

# wwPDB X-ray Structure Validation Summary Report (i)

Apr 18, 2024 – 04:10 pm BST

PDB ID : 8RUU

Title: Fabs derived from bimekizumab in complex with IL-17F

Authors: Adams, R.; Lawson, A.D.G.

Deposited on : 2024-01-31

Resolution : 2.81 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 : 1.8.4, 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)

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

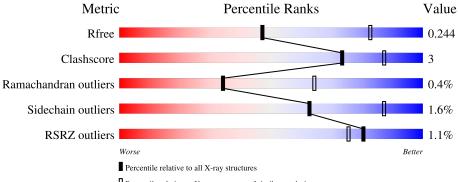
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.81 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.



Percentile relative to X-ray structures of similar resolution

Metric	Whole archive	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 o	chain	
1	В	228	86%		9% •
1	Н	228	88%		8% •
2	С	214	93%		6%
2	L	214	93%		6%
3	X	133	62%	11%	27%

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Mol	Chain	Length	Quality of chain					
3	Y	133	66%	11%	23%			
4	A	5	100%					



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16433 atoms, of which 8110 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 Immunoblobulin heavy chain.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	В	219	Total 3306	C 1065	H 1628	N 282	O 325	S 6	0	1	0
1	Н	220	Total 3328	C 1071	H 1641	N 284	O 326	S 6	0	1	0

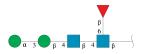
• Molecule 2 is a protein called Immunoblobulin light chain.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
2	С	213	20000	C 1037		N 280	O 333	S 5	0	0	0
2	L	213	Total 3264	C 1037	H 1609	N 280	O 333	S 5	0	0	0

• Molecule 3 is a protein called Interleukin-17F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	X	97	Total 1525	_		N 137	O 147	S 7	0	0	0
3	Y	102	Total 1610	C 499	H 801	N 148	O 155	S 7	0	0	0

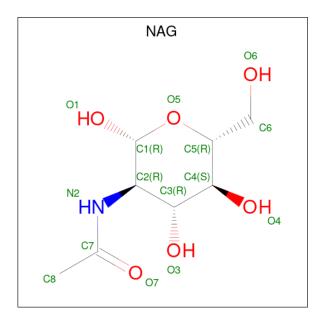
• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	A	5	Total 109	C 34	H 49	N 2	O 24	0	0	0



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



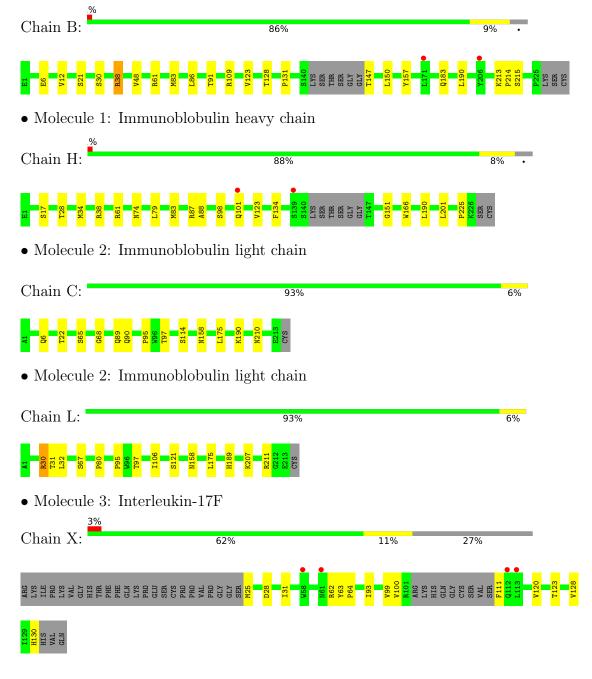
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	V	1	Total	С	Н	N	О	0	0
9	1	1	27	8	13	1	5	0	U



# 3 Residue-property plots (i)

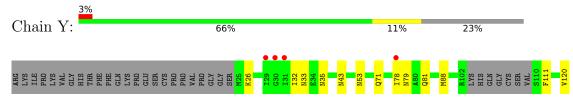
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Immunoblobulin heavy chain





• Molecule 3: Interleukin-17F





 $\bullet \ \, Molecule \ 4: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-experiments (1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-experiments (1-4)-[beta-L-fucopyranose-experiments (1-4)-[beta-L-fucopyranose-experimen$ 

Chain A:

NAG1 NAG2 BMA3 MAN4 FUL5



# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	99.15Å 141.75Å 145.56Å	Donositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	81.95 - 2.81	Depositor	
resolution (A)	81.95 - 2.81	EDS	
% Data completeness	99.9 (81.95-2.81)	Depositor	
(in resolution range)	99.9 (81.95-2.81)	EDS	
$R_{merge}$	0.05	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.77 (at 2.82Å)	Xtriage	
Refinement program	PHENIX 1.18.2_3874	Depositor	
$R, R_{free}$	0.204 , $0.241$	Depositor	
it, it free	0.205 , $0.244$	DCC	
$R_{free}$ test set	2442  reflections  (4.82%)	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	79.7	Xtriage	
Anisotropy	0.427	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36, 49.6	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	0.014 for -h,l,k	Xtriage	
$F_o, F_c$ correlation	0.94	EDS	
Total number of atoms	16433	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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, MAN, FUL, BMA

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	В	0.39	0/1722	0.59	0/2349	
1	Н	0.44	0/1731	0.61	0/2360	
2	С	0.39	0/1692	0.62	0/2299	
2	L	0.38	0/1692	0.57	0/2299	
3	X	0.37	0/776	0.57	0/1054	
3	Y	0.35	0/821	0.62	0/1113	
All	All	0.39	0/8434	0.60	0/11474	

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	В	1678	1628	1627	11	0
1	Н	1687	1641	1640	10	0
2	С	1655	1609	1609	7	0
2	L	1655	1609	1609	8	0
3	X	765	760	760	13	0
3	Y	809	801	802	13	0
4	A	60	49	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	14	13	13	3	0
All	All	8323	8110	8112	54	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 3.

The worst 5 of 54 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)
3:X:120:VAL:HG21	3:Y:120:VAL:HG21	1.47	0.96
3:Y:53:ASN:HD22	5:Y:201:NAG:H83	1.37	0.88
3:Y:53:ASN:ND2	5:Y:201:NAG:H83	1.90	0.85
2:L:80:PRO:HA	2:L:106:ILE:HD13	1.65	0.79
3:X:120:VAL:HG21	3:Y:120:VAL:CG2	2.22	0.66

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	В	$216/228 \ (95\%)$	210 (97%)	6 (3%)	0	100	100	
1	Н	217/228 (95%)	210 (97%)	7 (3%)	0	100	100	
2	С	211/214 (99%)	197 (93%)	13 (6%)	1 (0%)	29	59	
2	L	211/214 (99%)	196 (93%)	13 (6%)	2 (1%)	17	44	
3	X	93/133 (70%)	89 (96%)	4 (4%)	0	100	100	
3	Y	98/133 (74%)	95 (97%)	2 (2%)	1 (1%)	15	42	
All	All	1046/1150 (91%)	997 (95%)	45 (4%)	4 (0%)	34	64	

All (4) Ramachandran outliers are listed below:



Mol	Chain	$\operatorname{Res}$	Type
2	L	31	THR
2	L	30	ARG
3	Y	43	ASN
2	С	68	GLY

#### 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	В	185/191 (97%)	180 (97%)	5 (3%)	44	77	
1	Н	186/191 (97%)	180 (97%)	6 (3%)	39	71	
2	С	189/190 (100%)	188 (100%)	1 (0%)	88	96	
2	L	189/190 (100%)	187 (99%)	2 (1%)	73	91	
3	X	91/123 (74%)	91 (100%)	0	100	100	
3	Y	96/123 (78%)	94 (98%)	2 (2%)	53	82	
All	All	936/1008 (93%)	920 (98%)	16 (2%)	62	86	

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Y	35	ASN
2	L	207	LYS
1	Н	61	ARG
2	L	67	SER
1	Н	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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)

5 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	es Link	Bond lengths			Bond angles			
MIOI	vioi Type Chain ites	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
4	NAG	A	1	4,3	14,14,15	0.87	1 (7%)	17,19,21	1.61	3 (17%)	
4	NAG	A	2	4	14,14,15	1.14	2 (14%)	17,19,21	1.10	2 (11%)	
4	BMA	A	3	4	11,11,12	1.78	3 (27%)	15,15,17	1.40	2 (13%)	
4	MAN	A	4	4	11,11,12	0.95	0	15,15,17	1.62	3 (20%)	
4	FUL	A	5	4	10,10,11	2.14	3 (30%)	14,14,16	1.82	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
4	NAG	A	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	2/2/19/22	0/1/1/1
4	MAN	A	4	4	-	0/2/19/22	0/1/1/1
4	FUL	A	5	4	-	-	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
4	A	5	FUL	O5-C1	5.15	1.51	1.43
4	A	3	BMA	C1-C2	3.72	1.60	1.52
4	A	2	NAG	C1-C2	2.77	1.56	1.52
4	A	3	BMA	O5-C1	2.58	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
4	A	5	FUL	O5-C5	2.58	1.49	1.43

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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
4	A	1	NAG	C1-O5-C5	4.54	118.34	112.19
4	A	3	BMA	O2-C2-C3	-3.93	102.26	110.14
4	A	4	MAN	O2-C2-C3	-3.83	102.47	110.14
4	A	5	FUL	O5-C5-C4	3.33	115.50	109.52
4	A	4	MAN	C1-O5-C5	3.01	116.28	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

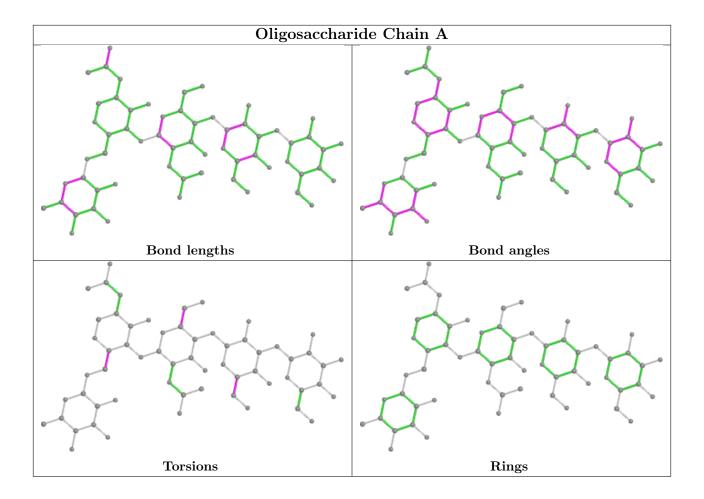
Mol	Chain	Res	Type	Atoms
4	A	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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)

#### 1 ligand 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	Mol Type	Chain	Pog	es Link	Bond lengths			Bond angles		
Moi Type C	Chain	Chain Res		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
5	NAG	Y	201	3	14,14,15	2.21	3 (21%)	17,19,21	1.93	3 (17%)

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	Y	201	3	-	4/6/23/26	0/1/1/1

#### All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
5	Y	201	NAG	O5-C1	6.97	1.54	1.43
5	Y	201	NAG	C1-C2	-2.77	1.48	1.52
5	Y	201	NAG	C4-C5	2.08	1.57	1.53

#### All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	Y	201	NAG	C1-O5-C5	6.23	120.64	112.19
5	Y	201	NAG	C2-N2-C7	2.73	126.78	122.90
5	Y	201	NAG	O4-C4-C5	2.09	114.49	109.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Y	201	NAG	O5-C5-C6-O6
5	Y	201	NAG	C4-C5-C6-O6
5	Y	201	NAG	C8-C7-N2-C2
5	Y	201	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	201	NAG	3	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,  $95^{th}$  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	<rsrz></rsrz>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	В	$219/228 \ (96\%)$	0.21	2 (0%) 84 80	58, 76, 106, 129	0
1	Н	220/228 (96%)	0.37	2 (0%) 84 80	58, 83, 121, 134	0
2	С	213/214 (99%)	0.23	0 100 100	54, 77, 105, 140	0
2	L	213/214 (99%)	0.39	0 100 100	51, 70, 110, 128	0
3	X	97/133 (72%)	0.43	4 (4%) 37 27	68, 101, 147, 156	0
3	Y	102/133 (76%)	0.59	4 (3%) 39 29	62, 98, 155, 165	0
All	All	$1064/1150 \ (92\%)$	0.34	12 (1%) 80 75	51, 80, 126, 165	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	31	ILE	6.0
3	Y	29	ILE	3.1
1	Н	101[A]	GLN	2.9
3	X	113	LEU	2.6
1	В	206	TYR	2.6

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

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

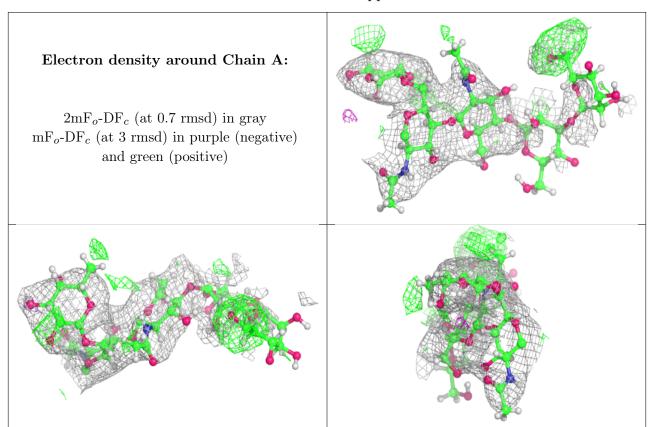
## 6.3 Carbohydrates (i)

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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
4	MAN	A	4	11/12	0.33	0.36	296,310,454,454	0
4	BMA	A	3	11/12	0.59	0.36	240,276,331,333	0
4	NAG	A	2	14/15	0.86	0.21	141,191,251,265	0
4	NAG	A	1	14/15	0.92	0.15	94,116,141,152	0
4	FUL	A	5	10/11	0.95	0.15	97,126,152,154	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,  $95^{th}$  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	Y	201	14/15	0.90	0.21	93,113,135,144	0



# 6.5 Other polymers (i)

There are no such residues in this entry.

