



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2025 – 01:07 PM EDT

PDB ID : 9C6Y / pdb\_00009c6y  
Title : Crystal structure of SARS-CoV-2 XBB.1.5 RBD bound to COV2-3906 Fab  
Authors : Buchman, C.D.; Crowe, J.E.  
Deposited on : 2024-06-10  
Resolution : 2.68 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.

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)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

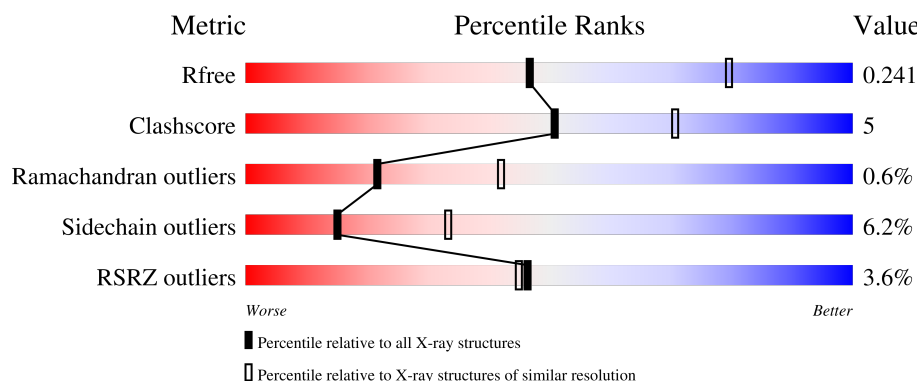
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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))
$R_{free}$	164625	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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	225	<div> <div>4%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	C	225	<div> <div>9%</div> <div>73%</div> <div>20%</div> <div>.</div> <div>.</div> </div>
2	B	216	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	D	216	<div> <div>%</div> <div>80%</div> <div>16%</div> <div>.</div> <div>.</div> </div>
3	E	216	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	216	<div><div></div><div>4%</div><div>81%</div><div>17%</div><div>••</div></div>
4	G	4	<div><div></div><div>50%</div><div>50%</div></div>
5	H	5	<div><div></div><div>40%</div><div>60%</div></div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10096 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 Heavy chain of COV2-3906 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1664	1059	272	329	4			
1	C	219	Total	C	N	O	S	0	0	0
			1600	1018	262	316	4			

- Molecule 2 is a protein called Light chain of COV2-3906 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1597	992	267	333	5			
2	D	213	Total	C	N	O	S	0	0	0
			1589	987	266	331	5			

- Molecule 3 is a protein called Spike protein S2'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1678	1083	280	307	8			
3	F	214	Total	C	N	O	S	0	0	0
			1682	1086	281	307	8			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	339	HIS	GLY	conflict	UNP P0DTC2
E	346	THR	ARG	conflict	UNP P0DTC2
E	365	PHE	TYR	conflict	UNP P0DTC2
E	368	ILE	LEU	conflict	UNP P0DTC2
E	371	PHE	SER	conflict	UNP P0DTC2
E	373	PRO	SER	conflict	UNP P0DTC2
E	375	PHE	SER	conflict	UNP P0DTC2
E	376	ALA	THR	conflict	UNP P0DTC2

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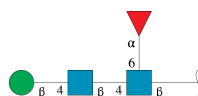
Chain	Residue	Modelled	Actual	Comment	Reference
E	392	TRP	PHE	conflict	UNP P0DTC2
E	395	ILE	VAL	conflict	UNP P0DTC2
E	405	ASN	ASP	conflict	UNP P0DTC2
E	408	SER	ARG	conflict	UNP P0DTC2
E	417	ASN	LYS	conflict	UNP P0DTC2
E	440	LYS	ASN	conflict	UNP P0DTC2
E	445	PRO	VAL	conflict	UNP P0DTC2
E	446	SER	GLY	conflict	UNP P0DTC2
E	460	LYS	ASN	conflict	UNP P0DTC2
E	477	ASN	SER	conflict	UNP P0DTC2
E	478	LYS	THR	conflict	UNP P0DTC2
E	484	ALA	GLU	conflict	UNP P0DTC2
E	486	PRO	PHE	conflict	UNP P0DTC2
E	490	SER	PHE	conflict	UNP P0DTC2
E	498	ARG	GLN	conflict	UNP P0DTC2
E	501	TYR	ASN	conflict	UNP P0DTC2
E	505	HIS	TYR	conflict	UNP P0DTC2
E	529	LEU	LYS	conflict	UNP P0DTC2
E	530	GLU	SER	conflict	UNP P0DTC2
E	531	VAL	THR	conflict	UNP P0DTC2
E	532	LEU	ASN	conflict	UNP P0DTC2
E	533	PHE	LEU	conflict	UNP P0DTC2
E	534	GLN	VAL	conflict	UNP P0DTC2
F	339	HIS	GLY	conflict	UNP P0DTC2
F	346	THR	ARG	conflict	UNP P0DTC2
F	365	PHE	TYR	conflict	UNP P0DTC2
F	368	ILE	LEU	conflict	UNP P0DTC2
F	371	PHE	SER	conflict	UNP P0DTC2
F	373	PRO	SER	conflict	UNP P0DTC2
F	375	PHE	SER	conflict	UNP P0DTC2
F	376	ALA	THR	conflict	UNP P0DTC2
F	392	TRP	PHE	conflict	UNP P0DTC2
F	395	ILE	VAL	conflict	UNP P0DTC2
F	405	ASN	ASP	conflict	UNP P0DTC2
F	408	SER	ARG	conflict	UNP P0DTC2
F	417	ASN	LYS	conflict	UNP P0DTC2
F	440	LYS	ASN	conflict	UNP P0DTC2
F	445	PRO	VAL	conflict	UNP P0DTC2
F	446	SER	GLY	conflict	UNP P0DTC2
F	460	LYS	ASN	conflict	UNP P0DTC2
F	477	ASN	SER	conflict	UNP P0DTC2
F	478	LYS	THR	conflict	UNP P0DTC2

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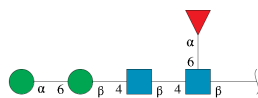
Chain	Residue	Modelled	Actual	Comment	Reference
F	484	ALA	GLU	conflict	UNP P0DTC2
F	486	PRO	PHE	conflict	UNP P0DTC2
F	490	SER	PHE	conflict	UNP P0DTC2
F	498	ARG	GLN	conflict	UNP P0DTC2
F	501	TYR	ASN	conflict	UNP P0DTC2
F	505	HIS	TYR	conflict	UNP P0DTC2
F	529	LEU	LYS	conflict	UNP P0DTC2
F	530	GLU	SER	conflict	UNP P0DTC2
F	531	VAL	THR	conflict	UNP P0DTC2
F	532	LEU	ASN	conflict	UNP P0DTC2
F	533	PHE	LEU	conflict	UNP P0DTC2
F	534	GLN	VAL	conflict	UNP P0DTC2

- Molecule 4 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
4	G	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

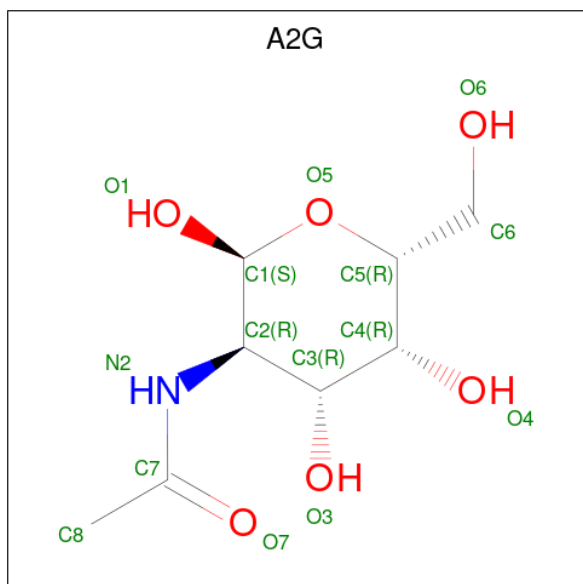
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 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
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula:  $C_8H_{15}NO_6$ ).



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

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

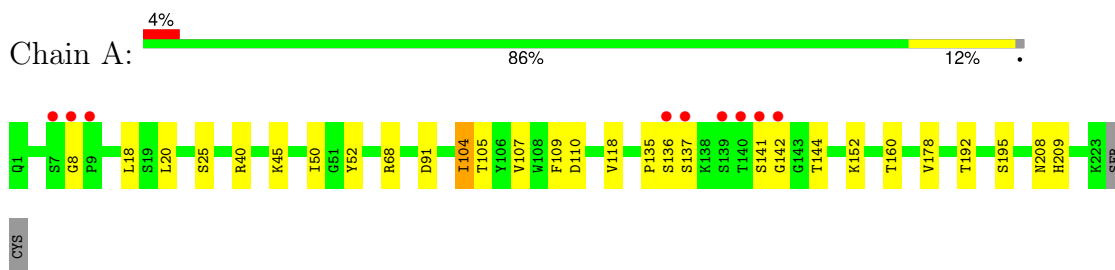
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	28	Total	O	0	0
			28	28		
10	B	26	Total	O	0	0
			26	26		
10	C	6	Total	O	0	0
			6	6		
10	D	12	Total	O	0	0
			12	12		
10	E	15	Total	O	0	0
			15	15		
10	F	7	Total	O	0	0
			7	7		

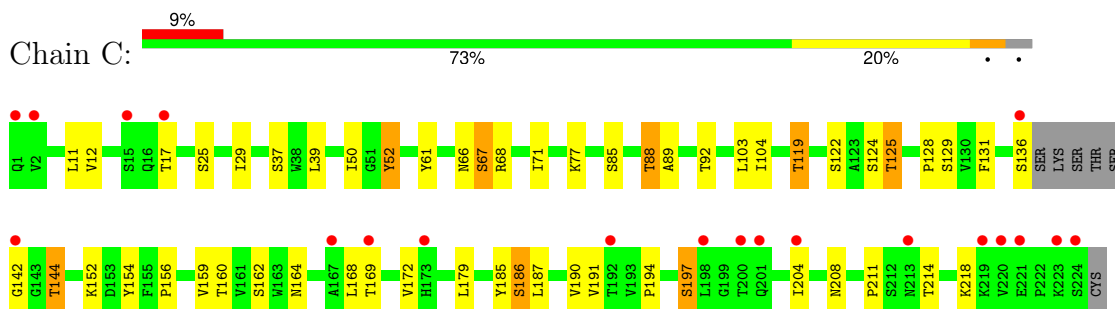
### 3 Residue-property plots [i](#)

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.

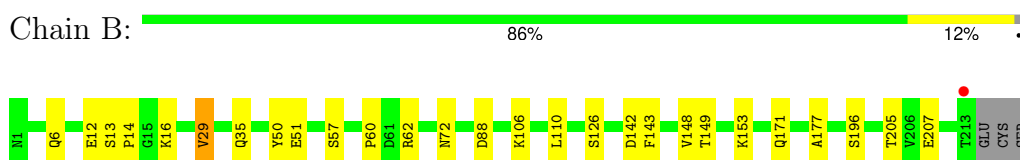
- Molecule 1: Heavy chain of COV2-3906 Fab



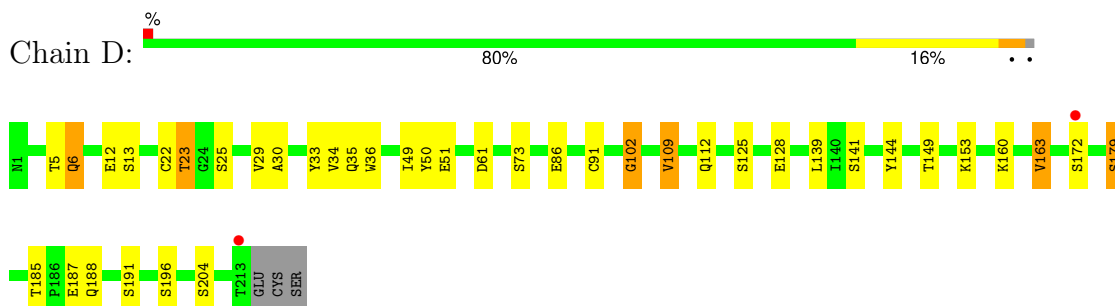
- Molecule 1: Heavy chain of COV2-3906 Fab



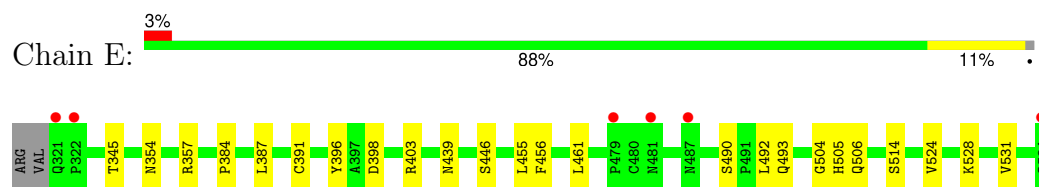
- Molecule 2: Light chain of COV2-3906 Fab



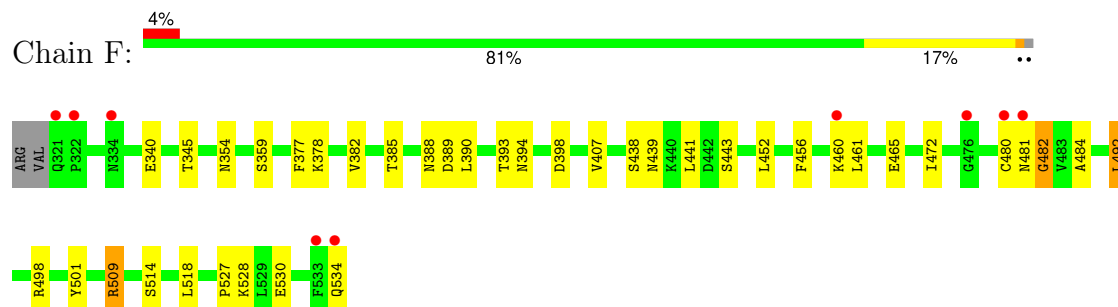
- Molecule 2: Light chain of COV2-3906 Fab



- Molecule 3: Spike protein S2'



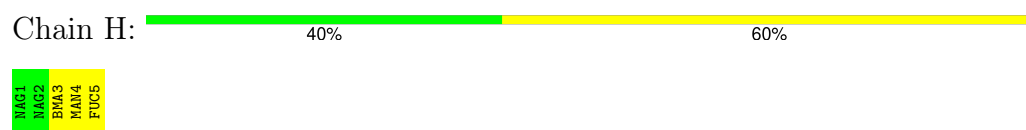
- Molecule 3: Spike protein S2'



- Molecule 4: 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



- Molecule 5: 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.97Å 170.85Å 231.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 2.68 48.50 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.50-2.68) 99.9 (48.50-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.207 , 0.242 0.210 , 0.241	Depositor DCC
$R_{free}$ test set	2000 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.3	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, A2G, SO4, NAG, CL, FUC

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	0.48	0/1708	0.67	0/2340
1	C	0.35	0/1643	0.56	0/2257
2	B	0.47	0/1637	0.65	0/2238
2	D	0.41	0/1629	0.62	1/2229 (0.0%)
3	E	0.37	0/1731	0.55	0/2367
3	F	0.36	0/1735	0.56	0/2371
All	All	0.41	0/10083	0.60	1/13802 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	102	GLY	N-CA-C	-5.07	106.75	112.33

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1664	0	1633	10	0
1	C	1600	0	1512	25	0
2	B	1597	0	1520	12	0
2	D	1589	0	1505	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1678	0	1571	13	0
3	F	1682	0	1582	23	0
4	G	49	0	43	1	0
5	H	60	0	52	0	0
6	B	10	0	0	0	0
6	E	10	0	0	0	0
6	F	5	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	E	14	0	13	0	0
8	F	14	0	13	0	0
9	E	14	0	12	0	0
9	F	14	0	12	0	0
10	A	28	0	0	0	0
10	B	26	0	0	0	0
10	C	6	0	0	0	0
10	D	12	0	0	0	0
10	E	15	0	0	0	0
10	F	7	0	0	0	0
All	All	10096	0	9468	99	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 5.

The worst 5 of 99 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:B:142:ASP:H	2:B:171:GLN:HE22	1.19	0.89
2:D:6:GLN:HE21	2:D:102:GLY:HA3	1.48	0.76
1:C:172:VAL:HG12	1:C:191:VAL:HG22	1.69	0.75
3:E:439:ASN:ND2	3:E:506:GLN:OE1	2.22	0.72
1:C:128:PRO:HB3	1:C:154:TYR:HB3	1.73	0.71

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	221/225 (98%)	209 (95%)	9 (4%)	3 (1%)	9	21
1	C	215/225 (96%)	202 (94%)	10 (5%)	3 (1%)	9	21
2	B	211/216 (98%)	206 (98%)	5 (2%)	0	100	100
2	D	211/216 (98%)	200 (95%)	11 (5%)	0	100	100
3	E	212/216 (98%)	197 (93%)	15 (7%)	0	100	100
3	F	212/216 (98%)	198 (93%)	12 (6%)	2 (1%)	14	32
All	All	1282/1314 (98%)	1212 (94%)	62 (5%)	8 (1%)	22	42

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ILE
1	A	141	SER
3	F	481	ASN
1	C	104	ILE
1	A	135	PRO

### 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	191/196 (97%)	180 (94%)	11 (6%)	17	36
1	C	175/196 (89%)	156 (89%)	19 (11%)	5	11
2	B	183/187 (98%)	176 (96%)	7 (4%)	28	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	181/187 (97%)	165 (91%)	16 (9%)	8	18
3	E	179/189 (95%)	175 (98%)	4 (2%)	47	73
3	F	180/189 (95%)	170 (94%)	10 (6%)	17	37
All	All	1089/1144 (95%)	1022 (94%)	67 (6%)	15	33

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	345	THR
3	F	393	THR
3	F	514	SER
1	C	103	LEU
1	C	88	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	487	ASN
3	F	417	ASN
1	C	3	GLN
1	C	5	GLN
1	C	164	ASN

### 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 ⓘ

9 monosaccharides are modelled in this entry.

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



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	G	1	4,3	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
4	NAG	G	2	4	14,14,15	0.79	1 (7%)	17,19,21	0.99	1 (5%)
4	BMA	G	3	4	11,11,12	2.55	6 (54%)	15,15,17	1.80	4 (26%)
4	FUC	G	4	4	10,10,11	1.76	3 (30%)	14,14,16	0.98	1 (7%)
5	NAG	H	1	5,3	14,14,15	0.65	0	17,19,21	0.58	0
5	NAG	H	2	5	14,14,15	0.51	0	17,19,21	0.74	0
5	BMA	H	3	5	11,11,12	1.96	5 (45%)	15,15,17	1.05	1 (6%)
5	MAN	H	4	5	11,11,12	2.06	2 (18%)	15,15,17	1.19	1 (6%)
5	FUC	H	5	5	10,10,11	1.36	2 (20%)	14,14,16	0.89	0

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

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

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	4	MAN	C2-C3	5.19	1.60	1.52
4	G	3	BMA	O5-C1	4.31	1.50	1.43
4	G	3	BMA	C2-C3	3.85	1.58	1.52
4	G	3	BMA	O5-C5	3.74	1.50	1.43
5	H	3	BMA	O5-C5	3.49	1.50	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	BMA	C1-O5-C5	4.90	118.76	112.19
4	G	2	NAG	C1-O5-C5	3.45	116.81	112.19
5	H	4	MAN	C1-C2-C3	2.94	113.92	109.64
5	H	3	BMA	O5-C5-C6	2.64	112.80	107.66
4	G	1	NAG	C1-O5-C5	2.61	115.68	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

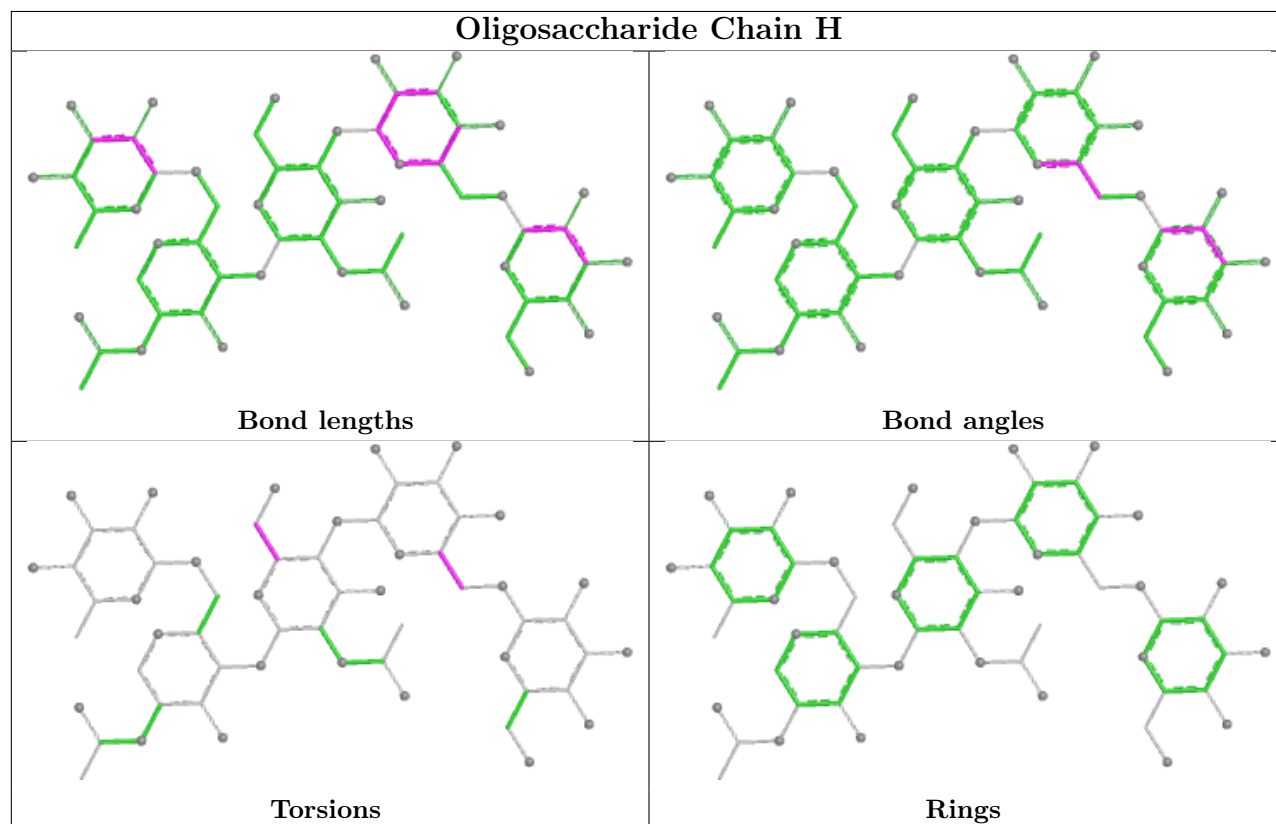
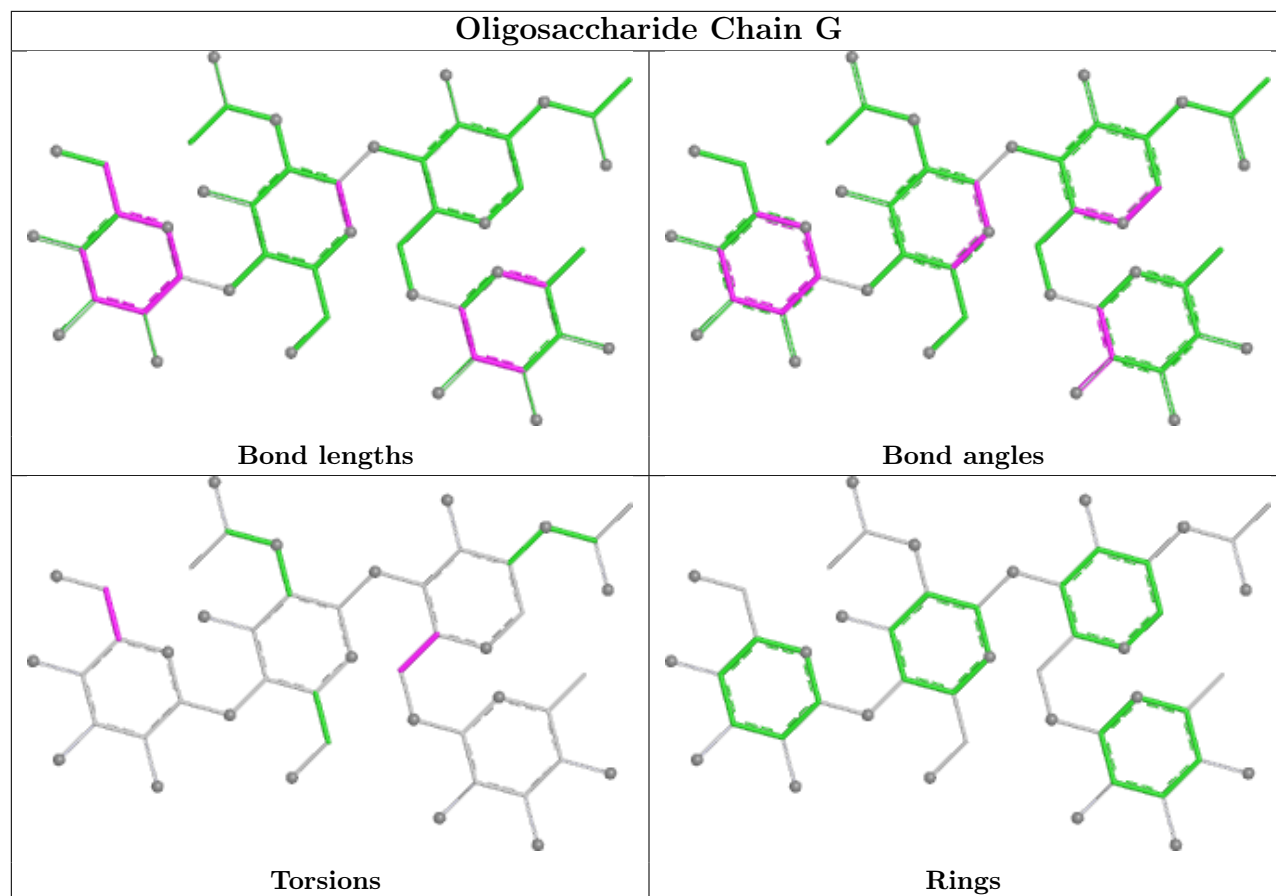
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	1	0
4	G	1	NAG	1	0

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



## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
6	SO4	E	603	-	4,4,4	0.35	0	6,6,6	0.13	0
6	SO4	B	302	-	4,4,4	0.35	0	6,6,6	0.23	0
6	SO4	B	301	-	4,4,4	0.37	0	6,6,6	0.19	0
8	NAG	F	601	3	14,14,15	0.72	0	17,19,21	0.69	0
6	SO4	E	604	-	4,4,4	0.28	0	6,6,6	0.13	0
8	NAG	E	601	3	14,14,15	0.71	1 (7%)	17,19,21	2.09	3 (17%)
9	A2G	F	602	3	14,14,15	1.38	1 (7%)	17,19,21	1.77	3 (17%)
9	A2G	E	602	3	14,14,15	1.60	2 (14%)	17,19,21	1.93	4 (23%)
6	SO4	F	603	-	4,4,4	0.29	0	6,6,6	0.16	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
8	NAG	F	601	3	-	2/6/23/26	0/1/1/1
9	A2G	F	602	3	-	3/6/23/26	0/1/1/1
8	NAG	E	601	3	-	2/6/23/26	0/1/1/1
9	A2G	E	602	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	602	A2G	C7-N2	3.89	1.46	1.34
9	E	602	A2G	C7-N2	3.81	1.46	1.34
8	E	601	NAG	O5-C1	2.15	1.47	1.43
9	E	602	A2G	C1-C2	2.13	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	601	NAG	C1-O5-C5	7.58	122.34	112.19
9	F	602	A2G	C4-C3-C2	-5.35	103.18	111.02
9	E	602	A2G	C4-C3-C2	-4.72	104.10	111.02
8	E	601	NAG	C3-C4-C5	3.12	115.89	110.23
9	E	602	A2G	O3-C3-C2	3.07	115.77	109.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	601	NAG	O5-C5-C6-O6
8	F	601	NAG	C4-C5-C6-O6
9	F	602	A2G	C4-C5-C6-O6
9	F	602	A2G	O5-C5-C6-O6
9	E	602	A2G	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	223/225 (99%)	-0.26	9 (4%) 43 41	42, 52, 81, 117	0
1	C	219/225 (97%)	0.29	20 (9%) 16 15	56, 79, 122, 140	0
2	B	213/216 (98%)	-0.35	1 (0%) 87 86	44, 55, 73, 86	0
2	D	213/216 (98%)	-0.19	2 (0%) 81 80	47, 69, 89, 99	0
3	E	214/216 (99%)	-0.06	6 (2%) 55 53	48, 66, 107, 128	0
3	F	214/216 (99%)	-0.04	9 (4%) 41 39	56, 68, 96, 113	0
All	All	1296/1314 (98%)	-0.10	47 (3%) 46 45	42, 65, 103, 140	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	224	SER	5.4
1	A	136	SER	5.3
3	E	481	ASN	5.2
1	A	139	SER	4.7
3	F	481	ASN	4.6

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

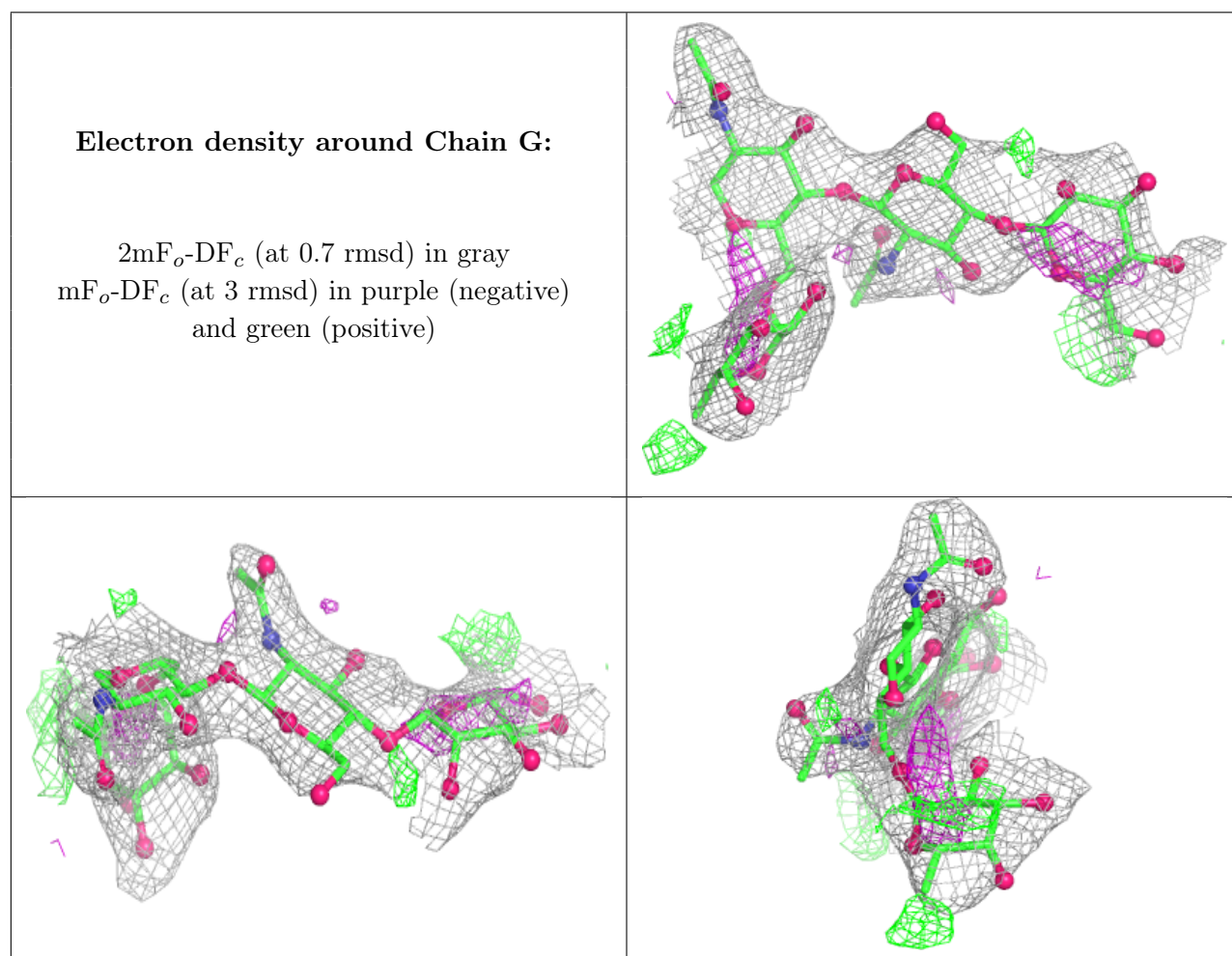
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

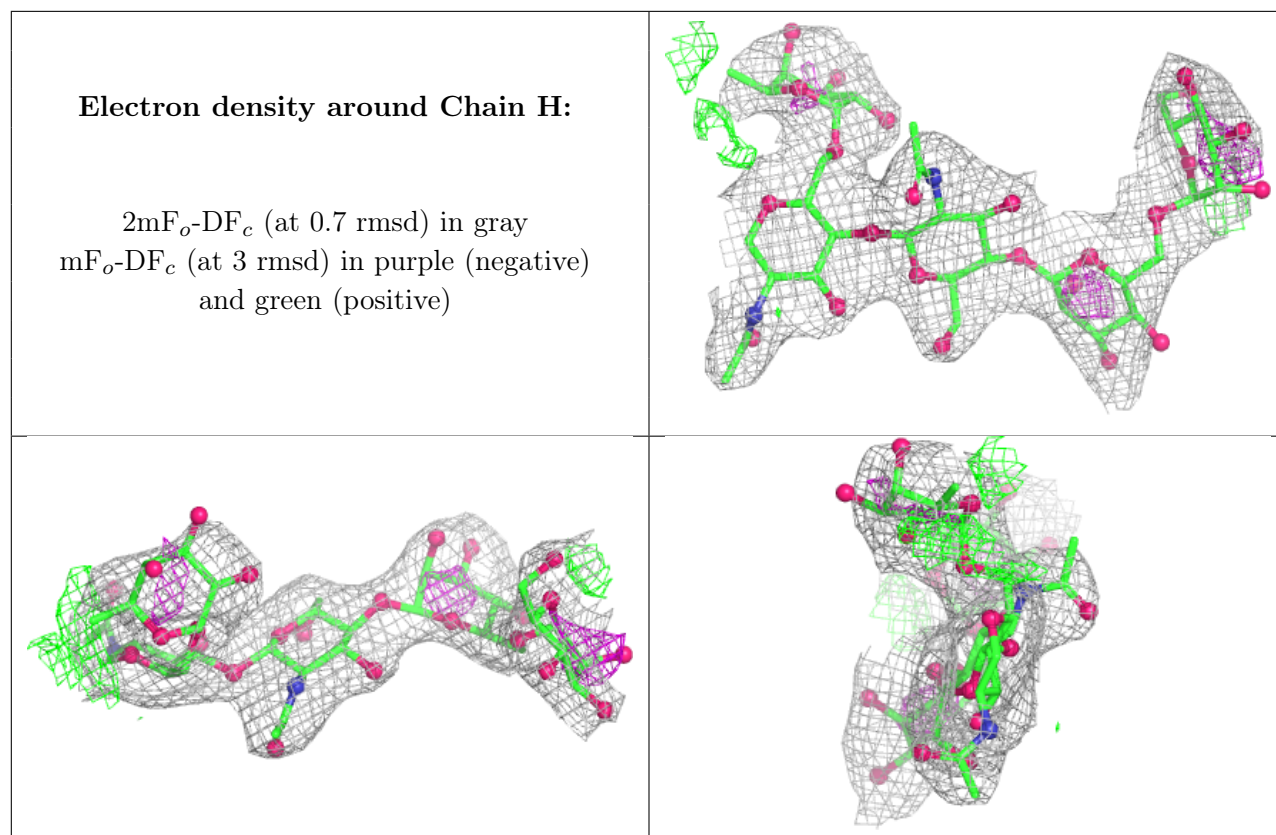
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FUC	G	4	10/11	0.37	0.21	104,107,112,114	0
4	BMA	G	3	11/12	0.39	0.23	104,110,113,114	0
5	MAN	H	4	11/12	0.54	0.17	100,106,108,112	0
5	FUC	H	5	10/11	0.55	0.20	99,104,108,109	0
5	BMA	H	3	11/12	0.73	0.14	98,101,106,111	0
4	NAG	G	1	14/15	0.78	0.13	71,91,99,105	0
4	NAG	G	2	14/15	0.79	0.15	91,100,109,109	0
5	NAG	H	1	14/15	0.85	0.12	71,83,91,93	0
5	NAG	H	2	14/15	0.93	0.10	79,89,93,98	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.







## 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( $\text{\AA}^2$ )	Q<0.9
8	NAG	E	601	14/15	0.42	0.20	89,97,102,102	0
8	NAG	F	601	14/15	0.64	0.19	89,97,101,103	0
9	A2G	E	602	14/15	0.73	0.18	70,74,78,79	0
9	A2G	F	602	14/15	0.80	0.16	64,73,75,78	0
6	SO4	B	302	5/5	0.88	0.22	87,94,96,104	0
6	SO4	B	301	5/5	0.92	0.20	82,83,94,98	0
6	SO4	F	603	5/5	0.97	0.08	76,78,85,87	0
7	CL	B	303	1/1	0.97	0.10	70,70,70,70	0
6	SO4	E	603	5/5	0.97	0.11	81,81,84,90	0
6	SO4	E	604	5/5	0.98	0.06	68,69,73,73	0
7	CL	D	301	1/1	0.98	0.11	58,58,58,58	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.