

wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 12:46 AM JST

PDB ID : 6ION

Title: The complex of C4.4A with its antibody 11H10 Fab fragment

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Deposited on : 2018-10-30

Resolution : 2.75 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

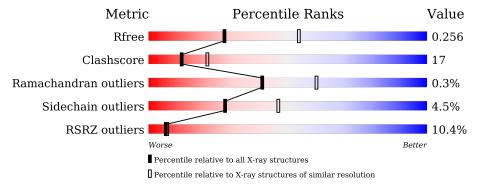
Validation Pipeline (wwPDB-VP) : 2.36

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 2.75 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 >=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 <=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	L	215	12%	33%	·.					
2	Н	220	13%	23%	• 5%					
3	A	201	63%	26%	• 8%					
4	В	2	100%							



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4603 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 anti-C4.4A antibody 11H10, light chain.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	L	213	Total 1630	C 1015	N 274	O 335	S 6	0	0	0

• Molecule 2 is a protein called anti-C4.4A antibody 11H10, heavy chain.

M	ol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	2	Н	208	Total 1575	C 1010	N 256	O 305	S 4	0	0	0

• Molecule 3 is a protein called Ly6/PLAUR domain-containing protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	185	Total 1342	C 814	N 241	O 268	S 19	0	0	0

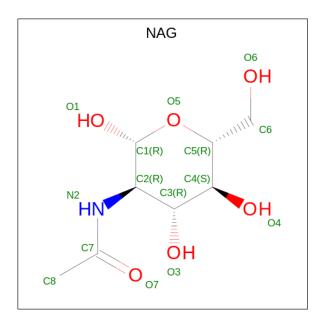
• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



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

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





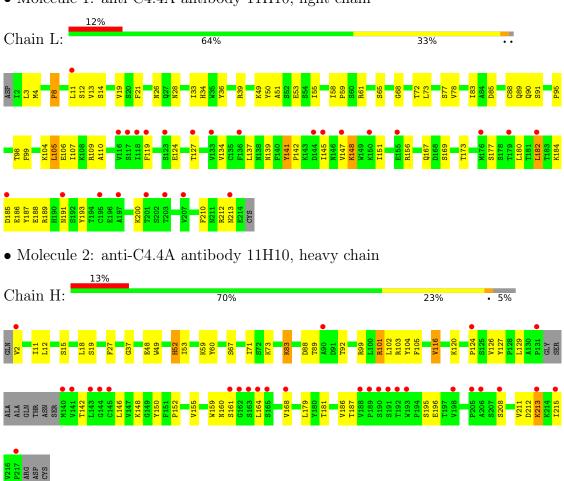
	\mathbf{Mol}	Chain	Residues	\mathbf{Atoms}				ZeroOcc	AltConf	
	5	Λ	1	Total	С	N	О	0	0	
	5	А	1	14	8	1	5	0	U	
Ī		Λ	1	Total	С	N	О	0	0	
	3	А	1	14	8	1	5	U	U	



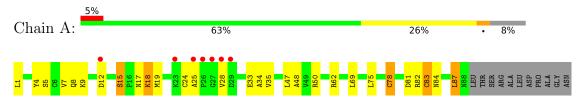
3 Residue-property plots (i)

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: anti-C4.4A antibody 11H10, light chain



• Molecule 3: Ly6/PLAUR domain-containing protein 3









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

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	51.86Å 63.96Å 107.71Å	Depositor
a, b, c, α , β , γ	90.00° 96.10° 90.00°	Depositor
Resolution (Å)	40.14 - 2.75	Depositor
Resolution (A)	$oxed{40.14 - 2.75}$	EDS
% Data completeness	99.0 (40.14-2.75)	Depositor
(in resolution range)	99.0 (40.14-2.75)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.34 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
P. P.	0.197 , 0.255	Depositor
R, R_{free}	0.196 , 0.256	DCC
R_{free} test set	926 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 46.3	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4603	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.47% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: 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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	L	0.57	0/1669	0.88	4/2273~(0.2%)	
2	Н	0.59	1/1621 (0.1%)	0.98	3/2228 (0.1%)	
3	A	0.72	2/1362 (0.1%)	1.11	8/1844 (0.4%)	
All	All	0.62	3/4652 (0.1%)	0.99	15/6345 (0.2%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
2	Н	116	VAL	CB-CG2	-5.32	1.41	1.52
3	A	78	CYS	CB-SG	-5.11	1.73	1.81
3	A	83	CYS	CB-SG	-5.10	1.73	1.81

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	A	69	LEU	CB-CG-CD2	-11.17	92.01	111.00
3	A	171	ARG	CG-CD-NE	-7.70	95.64	111.80
3	A	78	CYS	CA-CB-SG	-7.47	100.56	114.00
1	L	182	LEU	CA-CB-CG	6.50	130.24	115.30
3	A	83	CYS	CA-CB-SG	-6.36	102.55	114.00

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



All

All

4603

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1630	0	1523	75	0
2	Н	1575	0	1513	44	0
3	A	1342	0	1271	41	0
4	В	28	0	25	2	0
5	A	28	0	26	0	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 17.

155

0

4358

The worst 5 of 155 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:L:109:ARG:HG2	1:L:141:TYR:CD2	1.80	1.17
1:L:191:ASN:ND2	1:L:213:ASN:ND2	1.98	1.11
1:L:109:ARG:HG2	1:L:141:TYR:HD2	1.13	1.09
1:L:191:ASN:HD21	1:L:213:ASN:ND2	1.56	1.03
1:L:191:ASN:ND2	1:L:213:ASN:HD21	1.56	1.00

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	Perce	entiles
1	L	211/215 (98%)	204 (97%)	7 (3%)	0	100	100
2	Н	204/220 (93%)	198 (97%)	4 (2%)	2 (1%)	15	27
3	A	181/201 (90%)	168 (93%)	13 (7%)	0	100	100
All	All	596/636 (94%)	570 (96%)	24 (4%)	2 (0%)	41	60



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Н	102	LEU
2	Н	15	SER

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	L	185/192 (96%)	177 (96%)	8 (4%)	29 48
2	Н	176/191 (92%)	167 (95%)	9 (5%)	24 41
3	A	151/164 (92%)	145 (96%)	6 (4%)	31 51
All	All	512/547 (94%)	489 (96%)	23 (4%)	27 46

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Н	208	SER
3	A	15	SER
2	Н	213	LYS
3	A	78	CYS
1	L	177	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	Н	160	ASN
3	A	137	HIS
3	A	187	GLN
1	L	167	GLN
1	L	34	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)

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

5.5 Carbohydrates (i)

2 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	Trme	Chain	Dog Link		Bo	ond leng	ths	В	ond ang	cles
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	В	1	4,3	14,14,15	1.52	2 (14%)	17,19,21	1.82	2 (11%)
4	NAG	В	2	4	14,14,15	0.90	1 (7%)	17,19,21	0.99	1 (5%)

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	В	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	В	2	4	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
4	В	1	NAG	C1-C2	4.24	1.58	1.52
4	В	1	NAG	O5-C1	3.63	1.49	1.43
4	В	2	NAG	C1-C2	2.88	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
4	В	1	NAG	C1-O5-C5	6.65	121.20	112.19
4	В	2	NAG	C1-O5-C5	2.92	116.15	112.19
4	В	1	NAG	O4-C4-C5	2.51	115.52	109.30



There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	1	NAG	O5-C5-C6-O6
4	В	2	NAG	C4-C5-C6-O6
4	В	2	NAG	O5-C5-C6-O6
4	В	1	NAG	C4-C5-C6-O6
4	В	2	NAG	C1-C2-N2-C7

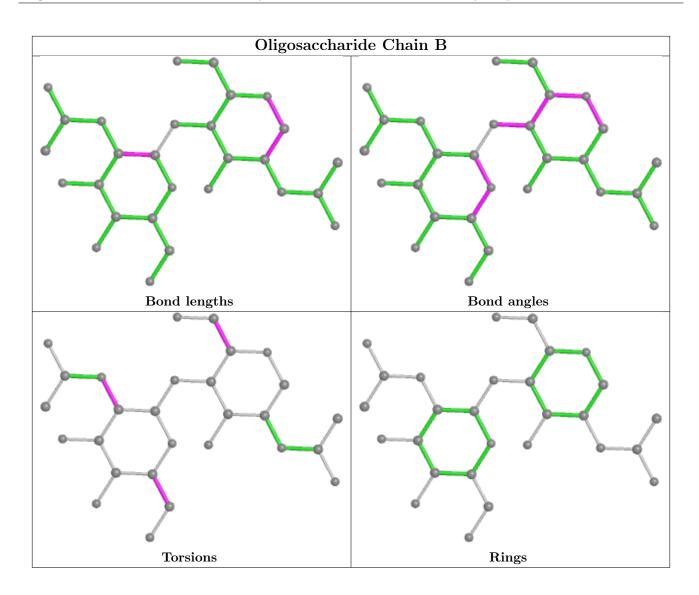
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	2	NAG	2	0
4	В	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 (i)

2 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	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Ola a ira	Clasies	Clasies	Chain De	Res	Link	Вс	ond leng	ths	В	ond ang	les
			nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2												
5	NAG	A	301	3	14,14,15	1.83	1 (7%)	17,19,21	1.24	3 (17%)												
5	NAG	A	302	3	14,14,15	0.84	1 (7%)	17,19,21	1.45	1 (5%)												



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.

Mo	l Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	301	3	-	1/6/23/26	0/1/1/1
5	NAG	A	302	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
5	A	301	NAG	O5-C1	-5.69	1.34	1.43
5	A	302	NAG	O5-C1	2.92	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	A	302	NAG	C1-O5-C5	5.10	119.11	112.19
5	A	301	NAG	C1-O5-C5	2.39	115.43	112.19
5	A	301	NAG	O3-C3-C2	2.16	113.93	109.47
5	A	301	NAG	C1-C2-N2	2.12	114.10	110.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	NAG	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^{th} 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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	L	213/215~(99%)	0.73	25 (11%) 4 5	37, 89, 140, 172	0
2	Н	208/220 (94%)	0.76	28 (13%) 3 3	34, 75, 137, 162	0
3	A	185/201 (92%)	0.49	10 (5%) 25 31	36, 57, 97, 132	0
All	All	606/636 (95%)	0.67	63 (10%) 6 7	34, 70, 135, 172	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Н	164	LEU	7.7
1	L	116	VAL	6.8
2	Н	191	SER	5.3
1	L	213	ASN	4.2
2	Н	217	PRO	4.1

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)

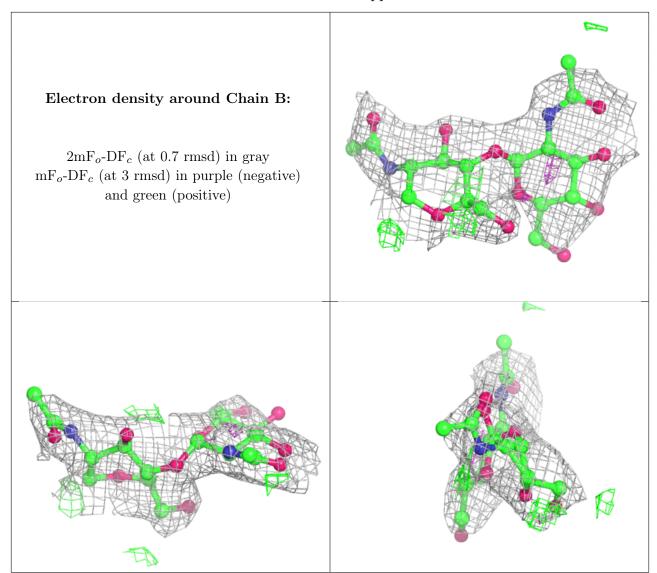
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	NAG	В	2	14/15	0.79	0.34	90,99,108,111	0
4	NAG	В	1	14/15	0.93	0.22	54,70,86,93	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-



charide. 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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	NAG	A	301	14/15	0.76	0.28	95,105,111,111	0
5	NAG	A	302	14/15	0.86	0.21	52,87,93,96	0



6.5 Other polymers (i)

There are no such residues in this entry.

