



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:07 AM UTC

PDB ID : 9ETH / pdb\_00009eth  
Title : Complex structure of IL-36R D1-D2 domain with 36R-P192 and BI655130 Fab  
Authors : Scheufler, C.; Wirth, E.; Lehmann, S.  
Deposited on : 2024-03-26  
Resolution : 2.30 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

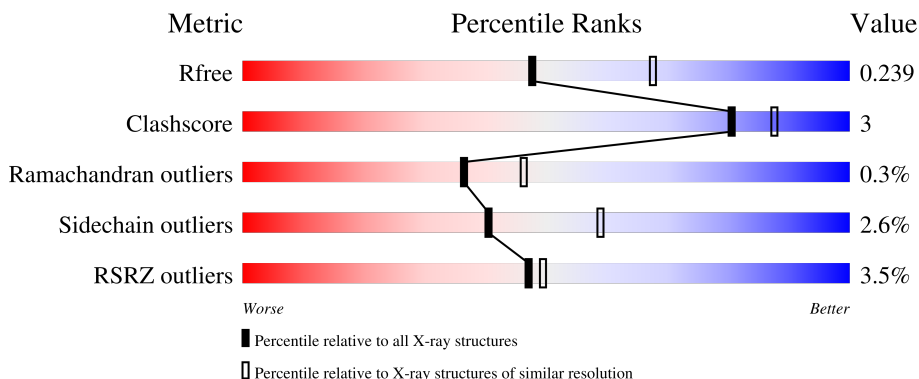
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



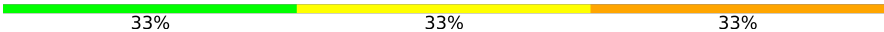
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	H	221	 2% 90% 7%
2	L	215	 3% 91% 7%
3	P	16	 6% 88% 6% 6%
4	R	207	 5% 82% 13% 5%
5	B	2	 100%

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Mol	Chain	Length	Quality of chain
6	C	6	 33% 33% 33%

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 5229 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 BI00655130 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	215	1620	1030	268	315	7	0	0	0

- Molecule 2 is a protein called BI00655130 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1623	1020	277	321	5	0	1	0

- Molecule 3 is a protein called ACE-PHE-VAL-GLU-5CW-3PN-TRP-ASP-TYR-VAL-CHG-6G5-SER-GLU-CYS-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	Cl	N	O				S
3	P	16	145	99	2	20	23	1	0	0	1

- Molecule 4 is a protein called Interleukin-1 receptor-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	R	197	1524	972	258	283	11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

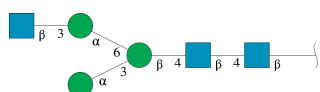
Chain	Residue	Modelled	Actual	Comment	Reference
R	221	HIS	-	expression tag	UNP Q9HB29
R	222	HIS	-	expression tag	UNP Q9HB29
R	223	HIS	-	expression tag	UNP Q9HB29
R	224	HIS	-	expression tag	UNP Q9HB29
R	225	HIS	-	expression tag	UNP Q9HB29
R	226	HIS	-	expression tag	UNP Q9HB29

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



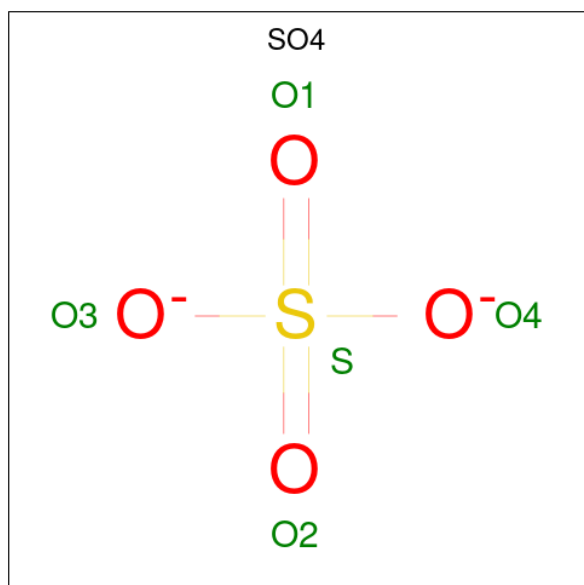
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	B	2	28	16	2	10	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	C	6	75	42	3	30	0	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	H	1	5	4	1	0	0

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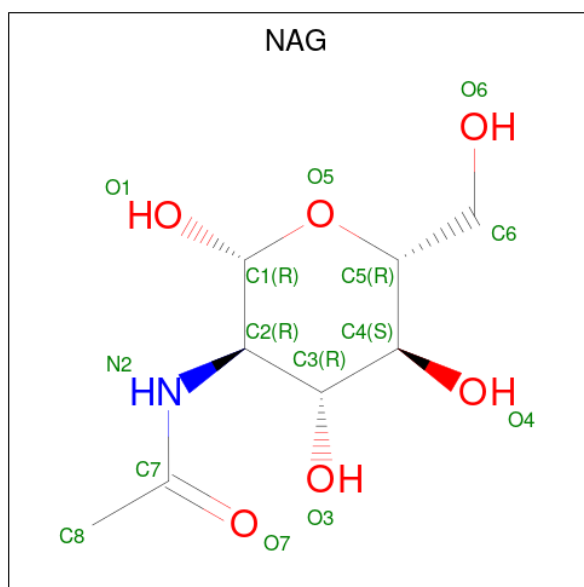
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	O	S	0	0
			5	4	1		
7	R	1	Total	O	S	0	0
			5	4	1		

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

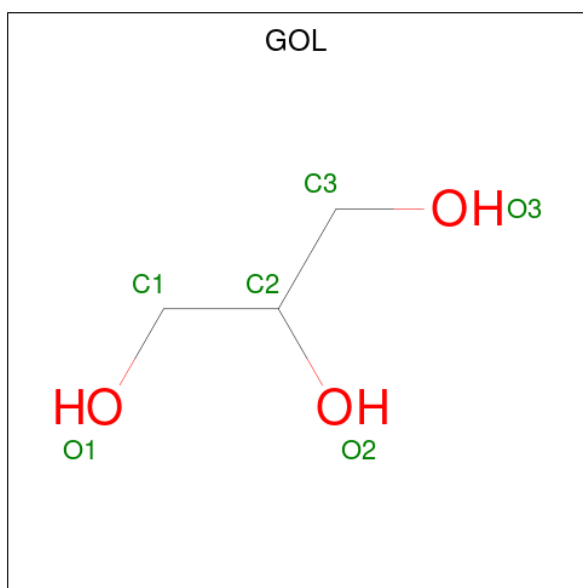
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Na	0	0
			1	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	R	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	R	1	Total	C O	0	0
			6	3 3		

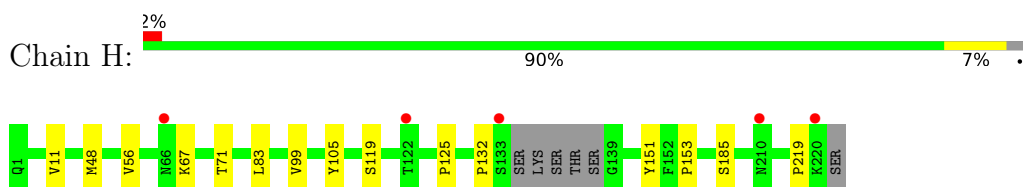
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	59	Total	O	0	0
			59	59		
11	L	50	Total	O	0	0
			50	50		
11	P	5	Total	O	0	0
			5	5		
11	R	39	Total	O	0	0
			39	39		

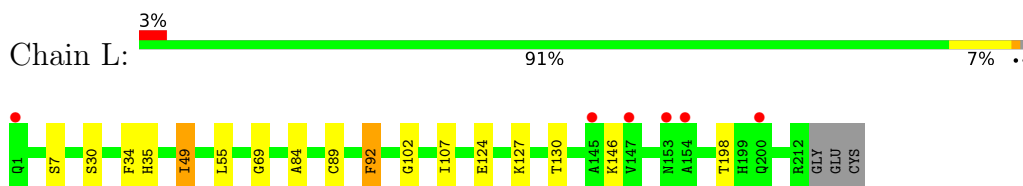
### 3 Residue-property plots [i](#)

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.

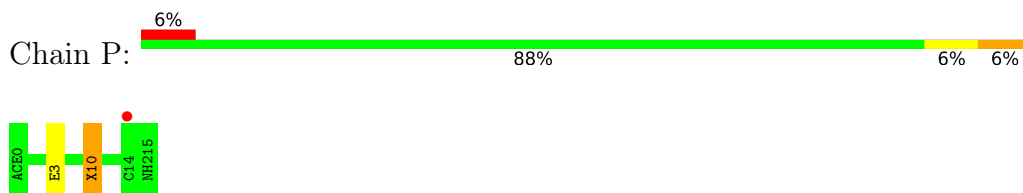
- Molecule 1: BI00655130 Fab heavy chain



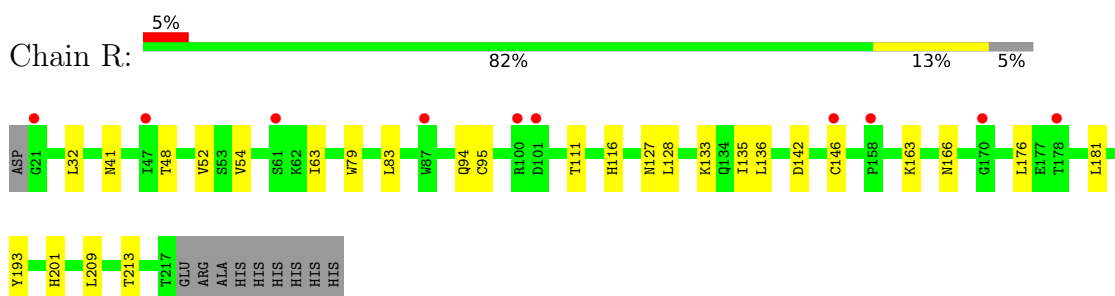
- Molecule 2: BI00655130 Fab light chain



- Molecule 3: ACE-PHE-VAL-GLU-5CW-3PN-TRP-ASP-TYR-VAL-CHG-6G5-SER-GLU-CYS-NH2



- Molecule 4: Interleukin-1 receptor-like 2

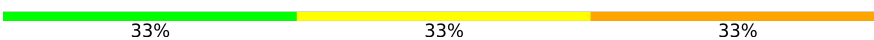


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

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

Chain C:  33% 33% 33%

MAG1  
MAG2  
MAG3  
MAG4  
MAG5  
MAG6

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.64Å 175.35Å 191.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.29 – 2.30 32.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	88.8 (32.29-2.30) 88.8 (32.29-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.29Å)	Xtrriage
Refinement program	BUSTER 2.11.8	Depositor
R, $R_{free}$	0.212 , 0.237 0.213 , 0.239	Depositor DCC
$R_{free}$ test set	1781 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.9	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	0.95	EDS
Total number of atoms	5229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: NH2, NA, 6G5, ACE, BMA, MAN, GOL, CHG, NAG, A1H6Z, SO4, 5CW

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	H	0.71	0/1663	0.96	1/2272 (0.0%)
2	L	0.63	0/1663	0.94	1/2265 (0.0%)
3	P	0.47	0/91	0.77	0/121
4	R	0.71	0/1563	1.02	1/2129 (0.0%)
All	All	0.68	0/4980	0.97	3/6787 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	67	LYS	N-CA-C	-6.83	104.95	113.55
2	L	102	GLY	N-CA-C	6.22	117.86	111.95
4	R	63	ILE	N-CA-C	5.39	112.89	107.55

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	H	1620	0	1568	6	0
2	L	1623	0	1546	7	0
3	P	145	0	94	1	0
4	R	1524	0	1442	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	28	0	25	0	0
6	C	75	0	64	3	0
7	H	15	0	0	0	0
7	L	20	0	0	0	0
7	R	5	0	0	0	0
8	H	1	0	0	0	0
9	R	14	0	13	0	0
10	R	6	0	8	2	0
11	H	59	0	0	0	0
11	L	50	0	0	0	0
11	P	5	0	0	0	0
11	R	39	0	0	0	0
All	All	5229	0	4760	26	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 3.

All (26) 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:H:11:VAL:HB	1:H:153:PRO:HG3	1.57	0.83
1:H:132:PRO:HG2	1:H:219:PRO:HB3	1.85	0.59
4:R:79:TRP:HE1	10:R:303:GOL:H11	1.69	0.57
1:H:125:PRO:HB3	1:H:151:TYR:HB3	1.90	0.53
3:P:3:GLU:HB2	3:P:10:CHG:H1	1.90	0.51
4:R:176:LEU:HD22	4:R:181:LEU:HD11	1.94	0.50
2:L:84:ALA:HB2	2:L:107:ILE:HG12	1.94	0.49
1:H:48:MET:HE1	1:H:83:LEU:HD21	1.95	0.48
4:R:41:ASN:HD22	6:C:1:NAG:H83	1.80	0.46
4:R:32:LEU:HD23	4:R:111:THR:HB	1.97	0.45
4:R:79:TRP:NE1	10:R:303:GOL:H11	2.30	0.44
4:R:116:HIS:CG	4:R:209:LEU:HD23	2.53	0.44
2:L:124:GLU:HA	2:L:127:LYS:HD3	2.00	0.44
6:C:5:NAG:H83	6:C:5:NAG:C1	2.48	0.43
4:R:136:LEU:HD22	4:R:142:ASP:HB3	2.00	0.43
1:H:99:VAL:HG21	2:L:92:PHE:HZ	1.83	0.42
4:R:128:LEU:HB3	4:R:133:LYS:HD3	2.02	0.42
2:L:34:PHE:CZ	2:L:89:CYS:HB2	2.55	0.41
4:R:163:LYS:HD3	4:R:193:TYR:CZ	2.55	0.41
4:R:54:VAL:HG13	4:R:95:CYS:SG	2.61	0.41
4:R:83:LEU:HD11	4:R:201:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:TYR:HB3	2:L:35:HIS:CE1	2.57	0.40
2:L:49:ILE:HD13	2:L:55:LEU:HD23	2.02	0.40
2:L:146:LYS:HB3	2:L:198:THR:HB	2.02	0.40
6:C:5:NAG:C1	6:C:5:NAG:C8	2.99	0.40
4:R:48:THR:HA	4:R:52:VAL:HG21	2.04	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	H	211/221 (96%)	207 (98%)	3 (1%)	1 (0%)	24	31
2	L	211/215 (98%)	207 (98%)	3 (1%)	1 (0%)	24	31
3	P	10/16 (62%)	10 (100%)	0	0	100	100
4	R	195/207 (94%)	182 (93%)	13 (7%)	0	100	100
All	All	627/659 (95%)	606 (97%)	19 (3%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	69	GLY
1	H	56	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	H	181/191 (95%)	178 (98%)	3 (2%)	53	72
2	L	178/188 (95%)	173 (97%)	5 (3%)	38	56
3	P	10/10 (100%)	10 (100%)	0	100	100
4	R	167/188 (89%)	161 (96%)	6 (4%)	31	47
All	All	536/577 (93%)	522 (97%)	14 (3%)	40	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	71	THR
1	H	119	SER
1	H	185	SER
2	L	7	SER
2	L	30	SER
2	L	49	ILE
2	L	92	PHE
2	L	130	THR
4	R	94	GLN
4	R	127	ASN
4	R	135	ILE
4	R	146	CYS
4	R	166	ASN
4	R	213	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	38	GLN
2	L	43	GLN
2	L	148	GLN
4	R	74	HIS
4	R	94	GLN
4	R	116	HIS
4	R	127	ASN
4	R	149	HIS
4	R	201	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
3	CHG	P	10	3	9,10,11	0.47	0	9,12,14	0.70	1 (11%)
3	A1H6Z	P	5	3	11,12,13	0.35	0	10,15,17	0.29	0
3	5CW	P	4	3	15,16,17	0.39	0	17,22,24	0.37	0
3	6G5	P	11	3	15,16,17	0.37	0	14,22,24	0.42	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CHG	P	10	3	-	1/5/14/16	0/1/1/1
3	A1H6Z	P	5	3	-	0/5/6/8	0/1/1/1
3	5CW	P	4	3	-	0/5/6/8	0/2/2/2
3	6G5	P	11	3	-	0/5/6/8	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	10	CHG	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	10	CHG	O-C-CA-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	10	CHG	1	0

## 5.5 Carbohydrates i

8 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	B	1	5,4	14,14,15	0.27	0	17,19,21	0.57	0
5	NAG	B	2	5	14,14,15	0.31	0	17,19,21	0.47	0
6	NAG	C	1	6,4	14,14,15	0.26	0	17,19,21	0.90	1 (5%)
6	NAG	C	2	6	14,14,15	0.27	0	17,19,21	0.50	0
6	BMA	C	3	6	11,11,12	0.24	0	15,15,17	0.49	0
6	MAN	C	4	6	11,11,12	0.29	0	15,15,17	0.72	1 (6%)
6	NAG	C	5	6	14,14,15	0.58	0	17,19,21	1.57	3 (17%)
6	MAN	C	6	6	11,11,12	0.26	0	15,15,17	0.66	1 (6%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	B	2	5	-	0/6/23/26	0/1/1/1
6	NAG	C	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	C	2	6	-	0/6/23/26	0/1/1/1
6	BMA	C	3	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	C	4	6	-	0/2/19/22	0/1/1/1
6	NAG	C	5	6	-	4/6/23/26	0/1/1/1
6	MAN	C	6	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	5	NAG	C1-O5-C5	4.44	118.14	112.19
6	C	5	NAG	C2-N2-C7	3.37	127.42	122.90
6	C	4	MAN	C1-O5-C5	2.53	115.57	112.19
6	C	5	NAG	C4-C3-C2	2.52	114.71	111.02
6	C	6	MAN	C1-O5-C5	2.30	115.27	112.19
6	C	1	NAG	C1-O5-C5	2.11	115.01	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

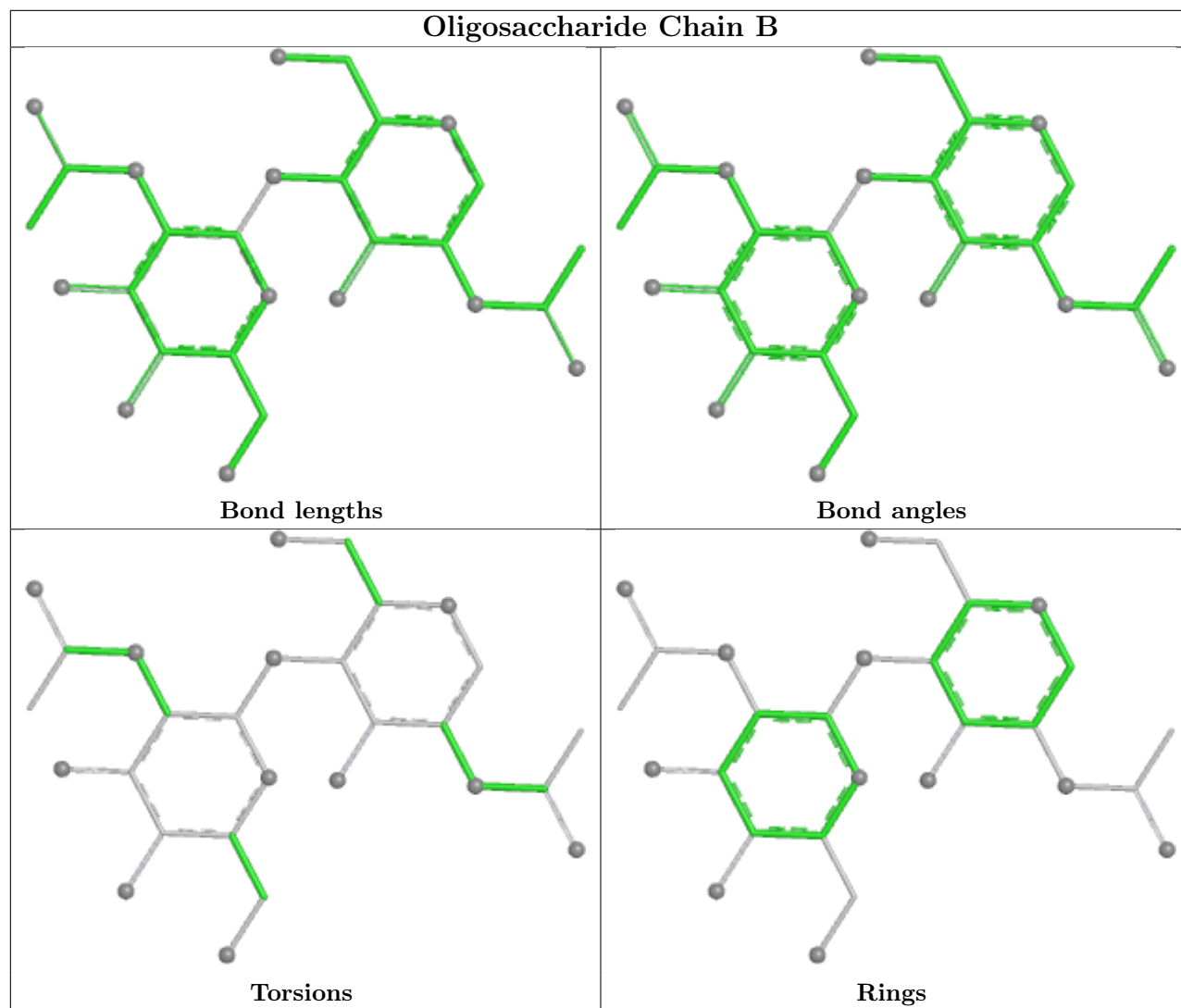
Mol	Chain	Res	Type	Atoms
6	C	1	NAG	C8-C7-N2-C2
6	C	1	NAG	O7-C7-N2-C2
6	C	5	NAG	C8-C7-N2-C2
6	C	5	NAG	O7-C7-N2-C2
6	C	5	NAG	C1-C2-N2-C7
6	C	5	NAG	C3-C2-N2-C7

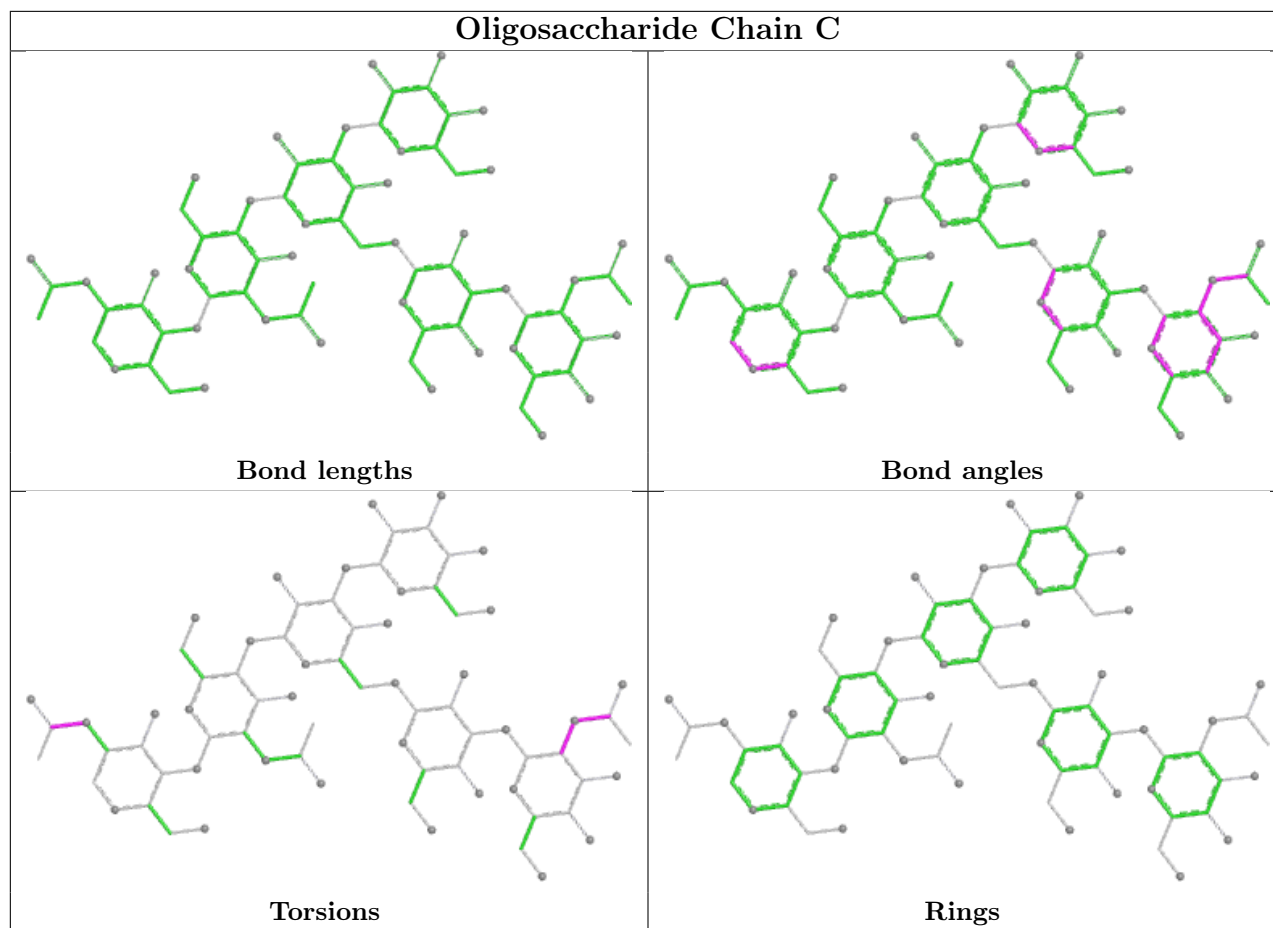
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1	NAG	1	0
6	C	5	NAG	2	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, 1 is monoatomic - leaving 10 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	SO4	H	301	8	4,4,4	0.27	0	6,6,6	0.41	0
7	SO4	H	302	-	4,4,4	0.29	0	6,6,6	0.20	0
7	SO4	R	302	-	4,4,4	0.28	0	6,6,6	0.19	0
9	NAG	R	301	4	14,14,15	0.27	0	17,19,21	0.66	0
7	SO4	H	303	-	4,4,4	0.28	0	6,6,6	0.36	0
7	SO4	L	303	-	4,4,4	0.32	0	6,6,6	0.20	0
10	GOL	R	303	-	5,5,5	0.07	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	L	302	-	4,4,4	0.29	0	6,6,6	0.21	0
7	SO4	L	304	-	4,4,4	0.28	0	6,6,6	0.16	0
7	SO4	L	301	-	4,4,4	0.29	0	6,6,6	0.32	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
10	GOL	R	303	-	-	1/4/4/4	-
9	NAG	R	301	4	-	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.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	R	303	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	R	303	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	H	215/221 (97%)	0.20	5 (2%) 61 63	32, 52, 77, 89	0
2	L	212/215 (98%)	0.36	6 (2%) 55 57	39, 64, 81, 91	1 (0%)
3	P	10/16 (62%)	0.47	1 (10%) 12 14	45, 55, 68, 70	0
4	R	197/207 (95%)	0.47	10 (5%) 33 35	44, 61, 77, 85	0
All	All	634/659 (96%)	0.34	22 (3%) 47 49	32, 59, 79, 91	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	101	ASP	5.1
2	L	145	ALA	3.8
1	H	122	THR	3.3
4	R	100	ARG	3.2
4	R	170	GLY	3.0
4	R	61	SER	3.0
4	R	21	GLY	2.8
3	P	14	CYS	2.6
2	L	200	GLN	2.5
1	H	220	LYS	2.4
2	L	147	VAL	2.4
1	H	133	SER	2.3
2	L	1	GLN	2.3
2	L	154	ALA	2.3
2	L	153	ASN	2.2
4	R	87	TRP	2.2
4	R	146	CYS	2.1
1	H	66	ASN	2.1
1	H	210	ASN	2.1
4	R	158	PRO	2.0
4	R	178	THR	2.0
4	R	47	ILE	2.0

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

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
3	6G5	P	11	15/16	0.88	0.11	48,51,54,58	0
3	A1H6Z	P	5	12/13	0.93	0.09	46,48,50,50	0
3	CHG	P	10	10/11	0.96	0.08	42,43,46,46	0
3	5CW	P	4	15/16	0.97	0.06	44,44,46,47	0

## 6.3 Carbohydrates [\(i\)](#)

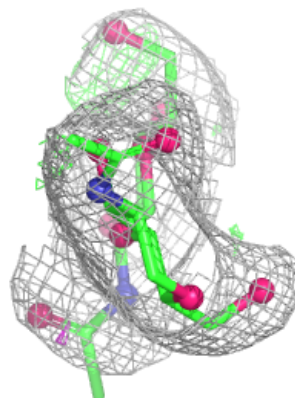
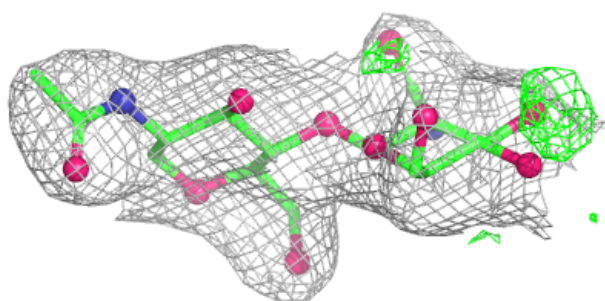
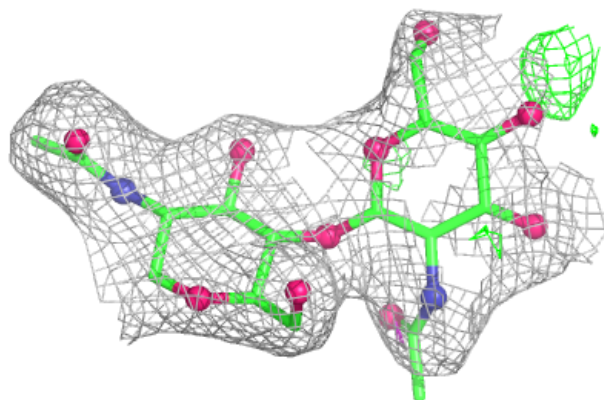
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	NAG	B	1	14/15	-	-	70,72,74,76	0
5	NAG	B	2	14/15	-	-	79,81,81,82	0
6	NAG	C	1	14/15	-	-	61,63,65,67	0
6	NAG	C	2	14/15	-	-	69,71,75,79	0
6	BMA	C	3	11/12	-	-	82,86,88,90	0
6	MAN	C	4	11/12	-	-	91,93,94,95	0
6	NAG	C	5	14/15	-	-	96,97,99,99	0
6	MAN	C	6	11/12	-	-	90,91,92,92	0

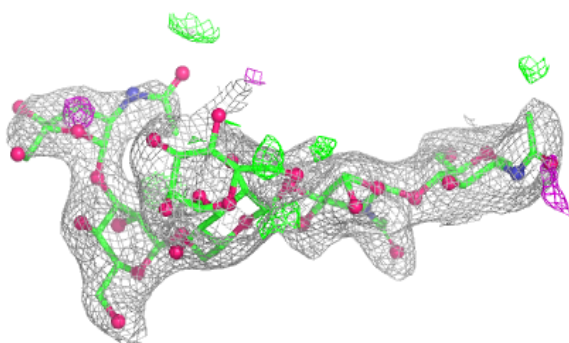
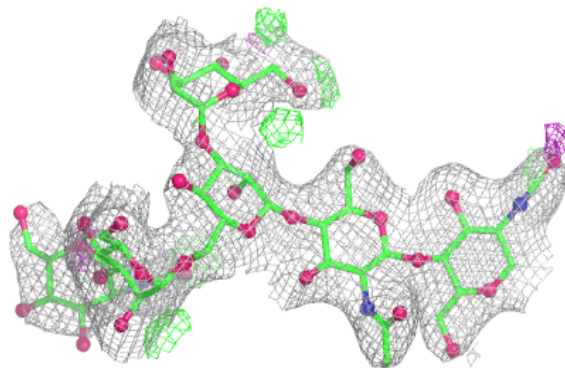
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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	SO4	L	304	5/5	0.66	0.11	167,167,167,167	0
7	SO4	L	301	5/5	0.67	0.10	114,114,114,114	0
9	NAG	R	301	14/15	0.68	0.16	93,94,95,95	0
7	SO4	L	302	5/5	0.73	0.13	126,127,127,127	0
7	SO4	R	302	5/5	0.78	0.08	125,125,125,125	0
7	SO4	L	303	5/5	0.79	0.12	102,102,102,102	0
10	GOL	R	303	6/6	0.83	0.15	74,75,75,75	0
7	SO4	H	303	5/5	0.85	0.08	127,127,127,127	0
7	SO4	H	302	5/5	0.86	0.11	102,102,102,103	0
8	NA	H	304	1/1	0.95	0.20	85,85,85,85	1
7	SO4	H	301	5/5	0.99	0.03	41,42,42,42	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.