



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 03:22 PM EST

PDB ID : 6MFP  
Title : Crystal Structure of the RV305 C1-C2 specific ADCC potent antibody  
DH677.3 Fab in complex with HIV-1 clade A/E gp120 and M48U1  
Authors : Tolbert, W.D.; Young, B.; Pazgier, M.  
Deposited on : 2018-09-11  
Resolution : 3.00 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

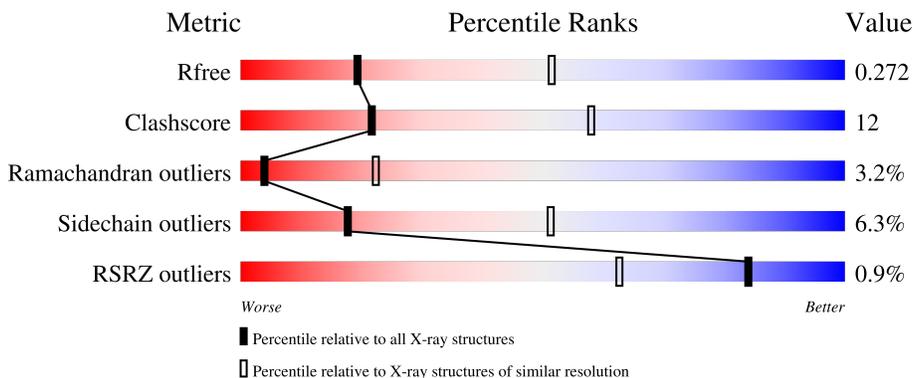
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	355	
1	G	355	
2	M	28	
2	N	28	
3	C	228	

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Mol	Chain	Length	Quality of chain
3	H	228	 66% 29% . .
4	D	214	 % 67% 29% .
4	L	214	 75% 23% .
5	B	3	 33% 67%

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	FUC	B	3	-	-	X	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12704 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 clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	341	2669	1675	463	509	22	0	0	0
1	A	341	2669	1675	463	509	22	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	42	VAL	-	see sequence details	UNP A0A0M3KKW9
G	43	PRO	-	see sequence details	UNP A0A0M3KKW9
G	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
A	42	VAL	-	see sequence details	UNP A0A0M3KKW9
A	43	PRO	-	see sequence details	UNP A0A0M3KKW9
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9

- Molecule 2 is a protein called M48U1 CD4 MIMETIC PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	N	28	209	133	38	32	6	0	0	1
2	M	28	209	133	38	32	6	0	0	1

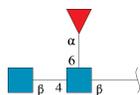
- Molecule 3 is a protein called DH677.3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	220	1665	1055	281	322	7	0	0	0
3	C	219	1661	1053	280	321	7	0	0	0

- Molecule 4 is a protein called DH677.3 Fab light chain.

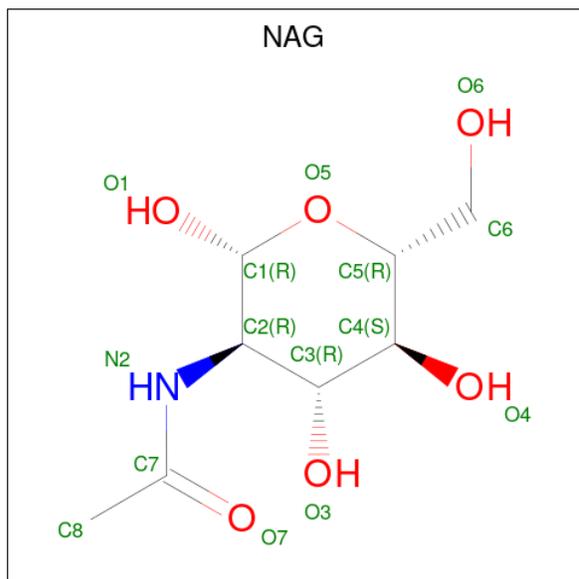
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	213	Total 1630	C 1020	N 273	O 333	S 4	0	0	0
4	D	213	Total 1630	C 1020	N 273	O 333	S 4	0	0	0

- Molecule 5 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
			Total	C	N	O			
5	B	3	Total 38	C 22	N 2	O 14	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	G	1	Total 14	C 8	N 1	O 5	0	0
6	G	1	Total 14	C 8	N 1	O 5	0	0
6	G	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

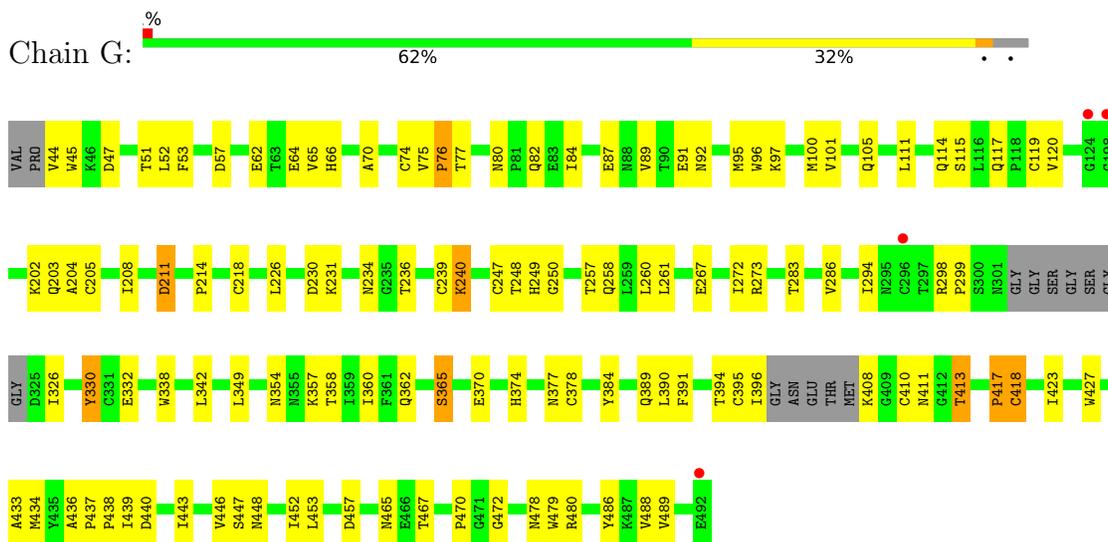
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	A	1	Total 1	Cl 1	0	0
7	D	1	Total 1	Cl 1	0	0

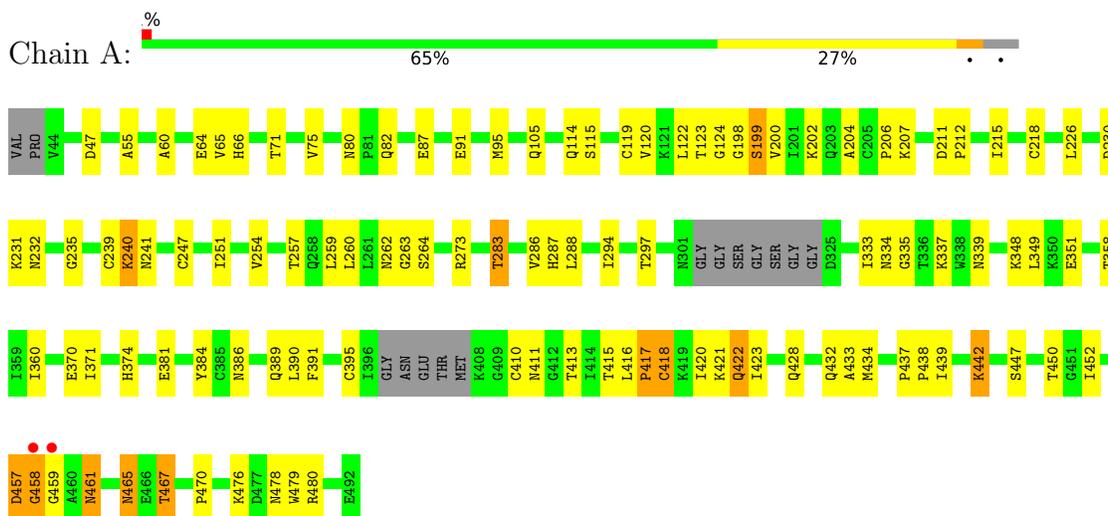
### 3 Residue-property plots [i](#)

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

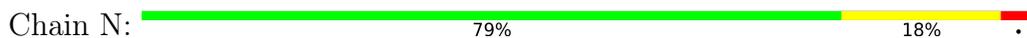
- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core



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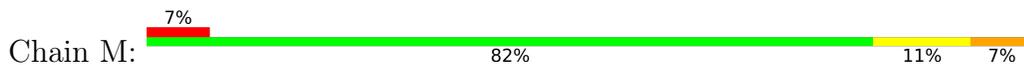


- Molecule 2: M48U1 CD4 MIMETIC PEPTIDE





- Molecule 2: M48U1 CD4 MIMETIC PEPTIDE



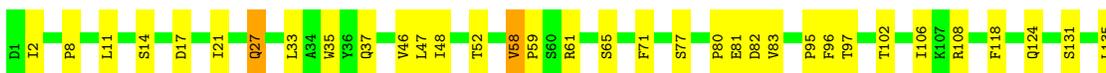
- Molecule 3: DH677.3 Fab heavy chain



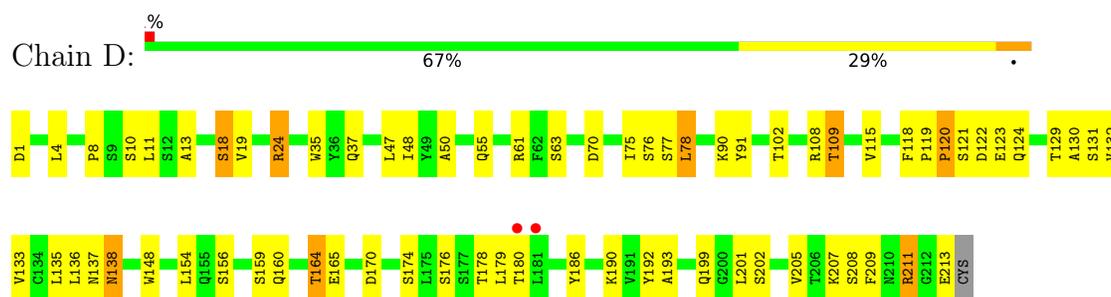
- Molecule 3: DH677.3 Fab heavy chain



- Molecule 4: DH677.3 Fab light chain



- Molecule 4: DH677.3 Fab light chain



- Molecule 5: 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 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.49Å 80.09Å 88.69Å 84.82° 82.33° 82.24°	Depositor
Resolution (Å)	39.60 – 3.00 39.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.9 (39.60-3.00) 89.0 (39.57-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.214 , 0.274 0.212 , 0.272	Depositor DCC
$R_{free}$ test set	1492 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.7	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: DPR, CL, NAG, U2X, FUC, MPT, NH2

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	0.63	0/2724	0.80	0/3697
1	G	0.64	0/2724	0.80	0/3697
2	M	0.69	0/176	0.80	0/231
2	N	0.69	0/176	0.75	0/231
3	C	0.66	0/1701	0.86	2/2319 (0.1%)
3	H	0.64	0/1705	0.80	0/2324
4	D	0.67	0/1665	0.80	0/2264
4	L	0.64	0/1665	0.79	0/2264
All	All	0.65	0/12536	0.81	2/17027 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1
2	N	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	147	PRO	N-CA-CB	-8.79	92.75	103.30
3	C	149	PRO	N-CA-CB	-5.66	96.38	102.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	23	U2X	Mainchain
2	N	23	U2X	Mainchain

## 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	2669	0	2605	62	0
1	G	2669	0	2605	68	0
2	M	209	0	212	1	0
2	N	209	0	212	5	0
3	C	1661	0	1631	56	0
3	H	1665	0	1635	42	0
4	D	1630	0	1578	44	0
4	L	1630	0	1578	33	0
5	B	38	0	34	9	0
6	A	154	0	143	1	0
6	G	154	0	143	2	0
6	H	14	0	13	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
All	All	12704	0	12389	298	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 12.

The worst 5 of 298 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)
3:C:146:PHE:CG	3:C:147:PRO:HD2	1.55	1.39
3:C:146:PHE:CD2	3:C:147:PRO:HD2	1.89	1.05
3:C:146:PHE:CG	3:C:147:PRO:CD	2.43	1.00
1:A:198:GLY:O	1:A:199:SER:HB2	1.59	0.99
1:A:207:LYS:HG3	1:A:439:ILE:HD11	1.64	0.80

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	335/355 (94%)	277 (83%)	41 (12%)	17 (5%)	2	12
1	G	335/355 (94%)	279 (83%)	43 (13%)	13 (4%)	3	17
2	M	24/28 (86%)	20 (83%)	2 (8%)	2 (8%)	1	4
2	N	24/28 (86%)	20 (83%)	2 (8%)	2 (8%)	1	4
3	C	215/228 (94%)	187 (87%)	21 (10%)	7 (3%)	4	21
3	H	216/228 (95%)	190 (88%)	21 (10%)	5 (2%)	6	30
4	D	211/214 (99%)	191 (90%)	17 (8%)	3 (1%)	11	43
4	L	211/214 (99%)	192 (91%)	17 (8%)	2 (1%)	17	55
All	All	1571/1650 (95%)	1356 (86%)	164 (10%)	51 (3%)	4	22

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	76	PRO
1	G	87	GLU
1	G	354	ASN
1	G	395	CYS
1	G	417	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	305/313 (97%)	294 (96%)	11 (4%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	305/313 (97%)	283 (93%)	22 (7%)	14	45
2	M	20/20 (100%)	19 (95%)	1 (5%)	24	60
2	N	20/20 (100%)	20 (100%)	0	100	100
3	C	183/191 (96%)	166 (91%)	17 (9%)	9	33
3	H	183/191 (96%)	170 (93%)	13 (7%)	14	46
4	D	185/186 (100%)	170 (92%)	15 (8%)	11	40
4	L	185/186 (100%)	176 (95%)	9 (5%)	25	61
All	All	1386/1420 (98%)	1298 (94%)	88 (6%)	18	51

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	48	MET
3	C	186	SER
3	C	69	LEU
3	C	115	SER
4	D	10	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	GLN
3	C	39	GLN
4	D	137	ASN
4	D	38	GLN
1	A	66	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	U2X	M	23	2	19,20,21	1.33	1 (5%)	22,25,27	1.09	2 (9%)
2	U2X	N	23	2	19,20,21	1.10	1 (5%)	22,25,27	1.04	1 (4%)

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
2	U2X	M	23	2	-	4/10/19/21	0/2/2/2
2	U2X	N	23	2	-	4/10/19/21	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	23	U2X	OH-CZ	3.69	1.46	1.37
2	N	23	U2X	OH-CZ	3.22	1.45	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	23	U2X	C7-OH-CZ	-3.39	110.74	117.93
2	M	23	U2X	C1-C2-C3	2.63	117.12	112.15
2	M	23	U2X	C4-C3-C2	2.41	115.23	109.33

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	23	U2X	CE1-CZ-OH-C7
2	N	23	U2X	CE2-CZ-OH-C7
2	M	23	U2X	CE1-CZ-OH-C7
2	M	23	U2X	CE2-CZ-OH-C7
2	M	23	U2X	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	23	U2X	1	0

## 5.5 Carbohydrates [i](#)

3 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	1	5,3	14,14,15	0.51	0	17,19,21	3.11	4 (23%)
5	NAG	B	2	5	14,14,15	0.65	1 (7%)	17,19,21	0.51	0
5	FUC	B	3	5	10,10,11	0.60	0	14,14,16	2.44	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1	5,3	-	1/6/23/26	0/1/1/1
5	NAG	B	2	5	-	0/6/23/26	0/1/1/1
5	FUC	B	3	5	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2	NAG	O5-C1	-2.34	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	NAG	C1-O5-C5	9.82	125.49	112.19
5	B	3	FUC	C1-C2-C3	5.27	116.15	109.67
5	B	3	FUC	O5-C1-C2	5.10	118.65	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	NAG	C3-C4-C5	4.23	117.79	110.24
5	B	1	NAG	C6-C5-C4	-4.21	103.14	113.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

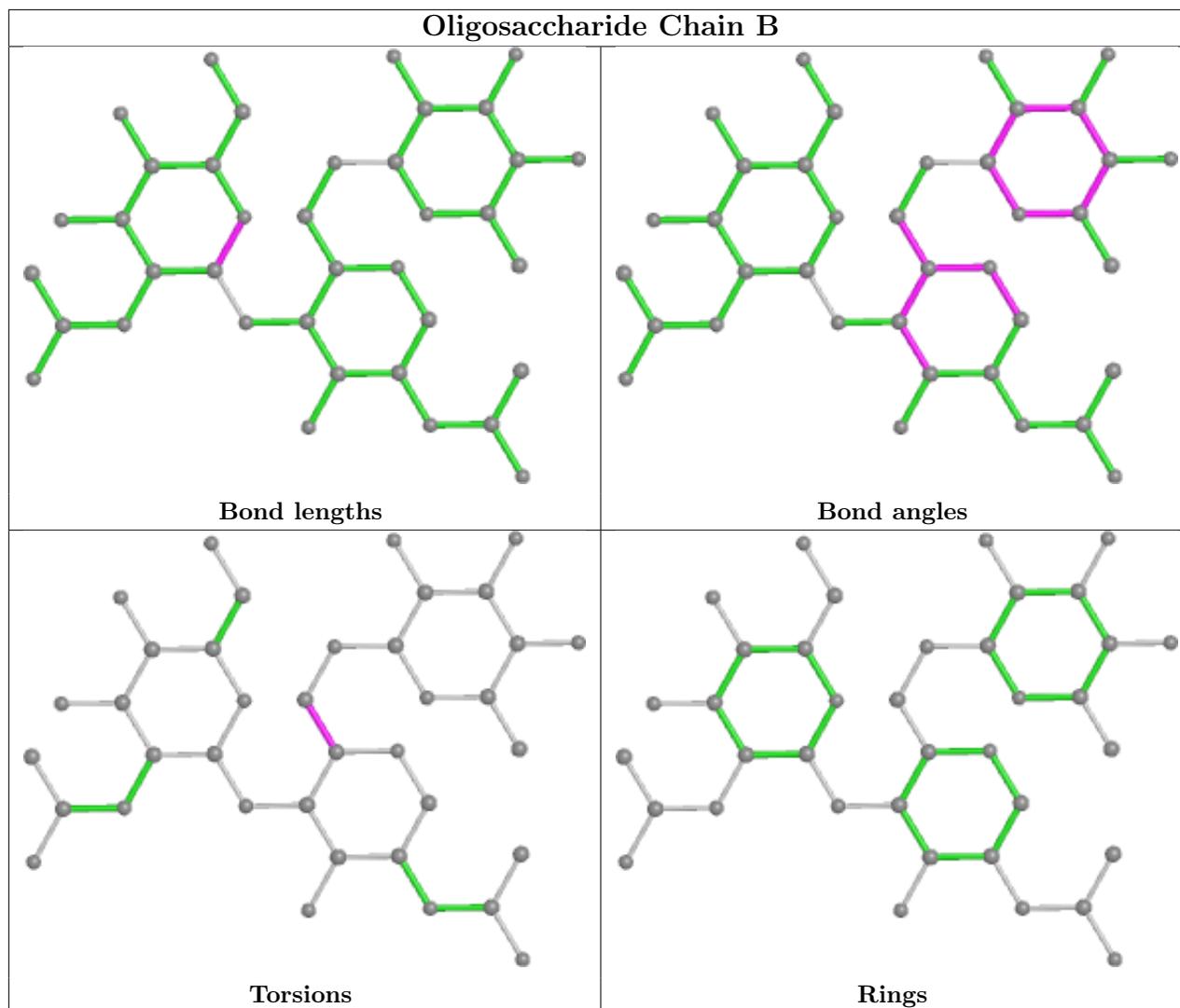
Mol	Chain	Res	Type	Atoms
5	B	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3	FUC	9	0
5	B	1	NAG	6	0

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



## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	NAG	G	502	1	14,14,15	0.35	0	17,19,21	1.79	2 (11%)
6	NAG	G	508	1	14,14,15	0.31	0	17,19,21	1.11	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	504	1	14,14,15	0.32	0	17,19,21	1.76	3 (17%)
6	NAG	A	505	1	14,14,15	0.37	0	17,19,21	1.17	2 (11%)
6	NAG	A	502	1	14,14,15	0.31	0	17,19,21	0.93	1 (5%)
6	NAG	G	506	1	14,14,15	0.38	0	17,19,21	0.88	0
6	NAG	A	511	1	14,14,15	0.35	0	17,19,21	0.87	1 (5%)
6	NAG	A	503	1	14,14,15	0.36	0	17,19,21	1.90	1 (5%)
6	NAG	G	503	1	14,14,15	0.41	0	17,19,21	0.87	1 (5%)
6	NAG	G	507	1	14,14,15	0.28	0	17,19,21	0.80	1 (5%)
6	NAG	G	501	1	14,14,15	0.26	0	17,19,21	0.55	0
6	NAG	A	509	1	14,14,15	0.40	0	17,19,21	1.25	3 (17%)
6	NAG	G	510	1	14,14,15	0.38	0	17,19,21	0.65	0
6	NAG	A	507	1	14,14,15	0.33	0	17,19,21	0.97	1 (5%)
6	NAG	A	501	1	14,14,15	0.22	0	17,19,21	0.80	0
6	NAG	G	505	1	14,14,15	0.33	0	17,19,21	1.83	5 (29%)
6	NAG	G	509	1	14,14,15	0.45	0	17,19,21	0.56	0
6	NAG	A	508	1	14,14,15	0.39	0	17,19,21	0.58	0
6	NAG	H	500	3	14,14,15	0.47	0	17,19,21	1.01	2 (11%)
6	NAG	A	506	1	14,14,15	0.34	0	17,19,21	1.73	2 (11%)
6	NAG	G	504	1	14,14,15	0.38	0	17,19,21	1.22	1 (5%)
6	NAG	A	510	1	14,14,15	0.44	0	17,19,21	0.60	0
6	NAG	G	511	1	14,14,15	0.72	1 (7%)	17,19,21	1.67	2 (11%)

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	NAG	G	502	1	-	2/6/23/26	0/1/1/1
6	NAG	G	508	1	-	2/6/23/26	0/1/1/1
6	NAG	A	504	1	-	1/6/23/26	0/1/1/1
6	NAG	A	505	1	-	2/6/23/26	0/1/1/1
6	NAG	A	502	1	-	1/6/23/26	0/1/1/1
6	NAG	G	506	1	-	0/6/23/26	0/1/1/1
6	NAG	A	511	1	-	2/6/23/26	0/1/1/1
6	NAG	A	503	1	-	2/6/23/26	0/1/1/1
6	NAG	G	503	1	-	0/6/23/26	0/1/1/1
6	NAG	G	507	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	501	1	-	0/6/23/26	0/1/1/1
6	NAG	A	509	1	-	0/6/23/26	0/1/1/1
6	NAG	G	510	1	-	2/6/23/26	0/1/1/1
6	NAG	A	507	1	-	0/6/23/26	0/1/1/1
6	NAG	A	501	1	-	2/6/23/26	0/1/1/1
6	NAG	G	505	1	-	5/6/23/26	0/1/1/1
6	NAG	G	509	1	-	2/6/23/26	0/1/1/1
6	NAG	A	508	1	-	0/6/23/26	0/1/1/1
6	NAG	H	500	3	-	2/6/23/26	0/1/1/1
6	NAG	A	506	1	-	5/6/23/26	0/1/1/1
6	NAG	G	504	1	-	0/6/23/26	0/1/1/1
6	NAG	A	510	1	-	2/6/23/26	0/1/1/1
6	NAG	G	511	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	511	NAG	C1-C2	2.39	1.55	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	503	NAG	C1-O5-C5	6.57	121.09	112.19
6	G	502	NAG	C1-O5-C5	6.40	120.87	112.19
6	A	504	NAG	C1-O5-C5	5.30	119.38	112.19
6	G	511	NAG	O5-C1-C2	4.75	118.78	111.29
6	A	506	NAG	C2-N2-C7	4.43	129.20	122.90

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	505	NAG	O5-C5-C6-O6
6	A	503	NAG	O5-C5-C6-O6
6	A	510	NAG	O5-C5-C6-O6
6	A	511	NAG	O5-C5-C6-O6
6	A	511	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	503	NAG	1	0
6	A	507	NAG	1	0
6	G	509	NAG	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	341/355 (96%)	-0.42	2 (0%) 89 72	56, 95, 156, 184	0
1	G	341/355 (96%)	-0.41	4 (1%) 79 54	58, 100, 151, 183	0
2	M	24/28 (85%)	-0.02	2 (8%) 11 3	93, 122, 137, 147	0
2	N	24/28 (85%)	-0.47	0 100 100	95, 115, 134, 159	0
3	C	219/228 (96%)	-0.26	4 (1%) 68 40	56, 97, 168, 189	0
3	H	220/228 (96%)	-0.23	0 100 100	76, 114, 143, 158	0
4	D	213/214 (99%)	-0.45	2 (0%) 84 63	54, 88, 158, 182	0
4	L	213/214 (99%)	-0.44	0 100 100	59, 95, 135, 151	0
All	All	1595/1650 (96%)	-0.37	14 (0%) 84 63	54, 100, 151, 189	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	211	VAL	4.8
2	M	27	VAL	4.3
1	A	459	GLY	3.9
1	G	492	GLU	3.9
3	C	208	ASP	3.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	DPR	M	21	7/8	0.95	0.24	91,94,96,97	0

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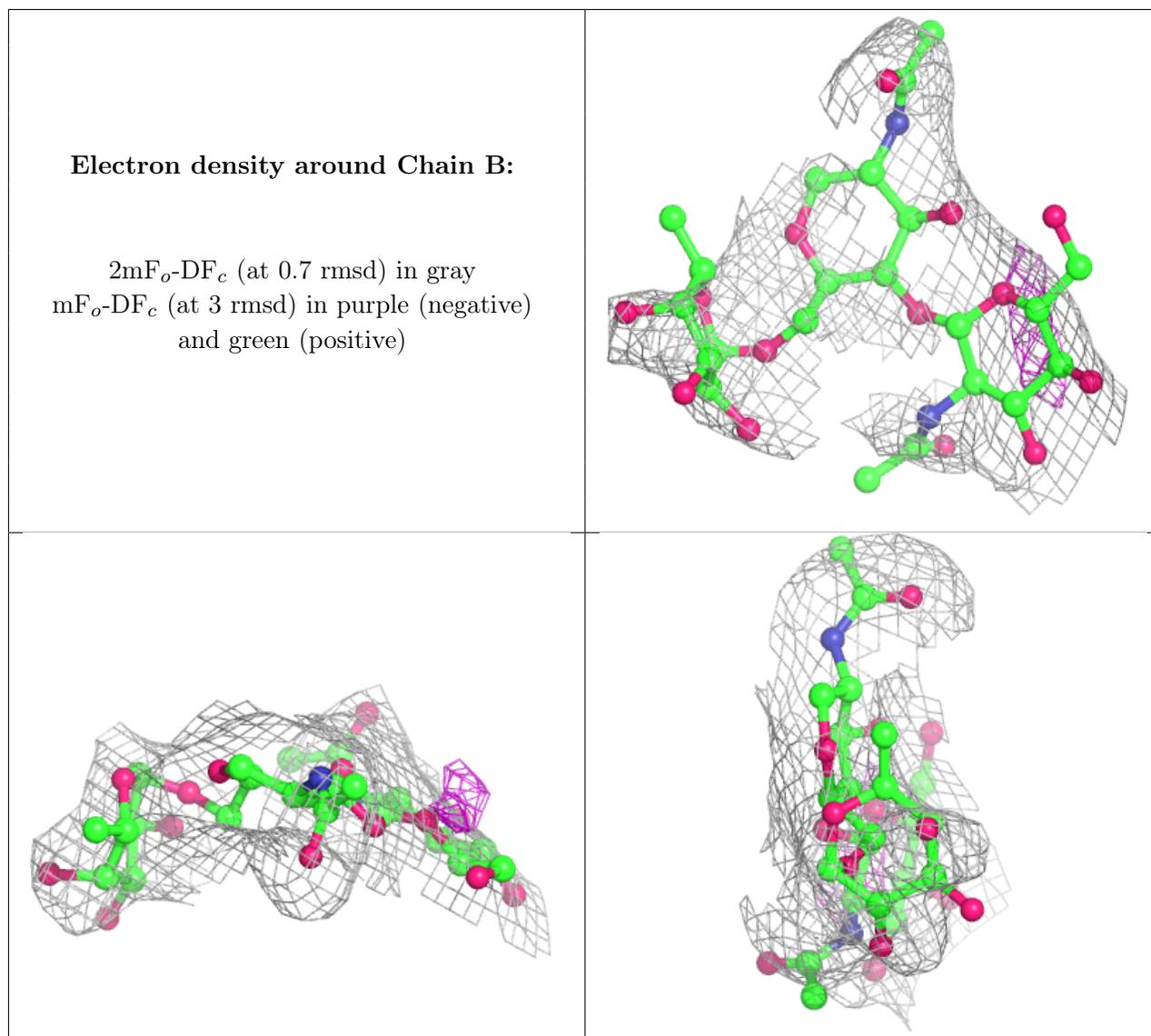
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	U2X	N	23	19/20	0.96	0.18	85,89,99,104	0
2	U2X	M	23	19/20	0.96	0.20	68,90,112,115	0
2	DPR	N	21	7/8	0.97	0.22	90,91,92,93	0

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	2	14/15	0.75	0.39	127,138,142,145	0
5	FUC	B	3	10/11	0.77	0.47	161,170,183,183	0
5	NAG	B	1	14/15	0.91	0.18	92,111,132,141	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(Å <sup>2</sup> )	Q < 0.9
6	NAG	H	500	14/15	0.74	0.29	114,134,149,153	0
6	NAG	G	511	14/15	0.78	0.32	106,118,136,141	0
7	CL	D	301	1/1	0.78	0.24	97,97,97,97	0
6	NAG	G	510	14/15	0.79	0.27	128,146,152,152	0
6	NAG	G	509	14/15	0.83	0.37	132,149,157,168	0
6	NAG	G	506	14/15	0.84	0.24	125,136,139,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CL	A	512	1/1	0.85	0.15	89,89,89,89	0
6	NAG	A	510	14/15	0.85	0.17	142,153,160,160	0
6	NAG	G	505	14/15	0.88	0.21	98,107,122,129	0
6	NAG	G	502	14/15	0.91	0.17	96,105,112,118	0
6	NAG	G	507	14/15	0.91	0.32	103,106,123,127	0
6	NAG	A	503	14/15	0.91	0.16	73,82,88,92	0
6	NAG	A	505	14/15	0.92	0.19	90,99,101,101	0
6	NAG	A	506	14/15	0.92	0.14	87,95,105,110	0
6	NAG	G	501	14/15	0.92	0.17	88,105,113,118	0
6	NAG	A	502	14/15	0.92	0.13	84,94,106,110	0
6	NAG	G	504	14/15	0.92	0.16	95,106,111,122	0
6	NAG	A	511	14/15	0.93	0.18	113,122,129,135	0
6	NAG	A	509	14/15	0.93	0.18	94,103,107,110	0
6	NAG	A	508	14/15	0.93	0.17	87,93,98,101	0
6	NAG	G	508	14/15	0.94	0.17	78,86,98,103	0
6	NAG	A	507	14/15	0.94	0.19	112,126,133,136	0
6	NAG	A	501	14/15	0.95	0.16	103,106,140,154	0
6	NAG	A	504	14/15	0.96	0.18	70,76,88,97	0
6	NAG	G	503	14/15	0.96	0.14	83,93,96,107	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.