



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 08:50 PM BST

PDB ID : 5BK3  
Title : Crystal structure of the neutralizing anti-circumsporozoite protein 580 anti-body  
Authors : Scally, S.W.; Bosch, A.; Triller, G.; Wardemann, H.; Julien, J.P.  
Deposited on : 2017-09-12  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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	:	2.13.1
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)	:	2.13.1

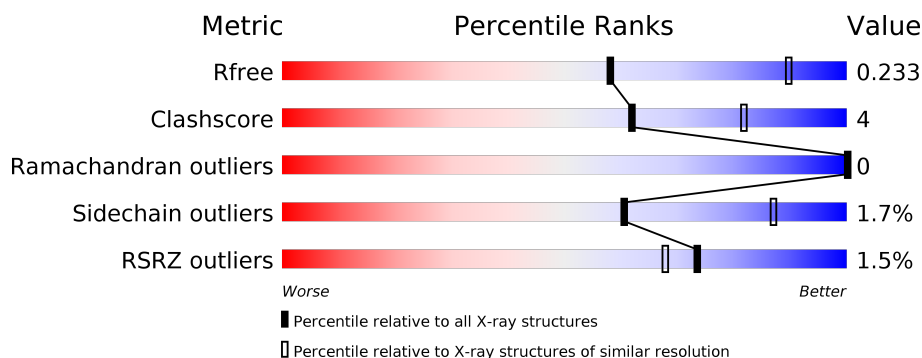
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	B	220	<div> <div>88%</div> <div>10% ..</div> </div>
1	D	220	<div> <div>3%</div> <div>88%</div> <div>11% .</div> </div>
1	F	220	<div> <div>4%</div> <div>89%</div> <div>10% .</div> </div>
1	L	220	<div> <div>86%</div> <div>13% .</div> </div>
2	A	228	<div> <div>84%</div> <div>11% .</div> </div>
2	C	228	<div> <div>2%</div> <div>86%</div> <div>9% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	228	
2	H	228	
3	G	3	
3	I	3	
4	J	2	
5	K	6	

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
3	NAG	I	2	-	-	-	X
6	GOL	B	306	-	-	-	X
6	GOL	F	307	-	-	-	X
6	GOL	L	304	-	-	-	X
7	SO4	B	309	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13490 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.

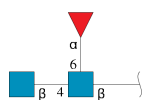
- Molecule 1 is a protein called 580 Antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1686	1057	284	340	5			
1	B	217	Total	C	N	O	S	0	0	0
			1686	1057	284	340	5			
1	D	217	Total	C	N	O	S	0	0	0
			1652	1034	277	336	5			
1	F	217	Total	C	N	O	S	0	0	0
			1661	1040	277	339	5			

- Molecule 2 is a protein called 580 Antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1619	1018	276	319	6			
2	A	219	Total	C	N	O	S	0	0	0
			1617	1016	275	320	6			
2	C	218	Total	C	N	O	S	0	0	0
			1610	1012	274	318	6			
2	E	218	Total	C	N	O	S	0	0	0
			1602	1007	272	317	6			

- Molecule 3 is an oligosaccharide called 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
3	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

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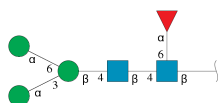
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	2	Total	C	N	O	0	0	0
			24	14	1	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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 6 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
6	L	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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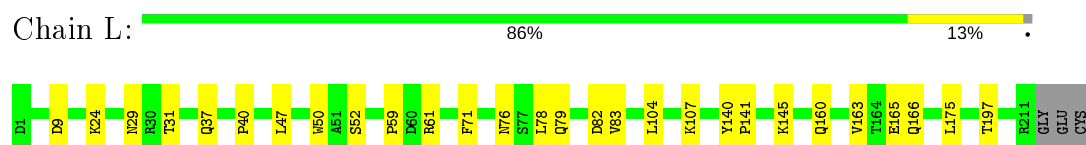
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		



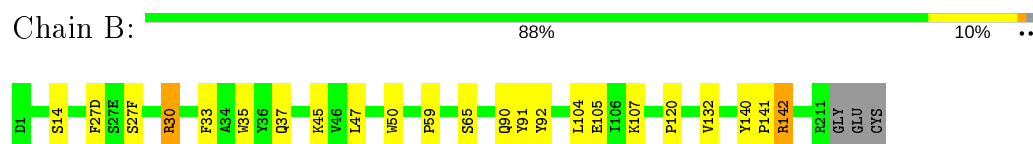
### 3 Residue-property plots [i](#)

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.

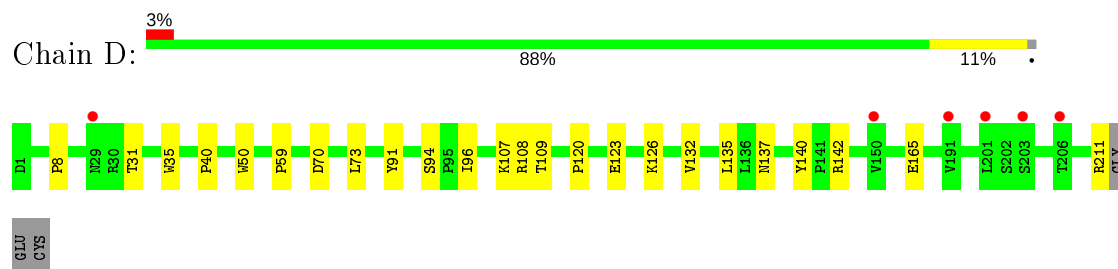
- Molecule 1: 580 Antibody, light chain



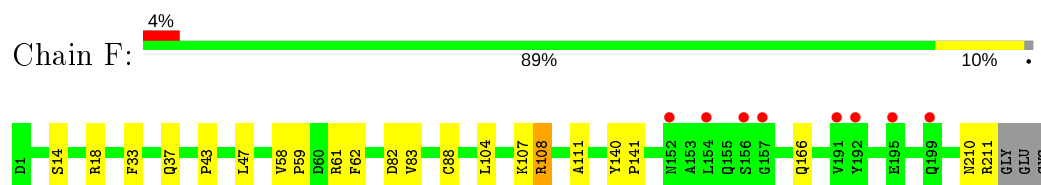
- Molecule 1: 580 Antibody, light chain



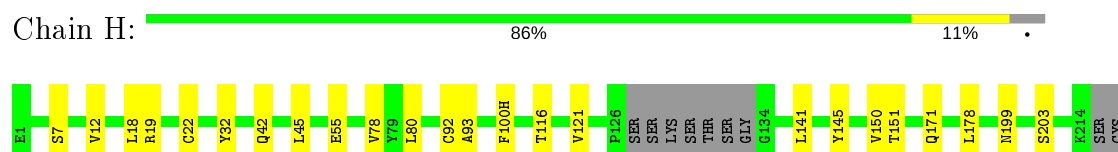
- Molecule 1: 580 Antibody, light chain




- Molecule 1: 580 Antibody, light chain

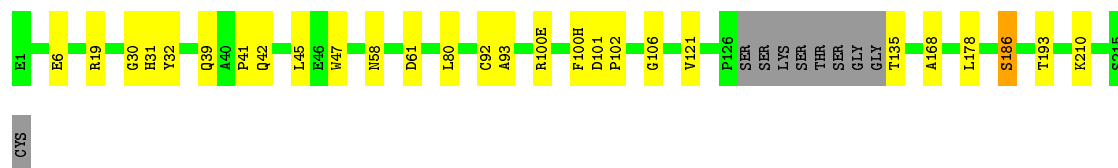


- Molecule 2: 580 Antibody, heavy chain




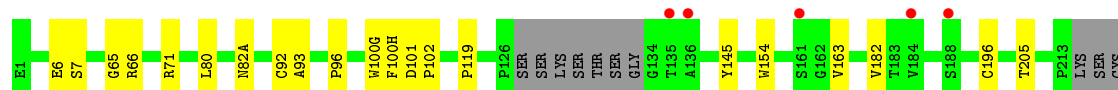
- Molecule 2: 580 Antibody, heavy chain

Chain A: 




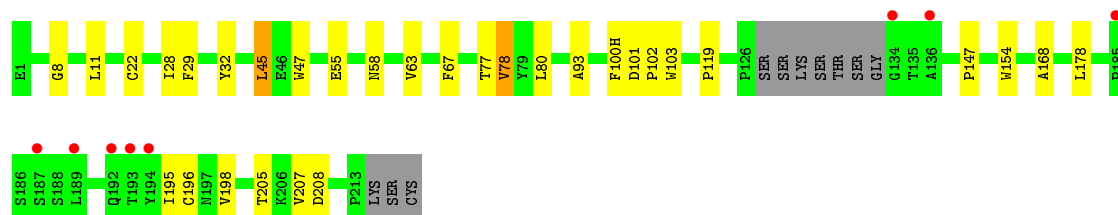
- Molecule 2: 580 Antibody, heavy chain

Chain C: 



- Molecule 2: 580 Antibody, heavy chain

Chain E: 



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

Chain G: 



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

Chain I: 



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

Chain J: 



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

Chain K:  33% 67%

MAN1	MAN2	MAN3	MAN4	MAN5	FUC6
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.36Å 179.57Å 140.43Å 90.00° 109.61° 90.00°	Depositor
Resolution (Å)	39.58 – 2.80 39.58 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.58-2.80) 92.5 (39.58-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.190 , 0.231 0.190 , 0.233	Depositor DCC
$R_{free}$ test set	2003 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: GOL, BMA, NAG, FUC, SO4, MAN

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	B	0.40	0/1724	0.56	0/2342
1	D	0.35	0/1690	0.56	0/2304
1	F	0.35	0/1699	0.55	0/2314
1	L	0.41	0/1724	0.58	0/2342
2	A	0.46	1/1657 (0.1%)	0.60	0/2259
2	C	0.42	0/1650	0.60	0/2249
2	E	0.40	0/1642	0.57	0/2240
2	H	0.52	1/1659 (0.1%)	0.64	0/2260
All	All	0.42	2/13445 (0.0%)	0.58	0/18310

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	92	CYS	CB-SG	-7.27	1.69	1.82
2	H	92	CYS	CB-SG	-5.72	1.72	1.81

There are no bond angle outliers.

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	B	1686	0	1627	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1652	0	1548	12	0
1	F	1661	0	1568	14	0
1	L	1686	0	1627	22	0
2	A	1617	0	1558	16	0
2	C	1610	0	1554	11	0
2	E	1602	0	1537	17	0
2	H	1619	0	1567	13	0
3	G	38	0	34	3	0
3	I	38	0	34	2	0
4	J	24	0	22	1	0
5	K	71	0	61	0	0
6	A	18	0	24	4	0
6	B	18	0	22	4	0
6	C	18	0	24	2	0
6	D	18	0	23	2	0
6	E	12	0	16	3	0
6	F	12	0	16	1	0
6	H	12	0	15	2	0
6	L	18	0	24	2	0
7	A	10	0	0	1	0
7	B	15	0	0	2	0
7	C	5	0	0	0	0
7	D	10	0	0	0	0
7	F	5	0	0	0	0
7	H	5	0	0	0	0
7	L	10	0	0	0	0
All	All	13490	0	12901	115	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.

The worst 5 of 115 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)
2:A:19:ARG:HH22	6:A:302:GOL:H32	1.48	0.79
1:D:50:TRP:HB3	4:J:2:FUC:H4	1.64	0.78
2:E:198:VAL:HB	2:E:207:VAL:HG23	1.73	0.71
1:D:59:PRO:HB3	6:D:304:GOL:H2	1.74	0.69
2:H:32:TYR:OH	6:H:301:GOL:O2	2.08	0.69

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	B	215/220 (98%)	208 (97%)	7 (3%)	0	100	100
1	D	215/220 (98%)	208 (97%)	7 (3%)	0	100	100
1	F	215/220 (98%)	209 (97%)	6 (3%)	0	100	100
1	L	215/220 (98%)	210 (98%)	5 (2%)	0	100	100
2	A	215/228 (94%)	207 (96%)	8 (4%)	0	100	100
2	C	214/228 (94%)	208 (97%)	6 (3%)	0	100	100
2	E	214/228 (94%)	208 (97%)	6 (3%)	0	100	100
2	H	215/228 (94%)	208 (97%)	7 (3%)	0	100	100
All	All	1718/1792 (96%)	1666 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	193/195 (99%)	189 (98%)	4 (2%)	53	84
1	D	184/195 (94%)	179 (97%)	5 (3%)	44	78
1	F	187/195 (96%)	185 (99%)	2 (1%)	73	92
1	L	193/195 (99%)	192 (100%)	1 (0%)	88	96
2	A	178/187 (95%)	174 (98%)	4 (2%)	52	83
2	C	177/187 (95%)	175 (99%)	2 (1%)	73	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	175/187 (94%)	171 (98%)	4 (2%)	50	82
2	H	178/187 (95%)	175 (98%)	3 (2%)	60	87
All	All	1465/1528 (96%)	1440 (98%)	25 (2%)	60	87

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	186	SER
1	D	70	ASP
2	E	78	VAL
1	D	31	THR
1	D	94	SER

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

Mol	Chain	Res	Type
1	L	160	GLN
1	D	137	ASN
2	C	204	ASN
2	E	3	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

14 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	$\# Z  > 2$
3	NAG	G	1	1,3	14,14,15	0.94	1 (7%)	17,19,21	0.69	0
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	0.73	1 (5%)
3	FUC	G	3	3	10,10,11	2.19	2 (20%)	14,14,16	2.03	4 (28%)
3	NAG	I	1	1,3	14,14,15	0.41	0	17,19,21	0.35	0
3	NAG	I	2	3	14,14,15	0.49	0	17,19,21	0.49	0
3	FUC	I	3	3	10,10,11	1.10	1 (10%)	14,14,16	1.09	1 (7%)
4	NAG	J	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.90	1 (5%)
4	FUC	J	2	4	10,10,11	1.26	2 (20%)	14,14,16	1.00	1 (7%)
5	NAG	K	1	1,5	14,14,15	0.36	0	17,19,21	0.90	1 (5%)
5	NAG	K	2	5	14,14,15	0.48	0	17,19,21	0.45	0
5	BMA	K	3	5	11,11,12	0.92	0	15,15,17	0.87	0
5	MAN	K	4	5	11,11,12	1.48	3 (27%)	15,15,17	0.93	0
5	MAN	K	5	5	11,11,12	1.03	0	15,15,17	0.95	1 (6%)
5	FUC	K	6	5	10,10,11	0.74	0	14,14,16	0.96	1 (7%)

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
3	NAG	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	FUC	G	3	3	-	-	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	J	2	4	-	-	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	2/2/19/22	0/1/1/1
5	MAN	K	5	5	-	0/2/19/22	0/1/1/1
5	FUC	K	6	5	-	-	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	FUC	C1-C2	5.63	1.65	1.52
3	G	3	FUC	C4-C5	2.91	1.59	1.52
3	G	1	NAG	O5-C1	-2.87	1.39	1.43
4	J	2	FUC	C1-C2	2.64	1.58	1.52
5	K	4	MAN	C4-C3	2.51	1.58	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	FUC	O2-C2-C1	5.18	119.74	109.15
3	G	3	FUC	O5-C1-C2	-3.10	105.98	110.77
4	J	1	NAG	C1-O5-C5	-2.72	108.51	112.19
4	J	2	FUC	O2-C2-C1	2.62	114.52	109.15
3	G	2	NAG	C1-O5-C5	2.59	115.70	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

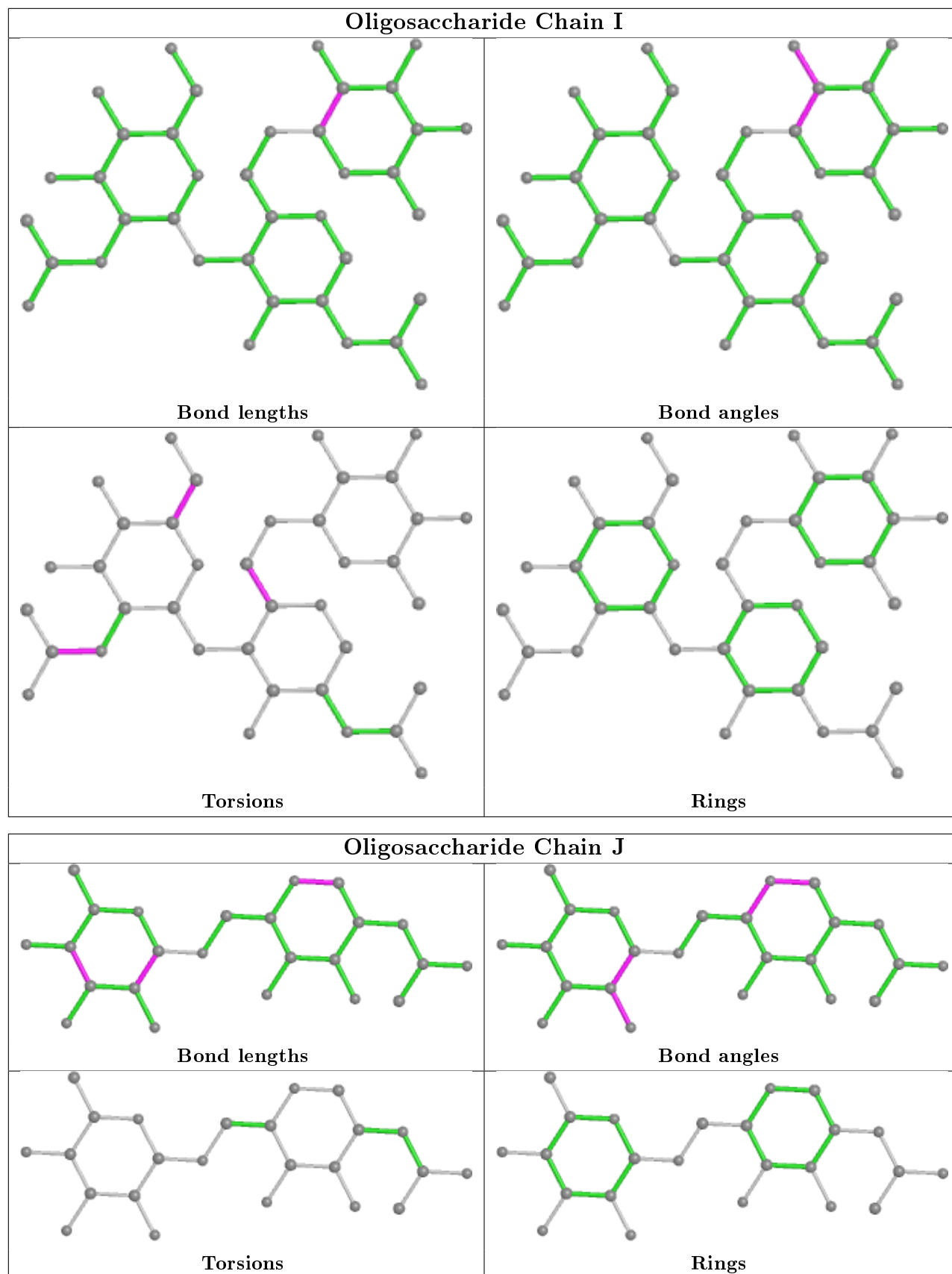
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
5	K	4	MAN	C4-C5-C6-O6

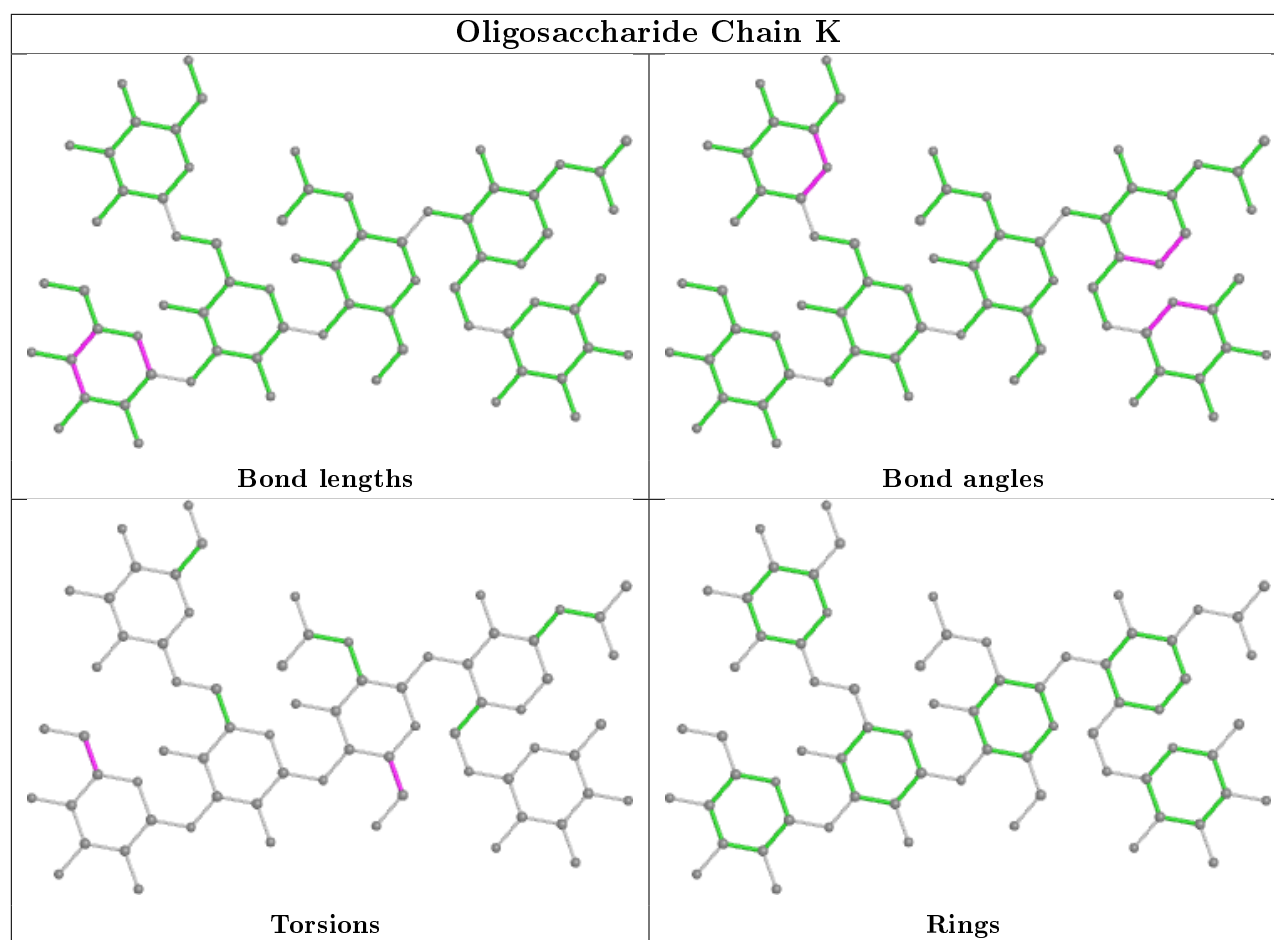
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	2	FUC	1	0
3	G	1	NAG	1	0
3	G	3	FUC	2	0
3	I	3	FUC	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](#)

33 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	GOL	A	302	-	5,5,5	1.15	0	5,5,5	0.91	0
6	GOL	C	302	-	5,5,5	1.07	0	5,5,5	0.81	0
6	GOL	D	304	-	5,5,5	0.95	0	5,5,5	0.95	0
6	GOL	F	307	-	5,5,5	0.93	0	5,5,5	0.91	0
6	GOL	H	302	-	5,5,5	0.95	0	5,5,5	0.95	0
6	GOL	L	305	-	5,5,5	0.91	0	5,5,5	1.06	0
6	GOL	B	305	-	5,5,5	1.58	1 (20%)	5,5,5	1.24	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	A	304	-	4,4,4	0.13	0	6,6,6	0.14	0
6	GOL	C	301	-	5,5,5	1.14	0	5,5,5	0.80	0
7	SO4	A	305	-	4,4,4	0.12	0	6,6,6	0.10	0
6	GOL	C	303	-	5,5,5	0.84	0	5,5,5	1.09	0
6	GOL	H	301	-	5,5,5	1.48	1 (20%)	5,5,5	0.68	0
6	GOL	D	305	-	5,5,5	0.92	0	5,5,5	1.03	0
6	GOL	E	302	-	5,5,5	0.88	0	5,5,5	1.04	0
7	SO4	D	306	-	4,4,4	0.14	0	6,6,6	0.16	0
6	GOL	A	303	-	5,5,5	0.81	0	5,5,5	0.99	0
7	SO4	L	307	-	4,4,4	0.15	0	6,6,6	0.22	0
7	SO4	B	307	-	4,4,4	0.14	0	6,6,6	0.11	0
7	SO4	B	309	-	4,4,4	0.15	0	6,6,6	0.15	0
6	GOL	A	301	-	5,5,5	1.11	0	5,5,5	1.12	0
6	GOL	B	304	-	5,5,5	1.29	1 (20%)	5,5,5	0.90	0
7	SO4	F	309	-	4,4,4	0.13	0	6,6,6	0.08	0
6	GOL	D	303	-	5,5,5	1.15	1 (20%)	5,5,5	0.85	0
7	SO4	B	308	-	4,4,4	0.17	0	6,6,6	0.21	0
7	SO4	C	304	-	4,4,4	0.16	0	6,6,6	0.11	0
6	GOL	L	306	-	5,5,5	1.18	0	5,5,5	1.06	0
7	SO4	H	303	-	4,4,4	0.13	0	6,6,6	0.15	0
7	SO4	L	308	-	4,4,4	0.12	0	6,6,6	0.12	0
6	GOL	B	306	-	5,5,5	0.95	0	5,5,5	0.91	0
7	SO4	D	307	-	4,4,4	0.19	0	6,6,6	0.20	0
6	GOL	F	308	-	5,5,5	0.88	0	5,5,5	1.10	0
6	GOL	E	301	-	5,5,5	0.97	0	5,5,5	0.71	0
6	GOL	L	304	-	5,5,5	0.88	0	5,5,5	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	304	-	-	2/4/4/4	-
6	GOL	A	302	-	-	2/4/4/4	-
6	GOL	E	301	-	-	4/4/4/4	-
6	GOL	C	302	-	-	2/4/4/4	-
6	GOL	D	303	-	-	2/4/4/4	-
6	GOL	D	304	-	-	3/4/4/4	-
6	GOL	F	307	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	303	-	-	2/4/4/4	-
6	GOL	L	306	-	-	3/4/4/4	-
6	GOL	A	301	-	-	2/4/4/4	-
6	GOL	B	306	-	-	0/4/4/4	-
6	GOL	L	305	-	-	2/4/4/4	-
6	GOL	B	305	-	-	0/4/4/4	-
6	GOL	H	301	-	-	0/4/4/4	-
6	GOL	H	302	-	-	4/4/4/4	-
6	GOL	F	308	-	-	4/4/4/4	-
6	GOL	C	303	-	-	2/4/4/4	-
6	GOL	D	305	-	-	2/4/4/4	-
6	GOL	C	301	-	-	0/4/4/4	-
6	GOL	E	302	-	-	0/4/4/4	-
6	GOL	L	304	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	305	GOL	O2-C2	-3.25	1.33	1.43
6	H	301	GOL	O2-C2	-2.72	1.35	1.43
6	B	304	GOL	O2-C2	-2.54	1.35	1.43
6	D	303	GOL	O2-C2	-2.25	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	305	GOL	O1-C1-C2	-2.09	100.19	110.20

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	302	GOL	O1-C1-C2-O2
6	A	302	GOL	O1-C1-C2-C3
6	C	302	GOL	O1-C1-C2-O2
6	C	302	GOL	O1-C1-C2-C3
6	F	307	GOL	O1-C1-C2-C3

There are no ring outliers.

20 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	302	GOL	1	0
6	C	302	GOL	1	0
6	D	304	GOL	1	0
6	F	307	GOL	1	0
6	H	302	GOL	1	0
6	L	305	GOL	1	0
6	B	305	GOL	2	0
7	A	305	SO4	1	0
6	C	303	GOL	1	0
6	H	301	GOL	1	0
6	D	305	GOL	1	0
6	E	302	GOL	1	0
6	A	303	GOL	1	0
7	B	309	SO4	1	0
6	A	301	GOL	2	0
6	B	304	GOL	1	0
7	B	308	SO4	1	0
6	B	306	GOL	1	0
6	E	301	GOL	2	0
6	L	304	GOL	1	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 [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	B	217/220 (98%)	-0.16	0 <span>100</span> <span>100</span>	32, 56, 83, 101	0
1	D	217/220 (98%)	0.18	6 (2%) <span>53</span> <span>43</span>	35, 69, 100, 124	0
1	F	217/220 (98%)	0.15	8 (3%) <span>41</span> <span>31</span>	37, 67, 116, 126	0
1	L	217/220 (98%)	-0.30	0 <span>100</span> <span>100</span>	30, 45, 68, 80	0
2	A	219/228 (96%)	-0.43	0 <span>100</span> <span>100</span>	32, 44, 67, 136	0
2	C	218/228 (95%)	-0.25	5 (2%) <span>60</span> <span>51</span>	26, 43, 88, 120	0
2	E	218/228 (95%)	-0.19	8 (3%) <span>41</span> <span>31</span>	34, 52, 107, 135	0
2	H	219/228 (96%)	-0.52	0 <span>100</span> <span>100</span>	19, 35, 61, 91	0
All	All	1742/1792 (97%)	-0.19	27 (1%) <span>73</span> <span>68</span>	19, 50, 98, 136	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	LEU	4.4
2	C	135	THR	3.5
2	C	188	SER	3.5
1	F	199	GLN	3.5
2	C	136	ALA	2.9

### 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,



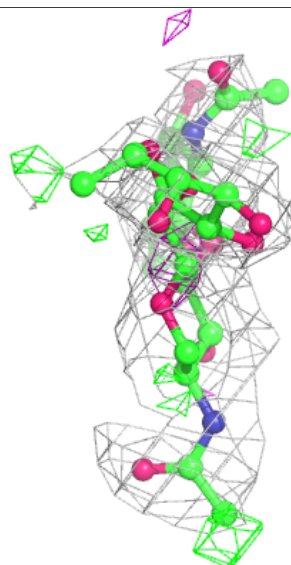
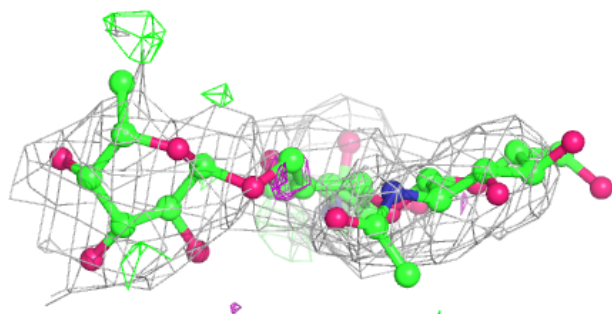
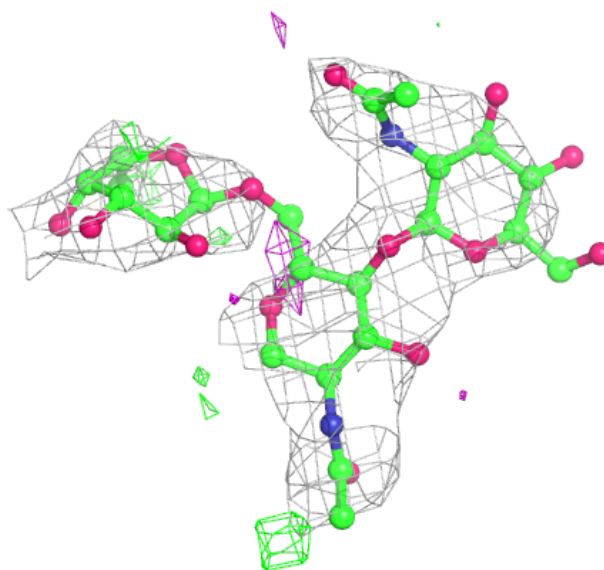
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	I	2	14/15	0.77	0.46	116,125,131,133	0
3	NAG	I	1	14/15	0.78	0.32	77,86,105,112	0
4	FUC	J	2	10/11	0.79	0.40	97,106,112,112	0
5	MAN	K	4	11/12	0.80	0.38	98,101,103,105	0
5	MAN	K	5	11/12	0.82	0.27	79,87,91,95	0
4	NAG	J	1	14/15	0.85	0.30	73,81,94,101	0
3	NAG	G	2	14/15	0.88	0.32	62,82,93,96	0
3	FUC	G	3	10/11	0.90	0.19	50,53,57,58	0
3	FUC	I	3	10/11	0.90	0.33	91,96,100,101	0
5	BMA	K	3	11/12	0.91	0.22	80,86,91,96	0
3	NAG	G	1	14/15	0.92	0.14	33,49,58,61	0
5	NAG	K	2	14/15	0.96	0.15	54,57,63,72	0
5	NAG	K	1	14/15	0.97	0.16	35,44,53,58	0
5	FUC	K	6	10/11	0.98	0.14	36,44,48,52	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.

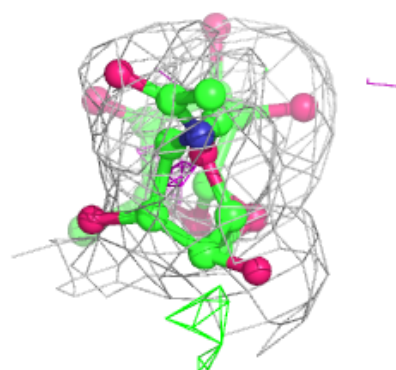
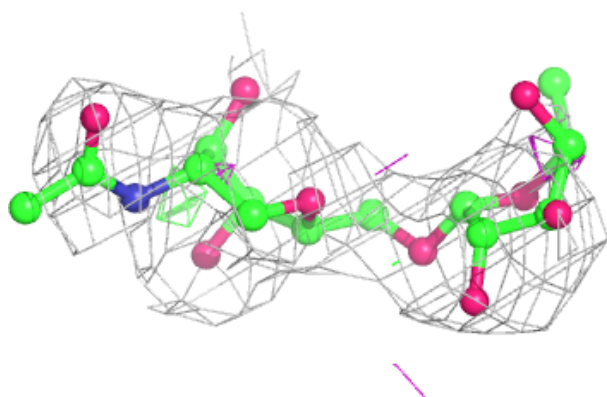
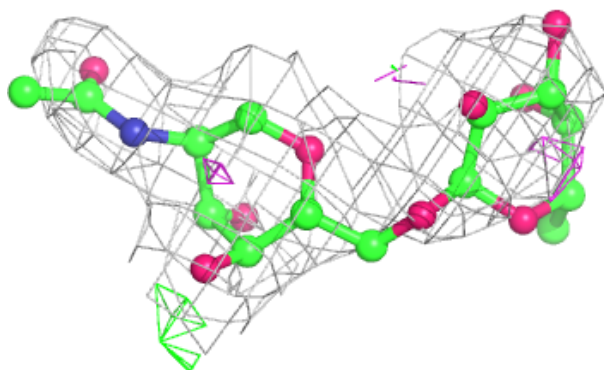
**Electron density around Chain I:**

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

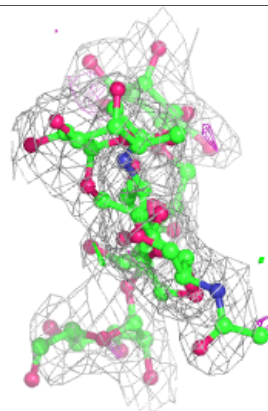
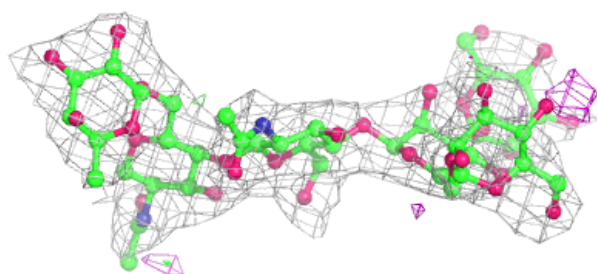
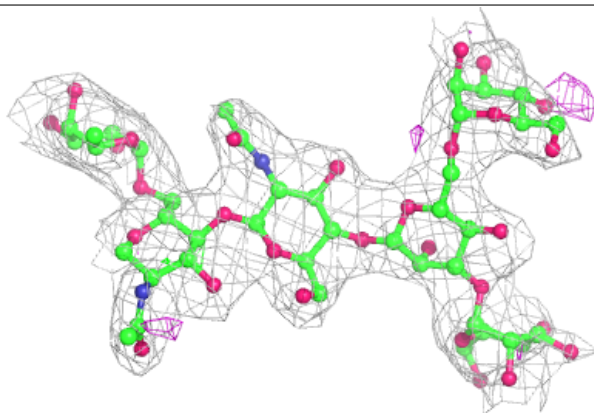


**Electron density around Chain J:**

$2mF_o-DF_c$  (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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	B	306	6/6	0.55	0.52	81,82,84,86	0
6	GOL	L	304	6/6	0.67	0.41	80,82,84,86	0
7	SO4	B	309	5/5	0.73	0.44	148,148,149,149	0
7	SO4	L	308	5/5	0.74	0.38	137,137,138,138	0
6	GOL	F	307	6/6	0.76	0.47	76,81,82,83	0
6	GOL	L	306	6/6	0.77	0.33	58,61,62,63	0
7	SO4	C	304	5/5	0.77	0.27	137,137,137,138	0
7	SO4	A	305	5/5	0.81	0.22	146,146,146,147	0
6	GOL	H	302	6/6	0.82	0.29	69,70,71,74	0
6	GOL	D	304	6/6	0.82	0.18	79,82,82,84	0
6	GOL	E	302	6/6	0.83	0.24	61,63,67,71	0
6	GOL	A	303	6/6	0.83	0.30	72,73,79,83	0
7	SO4	A	304	5/5	0.84	0.27	127,127,128,128	0
6	GOL	D	305	6/6	0.84	0.21	77,81,84,85	0
6	GOL	C	301	6/6	0.87	0.16	58,59,60,61	0
6	GOL	L	305	6/6	0.87	0.33	66,72,72,73	0
6	GOL	C	303	6/6	0.87	0.15	56,57,60,65	0
6	GOL	E	301	6/6	0.89	0.20	56,60,61,64	0
6	GOL	C	302	6/6	0.90	0.18	61,66,73,76	0
6	GOL	F	308	6/6	0.91	0.22	57,61,64,69	0
6	GOL	A	302	6/6	0.91	0.15	51,57,59,61	0
7	SO4	D	307	5/5	0.91	0.20	100,101,102,102	0
6	GOL	H	301	6/6	0.93	0.18	33,36,40,42	0
7	SO4	D	306	5/5	0.93	0.14	99,99,101,102	0
6	GOL	B	304	6/6	0.94	0.26	45,47,47,47	0
6	GOL	B	305	6/6	0.94	0.26	34,38,48,52	0
6	GOL	A	301	6/6	0.94	0.19	41,43,50,52	0
7	SO4	F	309	5/5	0.95	0.14	107,107,108,108	0
7	SO4	H	303	5/5	0.95	0.18	98,99,101,104	0
7	SO4	B	308	5/5	0.96	0.17	83,84,85,86	0
7	SO4	L	307	5/5	0.96	0.18	84,84,86,91	0
7	SO4	B	307	5/5	0.97	0.13	76,77,79,79	0
6	GOL	D	303	6/6	0.98	0.18	41,50,55,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.