



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:59 PM UTC

PDB ID : 8FFE / pdb\_00008ffe  
Title : Crystal structure of LRP6 E1E2 domains bound to YW210.09 Fab and engineered XWnt8 peptide  
Authors : Jude, K.M.; Tsutsumi, N.; Waghray, D.; Garcia, K.C.  
Deposited on : 2022-12-08  
Resolution : 1.72 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>.

---

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

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

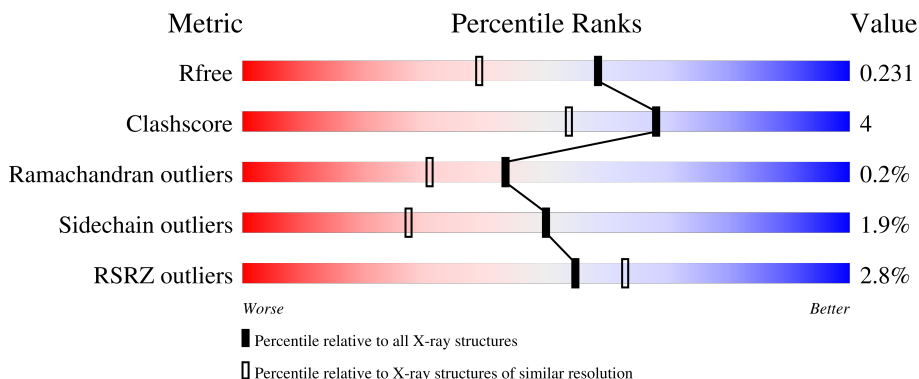
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	613	
2	H	276	
3	L	225	
4	B	4	
5	C	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
6	D	3	 67% 33%

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9116 atoms, of which 0 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 Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	4889	3096	842	927	24	0	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	632	HIS	-	expression tag	UNP O75581

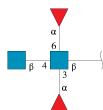
- Molecule 2 is a protein called YW210.09 Fab heavy chain with engineered XWnt8 NC peptide and linker.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	239	1796	1136	303	349	8	0	2	0

- Molecule 3 is a protein called YW210.09 Fab light chain.

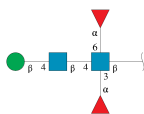
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	215	1639	1024	270	339	6	0	0	0

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



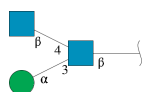
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	4	48	28	2	18	0	0	0

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



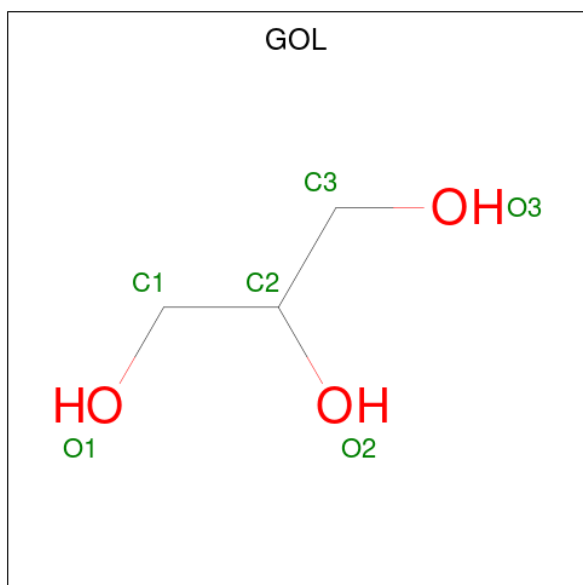
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	5	59	34	2	23	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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	N	O			
6	D	3	39	22	2	15	0	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0

*Continued on next page...*

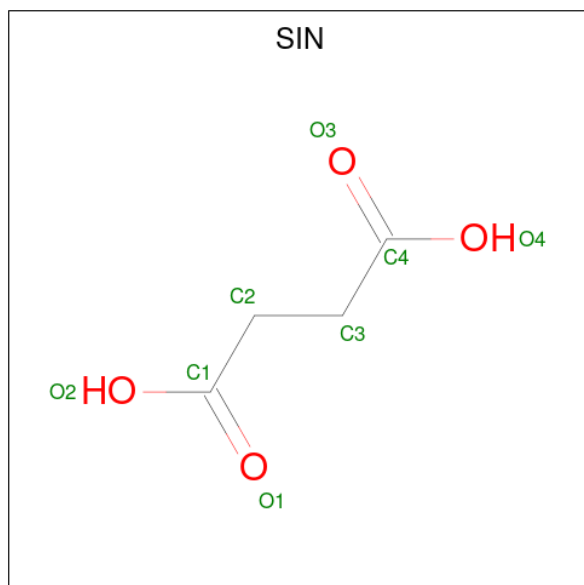
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	Na	0	0
			3	3		

- Molecule 9 is SUCCINIC ACID (CCD ID: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			8	4	4		

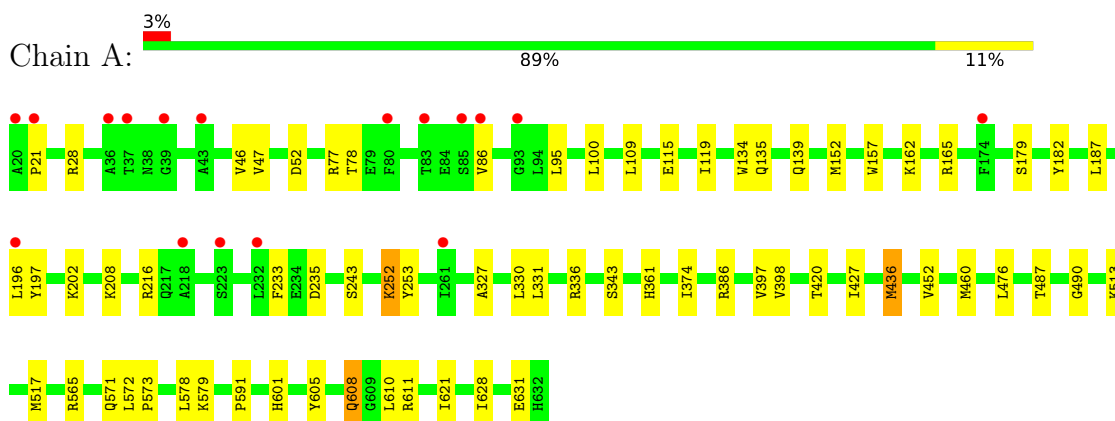
- Molecule 10 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
10	A	346	Total 347	O 347	0	1
10	H	130	Total 130	O 130	0	0
10	L	116	Total 116	O 116	0	0

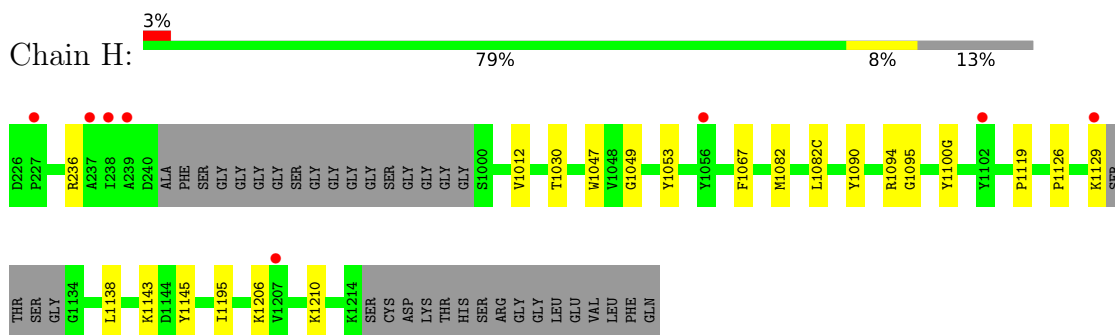
### 3 Residue-property plots [i](#)

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

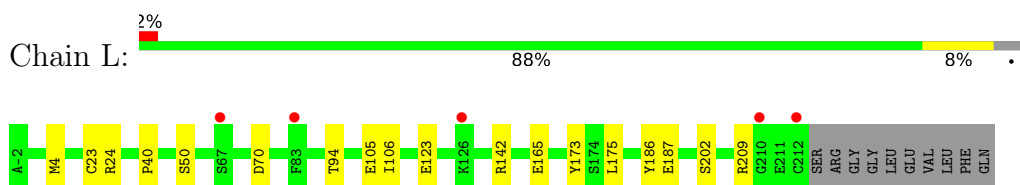
- Molecule 1: Low-density lipoprotein receptor-related protein 6



- Molecule 2: YW210.09 Fab heavy chain with engineered XWnt8 NC peptide and linker



- Molecule 3: YW210.09 Fab light chain



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





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

Chain C:



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

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.21Å 91.39Å 104.06Å 90.00° 103.67° 90.00°	Depositor
Resolution (Å)	44.37 – 1.72 44.37 – 1.72	Depositor EDS
% Data completeness (in resolution range)	90.6 (44.37-1.72) 83.5 (44.37-1.72)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.35 (at 1.72Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.185 , 0.231 0.185 , 0.231	Depositor DCC
$R_{free}$ test set	6043 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtrriage
Anisotropy	0.469	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: SIN, MAN, NAG, NA, BMA, FUC, GOL

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	0.40	0/5009	0.57	0/6819
2	H	0.41	0/1847	0.58	0/2520
3	L	0.37	0/1674	0.54	0/2277
All	All	0.39	0/8530	0.57	0/11616

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	4889	0	4728	40	0
2	H	1796	0	1733	12	0
3	L	1639	0	1587	10	0
4	B	48	0	43	1	0
5	C	59	0	52	1	0
6	D	39	0	34	0	0
7	A	30	0	40	7	0
7	H	6	0	8	0	0
7	L	6	0	8	0	0
8	A	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	8	0	4	0	0
10	A	347	0	0	3	0
10	H	130	0	0	0	0
10	L	116	0	0	2	0
All	All	9116	0	8237	60	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 4.

All (60) 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)
1:A:452:VAL:HA	7:A:702:GOL:H32	1.72	0.70
1:A:46:VAL:HG12	1:A:47:VAL:HG23	1.73	0.70
1:A:327:ALA:H	7:A:701:GOL:H12	1.60	0.67
1:A:235:ASP:HA	1:A:252:LYS:HD2	1.79	0.65
1:A:427:ILE:HG21	1:A:460:MET:HE1	1.84	0.59
1:A:621:ILE:HG21	1:A:628:ILE:HD12	1.85	0.58
1:A:611:ARG:NH1	10:A:803:HOH:O	2.37	0.56
3:L:105:GLU:HG2	3:L:106:ILE:N	2.19	0.56
1:A:476:LEU:HB2	1:A:605:TYR:O	2.06	0.55
2:H:1195:ILE:HD13	2:H:1210:LYS:HA	1.88	0.55
1:A:420:THR:HG22	1:A:427:ILE:HG12	1.90	0.54
1:A:513:LYS:HZ3	7:A:708:GOL:H11	1.73	0.53
1:A:100:LEU:HD11	1:A:109:LEU:HD11	1.90	0.53
1:A:78:THR:HG22	1:A:86:VAL:HA	1.90	0.53
3:L:142:ARG:NH1	10:L:402:HOH:O	2.42	0.53
1:A:187:LEU:HD11	1:A:196:LEU:HD11	1.92	0.52
1:A:208:LYS:NZ	10:A:807:HOH:O	2.42	0.52
2:H:1126:PRO:HG3	2:H:1138:LEU:HB3	1.91	0.51
1:A:513:LYS:NZ	7:A:708:GOL:H11	2.26	0.51
3:L:186:TYR:CE2	3:L:209:ARG:HD3	2.45	0.51
1:A:591:PRO:HB2	1:A:610:LEU:HD23	1.94	0.50
2:H:1047:TRP:CZ2	2:H:1049:GLY:HA2	2.46	0.50
1:A:330:LEU:HD21	7:A:701:GOL:H2	1.94	0.50
1:A:134:TRP:CD1	1:A:135:GLN:HG3	2.47	0.49
1:A:252:LYS:HD3	1:A:253:TYR:CZ	2.47	0.49
1:A:119:ILE:HG21	1:A:152:MET:HE1	1.94	0.49
1:A:374:ILE:O	1:A:386:ARG:HA	2.14	0.47
3:L:40:PRO:HG2	3:L:165:GLU:HG3	1.95	0.47
1:A:197:TYR:OH	1:A:252:LYS:HG3	2.13	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:VAL:HG12	1:A:398:VAL:HG23	1.97	0.46
1:A:436:MET:HE3	5:C:2:NAG:H82	1.98	0.46
3:L:4:MET:HE3	3:L:23:CYS:SG	2.56	0.45
1:A:517:MET:HE1	10:A:1062:HOH:O	2.17	0.45
1:A:28:ARG:HD3	1:A:52:ASP:OD1	2.17	0.45
1:A:436:MET:HG3	1:A:601:HIS:CD2	2.52	0.44
3:L:175:LEU:C	3:L:175:LEU:HD23	2.43	0.44
1:A:330:LEU:HD23	1:A:343:SER:HA	2.00	0.44
2:H:1119:PRO:HB3	2:H:1145:TYR:HB3	2.00	0.44
1:A:436:MET:HG3	1:A:601:HIS:HD2	1.83	0.43
2:H:1082:MET:HE1	2:H:1090:TYR:CZ	2.52	0.43
2:H:1030:THR:O	2:H:1053:TYR:HB3	2.18	0.43
1:A:343:SER:HB2	7:A:701:GOL:H32	2.00	0.43
2:H:1067:PHE:CZ	2:H:1082:MET:HE2	2.53	0.43
3:L:187:GLU:O	3:L:209:ARG:NH2	2.52	0.43
1:A:21:PRO:HB3	1:A:233:PHE:CD2	2.54	0.42
1:A:361:HIS:CE1	2:H:236:ARG:HD3	2.53	0.42
1:A:608:GLN:H	1:A:608:GLN:CD	2.28	0.42
1:A:579:LYS:HE3	7:A:702:GOL:H2	2.01	0.42
2:H:1012:VAL:HG11	2:H:1082(C):LEU:HD13	2.01	0.42
1:A:331:LEU:HD11	1:A:578:LEU:HG	2.00	0.42
3:L:24:ARG:NE	3:L:70:ASP:OD1	2.53	0.42
1:A:139:GLN:HB3	1:A:157:TRP:CE2	2.55	0.41
3:L:105:GLU:HG3	3:L:173:TYR:OH	2.20	0.41
2:H:1143:LYS:HE2	10:L:405:HOH:O	2.20	0.41
2:H:1094:ARG:HG2	2:H:1095:GLY:O	2.21	0.41
1:A:487:THR:HG22	4:B:1:NAG:H82	2.02	0.41
1:A:572:LEU:HD12	1:A:573:PRO:HD2	2.03	0.41
2:H:1100(G):TYR:OH	3:L:94:THR:OG1	2.26	0.41
1:A:95:LEU:HB2	1:A:115:GLU:HB3	2.02	0.40
1:A:182:TYR:HB3	1:A:202:LYS:HB3	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	615/613 (100%)	570 (93%)	42 (7%)	3 (0%)	24	11
2	H	235/276 (85%)	231 (98%)	4 (2%)	0	100	100
3	L	213/225 (95%)	209 (98%)	4 (2%)	0	100	100
All	All	1063/1114 (95%)	1010 (95%)	50 (5%)	3 (0%)	43	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	GLY
1	A	336[A]	ARG
1	A	336[B]	ARG

### 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	528/529 (100%)	516 (98%)	12 (2%)	44	21
2	H	197/218 (90%)	195 (99%)	2 (1%)	68	53
3	L	188/196 (96%)	185 (98%)	3 (2%)	55	34
All	All	913/943 (97%)	896 (98%)	17 (2%)	50	27

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	162	LYS
1	A	165	ARG
1	A	179	SER
1	A	216	ARG
1	A	243	SER
1	A	252	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	436	MET
1	A	565	ARG
1	A	571	GLN
1	A	608	GLN
1	A	631	GLU
2	H	1129	LYS
2	H	1206	LYS
3	L	50	SER
3	L	123	GLU
3	L	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	ASN
1	A	571	GLN
3	L	138	ASN
3	L	160	GLN

### 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
4	NAG	B	1	4,1	14,14,15	0.58	0	17,19,21	0.61	0
4	FUC	B	2	4	10,10,11	0.65	0	14,14,16	0.84	1 (7%)
4	NAG	B	3	4	14,14,15	0.25	0	17,19,21	0.41	0
4	FUC	B	4	4	10,10,11	1.14	0	14,14,16	1.00	1 (7%)
5	NAG	C	1	5,1	14,14,15	0.61	1 (7%)	17,19,21	0.48	0
5	NAG	C	2	5	14,14,15	0.37	0	17,19,21	0.49	0
5	BMA	C	3	5	11,11,12	0.86	0	15,15,17	0.87	1 (6%)
5	FUC	C	4	5	10,10,11	0.87	0	14,14,16	0.73	0
5	FUC	C	5	5	10,10,11	0.94	0	14,14,16	0.71	1 (7%)
6	NAG	D	1	6,1	14,14,15	0.38	0	17,19,21	0.59	0
6	MAN	D	2	6	11,11,12	0.93	0	15,15,17	0.97	1 (6%)
6	NAG	D	3	6	14,14,15	0.56	0	17,19,21	0.53	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
4	NAG	B	1	4,1	-	0/6/23/26	0/1/1/1
4	FUC	B	2	4	-	-	0/1/1/1
4	NAG	B	3	4	-	2/6/23/26	0/1/1/1
4	FUC	B	4	4	-	-	0/1/1/1
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	2/2/19/22	0/1/1/1
5	FUC	C	4	5	-	-	0/1/1/1
5	FUC	C	5	5	-	-	0/1/1/1
6	NAG	D	1	6,1	-	0/6/23/26	0/1/1/1
6	MAN	D	2	6	-	0/2/19/22	0/1/1/1
6	NAG	D	3	6	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	NAG	O5-C1	-2.10	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2	MAN	C1-O5-C5	2.51	115.56	112.19
5	C	3	BMA	C1-O5-C5	2.40	115.41	112.19
4	B	4	FUC	C1-O5-C5	2.07	117.84	112.97
4	B	2	FUC	C1-O5-C5	2.05	117.80	112.97
5	C	5	FUC	O2-C2-C1	2.01	113.81	109.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

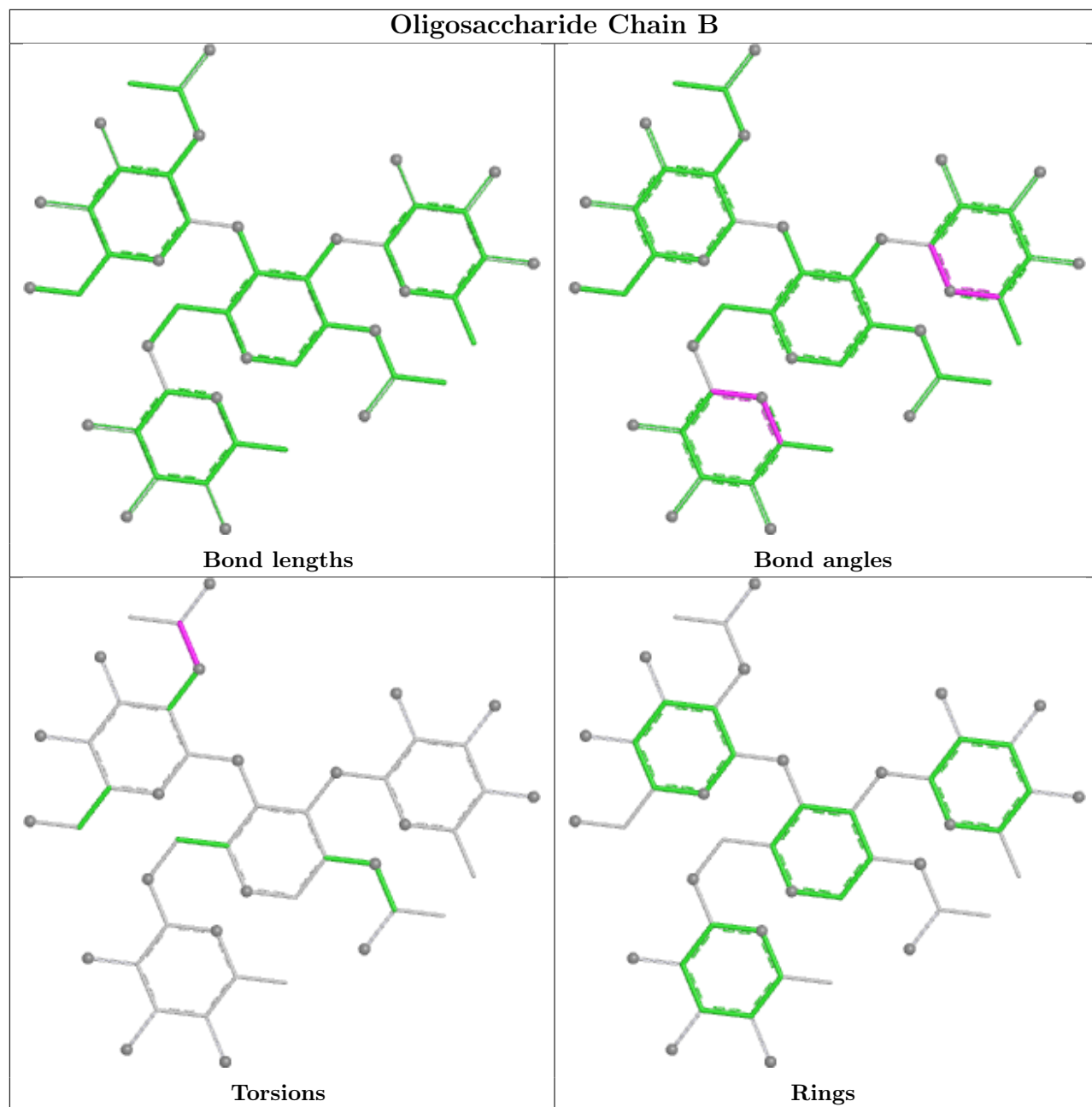
Mol	Chain	Res	Type	Atoms
4	B	3	NAG	C8-C7-N2-C2
4	B	3	NAG	O7-C7-N2-C2
5	C	3	BMA	C4-C5-C6-O6
5	C	3	BMA	O5-C5-C6-O6

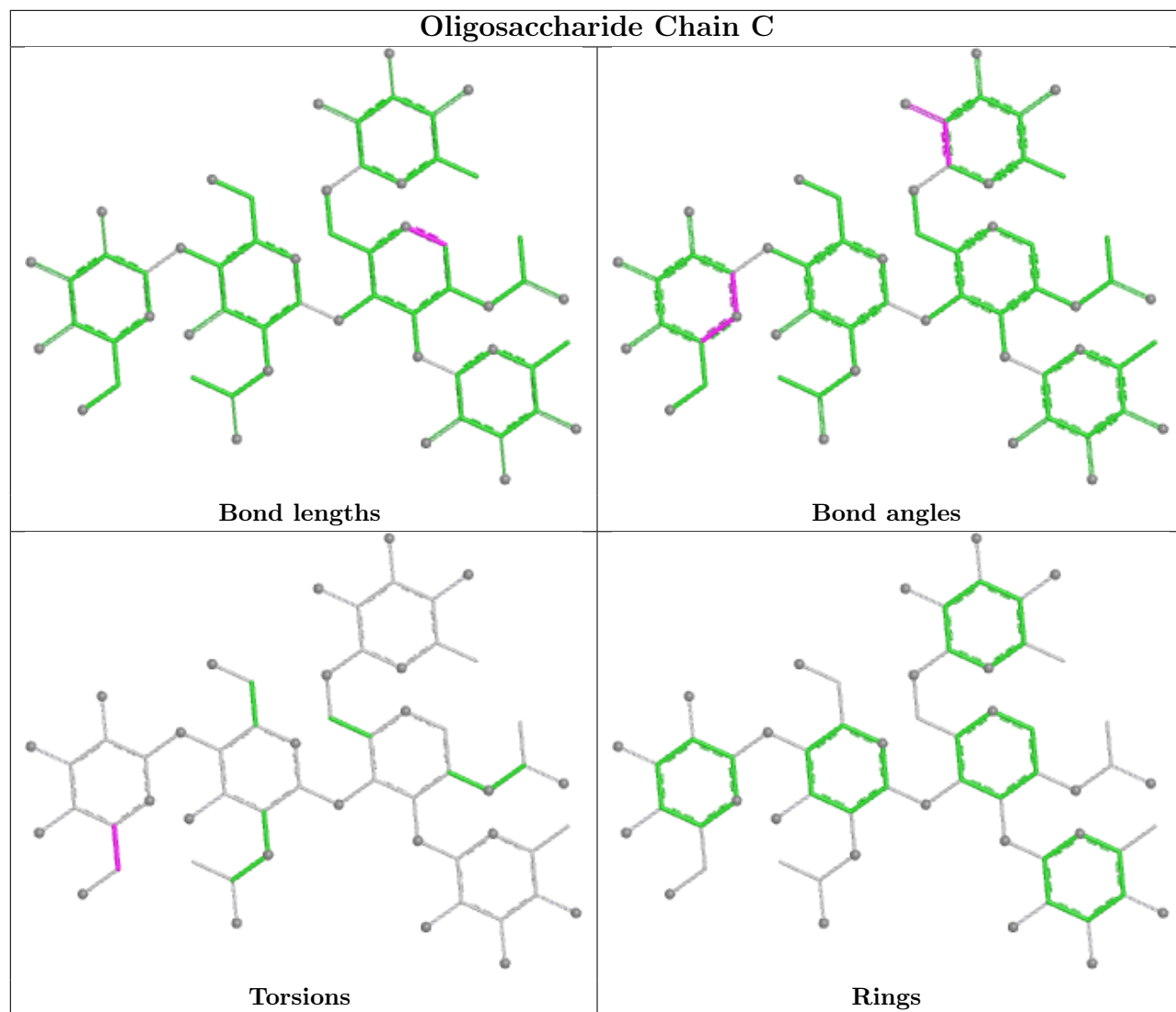
There are no ring outliers.

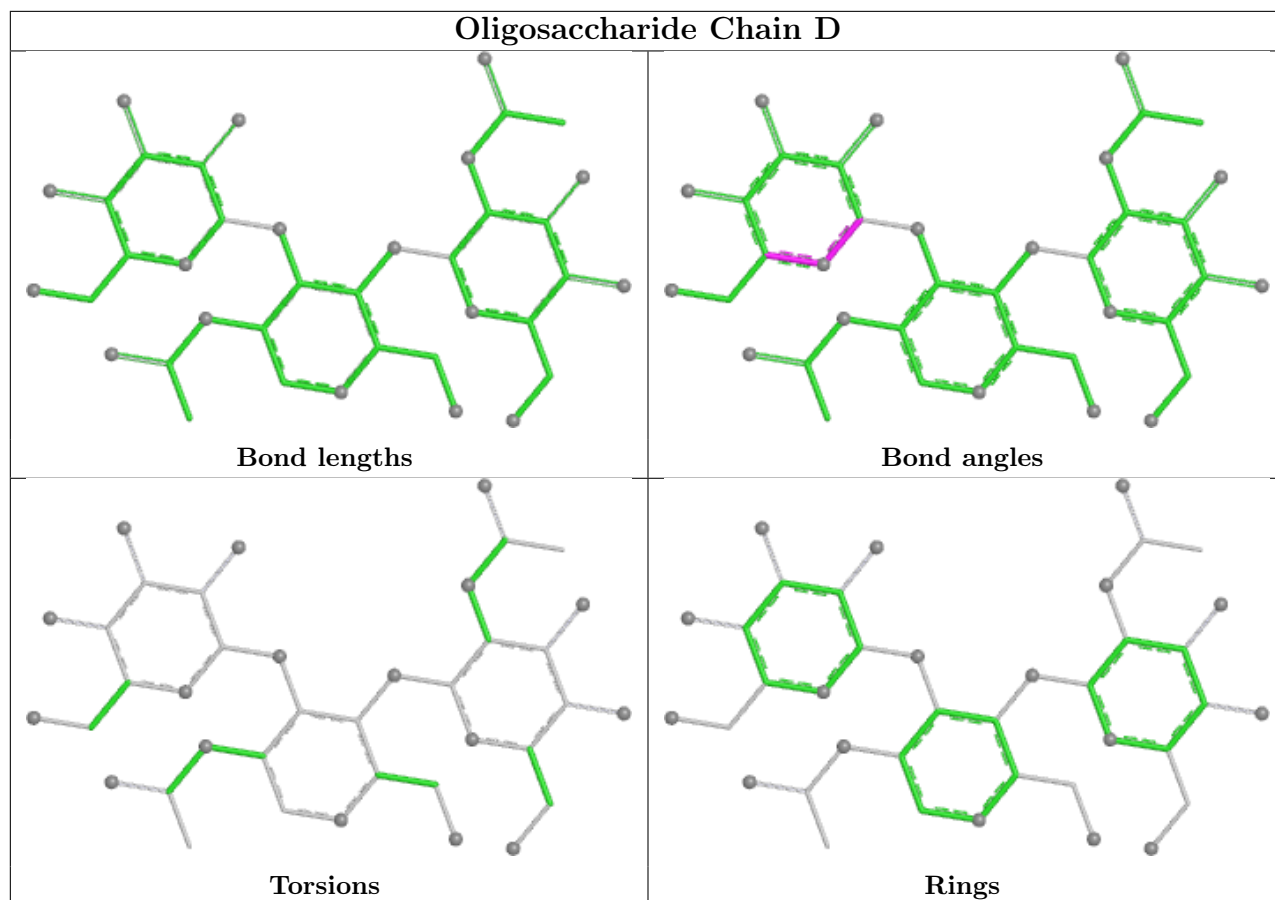
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	NAG	1	0
4	B	1	NAG	1	0

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







## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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
7	GOL	A	701	-	5,5,5	1.66	2 (40%)	5,5,5	0.84	0
7	GOL	A	703	-	5,5,5	1.07	0	5,5,5	0.96	0
7	GOL	A	702	-	5,5,5	1.99	2 (40%)	5,5,5	1.25	1 (20%)
7	GOL	H	1301	-	5,5,5	1.41	1 (20%)	5,5,5	0.78	0
7	GOL	L	301	-	5,5,5	0.86	0	5,5,5	1.11	1 (20%)
7	GOL	A	708	-	5,5,5	1.65	2 (40%)	5,5,5	1.15	0
9	SIN	L	302	-	7,7,7	1.02	0	8,8,8	1.41	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	A	704	-	5,5,5	1.13	0	5,5,5	0.84	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
7	GOL	A	701	-	-	1/4/4/4	-
7	GOL	A	703	-	-	1/4/4/4	-
7	GOL	A	702	-	-	1/4/4/4	-
7	GOL	H	1301	-	-	1/4/4/4	-
7	GOL	L	301	-	-	2/4/4/4	-
7	GOL	A	708	-	-	2/4/4/4	-
9	SIN	L	302	-	-	4/5/5/5	-
7	GOL	A	704	-	-	1/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	702	GOL	C1-C2	3.03	1.63	1.51
7	A	702	GOL	C3-C2	3.01	1.63	1.51
7	A	708	GOL	C3-C2	2.68	1.62	1.51
7	A	701	GOL	C1-C2	2.54	1.61	1.51
7	A	708	GOL	C1-C2	2.43	1.61	1.51
7	A	701	GOL	C3-C2	2.27	1.60	1.51
7	H	1301	GOL	C3-C2	2.05	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	302	SIN	O4-C4-C3	2.43	121.67	114.00
7	A	702	GOL	O2-C2-C3	2.08	117.79	109.18
7	L	301	GOL	C3-C2-C1	-2.03	104.34	111.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	708	GOL	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	A	703	GOL	C1-C2-C3-O3
7	A	704	GOL	O1-C1-C2-C3
7	L	301	GOL	O1-C1-C2-C3
7	A	702	GOL	O1-C1-C2-O2
7	H	1301	GOL	O2-C2-C3-O3
7	A	701	GOL	O2-C2-C3-O3
7	L	301	GOL	O1-C1-C2-O2
9	L	302	SIN	C2-C3-C4-O3
9	L	302	SIN	C2-C3-C4-O4
9	L	302	SIN	O2-C1-C2-C3
9	L	302	SIN	O1-C1-C2-C3
7	A	708	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	701	GOL	3	0
7	A	702	GOL	2	0
7	A	708	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	613/613 (100%)	0.19	17 (2%) 55 63	15, 34, 61, 112	4 (0%)
2	H	239/276 (86%)	0.23	8 (3%) 49 58	18, 34, 66, 102	2 (0%)
3	L	215/225 (95%)	0.20	5 (2%) 61 69	27, 36, 59, 100	0
All	All	1067/1114 (95%)	0.20	30 (2%) 55 63	15, 34, 63, 112	6 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	212	CYS	4.4
1	A	218	ALA	3.8
1	A	80	PHE	3.6
2	H	239	ALA	3.6
2	H	238	ILE	3.2
1	A	20	ALA	2.8
2	H	1056[A]	TYR	2.8
1	A	93	GLY	2.7
2	H	237	ALA	2.7
2	H	1102[A]	TYR	2.7
3	L	126	LYS	2.7
1	A	21	PRO	2.6
1	A	174	PHE	2.5
1	A	39	GLY	2.5
1	A	83	THR	2.5
2	H	227	PRO	2.4
1	A	36	ALA	2.4
1	A	232	LEU	2.4
1	A	43	ALA	2.4
3	L	67	SER	2.3
3	L	210	GLY	2.3
1	A	196	LEU	2.3
2	H	1207	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	85	SER	2.2
2	H	1129	LYS	2.2
1	A	37	THR	2.1
3	L	83	PHE	2.1
1	A	261	ILE	2.1
1	A	86	VAL	2.0
1	A	223	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](#)

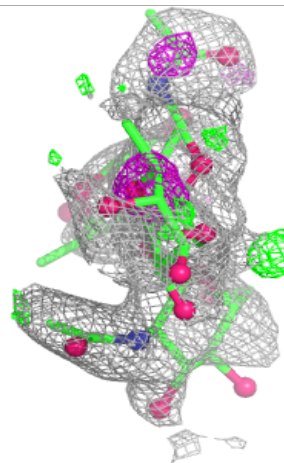
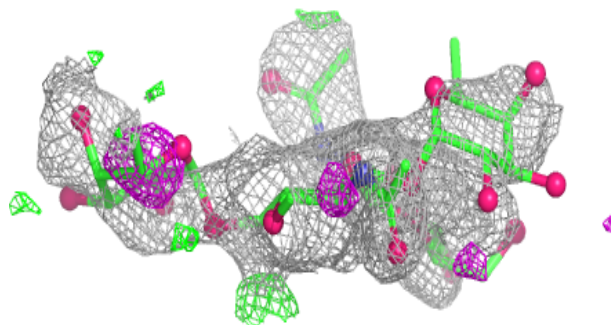
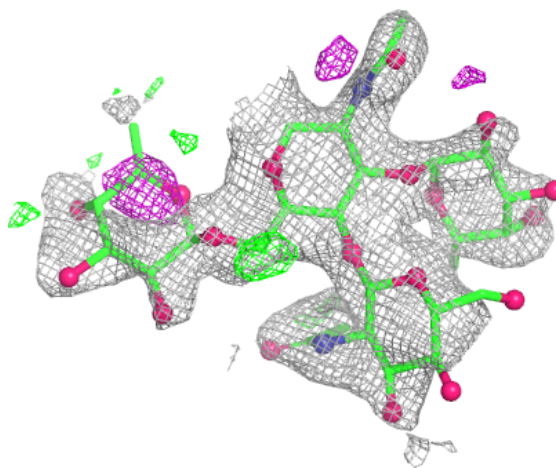
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	NAG	B	1	14/15	-	-	61,76,87,88	0
4	FUC	B	2	10/11	-	-	82,92,96,97	0
4	NAG	B	3	14/15	-	-	85,93,96,99	0
4	FUC	B	4	10/11	-	-	65,86,91,99	0
5	NAG	C	1	14/15	-	-	35,43,49,50	0
5	NAG	C	2	14/15	-	-	41,52,61,63	0
5	BMA	C	3	11/12	-	-	59,71,77,78	0
5	FUC	C	4	10/11	-	-	57,61,68,72	0
5	FUC	C	5	10/11	-	-	43,47,49,50	0
6	NAG	D	3	14/15	0.61	0.14	69,86,89,89	0
6	MAN	D	2	11/12	-	-	95,97,103,105	0
6	NAG	D	1	14/15	0.72	0.12	73,78,88,88	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.

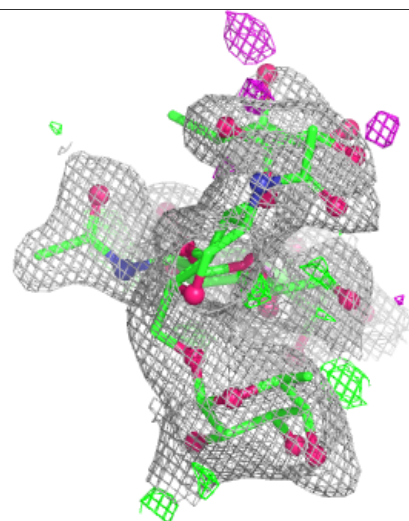
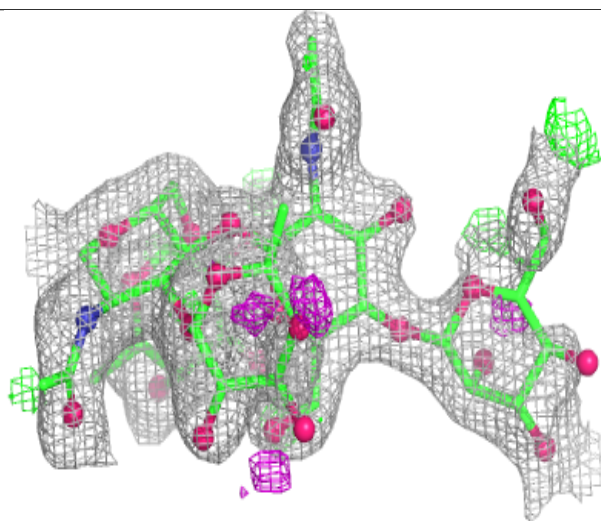
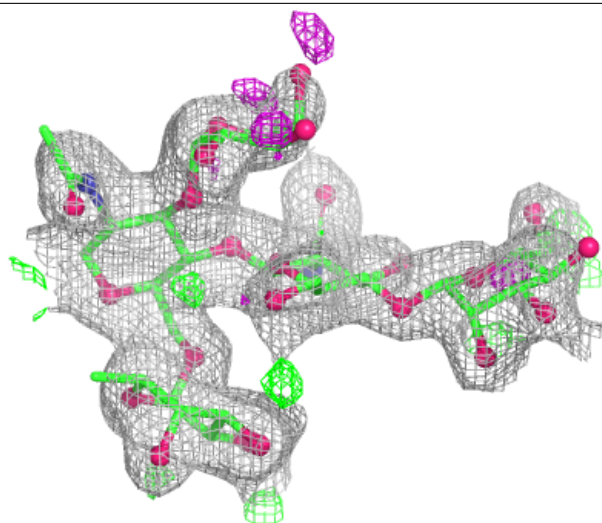
**Electron density around Chain B:**

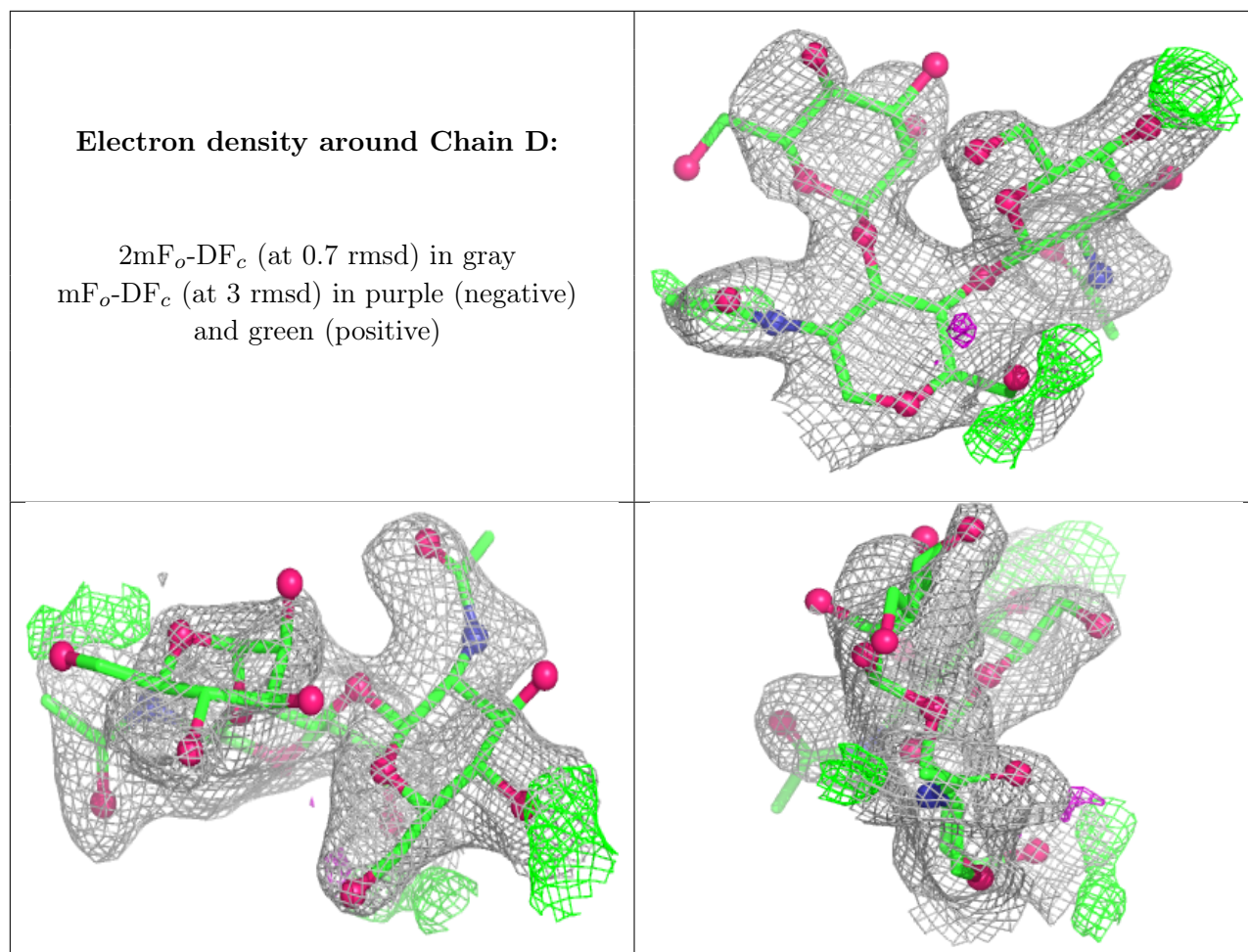
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain C:**

$2mF_o-DF_c$  (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
7	GOL	A	708	6/6	0.63	0.18	35,46,50,53	0
7	GOL	H	1301	6/6	0.71	0.16	51,55,60,62	0
9	SIN	L	302	8/8	0.71	0.15	46,54,62,64	0
7	GOL	A	701	6/6	0.79	0.14	38,44,46,51	0
7	GOL	A	704	6/6	0.84	0.12	41,47,48,51	0
7	GOL	A	702	6/6	0.85	0.14	31,36,42,47	0
7	GOL	A	703	6/6	0.86	0.11	44,45,51,52	0
7	GOL	L	301	6/6	0.90	0.09	47,48,50,53	0
8	NA	A	706	1/1	0.94	0.06	27,27,27,27	0
8	NA	A	705	1/1	0.96	0.05	32,32,32,32	0
8	NA	A	707	1/1	0.97	0.06	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.