



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2021 – 04:12 PM EDT

PDB ID : 3SDY  
Title : Crystal Structure of Broadly Neutralizing Antibody CR8020 Bound to the Influenza A H3 Hemagglutinin  
Authors : Ekiert, D.C.; Wilson, I.A.  
Deposited on : 2011-06-09  
Resolution : 2.85 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 : 2.18  
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) : 2.18

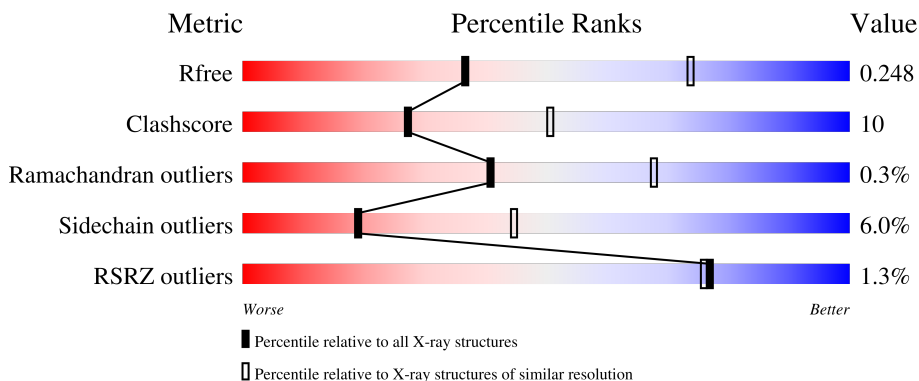
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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.





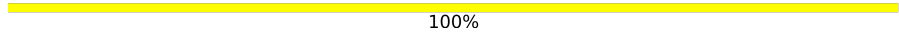
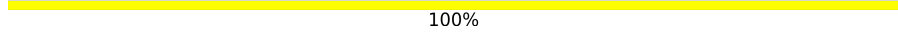
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	323	
2	B	176	
3	H	227	
4	L	216	
5	C	4	

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Mol	Chain	Length	Quality of chain
6	D	6	 83% 17%
7	E	4	 25% 25% 50%
8	F	2	 100%
9	G	4	 100%

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
5	NAG	C	2	-	-	-	X
6	FUC	D	6	X	-	-	-
9	BMA	G	3	-	-	-	X
9	FUC	G	4	X	-	-	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 14620 atoms, of which 7155 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	319	4868	1542	2407	433	473	13	2407	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	172	2696	863	1305	243	279	6	1305	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

- Molecule 3 is a protein called Antibody CR8020, Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	H	221	3286	1056	1617	276	330	7	1617	0	0

- Molecule 4 is a protein called Antibody CR8020, Light Chain.

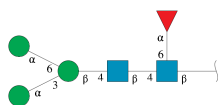
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	L	215	3255	1026	1609	285	328	7	1609	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	C	4	93	28	43	2	20	43	0	0

- Molecule 6 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
			Total	C	H	N	O			
6	D	6	133	40	62	2	29	62	0	0

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



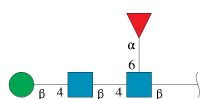
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
7	E	4	93	28	43	2	20	43	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



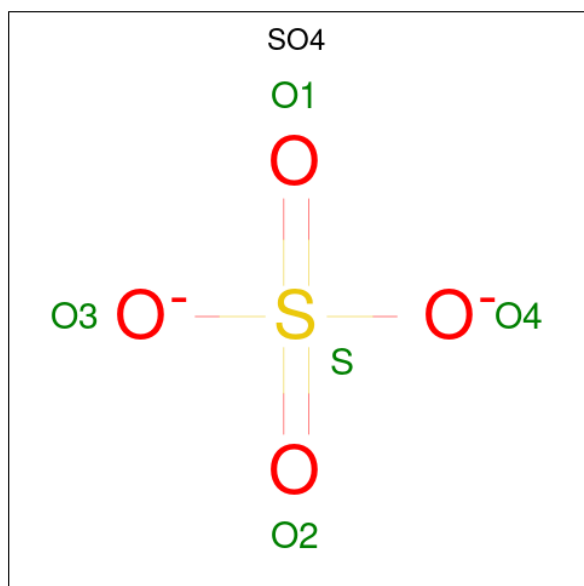
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
8	F	2	53	16	25	2	10	25	0	0

- Molecule 9 is an oligosaccharide called 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	
			Total	C	H	N				O
9	G	4	93	28	44	2	19	44	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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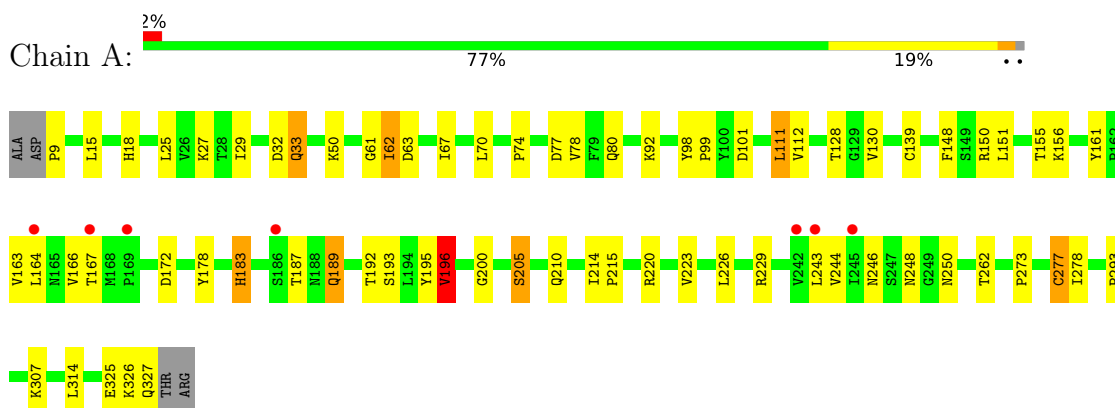
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
10	B	1	Total 5	O 4	S 1	0	0
10	B	1	Total 5	O 4	S 1	0	0
10	L	1	Total 5	O 4	S 1	0	0
10	L	1	Total 5	O 4	S 1	0	0
10	L	1	Total 5	O 4	S 1	0	0
10	L	1	Total 5	O 4	S 1	0	0
10	L	1	Total 5	O 4	S 1	0	0
10	L	1	Total 5	O 4	S 1	0	0

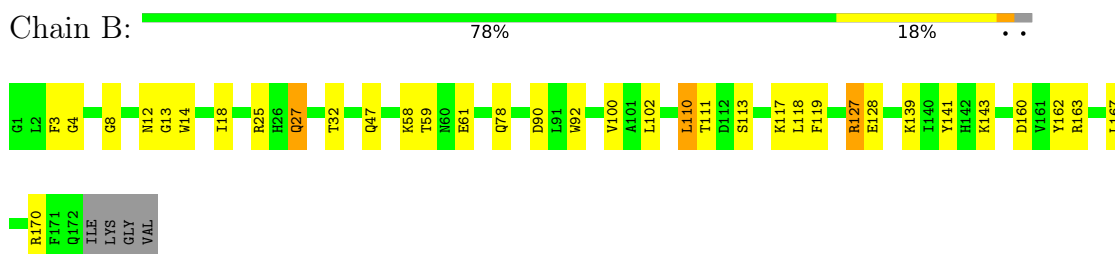
### 3 Residue-property plots

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.

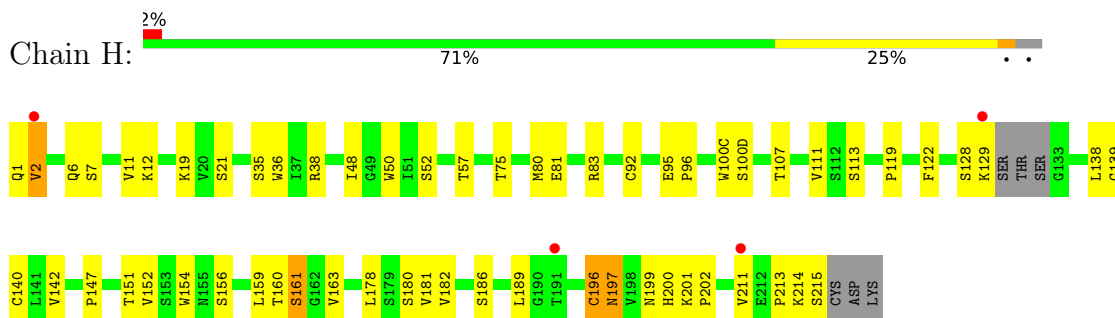
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 2: Hemagglutinin HA2 chain



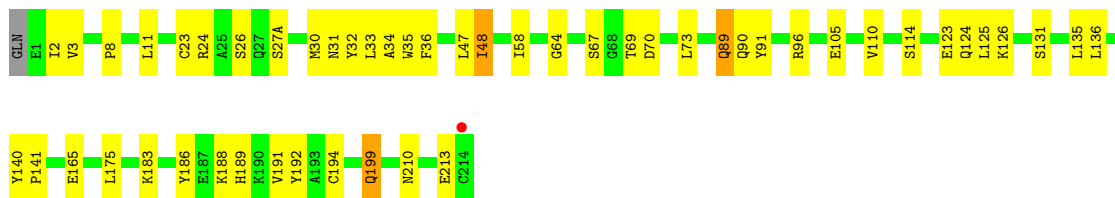
- Molecule 3: Antibody CR8020, Heavy Chain



- Molecule 4: Antibody CR8020, Light Chain







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

Chain C: 75% 25%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 6: 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 D: 83% 17%

MAG1  
MAG2  
BMA3  
MAN5  
FUC6

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

Chain E: 25% 25% 50%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

MAG1  
MAG2

- Molecule 9: 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 G: 100%

MAG1  
MAG2  
BMA3  
FUC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.75Å 197.75Å 197.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.61 – 2.85 46.61 – 2.85	Depositor EDS
% Data completeness (in resolution range)	88.1 (46.61-2.85) 99.3 (46.61-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.202 , 0.235 0.214 , 0.248	Depositor DCC
$R_{free}$ test set	3018 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.9	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.009 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: FUC, MAN, PCA, SO4, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/2518	0.50	0/3430
2	B	0.32	0/1415	0.49	0/1902
3	H	0.28	0/1705	0.50	0/2329
4	L	0.30	0/1680	0.52	0/2278
All	All	0.29	0/7318	0.50	0/9939

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2461	2407	2411	56	0
2	B	1391	1305	1306	27	0
3	H	1669	1617	1618	38	0
4	L	1646	1609	1612	37	0
5	C	50	43	43	1	0
6	D	71	62	61	3	0
7	E	50	43	43	3	0
8	F	28	25	25	0	0
9	G	49	44	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	5	0	0	0	0
10	B	15	0	0	1	0
10	L	30	0	0	0	0
All	All	7465	7155	7162	148	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 10.

The worst 5 of 148 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)
4:L:210:ASN:HB2	4:L:213:GLU:HG3	1.59	0.85
3:H:138:LEU:HD13	3:H:211:VAL:HG21	1.63	0.81
1:A:195:TYR:O	1:A:196:VAL:HG23	1.84	0.78
1:A:220:ARG:HD2	1:A:229:ARG:HG3	1.69	0.74
3:H:35:SER:HB2	3:H:95:GLU:HG3	1.75	0.69

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	317/323 (98%)	310 (98%)	5 (2%)	2 (1%)	25	53
2	B	170/176 (97%)	166 (98%)	4 (2%)	0	100	100
3	H	217/227 (96%)	206 (95%)	10 (5%)	1 (0%)	29	57
4	L	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
All	All	917/942 (97%)	888 (97%)	26 (3%)	3 (0%)	41	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	A	62	ILE
3	H	2	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/283 (99%)	262 (94%)	18 (6%)	17	41
2	B	146/149 (98%)	139 (95%)	7 (5%)	25	55
3	H	186/192 (97%)	176 (95%)	10 (5%)	22	49
4	L	184/185 (100%)	171 (93%)	13 (7%)	14	36
All	All	796/809 (98%)	748 (94%)	48 (6%)	19	45

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	92	CYS
4	L	2	ILE
3	H	113	SER
3	H	196	CYS
4	L	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
4	L	138	ASN
4	L	210	ASN
4	L	199	GLN
2	B	125	GLN
4	L	89	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](#)

1 non-standard protein/DNA/RNA residue is 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	PCA	H	1	3	7,8,9	2.20	2 (28%)	9,10,12	2.09	5 (55%)

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	PCA	H	1	3	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	PCA	CD-N	4.56	1.46	1.34
3	H	1	PCA	CA-N	3.44	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	PCA	OE-CD-CG	-3.07	121.41	126.76
3	H	1	PCA	CA-N-CD	-2.96	103.45	113.58
3	H	1	PCA	CG-CD-N	2.55	114.99	108.39
3	H	1	PCA	CB-CA-N	2.34	110.03	103.30
3	H	1	PCA	CB-CA-C	-2.27	109.57	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates i

20 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	C	1	1,5	14,14,15	0.54	0	17,19,21	1.66	2 (11%)
5	NAG	C	2	5	14,14,15	0.41	0	17,19,21	0.84	0
5	BMA	C	3	5	11,11,12	0.61	0	15,15,17	1.09	2 (13%)
5	MAN	C	4	5	11,11,12	0.62	0	15,15,17	1.06	2 (13%)
6	NAG	D	1	1,6	14,14,15	0.51	0	17,19,21	0.77	1 (5%)
6	NAG	D	2	6	14,14,15	0.53	0	17,19,21	0.73	0
6	BMA	D	3	6	11,11,12	0.61	0	15,15,17	0.97	1 (6%)
6	MAN	D	4	6	11,11,12	0.59	0	15,15,17	1.05	2 (13%)
6	MAN	D	5	6	11,11,12	0.59	0	15,15,17	1.12	1 (6%)
6	FUC	D	6	6	10,10,11	0.59	0	14,14,16	1.36	2 (14%)
7	NAG	E	1	1,7	14,14,15	0.55	0	17,19,21	1.14	1 (5%)
7	NAG	E	2	7	14,14,15	0.62	0	17,19,21	1.02	0
7	BMA	E	3	7	11,11,12	0.59	0	15,15,17	1.77	3 (20%)
7	MAN	E	4	7	11,11,12	0.63	0	15,15,17	0.90	0
8	NAG	F	1	1,8	14,14,15	0.49	0	17,19,21	0.84	1 (5%)
8	NAG	F	2	8	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
9	NAG	G	1	2,9	14,14,15	0.34	0	17,19,21	2.05	4 (23%)
9	NAG	G	2	9	14,14,15	0.57	0	17,19,21	0.79	1 (5%)
9	BMA	G	3	9	11,11,12	0.68	0	15,15,17	1.33	2 (13%)
9	FUC	G	4	9	10,10,11	0.91	1 (10%)	14,14,16	2.09	5 (35%)

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	C	1	1,5	-	3/6/23/26	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	MAN	C	4	5	-	0/2/19/22	0/1/1/1
6	NAG	D	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	BMA	D	3	6	-	2/2/19/22	0/1/1/1
6	MAN	D	4	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5	6	-	2/2/19/22	0/1/1/1
6	FUC	D	6	6	1/1/5/5	-	0/1/1/1
7	NAG	E	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1
7	BMA	E	3	7	-	2/2/19/22	0/1/1/1
7	MAN	E	4	7	-	0/2/19/22	0/1/1/1
8	NAG	F	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
9	NAG	G	1	2,9	-	3/6/23/26	0/1/1/1
9	NAG	G	2	9	-	2/6/23/26	0/1/1/1
9	BMA	G	3	9	-	2/2/19/22	0/1/1/1
9	FUC	G	4	9	1/1/5/5	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	4	FUC	O5-C1	-2.10	1.40	1.43

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	1	NAG	C1-O5-C5	6.21	120.60	112.19
5	C	1	NAG	C1-O5-C5	5.66	119.86	112.19
9	G	4	FUC	C1-C2-C3	-5.06	103.45	109.67
7	E	3	BMA	C1-C2-C3	4.85	115.63	109.67
6	D	5	MAN	O5-C5-C6	3.42	112.56	107.20

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
6	D	6	FUC	C1
9	G	4	FUC	C1

5 of 23 torsion outliers are listed below:

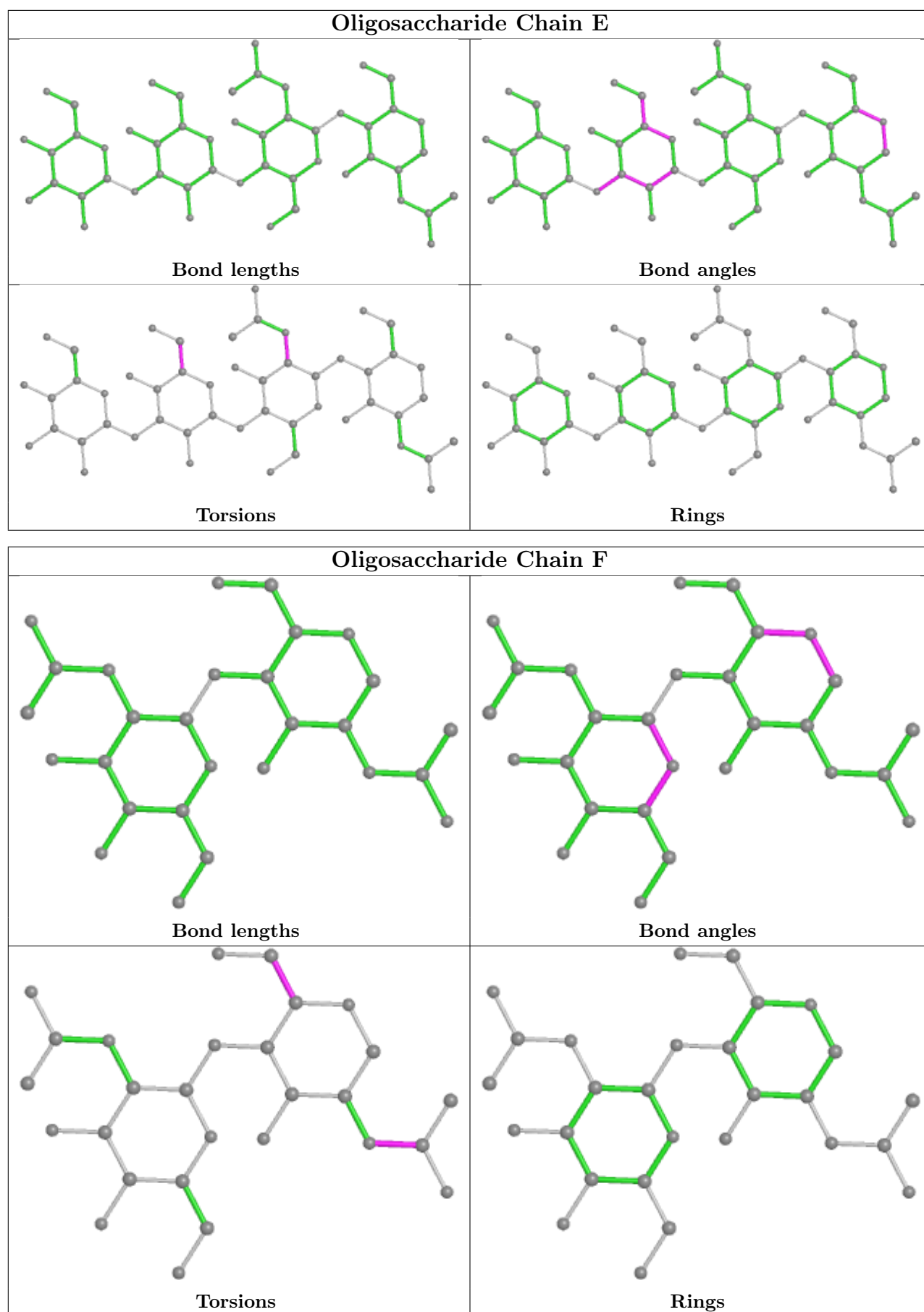
Mol	Chain	Res	Type	Atoms
9	G	1	NAG	C3-C2-N2-C7
5	C	3	BMA	O5-C5-C6-O6
5	C	3	BMA	C4-C5-C6-O6
6	D	3	BMA	O5-C5-C6-O6
9	G	2	NAG	C8-C7-N2-C2

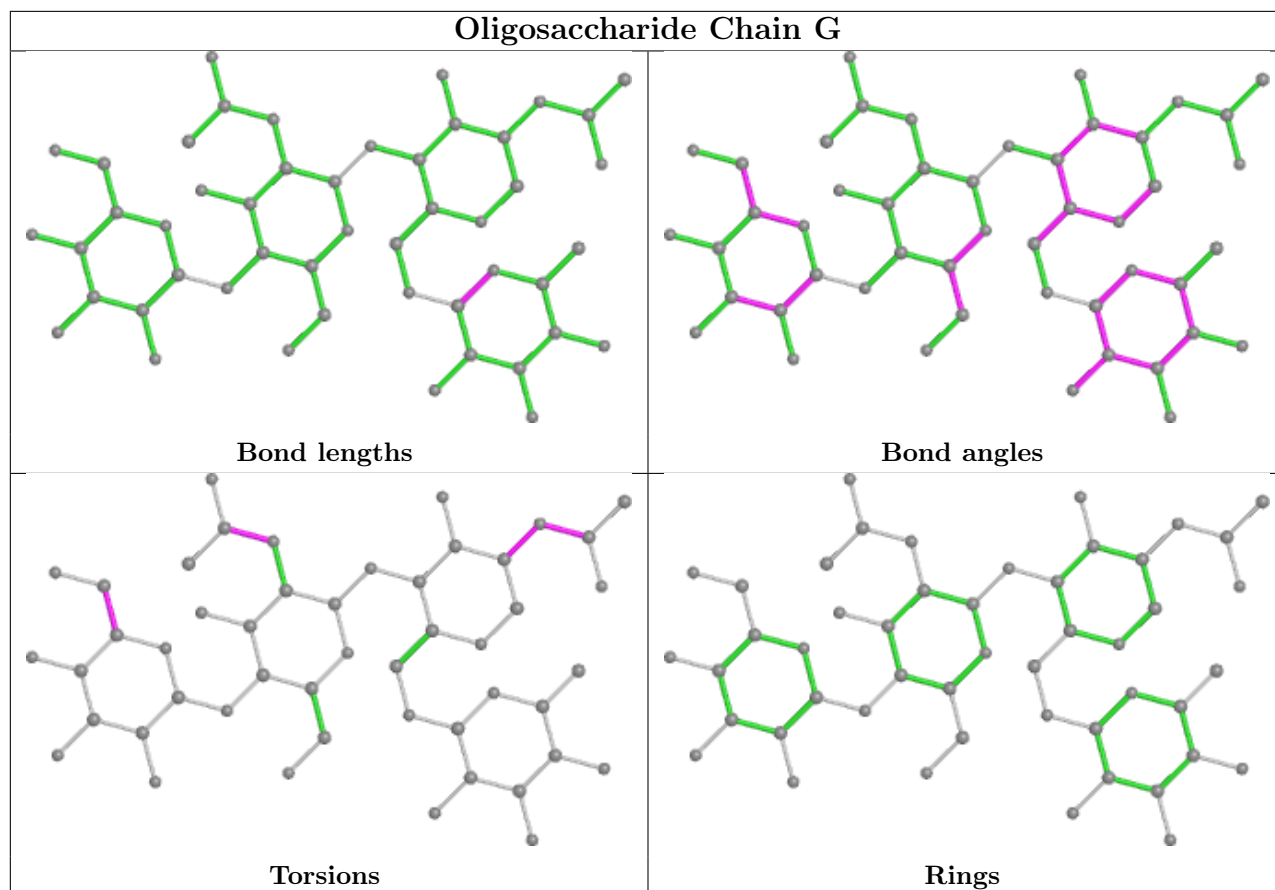
There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1	NAG	3	0
7	E	3	BMA	2	0
7	E	1	NAG	1	0
5	C	2	NAG	1	0
5	C	4	MAN	1	0
6	D	2	NAG	3	0
7	E	2	NAG	3	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](#)

10 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	$\# Z  > 2$
10	SO4	L	217	-	4,4,4	0.14	0	6,6,6	0.11	0
10	SO4	L	218	-	4,4,4	0.15	0	6,6,6	0.08	0
10	SO4	L	220	-	4,4,4	0.14	0	6,6,6	0.08	0
10	SO4	B	179	-	4,4,4	0.15	0	6,6,6	0.05	0
10	SO4	B	178	-	4,4,4	0.16	0	6,6,6	0.17	0
10	SO4	A	1	-	4,4,4	0.11	0	6,6,6	0.18	0
10	SO4	L	219	-	4,4,4	0.13	0	6,6,6	0.12	0
10	SO4	B	177	-	4,4,4	0.13	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	SO4	L	216	-	4,4,4	0.14	0	6,6,6	0.10	0
10	SO4	L	215	-	4,4,4	0.12	0	6,6,6	0.14	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	177	SO4	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	A	319/323 (98%)	-0.04	7 (2%) 62 59	55, 108, 165, 189	0
2	B	172/176 (97%)	-0.11	0 100 100	49, 77, 126, 160	0
3	H	220/227 (96%)	0.00	4 (1%) 68 66	63, 97, 150, 184	0
4	L	215/216 (99%)	-0.12	1 (0%) 91 90	64, 88, 121, 171	0
All	All	926/942 (98%)	-0.06	12 (1%) 77 76	49, 92, 153, 189	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	214	CYS	3.7
1	A	245	ILE	3.7
3	H	129	LYS	3.7
1	A	186	SER	2.5
3	H	211	VAL	2.4

### 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	PCA	H	1	8/9	0.77	0.34	140,152,171,171	5

### 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,

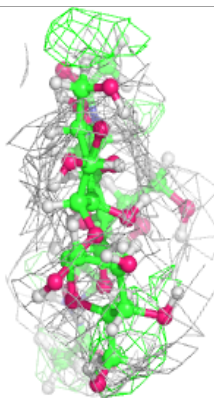
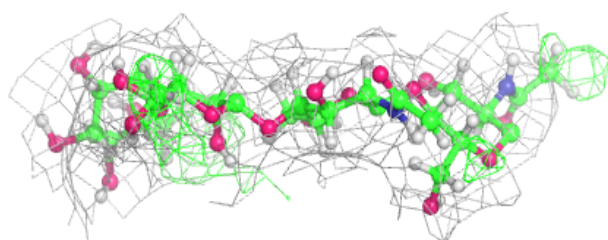
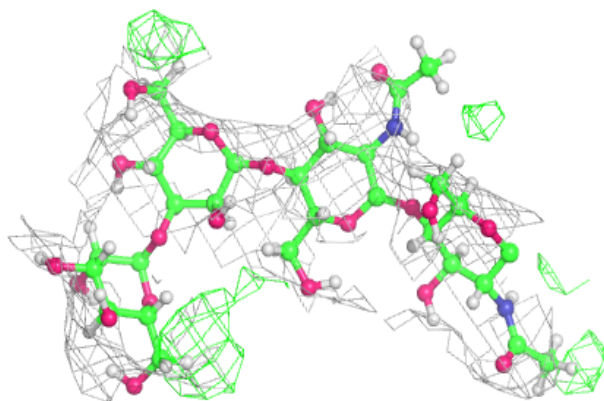
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BMA	C	3	11/12	0.19	0.38	184,202,216,217	9
9	BMA	G	3	11/12	0.57	0.42	181,194,205,213	10
5	MAN	C	4	11/12	0.60	0.30	177,196,206,209	10
7	MAN	E	4	11/12	0.74	0.34	215,230,238,239	10
5	NAG	C	2	14/15	0.74	0.41	130,161,175,185	12
5	NAG	C	1	14/15	0.80	0.20	121,155,178,194	12
7	BMA	E	3	11/12	0.82	0.32	186,191,204,216	9
8	NAG	F	2	14/15	0.84	0.14	115,144,159,167	13
9	NAG	G	2	14/15	0.86	0.23	118,156,178,194	12
6	NAG	D	1	14/15	0.86	0.16	110,122,138,143	11
7	NAG	E	2	14/15	0.88	0.38	164,171,177,185	12
6	MAN	D	5	11/12	0.89	0.29	130,145,154,156	10
6	BMA	D	3	11/12	0.90	0.18	110,122,137,142	8
7	NAG	E	1	14/15	0.90	0.14	153,169,175,176	12
9	FUC	G	4	10/11	0.92	0.27	9,9,133,160	11
6	NAG	D	2	14/15	0.93	0.14	111,122,135,137	12
6	FUC	D	6	10/11	0.94	0.12	9,9,131,135	11
6	MAN	D	4	11/12	0.94	0.17	93,114,127,142	10
9	NAG	G	1	14/15	0.94	0.13	89,121,136,148	11
8	NAG	F	1	14/15	0.95	0.13	90,107,119,137	12

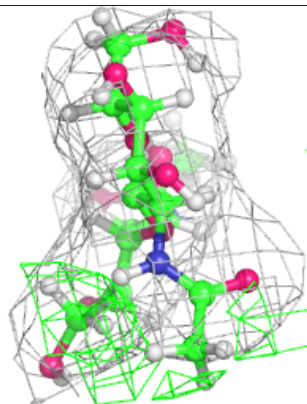
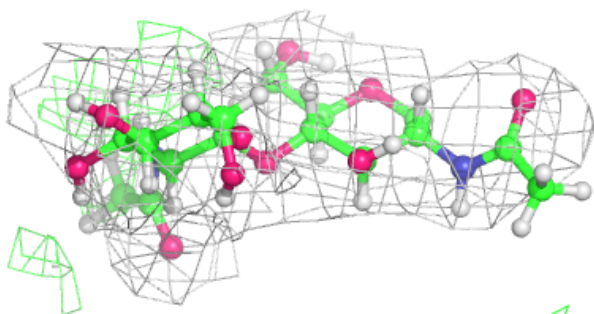
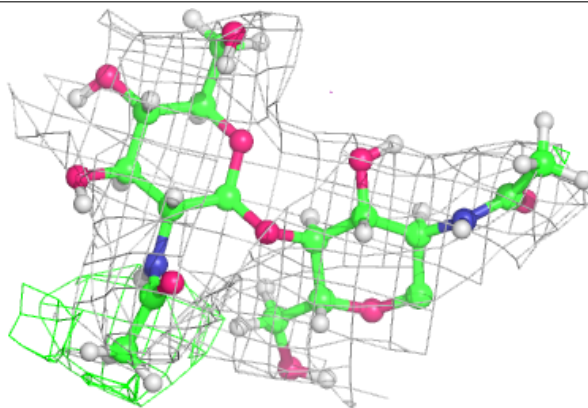
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

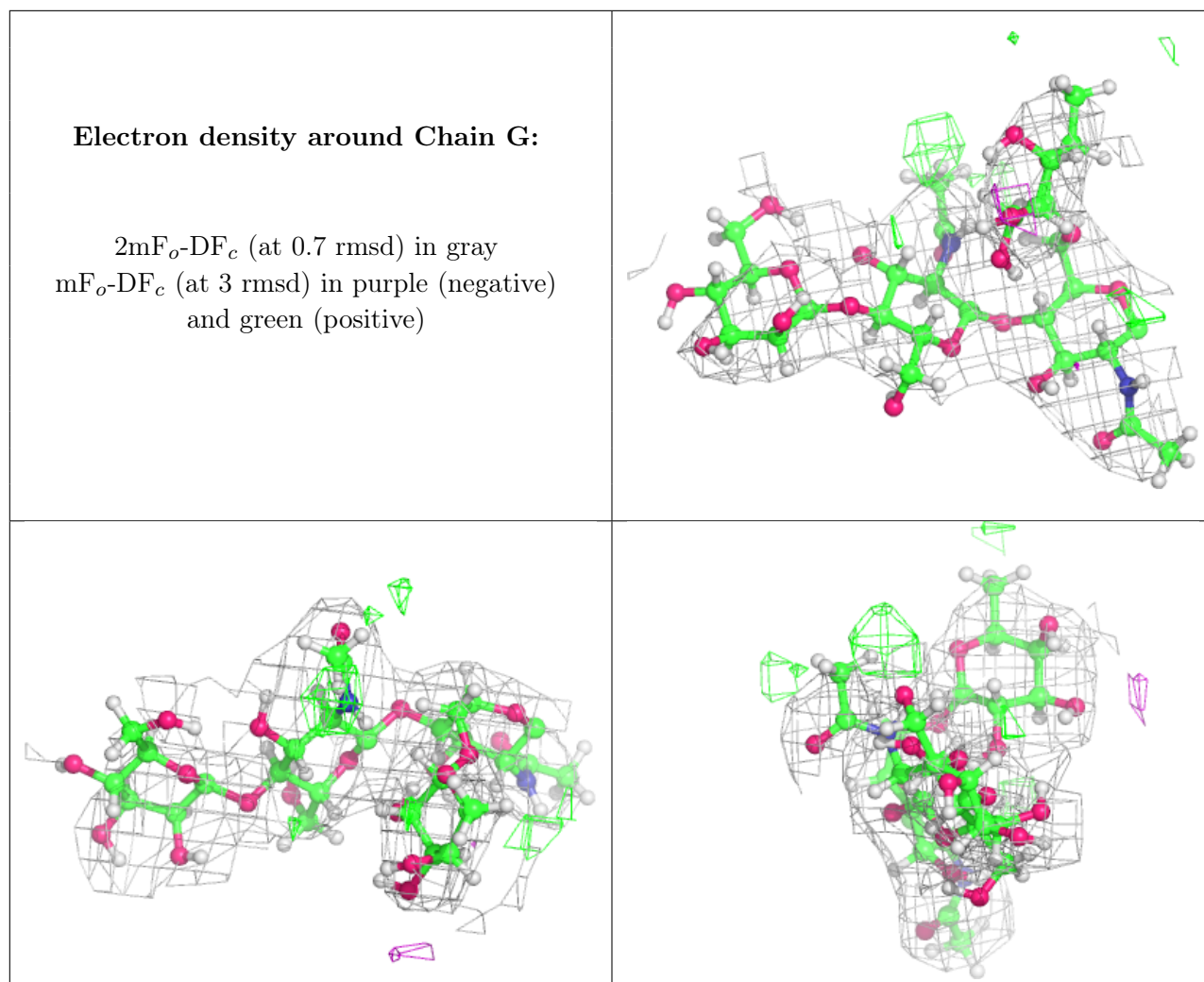
**Electron density around Chain E:**

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

**Electron density around Chain F:**

$2mF_o-DF_c$  (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
10	SO4	B	179	5/5	0.75	0.25	210,213,214,214	0
10	SO4	L	219	5/5	0.77	0.17	142,162,169,174	0
10	SO4	B	177	5/5	0.90	0.15	153,163,171,174	0
10	SO4	L	220	5/5	0.90	0.19	162,163,166,168	0
10	SO4	L	218	5/5	0.91	0.19	147,159,164,175	0
10	SO4	L	215	5/5	0.92	0.18	118,132,139,139	0
10	SO4	L	217	5/5	0.93	0.20	145,153,158,164	0
10	SO4	L	216	5/5	0.93	0.23	150,151,161,164	0
10	SO4	A	1	5/5	0.95	0.14	111,117,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	SO4	B	178	5/5	0.98	0.12	96,113,118,118	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.