	0.81	0	15,15,17	1.15	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.51	0	17,19,21	0.47	0
6	NAG	I	2	6	14,14,15	0.14	0	17,19,21	0.59	0
7	NAG	J	1	2,7	14,14,15	0.17	0	17,19,21	0.57	0
7	NAG	J	2	7	14,14,15	0.65	1 (7%)	17,19,21	0.53	0
7	BMA	J	3	7	11,11,12	0.70	0	15,15,17	0.88	1 (6%)
7	MAN	J	4	7	11,11,12	0.71	0	15,15,17	0.97	1 (6%)
6	NAG	K	1	2,6	14,14,15	0.56	0	17,19,21	0.42	0
6	NAG	K	2	6	14,14,15	0.18	0	17,19,21	0.62	0

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	2	NAG	O5-C1	-2.29	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4	MAN	C1-O5-C5	3.33	116.70	112.19
5	G	5	MAN	C1-O5-C5	2.69	115.83	112.19
7	J	4	MAN	C1-O5-C5	2.49	115.56	112.19
5	G	5	MAN	O2-C2-C3	-2.28	105.58	110.14
5	G	4	MAN	O2-C2-C3	-2.16	105.81	110.14
7	J	3	BMA	O2-C2-C3	-2.07	105.99	110.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

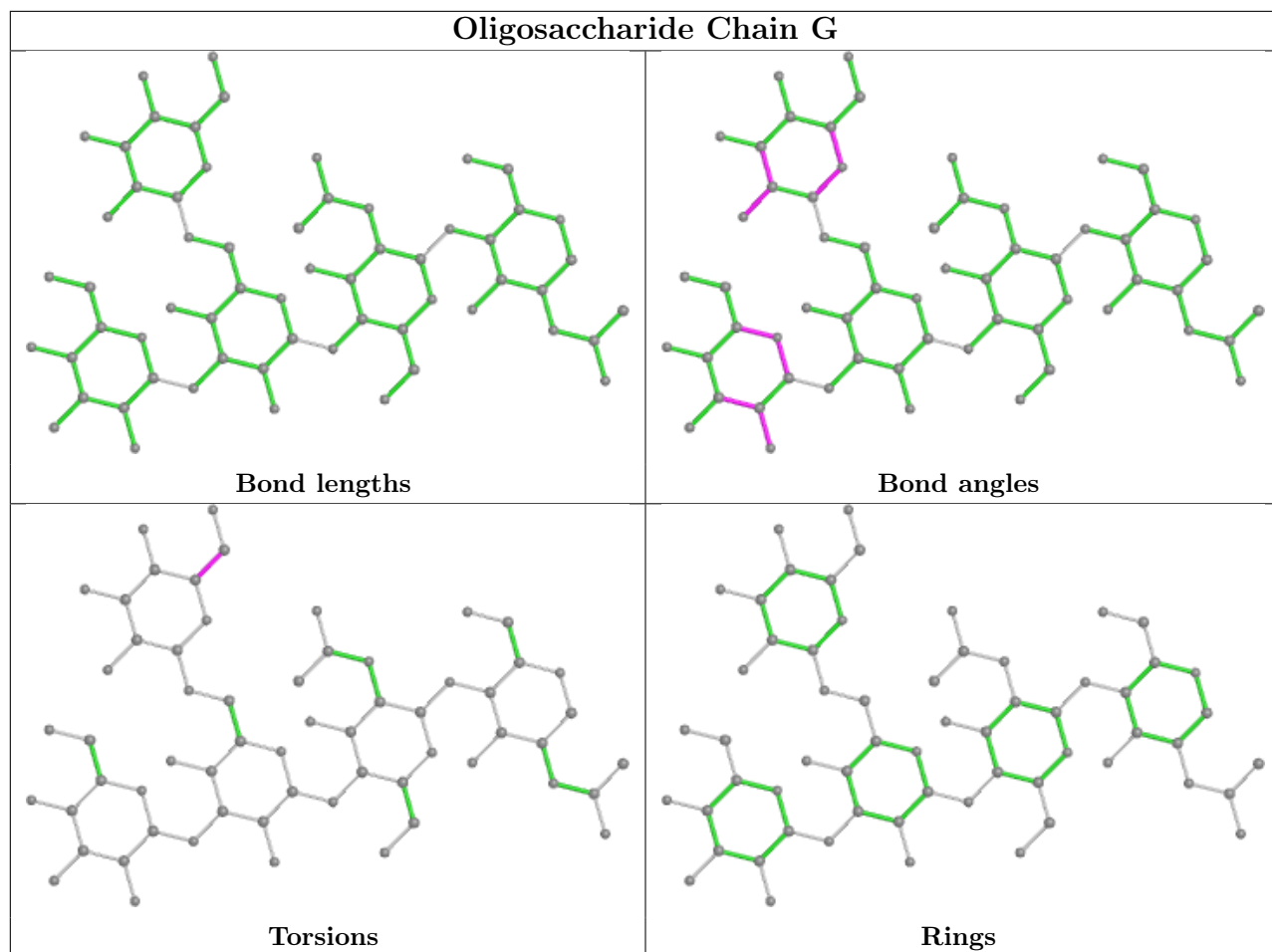
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	G	5	MAN	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6

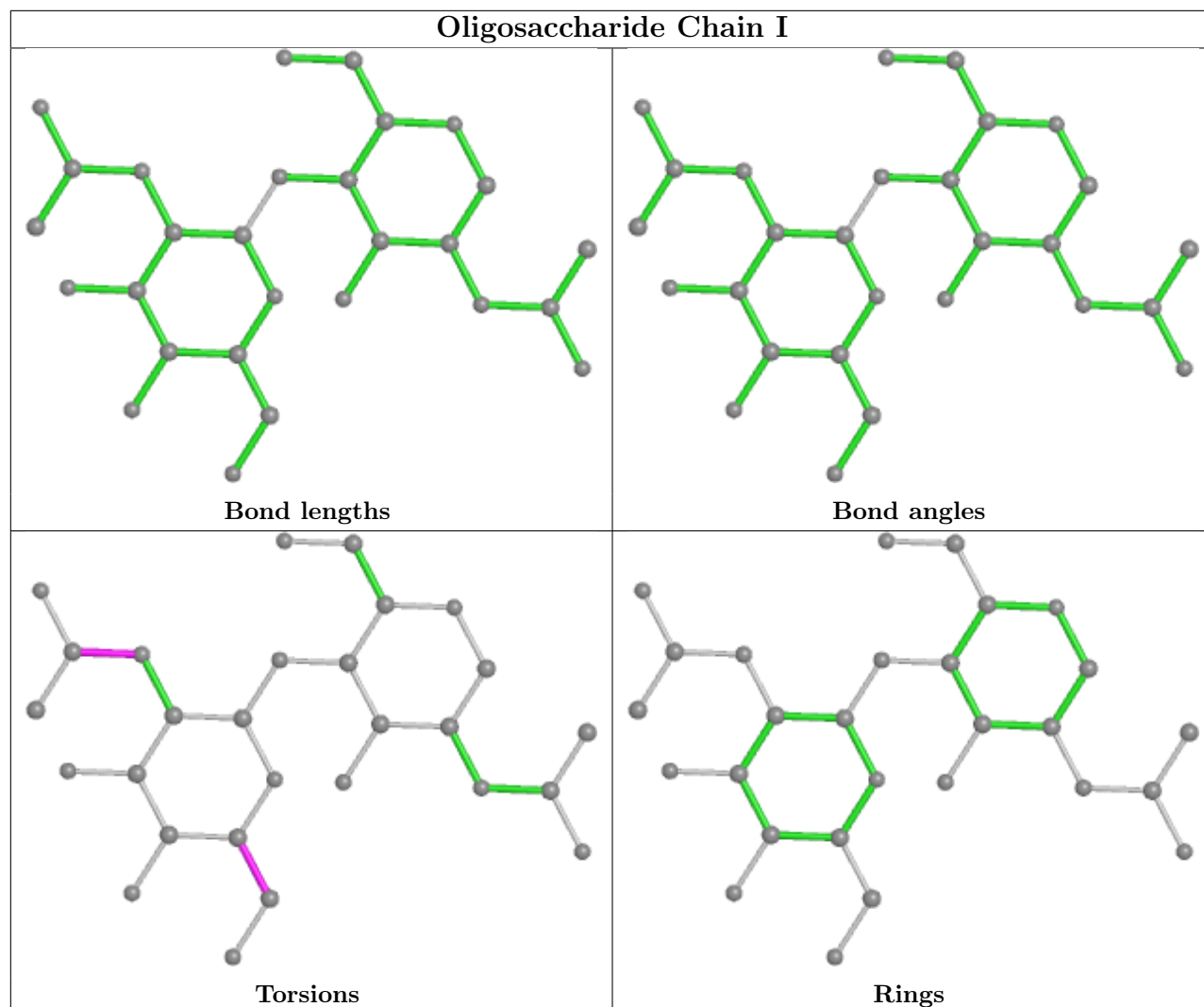
There are no ring outliers.

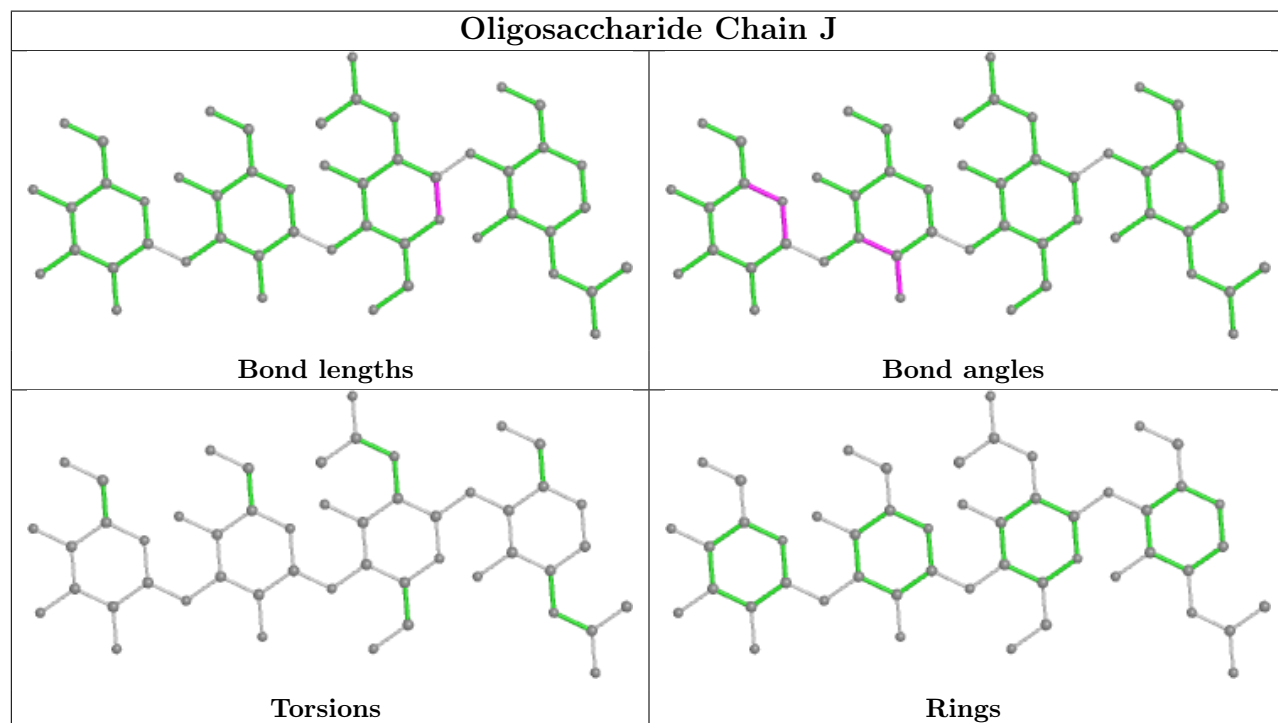
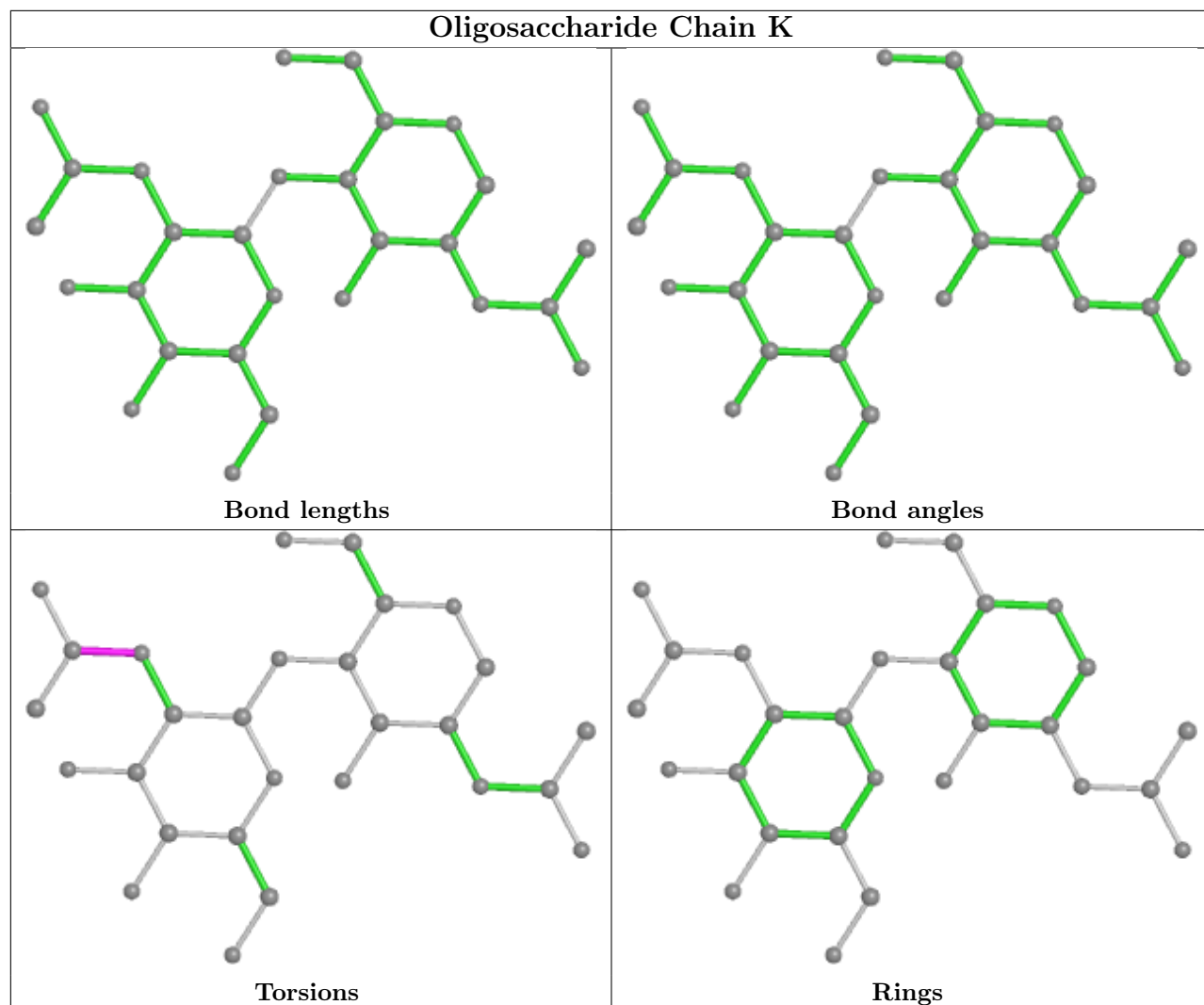
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	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

Of 28 ligands modelled in this entry, 16 are monoatomic - leaving 12 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	L	301	-	4,4,4	0.22	0	6,6,6	0.12	0
13	XQS	B	2005	11	28,28,28	0.79	0	33,38,38	2.06	8 (24%)
8	SO4	C	503	-	4,4,4	0.18	0	6,6,6	0.24	0
12	NAG	B	2004	2	14,14,15	0.45	0	17,19,21	0.57	0
8	SO4	A	502	-	4,4,4	0.22	0	6,6,6	0.27	0
8	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.23	0
8	SO4	A	503	-	4,4,4	0.16	0	6,6,6	0.18	0
12	NAG	D	2004	2	14,14,15	0.40	0	17,19,21	0.57	0
9	GOL	A	504	-	5,5,5	0.31	0	5,5,5	0.24	0
13	XQS	C	510	11	28,28,28	0.82	0	33,38,38	1.97	8 (24%)
8	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.18	0
8	SO4	C	501	-	4,4,4	0.22	0	6,6,6	0.21	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
13	XQS	B	2005	11	-	4/25/35/35	0/2/2/2
12	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
12	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
9	GOL	A	504	-	-	2/4/4/4	-
13	XQS	C	510	11	-	4/25/35/35	0/2/2/2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	2005	XQS	C13-C11-C10	-7.17	102.43	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	510	XQS	C13-C11-C10	-7.08	102.53	110.32
13	B	2005	XQS	C11-C13-N06	-4.55	103.91	110.82
13	C	510	XQS	C11-C13-N06	-4.31	104.27	110.82
13	B	2005	XQS	C14-C12-C10	-4.09	105.82	110.32
13	C	510	XQS	C14-N06-C13	3.32	119.02	112.62
13	B	2005	XQS	C14-N06-C13	2.75	117.91	112.62
13	C	510	XQS	C14-C12-C10	-2.71	107.34	110.32
13	B	2005	XQS	O01-C10-C12	2.66	118.08	109.05
13	C	510	XQS	O01-C10-C12	2.43	117.31	109.05
13	C	510	XQS	O03-C20-C17	-2.32	113.73	122.44
13	C	510	XQS	O02-C15-N06	2.29	124.35	121.67
13	B	2005	XQS	O03-C20-C17	-2.25	113.98	122.44
13	B	2005	XQS	C12-C14-N06	-2.22	107.45	110.82
13	C	510	XQS	C12-C10-C11	-2.09	107.70	111.74
13	B	2005	XQS	O02-C15-N06	2.06	124.08	121.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	504	GOL	O1-C1-C2-C3
13	C	510	XQS	O01-C17-C20-O05
9	A	504	GOL	O1-C1-C2-O2
13	C	510	XQS	O01-C17-C20-O03
13	B	2005	XQS	C12-C10-O01-C17
13	C	510	XQS	C11-C10-O01-C17
13	C	510	XQS	C12-C10-O01-C17
13	B	2005	XQS	O01-C17-C20-O03
13	B	2005	XQS	O01-C17-C20-O05
13	B	2005	XQS	C11-C10-O01-C17

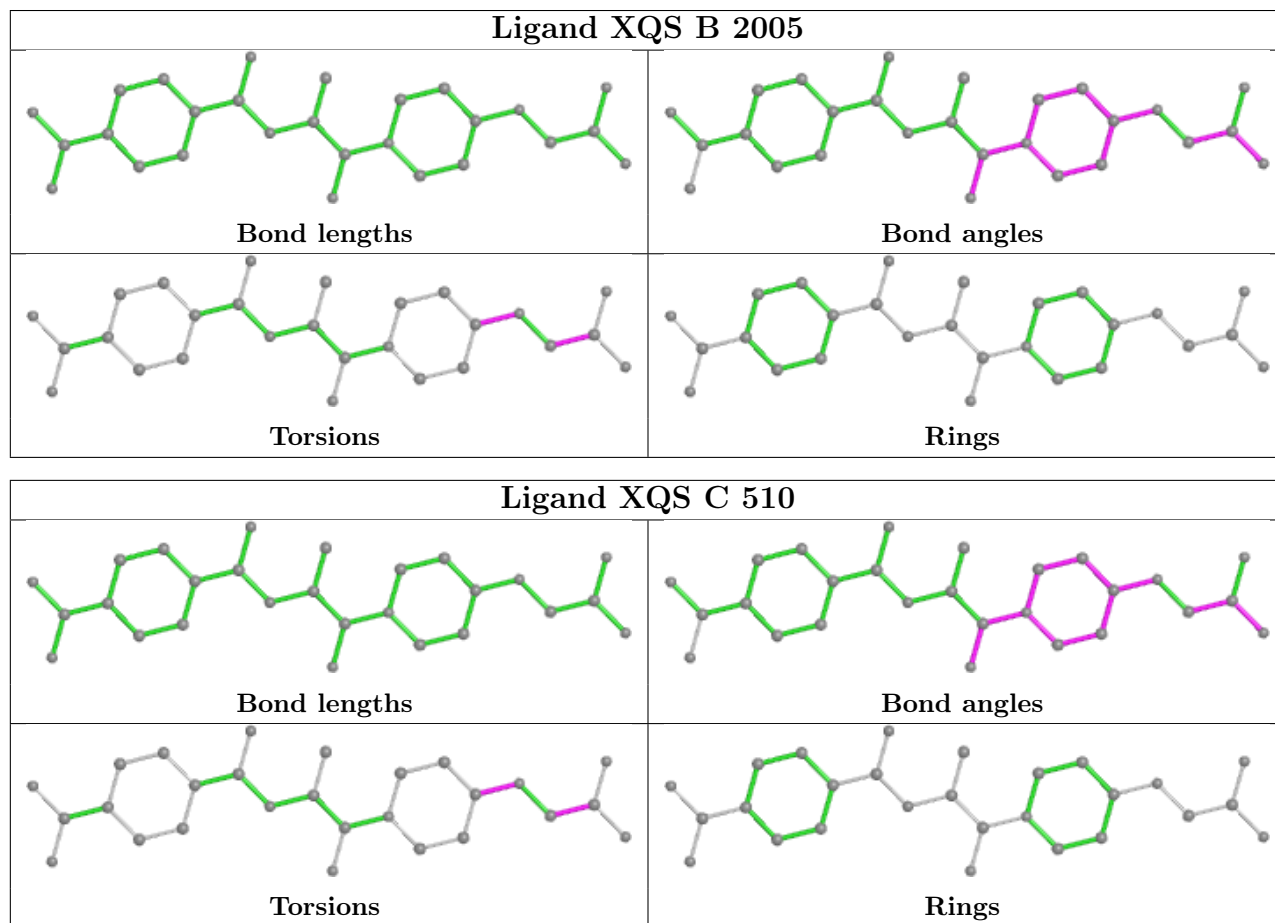
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	2005	XQS	1	0
13	C	510	XQS	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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%)	0.84	32 (7%) 16 24	27, 39, 62, 97	0
1	C	453/457 (99%)	0.74	39 (8%) 10 16	32, 52, 76, 104	0
2	B	466/472 (98%)	1.00	70 (15%) 2 3	27, 61, 124, 152	1 (0%)
2	D	471/472 (99%)	0.94	64 (13%) 3 4	35, 70, 120, 148	1 (0%)
3	E	214/221 (96%)	2.48	106 (49%) 0 0	57, 110, 168, 185	0
3	H	216/221 (97%)	0.99	36 (16%) 1 2	43, 87, 131, 149	0
4	F	214/214 (100%)	2.15	82 (38%) 0 0	60, 106, 160, 174	0
4	L	214/214 (100%)	0.62	13 (6%) 21 30	48, 78, 102, 133	0
All	All	2702/2728 (99%)	1.09	442 (16%) 1 2	27, 65, 137, 185	2 (0%)

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	201	CYS	14.2
3	E	212	VAL	11.8
3	E	134	CYS	10.6
2	B	33	LEU	10.5
3	E	210	THR	10.0
2	B	77	SER	9.9
4	F	148	TRP	9.9
2	D	469	SER	9.7
4	F	214	CYS	9.6
2	D	471	CYS	9.3
3	E	165	LEU	9.3
2	D	375	LEU	9.2
3	E	196	SER	8.9
3	E	144	LEU	8.8
4	F	147	LYS	8.8
4	F	126	THR	8.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	160	TRP	8.4
2	B	44	LEU	8.4
4	F	179	LEU	8.3
4	F	194	CYS	8.2
4	F	193	THR	8.2
4	F	115	VAL	8.1
4	F	130	ALA	8.1
4	F	181	LEU	8.1
3	E	194	TRP	8.0
3	E	219	ARG	8.0
4	L	214	CYS	7.8
3	E	216	ILE	7.7
3	E	142	VAL	7.3
2	B	36	PRO	7.3
3	E	199	ILE	7.3
4	F	125	LEU	7.2
4	F	206	VAL	7.1
3	E	132	PRO	6.8
2	B	1	GLY	6.8
4	F	159	VAL	6.8
2	D	44	LEU	6.8
4	F	204	PRO	6.8
3	H	189	VAL	6.8
3	E	193	THR	6.7
4	F	178	THR	6.7
4	F	195	GLU	6.4
3	E	200	THR	6.4
4	F	117	ILE	6.4
3	H	134	CYS	6.2
3	E	147	LEU	6.2
2	B	2	PRO	6.2
4	F	135	PHE	6.2
3	H	165	LEU	6.2
2	D	54	ILE	6.2
2	B	54	ILE	6.2
2	D	380	ILE	6.1
2	D	468	GLY	6.1
3	E	133	VAL	6.1
3	E	198	SER	6.1
4	F	150	ILE	6.0
4	F	205	ILE	6.0
4	F	133	VAL	6.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	454	VAL	5.9
2	B	8	ARG	5.9
4	F	213	GLU	5.9
2	D	33	LEU	5.9
4	F	132	VAL	5.8
3	E	195	PRO	5.8
3	H	133	VAL	5.6
4	F	146	VAL	5.6
2	B	34	GLY	5.6
4	F	136	LEU	5.6
3	E	92	ALA	5.6
4	F	157	ASN	5.5
2	D	470	GLN	5.5
2	B	32	PRO	5.5
2	B	49	CYS	5.5
3	E	16	ALA	5.4
4	F	134	CYS	5.4
3	E	203	VAL	5.3
3	E	192	SER	5.3
2	D	181	LYS	5.3
2	B	466	TRP	5.3
4	F	202	THR	5.3
4	F	160	LEU	5.3
3	E	129	PRO	5.2
3	H	198	SER	5.2
2	B	30	ALA	5.2
3	E	11	LEU	5.2
2	D	34	GLY	5.1
3	E	143	THR	5.1
2	B	451	GLY	5.1
2	D	8	ARG	5.1
4	F	209	PHE	5.1
2	B	10	VAL	5.1
3	E	156	VAL	5.1
4	F	144	ILE	5.0
2	D	35	SER	5.0
3	E	176	LEU	5.0
2	B	50	ALA	4.9
2	D	31	LEU	4.9
2	D	48	ASN	4.9
3	E	218	PRO	4.8
4	F	120	PRO	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	35	SER	4.8
4	F	186	TYR	4.8
3	H	138	THR	4.7
2	B	375	LEU	4.7
3	H	158	LEU	4.7
4	F	180	THR	4.7
1	C	1	LEU	4.7
4	F	197	THR	4.7
2	D	53	SER	4.6
2	D	36	PRO	4.6
2	D	2	PRO	4.6
4	F	122	SER	4.6
2	B	45	LEU	4.6
2	D	1	GLY	4.6
2	D	52	GLU	4.5
2	B	440	GLN	4.5
3	E	20	LEU	4.5
2	D	129[A]	TRP	4.5
1	A	337	PRO	4.5
3	E	158	LEU	4.5
2	D	32	PRO	4.5
2	D	376	ASN	4.4
4	F	156	GLN	4.4
3	E	83	LEU	4.4
4	F	201	SER	4.4
2	D	50	ALA	4.4
3	E	130	LEU	4.3
3	E	128	TYR	4.3
4	L	212	ASN	4.3
2	B	31	LEU	4.3
3	E	215	LYS	4.3
4	F	163	TRP	4.3
4	L	206	VAL	4.3
3	E	140	SER	4.2
3	E	148	VAL	4.2
4	L	213	GLU	4.2
3	E	191	SER	4.2
3	H	169	VAL	4.2
4	F	149	LYS	4.2
4	F	196	ALA	4.2
2	B	9	GLY	4.2
3	E	188	THR	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	29	GLU	4.2
2	D	40	LEU	4.2
2	B	4	ILE	4.2
3	E	114	SER	4.2
2	D	466	TRP	4.1
4	F	191	SER	4.1
3	E	205	HIS	4.1
4	F	151	ASP	4.0
3	E	12	VAL	4.0
2	B	28	ASP	4.0
3	H	207	ALA	4.0
2	D	58	VAL	4.0
3	E	169	VAL	4.0
3	E	131	ALA	4.0
4	F	118	PHE	4.0
2	D	30	ALA	4.0
4	F	208	SER	4.0
3	H	188	THR	3.9
1	A	339	ALA	3.9
1	C	130	CYS	3.9
4	F	154	GLU	3.9
3	E	183	LEU	3.9
3	H	218	PRO	3.8
3	E	206	PRO	3.8
2	D	55	GLU	3.8
2	B	181	LYS	3.8
4	L	205	ILE	3.8
4	F	212	ASN	3.8
2	B	376	ASN	3.8
3	E	54	ALA	3.8
4	F	210	ASN	3.8
4	F	207	LYS	3.8
4	F	83	PHE	3.7
4	F	182	THR	3.7
3	H	160	TRP	3.7
3	E	213	ASP	3.7
2	B	459	VAL	3.7
4	F	145	ASN	3.7
2	D	46	LYS	3.7
3	E	126	SER	3.6
2	D	7	THR	3.6
2	B	46	LYS	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	127	VAL	3.6
3	H	142	VAL	3.6
2	B	26	CYS	3.6
3	E	146	CYS	3.6
2	D	42	GLU	3.6
3	E	217	GLU	3.6
3	H	208	SER	3.6
2	D	79	GLN	3.6
3	H	216	ILE	3.5
3	E	177	GLN	3.5
2	D	39	ASP	3.5
2	D	450	ASN	3.5
2	D	22	MET	3.5
3	H	203	VAL	3.5
3	E	209	SER	3.5
4	F	127	SER	3.5
3	H	211	LYS	3.5
2	B	456	GLU	3.4
3	H	194	TRP	3.4
2	B	446	HIS	3.4
3	E	141	SER	3.4
1	A	338	HIS	3.4
3	E	168	GLY	3.4
2	B	69	LEU	3.4
2	B	452	ASN	3.4
3	E	163	GLY	3.4
2	B	48	ASN	3.4
2	B	67	ARG	3.4
4	F	119	PRO	3.3
2	D	28	ASP	3.3
3	E	175	VAL	3.3
2	B	450	ASN	3.3
3	E	204	ALA	3.3
4	F	111	ALA	3.3
2	B	51	PRO	3.3
3	H	144	LEU	3.3
3	E	186	SER	3.3
2	B	383	LEU	3.3
3	E	149	LYS	3.2
4	F	129	GLY	3.2
2	D	49	CYS	3.2
3	E	159	THR	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	130	CYS	3.2
2	D	378	GLU	3.2
3	E	17	SER	3.1
4	F	114	THR	3.1
3	E	153	PRO	3.1
3	E	187	VAL	3.1
2	D	45	LEU	3.1
4	F	200	THR	3.1
4	F	139	PHE	3.1
3	E	117	VAL	3.1
3	E	174	ALA	3.1
3	E	167	SER	3.1
3	H	195	PRO	3.1
1	C	131	PHE	3.1
3	H	166	SER	3.1
3	H	217	GLU	3.1
1	A	167	CYS	3.1
1	A	171	PHE	3.1
2	B	447	ARG	3.1
3	H	219	ARG	3.1
4	F	155	ARG	3.0
1	C	109	PRO	3.0
4	F	116	SER	3.0
2	B	379	VAL	3.0
3	E	189	VAL	3.0
1	C	171	PHE	3.0
2	D	51	PRO	3.0
3	E	155	PRO	3.0
2	B	76	ASP	2.9
3	E	211	LYS	2.9
3	E	115	VAL	2.9
1	C	107	CYS	2.9
4	F	131	SER	2.9
3	E	13	LYS	2.9
2	B	37	ARG	2.9
1	A	185	ALA	2.9
1	C	106	ALA	2.9
4	F	174	SER	2.9
3	E	145	GLY	2.9
4	F	190	ASN	2.9
4	F	107	LYS	2.9
2	B	265	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	336	GLY	2.8
2	B	458	GLY	2.8
3	E	84	SER	2.8
3	E	184	SER	2.8
4	F	177	SER	2.8
3	E	151	TYR	2.8
4	F	106	ILE	2.8
4	L	78	LEU	2.8
4	L	150	ILE	2.8
1	A	186	PRO	2.7
3	H	167	SER	2.7
2	B	377	ASN	2.7
3	E	181	TYR	2.7
2	D	9	GLY	2.7
4	F	14	SER	2.7
4	F	15	LEU	2.7
2	B	378	GLU	2.7
1	C	143	TYR	2.7
4	F	199	LYS	2.7
1	C	108	ALA	2.7
2	D	56	PHE	2.7
3	E	179	ASP	2.7
1	A	336	GLY	2.7
4	F	103	LYS	2.7
1	C	167	CYS	2.7
3	E	214	LYS	2.7
1	A	233	GLY	2.7
3	H	168	GLY	2.7
2	D	26	CYS	2.6
2	D	29	GLU	2.6
3	E	121	LYS	2.6
1	C	94	GLY	2.6
3	E	18	VAL	2.6
3	E	190	THR	2.6
3	E	208	SER	2.6
3	E	123	THR	2.6
1	C	237	TYR	2.6
3	H	130	LEU	2.6
4	L	126	THR	2.6
4	F	175	MET	2.6
1	C	335	ARG	2.6
1	C	95	ALA	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	143	ARG	2.6
3	H	193	THR	2.5
2	B	25	TRP	2.5
2	B	437	CYS	2.5
4	L	125	LEU	2.5
4	F	192	TYR	2.5
1	A	187	GLY	2.5
2	B	11	SER	2.5
4	L	117	ILE	2.5
2	B	262	LEU	2.5
3	H	147	LEU	2.5
3	E	91	THR	2.5
1	C	453	VAL	2.5
2	D	377	ASN	2.5
4	L	111	ALA	2.5
2	B	62	ARG	2.5
1	C	172	SER	2.5
3	E	85	SER	2.5
2	D	4	ILE	2.5
3	E	116	THR	2.5
3	H	209	SER	2.4
4	F	203	SER	2.4
1	C	196	ALA	2.4
2	B	266	VAL	2.4
4	F	113	PRO	2.4
3	E	86	LEU	2.4
3	E	164	SER	2.4
1	C	169	ALA	2.4
4	F	161	ASN	2.4
1	A	109	PRO	2.4
2	B	465	GLY	2.4
1	C	110	TRP	2.4
1	C	183	LEU	2.4
2	D	372	ALA	2.4
2	D	404	ARG	2.4
3	E	124	ALA	2.4
1	A	146	CYS	2.4
2	B	27	SER	2.4
1	C	337	PRO	2.4
2	B	455	PHE	2.4
4	F	185	GLU	2.4
3	H	201	CYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	150	GLY	2.3
3	E	180	LEU	2.3
1	A	170	GLY	2.3
2	B	64	LEU	2.3
3	E	25	SER	2.3
2	B	370	PHE	2.3
3	E	65	GLN	2.3
1	A	169	ALA	2.3
3	E	68	ALA	2.3
4	F	109	ALA	2.3
1	C	170	GLY	2.3
3	E	29	ILE	2.3
2	D	178	TYR	2.3
3	H	200	THR	2.3
3	H	210	THR	2.3
2	B	39	ASP	2.3
2	B	380	ILE	2.3
2	D	24	ALA	2.3
1	A	183	LEU	2.3
2	D	262	LEU	2.3
2	B	268	PRO	2.3
1	C	47	GLN	2.3
2	B	52	GLU	2.2
1	C	126	PRO	2.2
3	H	196	SER	2.2
2	D	399	ILE	2.2
4	L	105	GLU	2.2
1	A	172	SER	2.2
2	D	257	ALA	2.2
1	C	93	LEU	2.2
1	A	234	TYR	2.2
1	C	166	TYR	2.2
1	C	236	GLY	2.2
2	D	6	THR	2.2
2	B	53	SER	2.2
1	C	421	LEU	2.2
2	D	467	LEU	2.2
4	F	176	SER	2.2
4	L	184	ASP	2.2
1	C	70	PHE	2.2
2	D	263	ALA	2.2
3	E	207	ALA	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	320	ARG	2.2
1	A	107	CYS	2.2
2	B	448	CYS	2.2
2	D	258	LEU	2.2
1	A	258	PRO	2.2
1	A	96	SER	2.2
1	C	129	SER	2.2
1	A	237	TYR	2.1
1	A	255	VAL	2.1
1	A	47	GLN	2.1
1	A	235	TRP	2.1
3	E	88	SER	2.1
3	H	177	GLN	2.1
3	H	192	SER	2.1
1	A	108	ALA	2.1
2	D	47	ASP	2.1
4	F	79	ASP	2.1
3	E	197	GLN	2.1
3	E	118	SER	2.1
1	C	320	ARG	2.1
1	C	141	ALA	2.1
2	B	63	VAL	2.1
2	D	440	GLN	2.1
1	C	186	PRO	2.1
1	C	311	PRO	2.1
3	E	119	SER	2.1
2	D	63	VAL	2.1
3	E	202	ASN	2.1
2	B	264	GLY	2.1
1	A	95	ALA	2.1
1	C	105	VAL	2.1
4	F	153	SER	2.1
1	C	145	PRO	2.1
2	B	57	PRO	2.1
1	C	2	ASN	2.1
3	H	143	THR	2.1
1	A	381	GLY	2.1
2	D	41	LYS	2.0
2	B	6	THR	2.0
1	A	110	TRP	2.0
2	B	19	VAL	2.0
2	B	79	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	239	VAL	2.0
2	D	25	TRP	2.0
3	E	5	GLN	2.0
4	F	100	GLY	2.0
1	A	420	SER	2.0
3	E	122	THR	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](#)

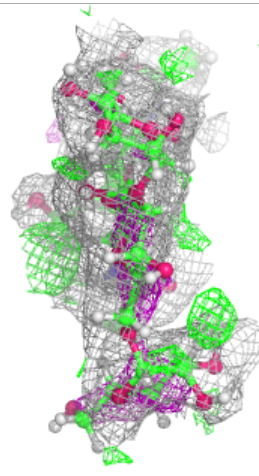
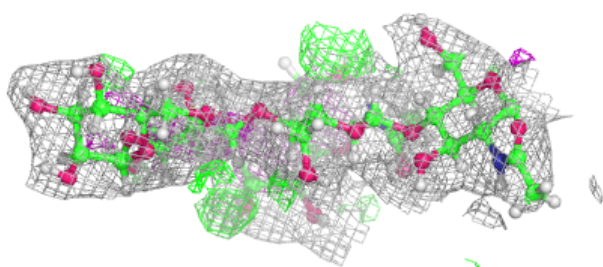
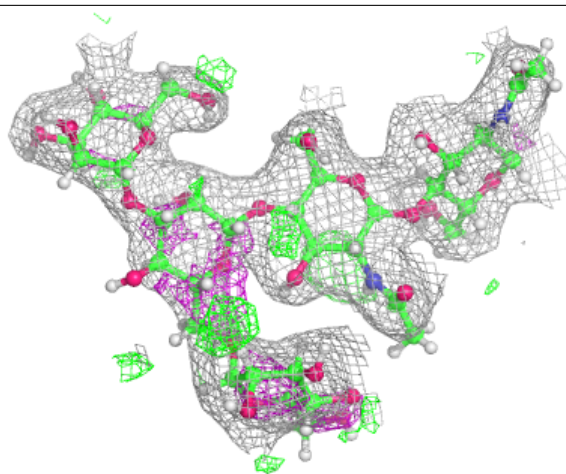
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 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
5	MAN	G	5	11/12	0.69	0.32	71,88,113,113	0
7	BMA	J	3	11/12	0.81	0.32	73,94,102,117	0
5	BMA	G	3	11/12	0.83	0.25	57,85,105,106	0
5	MAN	G	4	11/12	0.84	0.19	51,77,94,106	0
7	MAN	J	4	11/12	0.84	0.35	58,92,110,111	0
7	NAG	J	2	14/15	0.86	0.27	53,74,114,117	0
6	NAG	K	1	14/15	0.88	0.29	67,82,95,105	0
6	NAG	I	1	14/15	0.88	0.25	62,79,93,95	0
6	NAG	K	2	14/15	0.89	0.35	70,92,110,121	0
6	NAG	I	2	14/15	0.91	0.31	70,94,106,128	0
5	NAG	G	2	14/15	0.94	0.10	56,74,101,103	0
5	NAG	G	1	14/15	0.95	0.13	40,57,71,85	0
7	NAG	J	1	14/15	0.96	0.13	46,58,82,83	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:**

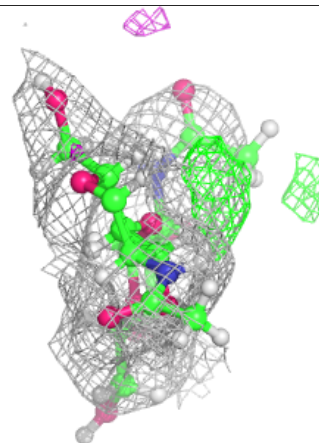
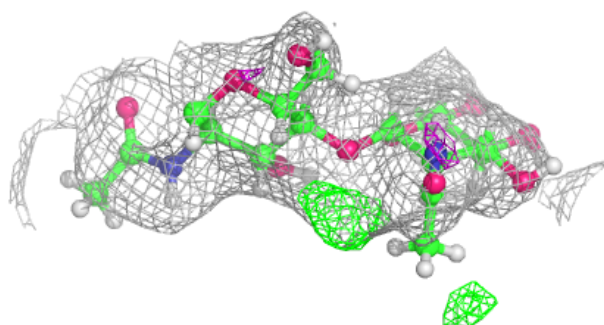
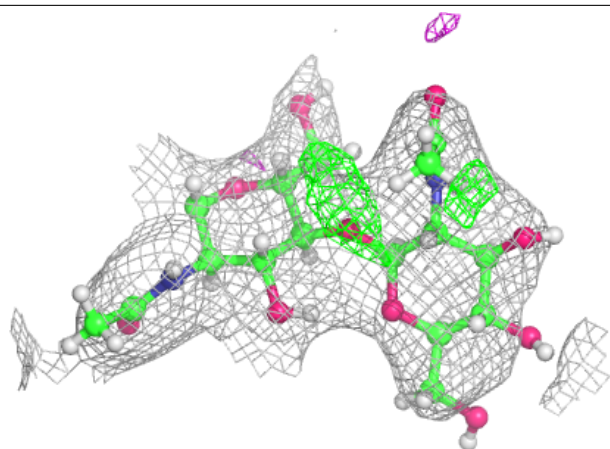
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



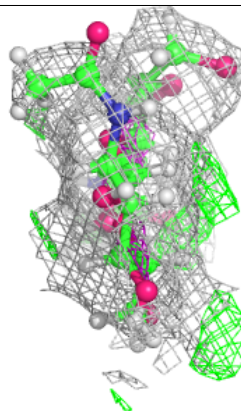
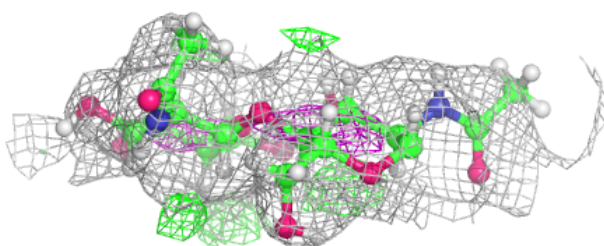
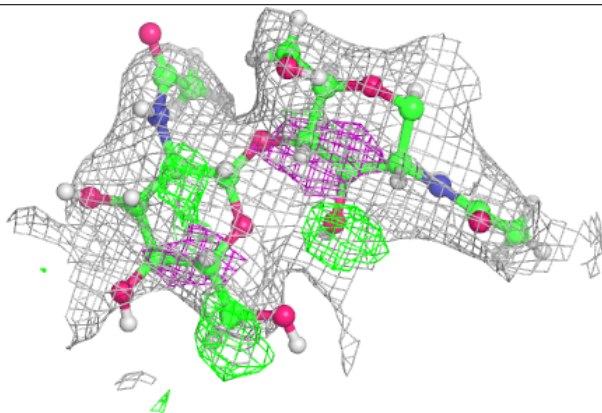


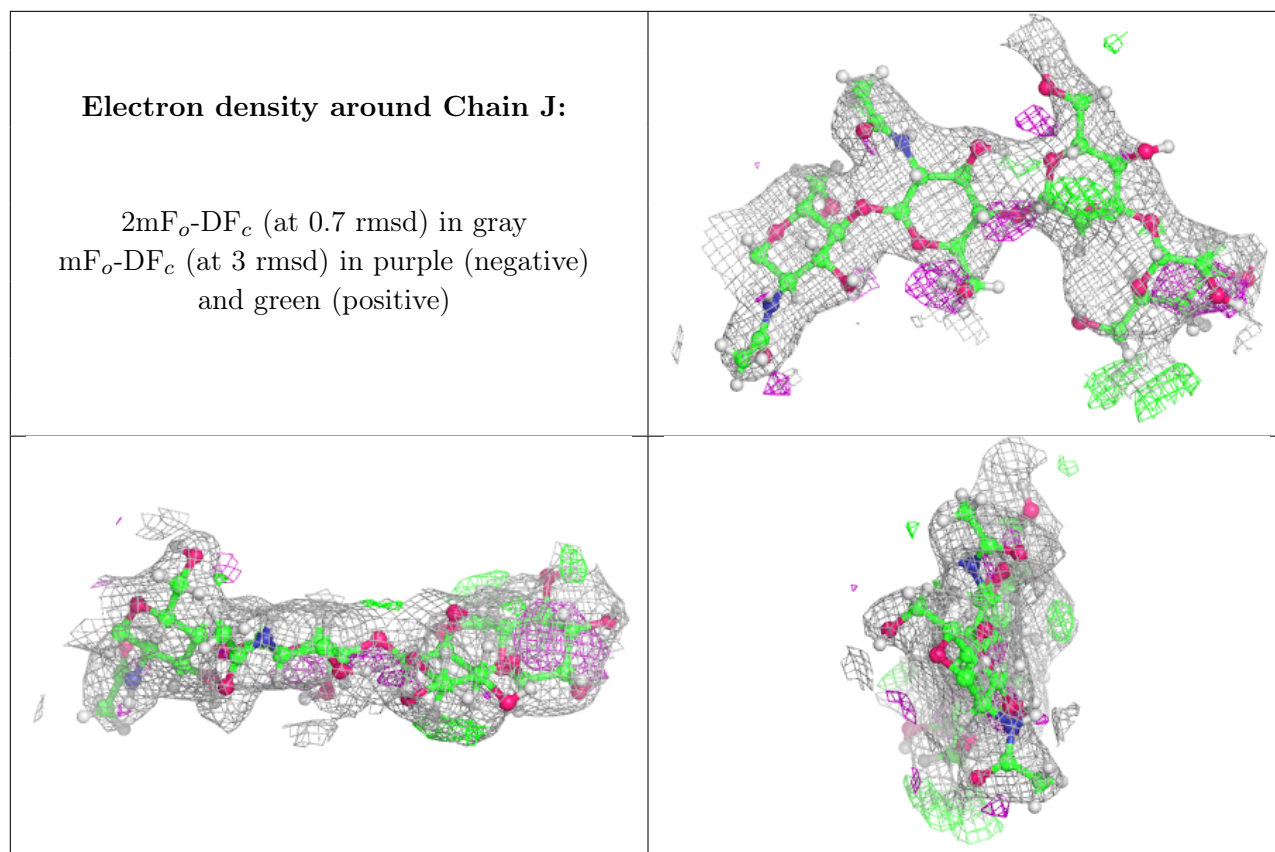
**Electron density around Chain I:**

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

**Electron density around Chain K:**

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





## 6.4 Ligands [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.

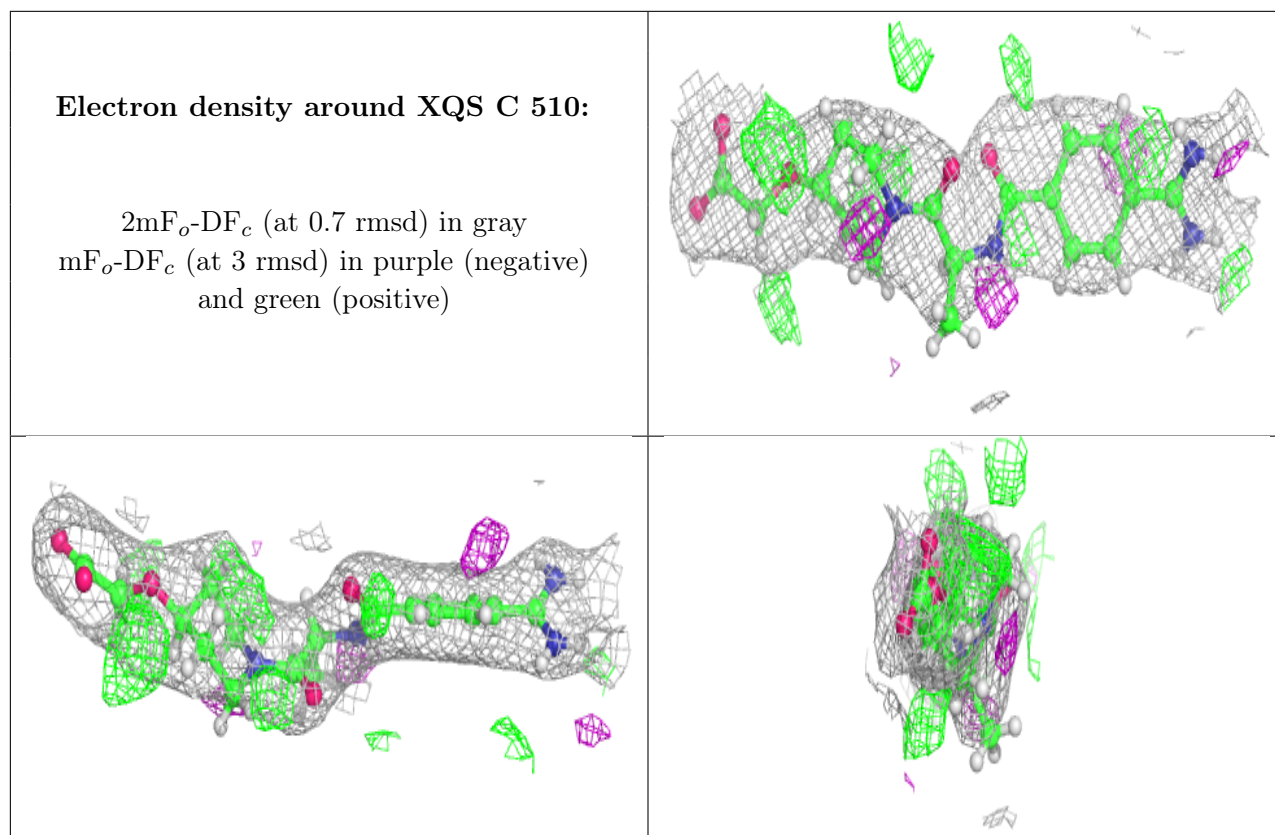
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	CL	C	505	1/1	0.35	0.36	136,136,136,136	0
14	CL	C	504	1/1	0.48	0.67	101,101,101,101	0
10	CA	C	506	1/1	0.74	0.15	108,108,108,108	0
12	NAG	B	2004	14/15	0.84	0.34	75,90,111,118	0
8	SO4	C	502	5/5	0.87	0.20	70,78,102,172	0
12	NAG	D	2004	14/15	0.88	0.29	64,80,103,121	0
8	SO4	A	502	5/5	0.89	0.23	51,54,88,128	0
8	SO4	C	501	5/5	0.89	0.17	57,74,88,168	0
8	SO4	A	501	5/5	0.89	0.29	58,84,105,171	0
8	SO4	L	301	5/5	0.89	0.14	66,70,77,146	0
9	GOL	A	504	6/6	0.89	0.27	31,71,87,92	0
11	MG	D	2001	1/1	0.91	0.20	30,30,30,30	0
11	MG	B	2001	1/1	0.92	0.30	30,30,30,30	0
8	SO4	C	503	5/5	0.92	0.15	60,74,79,139	0

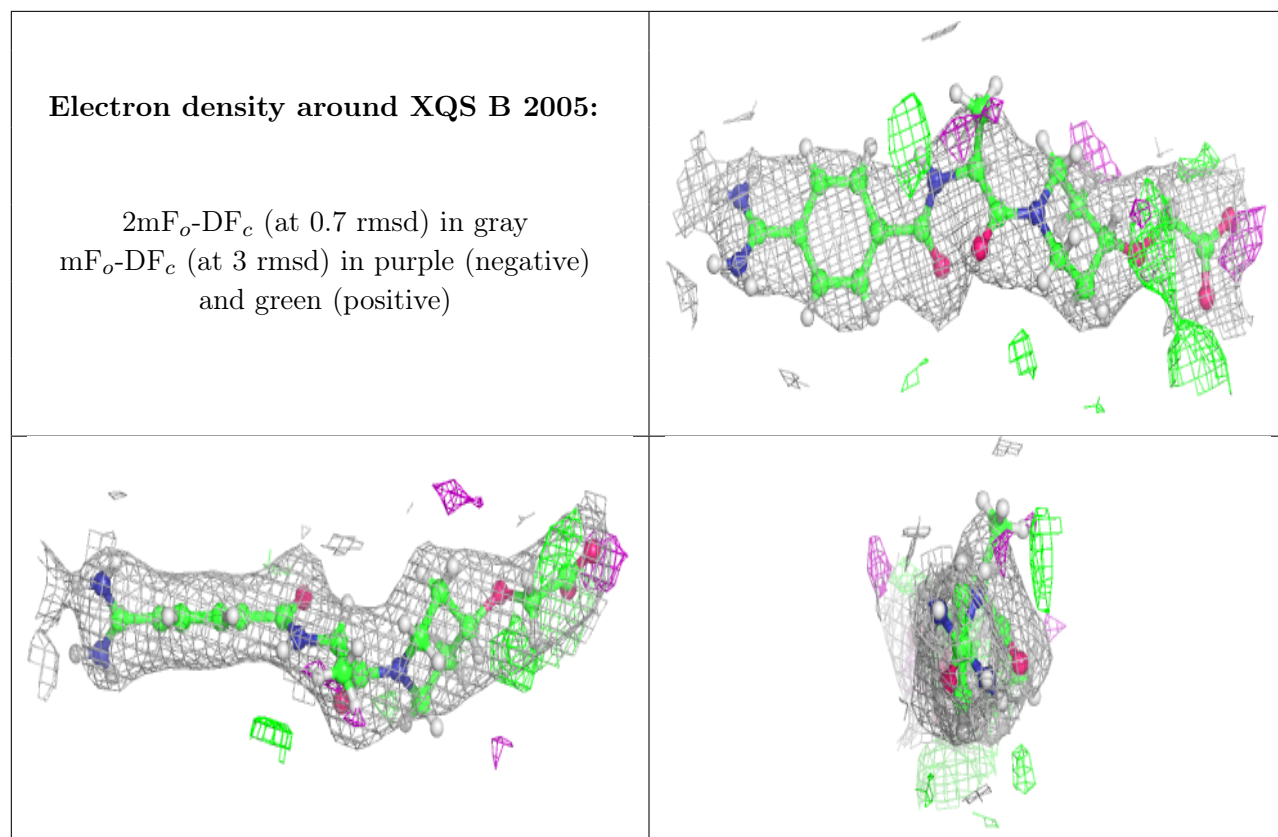
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	XQS	C	510	27/27	0.93	0.18	30,47,76,79	0
13	XQS	B	2005	27/27	0.94	0.22	30,39,69,77	0
10	CA	D	2002	1/1	0.94	0.13	48,48,48,48	0
10	CA	A	506	1/1	0.95	0.11	30,30,30,30	0
10	CA	A	505	1/1	0.96	0.13	57,57,57,57	0
10	CA	C	509	1/1	0.97	0.15	47,47,47,47	0
10	CA	B	2002	1/1	0.97	0.15	67,67,67,67	0
10	CA	A	508	1/1	0.98	0.17	30,30,30,30	0
10	CA	C	508	1/1	0.98	0.14	47,47,47,47	0
10	CA	A	507	1/1	0.98	0.19	30,30,30,30	0
10	CA	B	2003	1/1	0.98	0.20	30,30,30,30	0
10	CA	D	2003	1/1	0.99	0.21	43,43,43,43	0
10	CA	C	507	1/1	0.99	0.09	54,54,54,54	0
8	SO4	A	503	5/5	0.99	0.15	51,58,64,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.