

wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 12:10 PM JST

PDB ID : 8XC4

Title: Nipah virus attachment glycoprotein head domain in complex with a broadly

neutralizing antibody 1E5

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Deposited on : 2023-12-08

Resolution : 3.24 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

buster-report : 1.1.7 (2018)

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)

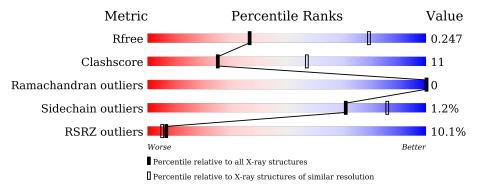
Validation Pipeline (wwPDB-VP) : 2.36

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 3.24 Å.

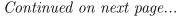
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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	A	439	74%	22%	
1	11	400	2%	2270	• •
1	В	439	72%	24%	• •
2	$^{\rm C}$	242	71%	23%	5%
2	E	242	32% 71%	23%	5%
3	D	214	74%	24%	•
	_		38%	21,70	
3	F	214	72%	26%	•





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Mol	Chain			Q	uality of chain						
4	G	4		750	_	250/					
4	G	4		75%		25%					
5	Н	5		80%							
5	K	5	20%		60%	20%					
6	I	3			100%						
6	L	3	33%		67%						
7	J	5	20%	20%	60%						

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	BMA	G	3	-	-	-	X
4	FUC	G	4	-	-	-	X
6	BMA	I	3	-	-	-	X
7	FUC	J	4	-	-	-	X
7	FUC	J	5	-	-	-	X
8	NAG	A	701	-	-	-	X
8	NAG	В	701	-	-	-	X



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13778 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 Glycoprotein.

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms		ZeroOcc	AltConf	Trace	
1	A	428	Total 3383	C 2153	N 566	O 643	S 21	0	0	0
1	В	428	Total 3383	C 2153	N 566	O 643	S 21	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	HIS	-	expression tag	UNP Q4VCP5
A	165	HIS	-	expression tag	UNP Q4VCP5
A	166	HIS	-	expression tag	UNP Q4VCP5
A	167	HIS	-	expression tag	UNP Q4VCP5
A	168	HIS	-	expression tag	UNP Q4VCP5
A	169	HIS	-	expression tag	UNP Q4VCP5
A	170	GLY	_	expression tag	UNP Q4VCP5
A	171	SER	-	expression tag	UNP Q4VCP5
A	172	GLY	-	expression tag	UNP Q4VCP5
A	173	GLY	-	expression tag	UNP Q4VCP5
A	174	GLY	-	expression tag	UNP Q4VCP5
A	175	SER	-	expression tag	UNP Q4VCP5
В	164	HIS	-	expression tag	UNP Q4VCP5
В	165	HIS	-	expression tag	UNP Q4VCP5
В	166	HIS	-	expression tag	UNP Q4VCP5
В	167	HIS	-	expression tag	UNP Q4VCP5
В	168	HIS	-	expression tag	UNP Q4VCP5
В	169	HIS	-	expression tag	UNP Q4VCP5
В	170	GLY	-	expression tag	UNP Q4VCP5
В	171	SER	-	expression tag	UNP Q4VCP5
В	172	GLY	-	expression tag	UNP Q4VCP5
В	173	GLY	-	expression tag	UNP Q4VCP5
В	174	GLY	-	expression tag	UNP Q4VCP5
В	175	SER	-	expression tag	UNP Q4VCP5



•	Molecule	2 is	a	protein	called	1E5-VH.
_	TITOTOGGIO	_ 10	~	PICCIII	COLLECT	110 111.

Mol	Chain	Residues		Ato	oms		ZeroOcc	AltConf	Trace	
2	С	229	Total 1727	C 1099	- 1	O 342	S 5	0	0	0
2	Е	229	Total 1727	C 1099	N 281	O 342	S 5	0	0	0

• Molecule 3 is a protein called 1E5-VL.

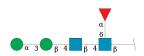
Mol	Chain	Residues		Ato	oms		ZeroOcc	AltConf	Trace	
2	D	211	Total	С	N	О	S	0	0	0
3	D	211	1612	1008	268	331	5	0	U	
9	E	211	Total	С	N	О	S	0	0	0
)	Г	211	1612	1008	268	331	5	U	U	U

• Molecule 4 is an oligosaccharide called 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.



\mathbf{N}	lol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
	4	G	4	Total 49	C 28	N 2	O 19	0	0	0

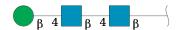
• Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns	ZeroOcc	AltConf	Trace
5	Н	5	Total 60			0	0	0
5	K	5	Total 60		N 2	0	0	0

• Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





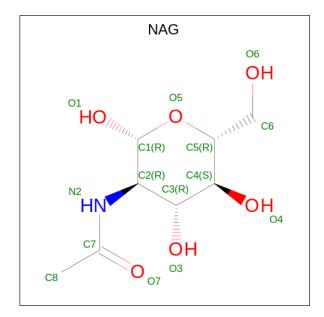
M	Iol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
(6	I	3	Total 39	C 22			0	0	0
(6	L	3	Total 39	C 22		O 15	0	0	0

• Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
7	J	5	Total 59		N 2		0	0	0

• Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).





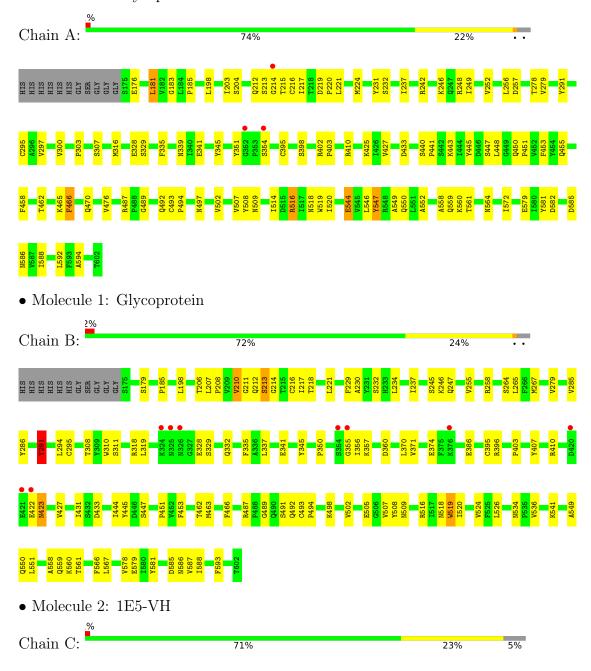
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 14 8 1 5	0	0
8	В	1	Total C N O 14 8 1 5	0	0



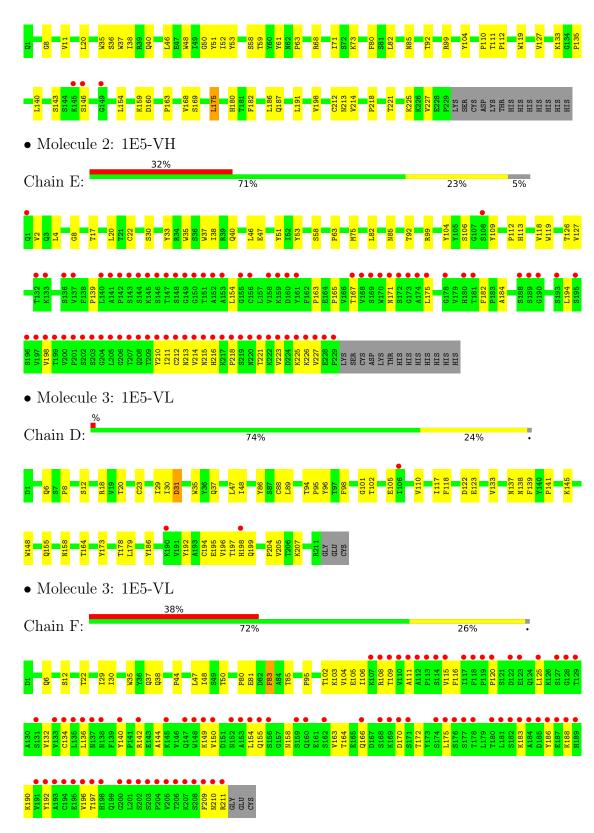
3 Residue-property plots (i)

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: Glycoprotein







• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alp ha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 75% 25%





 $\bullet \ \, Molecule \ 5: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6) 2-acetami$

Chain H: 80% 20%



• Molecule 5: alpha-D-mannopyranose-(1-3)-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-(1-6)

Chain K: 20% 60% 20%

NAG1 NAG2 BMA3 MAN4 FUC5

• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

NAG1 NAG2 BMA3

Chain L: 33% 67%



 $\bullet \ \, Molecule \ 7: \ beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]\\ 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]\\ 2-ace$

Chain J: 20% 20% 60%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	193.42Å 193.42Å 198.11Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.69 - 3.24	Depositor
Resolution (A)	33.69 - 3.24	EDS
% Data completeness	95.7 (33.69-3.24)	Depositor
(in resolution range)	95.7 (33.69-3.24)	EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.48 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
D.D.	0.218 , 0.247	Depositor
R, R_{free}	0.221 , 0.247	DCC
R_{free} test set	2001 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 57.1	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Atriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13778	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.18% 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, BMA, MAN, FUC

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	В	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.37	0/3463	0.65	1/4708 (0.0%)
1	В	0.39	0/3463	0.69	6/4708 (0.1%)
2	С	0.35	0/1778	0.66	$1/2437 \ (0.0\%)$
2	Е	0.29	0/1778	0.59	0/2437
3	D	0.34	0/1645	0.66	$1/2234 \ (0.0\%)$
3	F	0.35	0/1645	0.75	3/2234 (0.1%)
All	All	0.36	0/13772	0.67	$12/18758 \ (0.1\%)$

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	В	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	F	209	PHE	CB-CG-CD2	-10.97	113.12	120.80
3	F	209	PHE	CB-CG-CD1	8.59	126.81	120.80
1	A	466	PHE	CB-CG-CD2	-7.76	115.37	120.80
1	В	291	TYR	CA-CB-CG	7.54	127.73	113.40
3	F	38	GLN	C-N-CA	7.33	140.02	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	516	ARG	Sidechain
1	В	291	TYR	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	A	3383	0	3309	67	3
1	В	3383	0	3309	77	3
2	С	1727	0	1672	41	0
2	Ε	1727	0	1672	46	0
3	D	1612	0	1576	38	0
3	F	1612	0	1575	45	0
4	G	49	0	43	0	0
5	Н	60	0	52	0	0
5	K	60	0	52	1	0
6	I	39	0	34	1	0
6	L	39	0	34	0	0
7	J	59	0	52	2	0
8	A	14	0	13	0	0
8	В	14	0	13	0	0
All	All	13778	0	13406	292	3

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 11.

The worst 5 of 292 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
2:C:92:THR:HG22	2:C:127:VAL:H	1.25	1.00
3:F:150:VAL:HG23	3:F:155:GLN:HG3	1.52	0.91
3:F:190:LYS:HG3	3:F:210:ASN:HB3	1.58	0.86
1:A:586:ASN:ND2	3:F:30:ILE:O	2.14	0.81
2:C:63:PRO:HD2	3:D:95:PRO:HG3	1.64	0.79

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:544:GLU:OE1	1:B:386:GLU:OE2[4_554]	1.62	0.58
1:A:544:GLU:OE1	1:B:386:GLU:CD[4_554]	2.03	0.17
1:A:544:GLU:OE1	1:B:386:GLU:OE1[4_554]	2.05	0.15

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	$426/439 \ (97\%)$	403 (95%)	23 (5%)	0	100 100
1	В	426/439 (97%)	397 (93%)	29 (7%)	0	100 100
2	С	227/242 (94%)	217 (96%)	10 (4%)	0	100 100
2	Е	227/242 (94%)	218 (96%)	9 (4%)	0	100 100
3	D	209/214 (98%)	201 (96%)	8 (4%)	0	100 100
3	F	209/214 (98%)	198 (95%)	11 (5%)	0	100 100
All	All	1724/1790 (96%)	1634 (95%)	90 (5%)	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	385/392~(98%)	378 (98%)	7 (2%)	59	80
1	В	385/392 (98%)	376 (98%)	9 (2%)	50	76
2	\mathbf{C}	$197/210\ (94\%)$	197 (100%)	0	100	100

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	.,	10	1

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	${f E}$	197/210 (94%)	197 (100%)	0	100	100	
3	D	186/188 (99%)	185 (100%)	1 (0%)	88	94	
3	F	186/188 (99%)	185 (100%)	1 (0%)	88	94	
All	All	1536/1580 (97%)	1518 (99%)	18 (1%)	71	86	

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	518	ASN
3	F	83	PHE
3	D	31	ASP
1	В	213	SER
1	В	433	ASP

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

Mol	Chain	Res	Type
3	D	138	ASN
3	F	155	GLN
3	F	158	ASN
3	D	27	GLN
1	В	559	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)

25 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	Во	Bond lengths			Bond angles			
MIOI	Type		nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
4	NAG	G	1	4,1	14,14,15	0.52	0	17,19,21	0.52	0		
4	NAG	G	2	4	14,14,15	0.37	0	17,19,21	0.50	0		
4	BMA	G	3	4	11,11,12	0.78	0	15,15,17	0.86	0		
4	FUC	G	4	4	10,10,11	1.47	3 (30%)	14,14,16	2.24	4 (28%)		
5	NAG	Н	1	5,1	14,14,15	0.29	0	17,19,21	0.42	0		
5	NAG	Н	2	5	14,14,15	0.30	0	17,19,21	0.36	0		
5	BMA	Н	3	5	11,11,12	0.50	0	15,15,17	0.81	0		
5	MAN	Н	4	5	11,11,12	0.88	0	15,15,17	0.93	0		
5	FUC	Н	5	5	10,10,11	1.19	1 (10%)	14,14,16	1.07	1 (7%)		
6	NAG	I	1	6,1	14,14,15	0.31	0	17,19,21	0.66	0		
6	NAG	I	2	6	14,14,15	0.73	1 (7%)	17,19,21	1.16	1 (5%)		
6	BMA	I	3	6	11,11,12	0.63	0	15,15,17	1.54	3 (20%)		
7	NAG	J	1	7,1	14,14,15	0.89	1 (7%)	17,19,21	1.78	6 (35%)		
7	NAG	J	2	7	14,14,15	0.28	0	17,19,21	0.95	2 (11%)		
7	BMA	J	3	7	11,11,12	0.87	0	15,15,17	1.11	1 (6%)		
7	FUC	J	4	7	10,10,11	1.04	0	14,14,16	1.01	1 (7%)		
7	FUC	J	5	7	10,10,11	0.72	0	14,14,16	0.87	0		
5	NAG	K	1	5,1	14,14,15	1.66	1 (7%)	17,19,21	1.04	2 (11%)		
5	NAG	K	2	5	14,14,15	0.44	0	17,19,21	0.45	0		
5	BMA	K	3	5	11,11,12	0.78	0	15,15,17	0.89	0		
5	MAN	K	4	5	11,11,12	0.79	0	15,15,17	1.05	1 (6%)		
5	FUC	K	5	5	10,10,11	1.44	3 (30%)	14,14,16	1.03	1 (7%)		
6	NAG	L	1	6,1	14,14,15	0.83	1 (7%)	17,19,21	1.15	1 (5%)		
6	NAG	L	2	6	14,14,15	0.27	0	17,19,21	0.49	0		
6	BMA	L	3	6	11,11,12	0.91	1 (9%)	15,15,17	1.04	1 (6%)		

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	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Н	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Н	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Н	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Н	4	5	-	0/2/19/22	0/1/1/1
5	FUC	Н	5	5	-	-	0/1/1/1
6	NAG	I	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	Ι	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
7	NAG	J	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	FUC	J	4	7	-	-	0/1/1/1
7	FUC	J	5	7	-	-	0/1/1/1
5	NAG	K	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	FUC	K	5	5	-	-	0/1/1/1
6	NAG	L	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}({ ext{ iny A}})$
5	K	1	NAG	O5-C1	-5.99	1.34	1.43
4	G	4	FUC	C4-C5	2.71	1.58	1.52
5	K	5	FUC	C1-C2	2.71	1.58	1.52
5	Н	5	FUC	C1-C2	2.56	1.58	1.52
6	Ĺ	1	NAG	O5-C1	-2.49	1.39	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	G	4	FUC	O5-C5-C4	5.08	118.63	109.52
4	G	4	FUC	C3-C4-C5	4.11	116.18	109.77
7	J	1	NAG	O3-C3-C2	4.00	117.74	109.47
6	I	3	BMA	C1-O5-C5	3.85	117.40	112.19
4	G	4	FUC	C1-O5-C5	3.67	121.10	112.78

There are no chirality outliers.



5 of 20 torsion outliers are listed below:

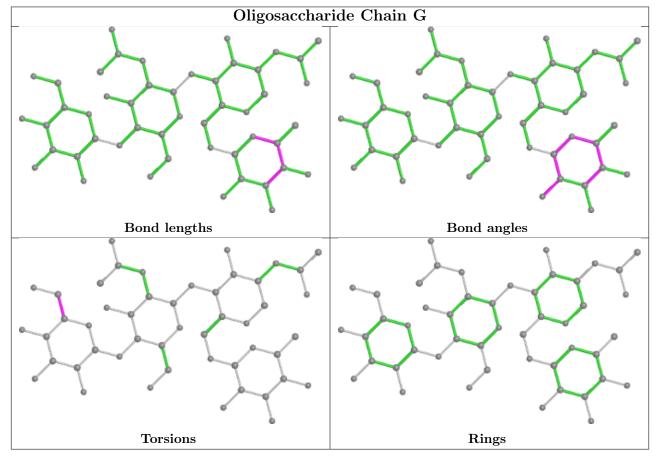
Mol	Chain	Res	Type	Atoms
5	Н	1	NAG	O5-C5-C6-O6
5	Н	1	NAG	C4-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
7	J	1	NAG	C4-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6

There are no ring outliers.

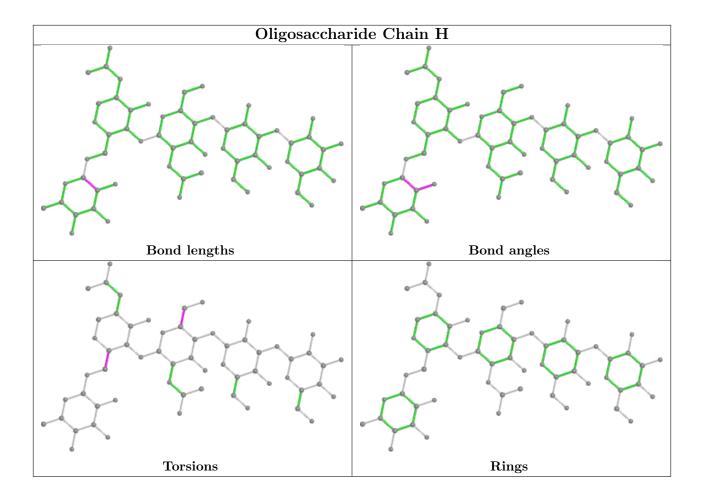
6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	5	FUC	1	0
6	I	1	NAG	1	0
7	J	4	FUC	1	0
7	J	2	NAG	1	0
7	J	1	NAG	1	0
5	K	2	NAG	1	0

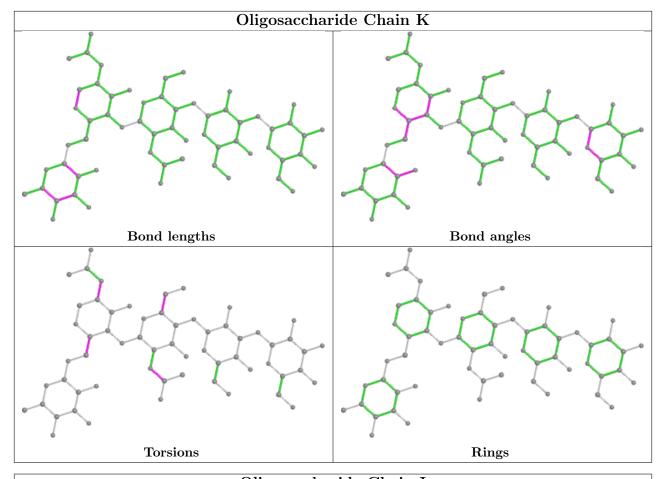
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

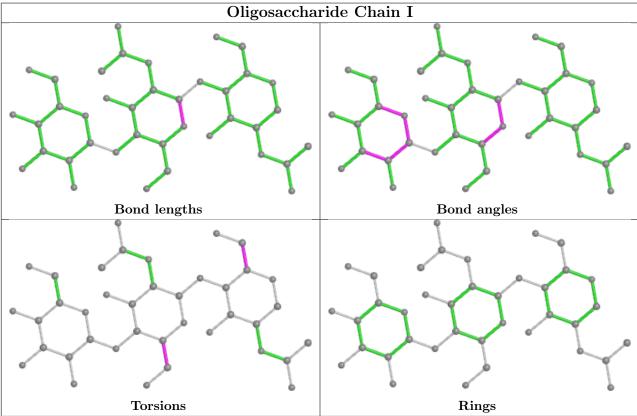




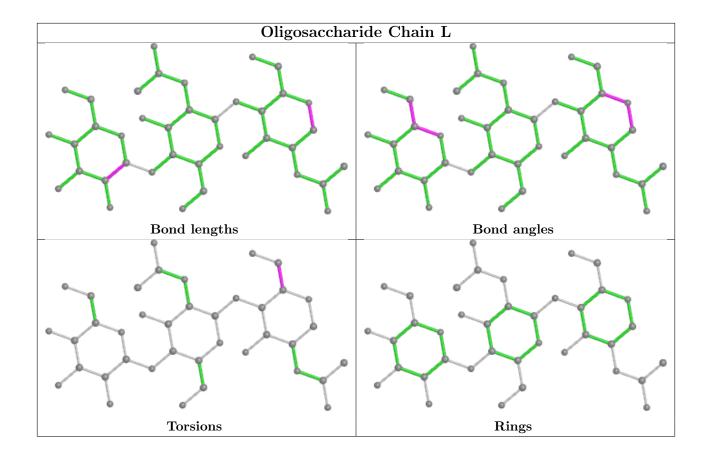




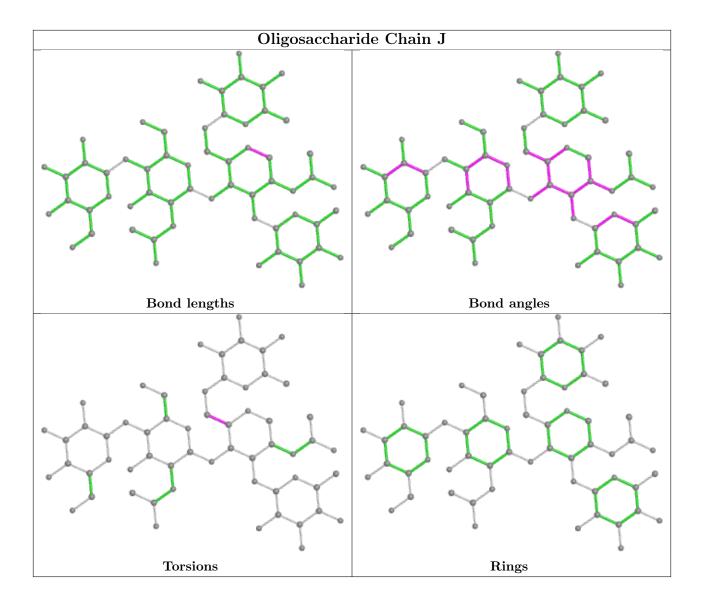












5.6 Ligand geometry (i)

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 Ch		Chain	Chain Res		Bo	Bond lengths			Bond angles		
WIOI	туре	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
8	NAG	A	701	1	14,14,15	0.41	0	17,19,21	0.47	0	
8	NAG	В	701	1	14,14,15	0.20	0	17,19,21	0.50	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
8	NAG	A	701	1	-	2/6/23/26	0/1/1/1
8	NAG	В	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

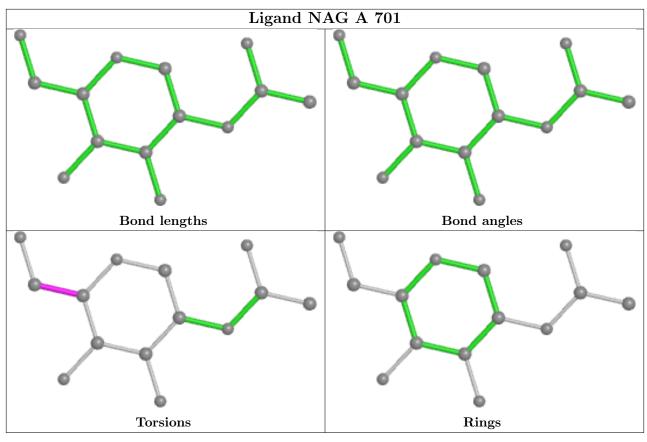
Mol	Chain	Res	Type	Atoms
8	A	701	NAG	C4-C5-C6-O6
8	В	701	NAG	C4-C5-C6-O6
8	A	701	NAG	O5-C5-C6-O6
8	В	701	NAG	O5-C5-C6-O6

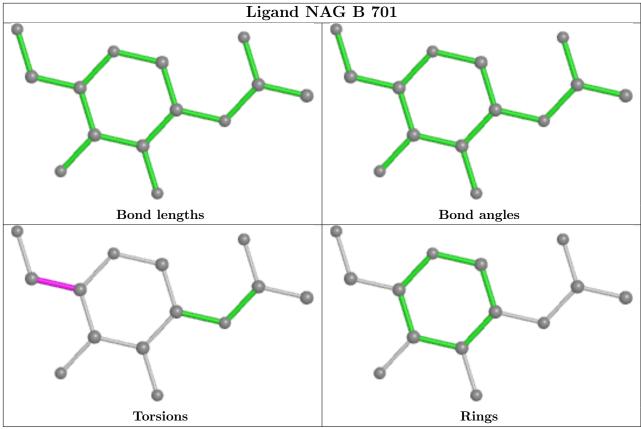
There are no ring outliers.

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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>	# RSRZ > 2	$OWAB(\AA^2)$	Q < 0.9
1	A	428/439 (97%)	-0.12	3 (0%) 87 83	56, 76, 117, 238	0
1	В	428/439 (97%)	-0.02	9 (2%) 63 53	60, 80, 135, 209	0
2	С	229/242 (94%)	-0.07	3 (1%) 77 68	61, 88, 149, 257	0
2	E	229/242 (94%)	1.78	77 (33%) 0 0	72, 123, 344, 420	0
3	D	211/214 (98%)	0.02	3 (1%) 75 66	59, 86, 154, 185	0
3	F	211/214 (98%)	1.87	81 (38%) 0 0	71, 146, 306, 416	0
All	All	1736/1790 (96%)	0.42	176 (10%) 7 5	56, 87, 278, 420	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Е	147	THR	16.0
2	Е	195	SER	13.7
3	F	177	SER	13.1
2	Е	227	VAL	12.9
2	Е	209	THR	11.5

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)

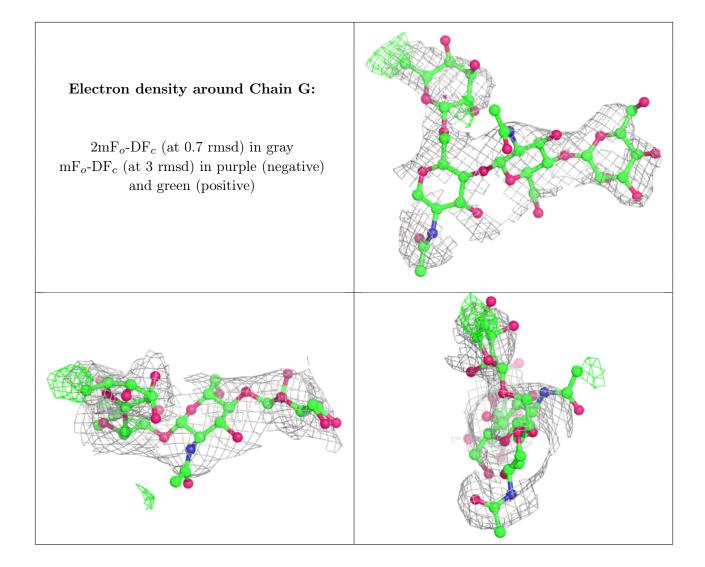
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



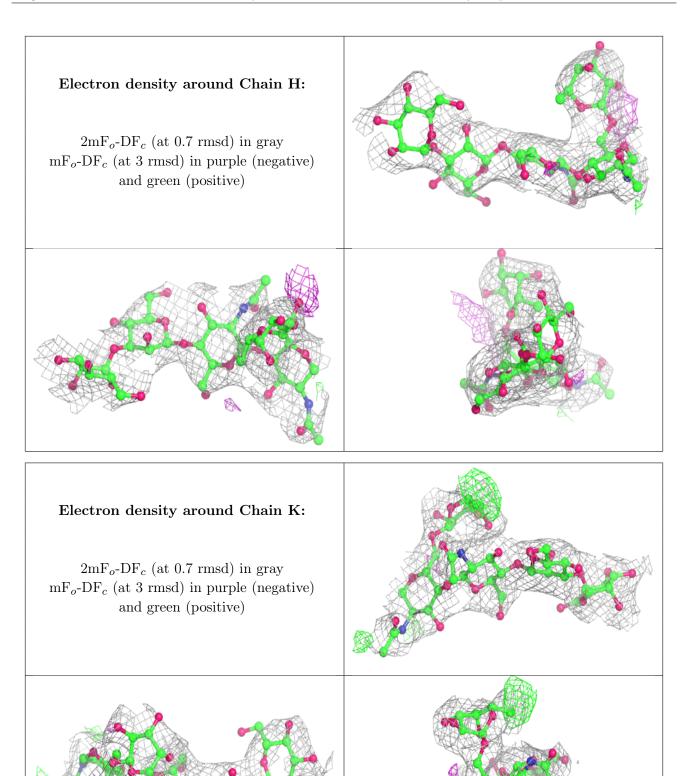
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
4	FUC	G	4	10/11	0.51	0.62	144,162,164,164	0
7	FUC	J	5	10/11	0.51	0.87	220,224,227,227	0
7	FUC	J	4	10/11	0.66	0.65	180,192,195,198	0
4	BMA	G	3	11/12	0.68	0.56	184,187,195,196	0
6	BMA	I	3	11/12	0.71	0.54	154,168,170,173	0
5	FUC	K	5	10/11	0.72	0.28	119,134,139,147	0
6	BMA	L	3	11/12	0.80	0.33	148,162,168,172	0
7	BMA	J	3	11/12	0.80	0.38	156,161,165,166	0
6	NAG	I	2	14/15	0.81	0.37	145,152,160,167	0
7	NAG	J	1	14/15	0.82	0.44	144,160,179,190	0
5	NAG	K	1	14/15	0.82	0.28	98,106,122,124	0
5	FUC	Н	5	10/11	0.84	0.43	100,110,114,119	0
5	MAN	Н	4	11/12	0.85	0.33	172,179,183,186	0
7	NAG	J	2	14/15	0.87	0.40	167,172,177,184	0
6	NAG	L	2	14/15	0.87	0.45	112,135,151,163	0
5	MAN	K	4	11/12	0.87	0.44	175,183,185,186	0
5	BMA	Н	3	11/12	0.87	0.45	175,179,187,188	0
6	NAG	I	1	14/15	0.88	0.23	114,122,134,140	0
6	NAG	L	1	14/15	0.91	0.28	114,117,128,136	0
5	BMA	K	3	11/12	0.91	0.45	145,159,169,175	0
4	NAG	G	1	14/15	0.91	0.23	101,116,147,150	0
4	NAG	G	2	14/15	0.91	0.48	159,166,171,179	0
5	NAG	Н	2	14/15	0.92	0.35	97,128,142,162	0
5	NAG	K	2	14/15	0.92	0.43	110,127,141,150	0
5	NAG	Н	1	14/15	0.93	0.25	94,103,110,111	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.





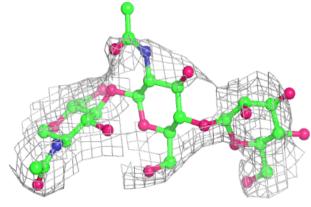


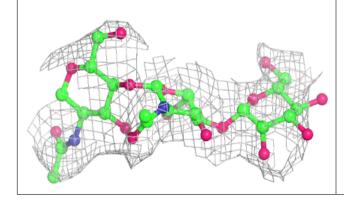


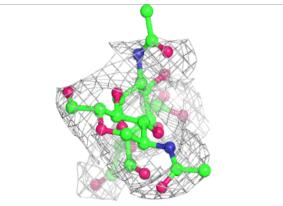


Electron density around Chain I:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

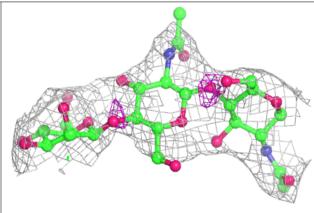


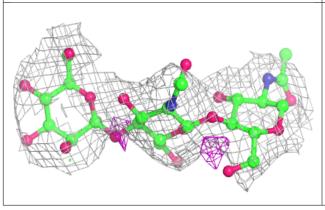


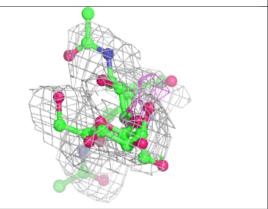


Electron density around Chain L:

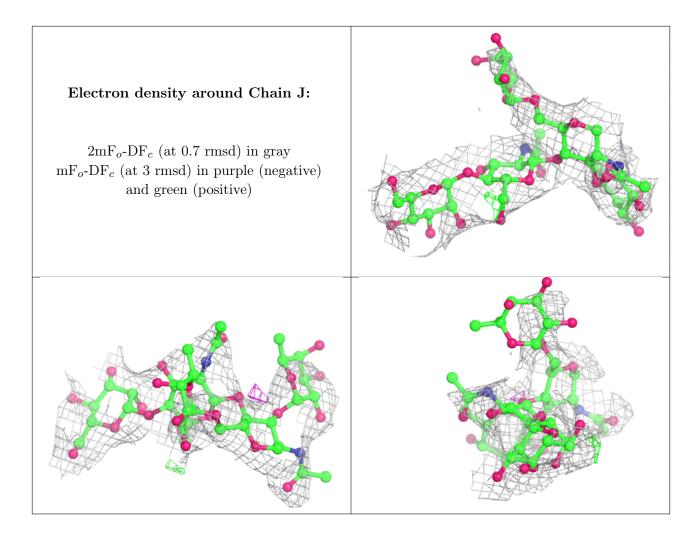
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











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	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
8	NAG	В	701	14/15	0.75	0.55	150,166,172,174	0
8	NAG	A	701	14/15	0.76	0.57	134,150,155,156	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around NAG B 701: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around NAG A 701: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

