

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

#### Oct 23, 2023 – 02:39 AM EDT

PDB ID : 3ASR

Title : Crystal structure of P domain from Norovirus Funabashi258 stain in the com-

plex with Lewis-a

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Deposited on : 2010-12-17

Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

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)

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

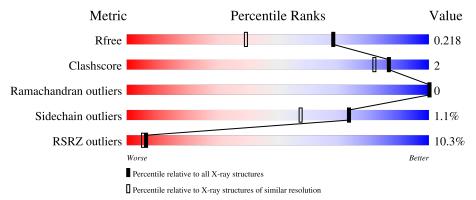
Validation Pipeline (wwPDB-VP) : 2.36

## 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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	
		224	9%	
1	A	326	90%	5% 5%
	_		10%	
1	В	326	85%	7% 7%
	61	_		
2	C	3	67%	33%
2	D	3	100%	

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
4	NPO	В	1001	-	-	-	X



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5218 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 Capsid protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	311	Total 2387	C 1527	N 402	O 449	S 9	0	1	0
1	В	302	Total 2322		N 391	O 434	S 9	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	GLY	-	expression tag	UNP Q8JW44
A	217	PRO	-	expression tag	UNP Q8JW44
A	218	LEU	-	expression tag	UNP Q8JW44
A	219	GLY	-	expression tag	UNP Q8JW44
A	220	SER	-	expression tag	UNP Q8JW44
В	216	GLY	-	expression tag	UNP Q8JW44
В	217	PRO	-	expression tag	UNP Q8JW44
В	218	LEU	-	expression tag	UNP Q8JW44
В	219	GLY	-	expression tag	UNP Q8JW44
В	220	SER	-	expression tag	UNP Q8JW44

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



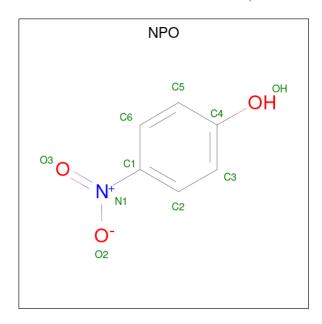
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	С	3	Total C N O 36 20 1 15	0	0	0
2	D	3	Total C N O 35 20 1 14	0	0	0



• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	В	1	Total Na 1 1	0	0

• Molecule 4 is P-NITROPHENOL (three-letter code: NPO) (formula:  $C_6H_5NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	С	N	О	0	0
- 4		1	10	6	1	3		

• Molecule 5 is water.

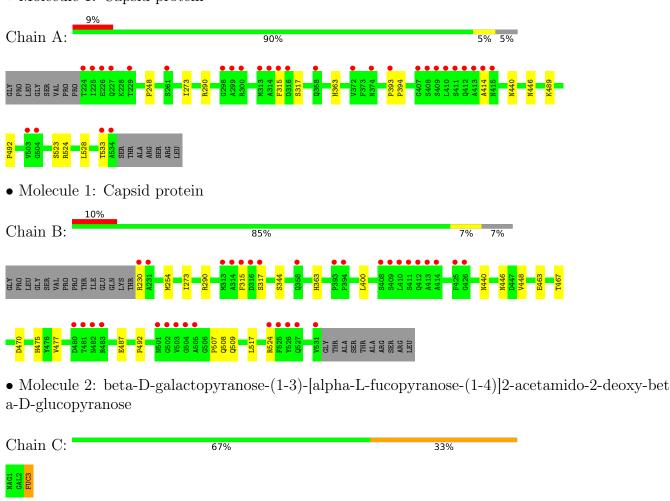
$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	224	Total O 224 224	0	0
5	В	202	Total O 202 202	0	0



## 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: Capsid protein



Chain D:

a-D-glucopyranose

100%

NAG1 GAL2 FUC3



• Molecule 2: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-bet

# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 31	Depositor	
Cell constants	74.73Å 74.73Å 107.04Å	Donositon	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	31.25 - 1.60	Depositor	
rtesolution (A)	31.25 - 1.60	EDS	
% Data completeness	98.6 (31.25-1.60)	Depositor	
(in resolution range)	98.6 (31.25-1.60)	EDS	
$R_{merge}$	0.06	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.89  (at  1.60Å)	Xtriage	
Refinement program	REFMAC 5.5.0109	Depositor	
$R, R_{free}$	0.201 , $0.218$	Depositor	
	0.197 , 0.218	DCC	
$R_{free}$ test set	4398 reflections $(5.03%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage	
Anisotropy	0.025	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.47, 64.4	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.46, < L^2> = 0.28$	Xtriage	
	0.023 for -h,-k,l		
Estimated twinning fraction	0.045  for h,-h-k,-l	Xtriage	
	0.035  for -k,-h,-l		
$F_o, F_c$ correlation	0.96	EDS	
Total number of atoms	5218	wwPDB-VP	
Average B, all atoms $(\mathring{A}^2)$	27.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.68% 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: FUC, GAL, NPO, NAG, NA

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		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.37	0/2463	0.52	0/3372	
1	В	0.37	0/2398	0.52	0/3284	
All	All	0.37	0/4861	0.52	0/6656	

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	A	2387	0	2316	7	0
1	В	2322	0	2249	14	0
2	С	36	0	33	1	0
2	D	35	0	31	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	В	10	0	4	0	0
5	A	224	0	0	0	0
5	В	202	0	0	0	0
All	All	5218	0	4633	20	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 2.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom 9	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
1:A:248:PRO:O	1:B:290:ARG:NH2	2.27	0.67
1:B:254:MET:HG2	1:B:507:PRO:HB2	1.79	0.64
1:B:440:ASN:HD22	1:B:446:ASN:ND2	2.02	0.58
1:B:467:THR:HG21	1:B:492:PRO:HG3	1.86	0.58
1:B:400:LEU:HD13	1:B:448:VAL:HG22	1.86	0.57
1:A:315:PHE:HA	1:A:363:HIS:CE1	2.40	0.57
1:B:477:VAL:HG21	1:B:517:LEU:HD12	1.88	0.55
1:B:508:GLN:HG2	1:B:509:GLN:HE21	1.72	0.55
1:A:440:ASN:HD22	1:A:446:ASN:ND2	2.06	0.54
1:B:230:ARG:HD3	1:B:463:GLU:OE1	2.08	0.53
1:A:363:HIS:CE1	1:A:414:ALA:H	2.28	0.52
1:B:470:ASP:HB2	1:B:524:ARG:N	2.25	0.50
1:A:273:ILE:HG12	1:A:492:PRO:HA	1.94	0.48
1:B:273:ILE:HG12	1:B:492:PRO:HA	1.97	0.46
1:B:470:ASP:HB3	1:B:524:ARG:HB3	1.99	0.43
1:B:344:SER:HB2	2:C:3:FUC:H2	2.00	0.43
1:A:393:PRO:HA	1:A:394:PRO:HD3	1.92	0.41
1:B:315:PHE:HA	1:B:363:HIS:NE2	2.35	0.41
1:A:489:LYS:HG3	1:A:528:LEU:HD21	2.03	0.41
1:B:475:HIS:CD2	1:B:487:GLU:HG2	2.57	0.40

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	A	310/326~(95%)	307 (99%)	3 (1%)	0	100	100
1	В	301/326 (92%)	297 (99%)	4 (1%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
All	All	611/652 (94%)	604 (99%)	7 (1%)	0	100	100

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	Rotameric Outliers		Percentiles		
1	A	266/277 (96%)	261 (98%)	5 (2%)	57 34		
1	В	259/277 (94%)	258 (100%)	1 (0%)	91 84		
All	All	525/554 (95%)	519 (99%)	6 (1%)	73 57		

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	ARG
1	A	317	SER
1	A	523	SER
1	A	524	ARG
1	A	533	THR
1	В	317	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	363	HIS
1	A	374	ASN
1	A	415	ASN
1	A	446	ASN
1	A	527	GLN
1	В	296	ASN
1	В	374	ASN
1	В	415	ASN



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Mol	Chain	Res	Type
1	В	446	ASN
1	В	509	GLN

#### 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)

6 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	Tune	Chain	Res	Link	Во	nd leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	С	1	2	15,15,15	0.41	0	21,21,21	0.74	0
2	GAL	С	2	2	11,11,12	0.54	0	15,15,17	0.83	0
2	FUC	С	3	2	10,10,11	0.64	0	14,14,16	0.90	1 (7%)
2	NAG	D	1	2,4	14,14,15	0.50	0	17,19,21	0.76	0
2	GAL	D	2	2	11,11,12	0.49	0	15,15,17	0.79	0
2	FUC	D	3	2	10,10,11	0.54	0	14,14,16	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	С	1	2	-	0/6/26/26	0/1/1/1
2	GAL	С	2	2	-	0/2/19/22	0/1/1/1
2	FUC	С	3	2	-	-	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	С	3	FUC	C1-C2-C3	2.03	112.16	109.67

There are no chirality outliers.

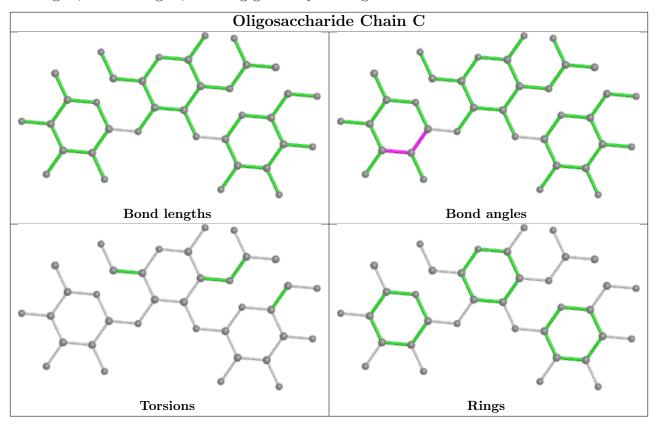
There are no torsion outliers.

There are no ring outliers.

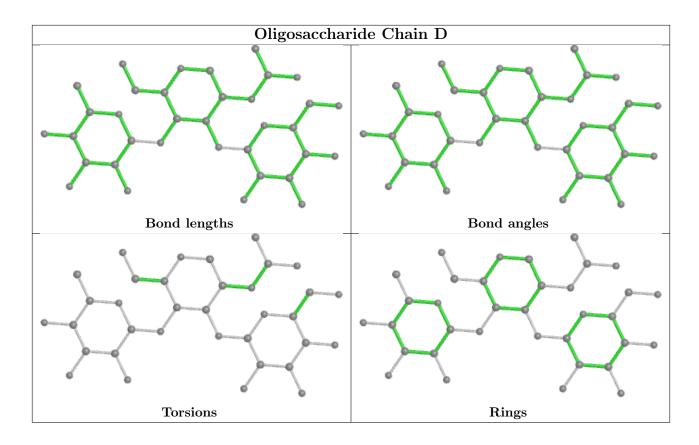
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	3	FUC	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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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			$\mathbf{B}$	Bond angles		
IVIOI	туре	Cham	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts $  RMSZ   \#  Z  > 1$	# Z  > 2		
4	NPO	В	1001	2	9,10,10	0.77	0	11,13,13	0.46	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.

$\mathbf{Mol}$	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NPO	В	1001	2	-	2/2/4/4	0/1/1/1



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	1001	NPO	C2-C1-N1-O3
4	В	1001	NPO	C6-C1-N1-O3

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	<RSRZ $>$	# RSRZ > 2		$OWAB(A^2)$	Q<0.9	
1	A	311/326 (95%)	0.67	30 (9%)	8	7	16, 25, 39, 47	0
1	В	302/326~(92%)	0.69	33 (10%)	5	4	17, 25, 40, 45	0
All	All	613/652 (94%)	0.68	63 (10%)	6	5	16, 25, 40, 47	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	LEU	14.1
1	A	225	ILE	12.9
1	A	315	PHE	12.7
1	В	503	VAL	11.8
1	В	315	PHE	11.1
1	В	410	LEU	9.9
1	В	525	PHE	9.0
1	A	224	THR	9.0
1	В	409	SER	8.7
1	A	409	SER	8.3
1	A	534	ALA	7.4
1	В	231	ALA	7.1
1	В	314	ALA	7.0
1	A	411	SER	6.9
1	В	412	GLN	6.6
1	В	504	GLY	6.5
1	A	503	VAL	6.5
1	A	314	ALA	6.4
1	В	425	PHE	6.2
1	A	316	ASP	5.7
1	A	412	GLN	5.7
1	A	229	THR	5.6
1	В	524	ARG	5.2
1	В	502	GLY	5.2



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1     B     313     MET       1     B     230     ARG       1     A     414     ALA       1     A     408     SER	5.1 5.0 4.8 4.7 4.5
1 B 230 ARG 1 A 414 ALA 1 A 408 SER	4.8 4.7 4.5
1 A 414 ALA 1 A 408 SER	4.7 4.5
1 A 408 SER	4.5
1 A 226 GLU	
	4.4
1 B 483 ARG	4.1
1 A 227 GLN	4.1
1 B 501 ASN	4.1
1 A 374 ASN	4.0
1 B 411 SER	4.0
1 A 533 THR	3.9
1 B 481 THR	3.9
1 B 480 ASP	3.8
1 A 313 MET	3.6
1 A 413 ALA	3.5
1 B 408 SER	3.4
1 B 482 ASN	3.4
1 B 393 PRO	3.3
1 B 316 ASP	3.1
1 B 527 GLN	3.1
1 A 358 GLN	2.9
1 B 317 SER	2.8
1 A 372 VAL	2.8
1 B 505 ALA	2.7
1 A 261 SER	2.7
1 B 531 VAL	2.6
1 A 415 ASN	2.5
1 A 298 GLY	2.4
1 A 300 ARG	2.4
1 B 358 GLN	2.4
1 A 299 ALA	2.4
1 B 394 PRO	2.3
	2.2
1 A 407 GLY	2.2
1 B 426 GLY	2.2
1 A 393 PRO	2.1
1 B 414 ALA	2.1
1 B 526 TYR	2.1



#### 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.

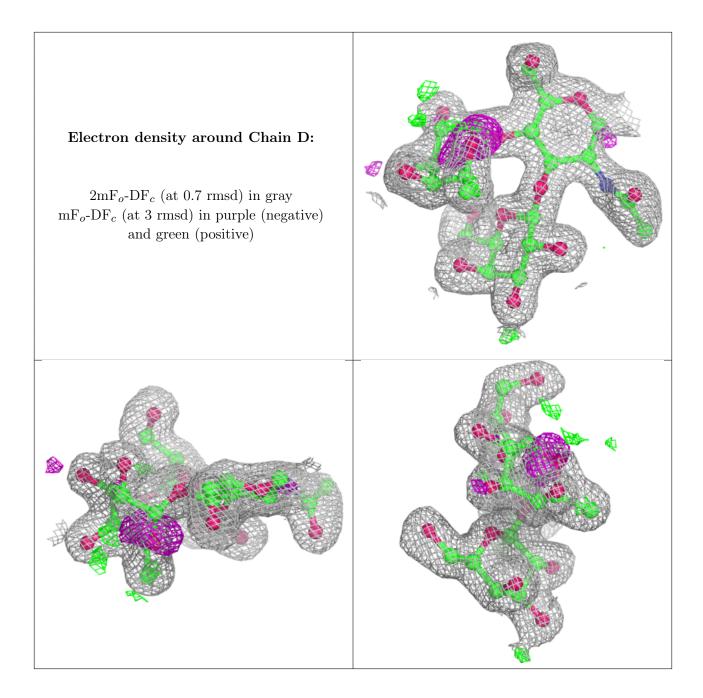
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	FUC	D	3	10/11	0.60	0.28	30,31,32,32	0
2	FUC	С	3	10/11	0.68	0.15	38,39,40,41	0
2	GAL	С	2	11/12	0.73	0.17	37,38,39,40	0
2	NAG	С	1	15/15	0.77	0.20	40,42,44,44	0
2	NAG	D	1	14/15	0.86	0.26	31,35,37,37	0
2	GAL	D	2	11/12	0.87	0.15	25,27,30,31	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.



# Electron density around Chain C: $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





## 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	$\operatorname{Res}$	Atoms	RSCC	RSR	${f B-factors}({f A}^2)$	Q<0.9
4	NPO	В	1001	10/10	0.63	0.41	43,47,50,50	0
3	NA	A	701	1/1	0.94	0.12	35,35,35,35	0
3	NA	В	701	1/1	0.99	0.15	28,28,28,28	0



# 6.5 Other polymers (i)

There are no such residues in this entry.

