

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

#### Jun 17, 2024 – 12:09 PM EDT

PDB ID	:	8TTM
Title	:	IgG1 Fc Heterodimer combYSelect1
Authors	:	Azzam, T.; Du, J.J.; Sundberg, E.J.
Deposited on	:	2023-08-14
Resolution	:	2.51  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:

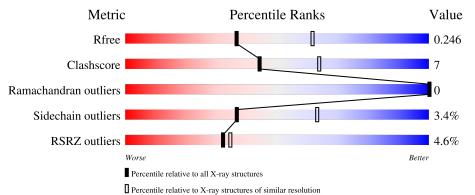
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 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 2.51 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	А	232	.% •	78%	10% • 11%	-
2	В	232	7%	72%	15% • 11%	-
3	С	8	12%	75%	12%	
3	D	8	25%	62%	12%	

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
3	FUC	D	8	-	-	-	Х



#### 8TTM

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3545 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	А	207	Total 1672	C 1067	N 279	O 320	S 6	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	SER	LYS	engineered mutation	UNP P0DOX5
А	411	TYR	THR	engineered mutation	UNP P0DOX5

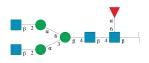
• Molecule 2 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	207	Total 1669	C 1066	N 279	0 318	S 6	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	368	SER	LEU	engineered mutation	UNP P0DOX5
В	399	TYR	ASP	engineered mutation	UNP P0DOX5

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp ha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-man nopyranose-(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	I	4ton	ns		ZeroOcc	AltConf	Trace
2	С	0	Total	С	Ν	0	0	0	0
5	U	0	99	56	4	39	0	0	0
2	Л	0	Total	С	Ν	0	0	0	0
0		0	99	56	4	39	0	U	U

• Molecule 4 is water.

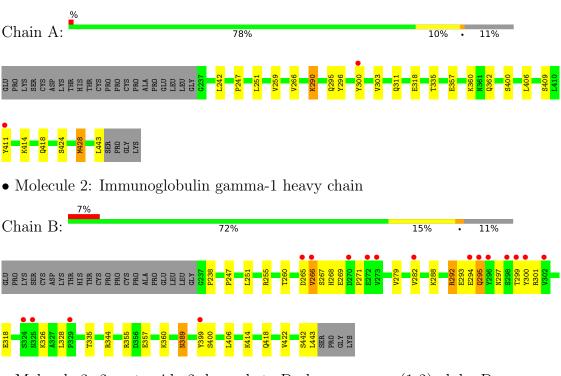
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	5	Total O 5 5	0	0
4	В	1	Total O 1 1	0	0



# 3 Residue-property plots (i)

• Molecule 1: Immunoglobulin gamma-1 heavy chain

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.



 $\label{eq:constraint} \bullet \mbox{Molecule 3: } 2\mbox{-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]2-acetamido-2-deoxy-be$ 



 $\label{eq:solution} \bullet \mbox{Molecule 3: } 2\mbox{-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]2-ace$ 

Chain D: 25%



12%

62%





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	49.78Å 79.39Å 142.90Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	40.88 - 2.51	Depositor
	40.85 - 2.51	EDS
% Data completeness	98.1 (40.88-2.51)	Depositor
(in resolution range)	98.2(40.85-2.51)	EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.58 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PDB-REDO, PHENIX v1.21	Depositor
$R, R_{free}$	0.202 , $0.242$	Depositor
It, It <sub>free</sub>	0.211 , $0.246$	DCC
$R_{free}$ test set	1970 reflections $(10.00\%)$	wwPDB-VP
Wilson B-factor ( $Å^2$ )	60.2	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32 , $44.9$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3545	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 6.41% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<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: FUC, BMA, NAG, MAN

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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.50	0.50 1/1720 (0.1%)		0/2345	
2	В	0.49	0/1720	0.71	0/2344	
All	All	0.50	1/3440~(0.0%)	0.69	0/4689	

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	В	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	428	MET	SD-CE	5.98	2.11	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	255	ARG	Sidechain
2	В	292	ARG	Sidechain
2	В	344	ARG	Sidechain
2	В	355	ARG	Sidechain



## 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	А	1672	0	1627	23	0
2	В	1669	0	1633	31	0
3	С	99	0	85	1	0
3	D	99	0	85	2	0
4	А	5	0	0	0	0
4	В	1	0	0	0	0
All	All	3545	0	3430	46	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 7.

The worst 5 of 46 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)
1:A:428:MET:CE	1:A:428:MET:SD	2.11	1.39
1:A:411[B]:TYR:CD2	2:B:399[B]:TYR:OH	2.07	1.07
2:B:294:GLU:O	2:B:299:THR:O	1.79	1.00
1:A:411[B]:TYR:HD2	2:B:399[B]:TYR:HH	1.13	0.92
1:A:411[A]:TYR:CZ	2:B:399[A]:TYR:HE1	1.96	0.83

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	А	206/232~(89%)	204 (99%)	2(1%)	0	100 100	

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	Chain	Analysed	Favoured	Allowed	Outliers	Percer	ntiles
2	В	206/232~(89%)	202~(98%)	4 (2%)	0	100	100
All	All	412/464 (89%)	406 (98%)	6(2%)	0	100	100

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There are no Ramachandran outliers to report.

#### 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	Analysed Rotameric Outliers		Percentiles
1	А	194/215~(90%)	189~(97%)	5(3%)	46 72
2	В	194/215~(90%)	186 (96%)	8 (4%)	30 55
All	All	388/430~(90%)	375~(97%)	13 (3%)	37 63

5 of 13 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	В	288	LYS
2	В	292	ARG
2	В	400	SER
2	В	326	LYS
2	В	389	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	А	295	GLN
1	А	419	GLN
1	А	421	ASN
2	В	389	ASN

#### 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)

16 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	Bo	ond leng		В	ond ang	les
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	NAG	С	1	$1,\!3$	$14,\!14,\!15$	0.41	0	$17,\!19,\!21$	1.02	1 (5%)
3	NAG	С	2	3	$14,\!14,\!15$	0.40	0	$17,\!19,\!21$	0.96	1 (5%)
3	BMA	С	3	3	11,11,12	0.47	0	$15,\!15,\!17$	0.77	1 (6%)
3	MAN	С	4	3	11,11,12	0.30	0	$15,\!15,\!17$	0.88	1 (6%)
3	NAG	С	5	3	14,14,15	0.42	0	17,19,21	1.09	2 (11%)
3	MAN	С	6	3	11,11,12	0.49	0	$15,\!15,\!17$	0.82	0
3	NAG	С	7	3	$14,\!14,\!15$	0.39	0	$17,\!19,\!21$	1.04	1 (5%)
3	FUC	С	8	3	10,10,11	0.45	0	$14,\!14,\!16$	0.73	1 (7%)
3	NAG	D	1	2,3	$14,\!14,\!15$	0.41	0	17,19,21	0.51	0
3	NAG	D	2	3	$14,\!14,\!15$	0.44	0	$17,\!19,\!21$	0.89	1 (5%)
3	BMA	D	3	3	$11,\!11,\!12$	0.52	0	$15,\!15,\!17$	1.12	2 (13%)
3	MAN	D	4	3	11,11,12	0.43	0	$15,\!15,\!17$	0.77	0
3	NAG	D	5	3	14,14,15	0.43	0	17,19,21	0.96	2 (11%)
3	MAN	D	6	3	11,11,12	0.33	0	$15,\!15,\!17$	0.94	1 (6%)
3	NAG	D	7	3	$14,\!14,\!15$	0.41	0	$17,\!19,\!21$	1.14	2 (11%)
3	FUC	D	8	3	10,10,11	0.31	0	$14,\!14,\!16$	0.48	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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
3	NAG	С	1	$1,\!3$	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	С	2	3	-	0/6/23/26	0/1/1/1
3	BMA	С	3	3	-	0/2/19/22	0/1/1/1
3	MAN	С	4	3	-	2/2/19/22	0/1/1/1
3	NAG	С	5	3	-	2/6/23/26	0/1/1/1
3	MAN	С	6	3	-	1/2/19/22	0/1/1/1
3	NAG	С	7	3	-	2/6/23/26	0/1/1/1
3	FUC	С	8	3	-	-	0/1/1/1
3	NAG	D	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	NAG	D	7	3	-	3/6/23/26	0/1/1/1
3	FUC	D	8	3	-	-	0/1/1/1

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There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	7	NAG	O3-C3-C2	-3.23	102.78	109.47
3	С	5	NAG	O5-C1-C2	3.03	116.08	111.29
3	D	7	NAG	C1-C2-N2	2.82	115.31	110.49
3	С	5	NAG	C2-N2-C7	2.79	126.88	122.90
3	D	3	BMA	C1-C2-C3	2.74	113.03	109.67

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	7	NAG	C8-C7-N2-C2
3	D	7	NAG	O7-C7-N2-C2
3	D	5	NAG	C8-C7-N2-C2

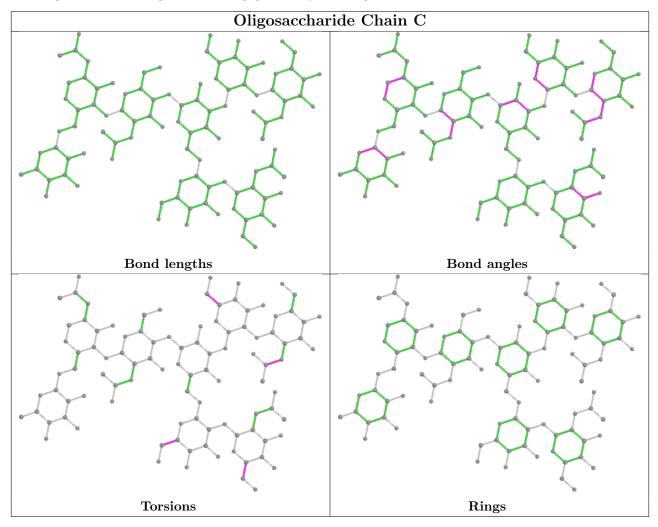
There are no ring outliers.

3 monomers are involved in 3 short contacts:



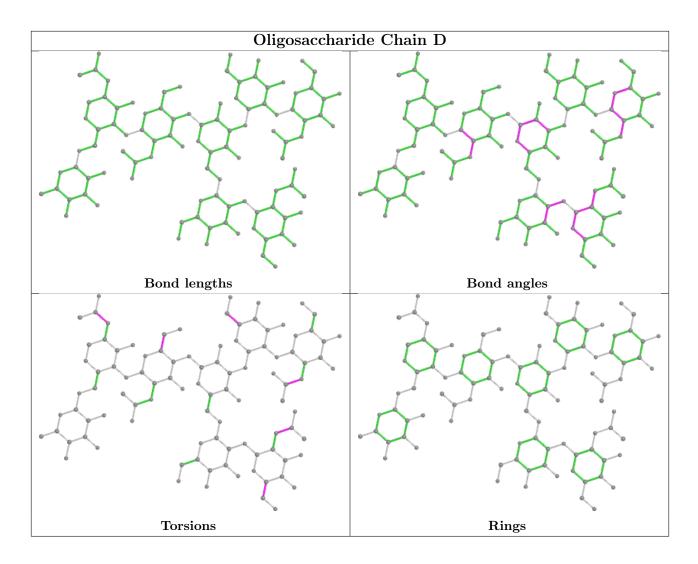
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
3	D	7	NAG	1	0
3	С	1	NAG	1	0

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)

There are no ligands in this entry.

## 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	$\langle RSRZ \rangle$	<RSRZ $>$ $#$ RSRZ $>$ 2		Q < 0.9
1	А	207/232~(89%)	0.27	2 (0%) 82 84	41, 63, 108, 121	0
2	В	207/232 (89%)	0.69	17 (8%) 11 11	43, 76, 140, 167	0
All	All	414/464~(89%)	0.48	19 (4%) 32 34	41, 69, 124, 167	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	296	TYR	7.3
2	В	300	TYR	5.6
2	В	273	VAL	5.3
2	В	294	GLU	3.9
2	В	295	GLN	3.9

## 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	$B-factors(Å^2)$	Q<0.9
3	NAG	С	5	14/15	0.77	0.22	110,116,122,133	0
3	NAG	D	5	14/15	0.78	0.29	108,140,147,152	0
3	FUC	D	8	10/11	0.78	0.43	135,146,150,156	0
3	NAG	D	1	14/15	0.80	0.28	123,137,144,147	0
3	MAN	D	6	11/12	0.83	0.14	90,102,107,113	0

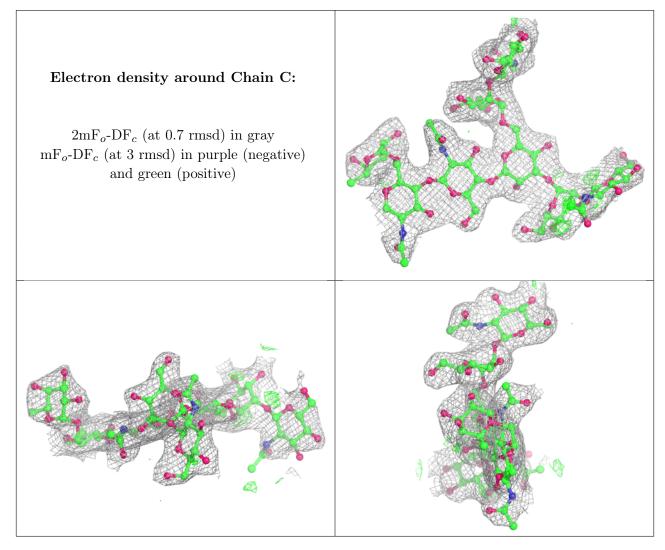
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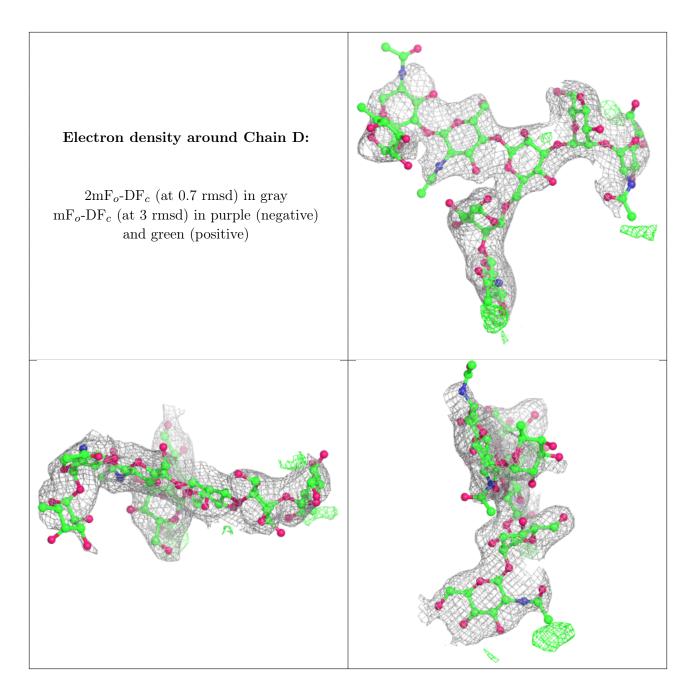
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	$Q{<}0.9$
3	FUC	С	8	10/11	0.86	0.20	92,98,104,109	0
3	MAN	D	4	11/12	0.88	0.15	88,116,147,147	0
3	NAG	D	2	14/15	0.91	0.19	102,117,122,128	0
3	BMA	D	3	11/12	0.91	0.12	107,118,122,125	0
3	NAG	D	7	14/15	0.92	0.13	81,95,106,110	0
3	NAG	С	7	14/15	0.92	0.11	67,80,89,89	0
3	MAN	С	4	11/12	0.94	0.11	70,78,88,96	0
3	NAG	С	1	14/15	0.94	0.16	76,82,94,95	0
3	MAN	С	6	11/12	0.95	0.09	66,75,83,85	0
3	BMA	С	3	11/12	0.96	0.12	61,65,74,75	0
3	NAG	С	2	14/15	0.97	0.14	63,70,74,80	0

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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)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.

