

wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 11:37 PM EDT

:	6WXA
:	Crystal structure of truncated Streptococcal bacteriophage hyaluronidase com-
	plexed with unsaturated hyaluronan hexa-saccharides
:	Deivanayagam, C.; Schormann, N.
	2020-05-10
:	2.30 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:

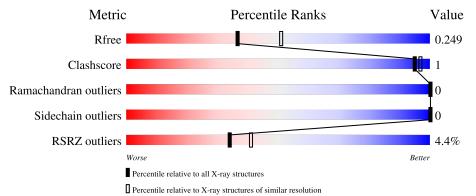
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.35.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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		20.2	5%	
1	A	293	91%	• 6%
1	В	293	4% 92%	• 6%
1	С	293	3% 92%	• 6%
2	D	6	83%	17%
2	G	6	67%	33%



Mol	Chain	Length	Quality of chain							
3	Е	5	100%							
4	F	4	75%	25%						
4	Н	4	75%	25%						



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6656 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	276	Total 2075	C 1284	N 365	O 419	${ m S} 7$	0	1	0
1	В	275	Total 2062	C 1277	N 363	0 415	${f S}7$	0	0	0
1	С	274	Total 2053	C 1271	N 361	0 414	S 7	0	0	0

• Molecule 1 is a protein called Hyaluronan lyase.

There are 24	discrepancies	hetween	the modelled	and	reference sequences:
There are 24	uiscrepancies	Detween	the modelled	anu	reference sequences.

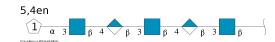
Chain	Residue	Modelled	Actual	Comment	Reference
А	372	LEU	-	expression tag	UNP P15316
А	373	GLU	-	expression tag	UNP P15316
А	374	HIS	-	expression tag	UNP P15316
А	375	HIS	-	expression tag	UNP P15316
А	376	HIS	-	expression tag	UNP P15316
А	377	HIS	-	expression tag	UNP P15316
А	378	HIS	-	expression tag	UNP P15316
А	379	HIS	-	expression tag	UNP P15316
В	372	LEU	-	expression tag	UNP P15316
В	373	GLU	-	expression tag	UNP P15316
В	374	HIS	-	expression tag	UNP P15316
В	375	HIS	-	expression tag	UNP P15316
В	376	HIS	-	expression tag	UNP P15316
В	377	HIS	-	expression tag	UNP P15316
В	378	HIS	-	expression tag	UNP P15316
В	379	HIS	-	expression tag	UNP P15316
С	372	LEU	-	expression tag	UNP P15316
С	373	GLU	-	expression tag	UNP P15316
С	374	HIS	-	expression tag	UNP P15316
С	375	HIS	-	expression tag	UNP P15316
С	376	HIS	-	expression tag	UNP P15316
С	377	HIS	-	expression tag	UNP P15316
С	378	HIS	-	expression tag	UNP P15316
	-			O i 1	on nort nago

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WIDE

Chain	Residue	Modelled	Actual	Comment	Reference	
С	379	HIS	-	expression tag	UNP P15316	

• Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1 -3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-aceta mido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	6	Total C N O 78 42 3 33	0	0	0
2	G	6	Total C N O 78 42 3 33	0	0	0

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-bet a-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-gl ucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total 67	C 36	N 3	O 28	0	0	0

• Molecule 4 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1 -3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues				ZeroOcc	AltConf	Trace
4	F	4	Total 52		N 2	0	0	0



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
4	Н	4	Total C 52 28	N 2	O 22	0	0	0

• Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Ni 1 1	0	0

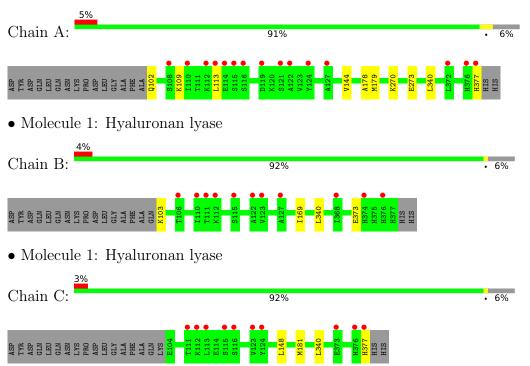
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	39	Total O 39 39	0	0
6	В	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	0	0
6	С	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	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: Hyaluronan lyase

 $\label{eq:model} \bullet \mbox{ Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-beta-D-glucopyranose (1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-beta-D-glucopyranose (1-4)-beta-D-g$

Chain D:	83%	17%
NAG1 BDP2 NAG3 BDP4 GCD6 GCD6		

 $\label{eq:model} \bullet \mbox{Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranose acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranose acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranose acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranose acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranose acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose anose-(1-4)-beta-D-glucopyranose acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose acid-(1-3)-2-acetamido-2-deoxy-b$

PROTEIN DATA BANK

Chain G:	67%		33%
		W_ORLDWIDE	
		WOKE DWIDE	

NAG1 BDP2 NAG3 BDP4 NAG5 NAG5 GCD6

 $\label{eq:constraint} \bullet \mbox{Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose \mbox{(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose} \label{eq:constraint}$

Chain E:

100%

NAG1 BDP2 NAG3 BDP4 NAG5

 \bullet Molecule 4: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyr anose

Chain F:	75%	25%
NAG1 BDP2 MAG3 GCD4 GCD4		

 \bullet Molecule 4: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyr anose

Chain H: 75% 25%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	67.30Å 86.49Å 168.23Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.91 - 2.30	Depositor
	44.91 - 2.30	EDS
% Data completeness	99.5(44.91-2.30)	Depositor
(in resolution range)	99.6(44.91-2.30)	EDS
R_{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.20 (at 2.29 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.210 , 0.243	Depositor
It, Itfree	0.213 , 0.249	DCC
R_{free} test set	2231 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor ($Å^2$)	41.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 27.5	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6656	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: NI, NAG, BDP, GCD

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		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.72	0/2102	0.80	0/2822	
1	В	0.71	0/2089	0.80	0/2804	
1	С	0.73	0/2080	0.80	0/2793	
All	All	0.72	0/6271	0.80	0/8419	

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	А	2075	0	2095	14	0
1	В	2062	0	2090	5	0
1	С	2053	0	2077	7	0
2	D	78	0	55	0	0
2	G	78	0	55	0	0
3	Е	67	0	51	0	0
4	F	52	0	37	0	0
4	Н	52	0	37	0	0
5	В	1	0	0	0	0
6	A	39	0	0	0	0



Mol	0	Non-H	1 0	H(added)	Clashes	Symm-Clashes
6	В	47	0	0	0	0
6	С	52	0	0	0	0
All	All	6656	0	6497	16	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 1.

The worst 5 of 16 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:270:LYS:HE3	1:A:273:GLU:OE1	1.78	0.83
1:A:270:LYS:HE3	1:A:273:GLU:CD	2.00	0.81
1:A:178:ALA:HB3	1:C:181:MET:HE3	1.63	0.80
1:B:373:GLU:HG2	1:B:373:GLU:O	1.86	0.76
1:A:270:LYS:HG2	1:A:270:LYS:O	1.99	0.61

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	ntiles
1	А	275/293~(94%)	269~(98%)	6(2%)	0	100	100
1	В	273/293~(93%)	266~(97%)	7 (3%)	0	100	100
1	С	272/293~(93%)	267~(98%)	5(2%)	0	100	100
All	All	820/879~(93%)	802 (98%)	18 (2%)	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	А	226/240~(94%)	226 (100%)	0	100 100		
1	В	225/240~(94%)	225~(100%)	0	100 100		
1	С	224/240 (93%)	224 (100%)	0	100 100		
All	All	675/720~(94%)	675 (100%)	0	100 100		

There are no protein residues with a non-rotameric sidechain to report.

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains 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)

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	Mol Type Chain Res		Tipk	Bond lengths			Bond angles			
Moi Type C	Chain Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
2	NAG	D	1	2	15,15,15	0.16	0	21,21,21	0.40	0



Mol	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BDP	D	2	2	12,12,13	0.29	0	14,17,19	0.62	0
2	NAG	D	3	2	14,14,15	0.28	0	17,19,21	0.58	0
2	BDP	D	4	2	12,12,13	1.09	2 (16%)	$14,\!17,\!19$	0.90	1 (7%)
2	NAG	D	5	2	14,14,15	0.31	0	17,19,21	0.45	0
2	GCD	D	6	2	10,11,12	0.31	0	$13,\!15,\!17$	0.74	0
3	NAG	Е	1	3	$15,\!15,\!15$	0.23	0	21,21,21	0.54	0
3	BDP	Ε	2	3	12,12,13	0.32	0	$14,\!17,\!19$	0.50	0
3	NAG	Е	3	3	14,14,15	0.24	0	17,19,21	0.49	0
3	BDP	Е	4	3	12,12,13	0.42	0	$14,\!17,\!19$	1.00	0
3	NAG	Ε	5	3	14,14,15	0.30	0	$17,\!19,\!21$	0.54	0
4	NAG	F	1	4	$15,\!15,\!15$	0.14	0	21,21,21	0.37	0
4	BDP	F	2	4	12,12,13	0.32	0	$14,\!17,\!19$	0.45	0
4	NAG	F	3	4	14,14,15	0.38	0	17,19,21	0.65	0
4	GCD	F	4	4	10,11,12	2.46	4 (40%)	$13,\!15,\!17$	1.55	2 (15%)
2	NAG	G	1	2	$15,\!15,\!15$	0.32	0	21,21,21	1.14	3 (14%)
2	BDP	G	2	2	12,12,13	0.40	0	$14,\!17,\!19$	0.78	0
2	NAG	G	3	2	14,14,15	0.29	0	17,19,21	0.74	0
2	BDP	G	4	2	12,12,13	0.39	0	$14,\!17,\!19$	0.83	1 (7%)
2	NAG	G	5	2	14,14,15	0.32	0	17,19,21	0.52	0
2	GCD	G	6	2	10,11,12	0.29	0	$13,\!15,\!17$	1.04	0
4	NAG	Н	1	4	15,15,15	0.22	0	21,21,21	0.48	0
4	BDP	Н	2	4	12,12,13	0.31	0	14,17,19	0.52	0
4	NAG	Н	3	4	14,14,15	0.26	0	17,19,21	0.69	0
4	GCD	Н	4	4	10,11,12	0.20	0	13,15,17	2.85	5 (38%)

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	D	1	2	-	0/6/26/26	0/1/1/1
2	BDP	D	2	2	-	0/4/21/24	0/1/1/1
2	NAG	D	3	2	-	0/6/23/26	0/1/1/1
2	BDP	D	4	2	-	3/4/21/24	0/1/1/1
2	NAG	D	5	2	-	0/6/23/26	0/1/1/1
2	GCD	D	6	2	-	0/4/17/20	0/1/1/1
3	NAG	Е	1	3	-	0/6/26/26	0/1/1/1
3	BDP	Е	2	3	-	0/4/21/24	0/1/1/1
3	NAG	Е	3	3	-	0/6/23/26	0/1/1/1
3	BDP	Ε	4	3	-	0/4/21/24	0/1/1/1



6WXA	
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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Е	5	3	_	0/6/23/26	0/1/1/1
4	NAG	F	1	4	_	0/6/26/26	0/1/1/1
4	BDP	F	2	4	_	0/4/21/24	0/1/1/1
4	NAG	F	3	4	-	0/6/23/26	0/1/1/1
4	GCD	F	4	4	-	2/4/17/20	0/1/1/1
2	NAG	G	1	2	-	2/6/26/26	0/1/1/1
2	BDP	G	2	2	-	2/4/21/24	0/1/1/1
2	NAG	G	3	2	-	0/6/23/26	0/1/1/1
2	BDP	G	4	2	-	1/4/21/24	0/1/1/1
2	NAG	G	5	2	-	2/6/23/26	0/1/1/1
2	GCD	G	6	2	-	0/4/17/20	0/1/1/1
4	NAG	Н	1	4	-	0/6/26/26	0/1/1/1
4	BDP	Н	2	4	-	0/4/21/24	0/1/1/1
4	NAG	Н	3	4	-	0/6/23/26	0/1/1/1
4	GCD	Н	4	4	-	2/4/17/20	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
4	F	4	GCD	O5-C1	-5.40	1.37	1.45
4	F	4	GCD	O5-C5	4.20	1.43	1.37
2	D	4	BDP	O6B-C6	-3.00	1.20	1.30
4	F	4	GCD	O6B-C6	-2.35	1.23	1.30
4	F	4	GCD	C5-C6	-2.17	1.43	1.48

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

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Н	4	GCD	C2-C3-C4	-8.31	100.95	112.32
4	Н	4	GCD	C3-C4-C5	-3.34	115.95	121.60
4	F	4	GCD	C2-C3-C4	-2.80	108.49	112.32
2	G	1	NAG	O5-C5-C4	2.79	114.77	109.69
2	G	1	NAG	C3-C4-C5	2.78	115.19	110.24

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	5	NAG	C8-C7-N2-C2
2	G	5	NAG	O7-C7-N2-C2



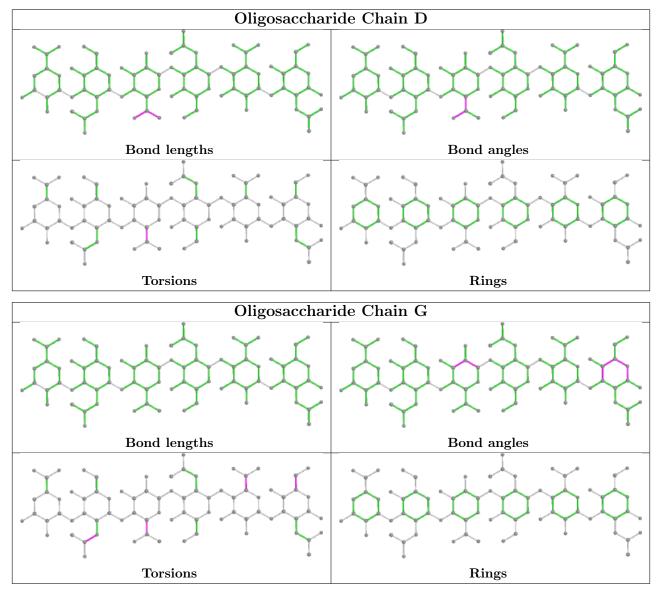
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Mol	Chain	Res	Type	Atoms
4	F	4	GCD	O5-C5-C6-O6A
2	G	1	NAG	C4-C5-C6-O6
4	F	4	GCD	O5-C5-C6-O6B

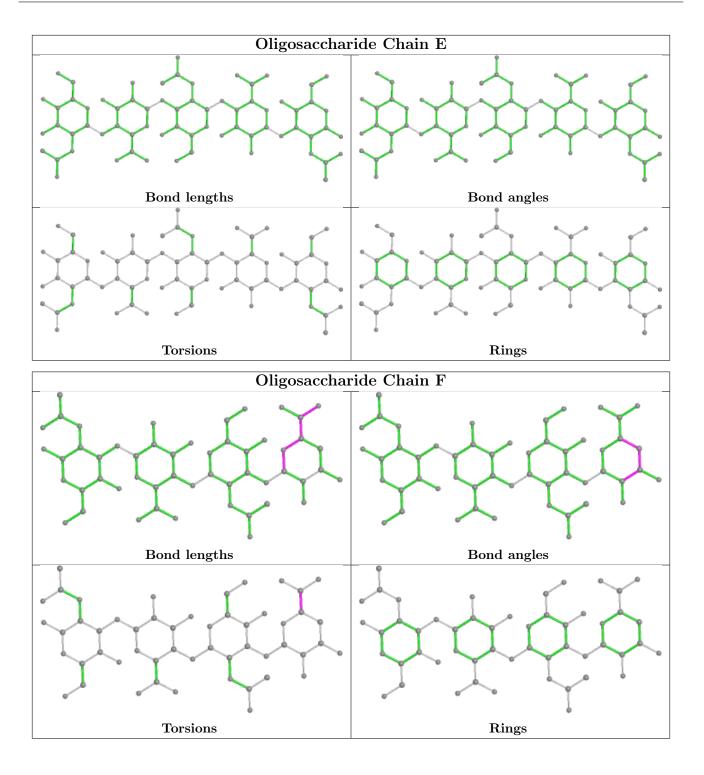
There are no ring outliers.

No monomer is involved in short contacts.

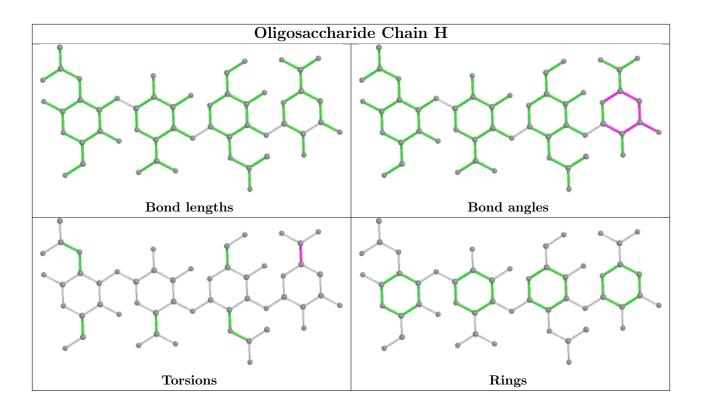
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	# RS	RZ>2	$OWAB(Å^2)$	Q<0.9
1	А	276/293~(94%)	0.16	15 (5%)	25 32	32, 47, 87, 128	0
1	В	275/293~(93%)	0.15	11 (4%)	38 45	31, 45, 87, 115	0
1	С	274/293~(93%)	0.15	10 (3%)	42 49	30, 45, 95, 117	0
All	All	825/879~(93%)	0.16	36 (4%)	34 41	30, 46, 90, 128	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	376	HIS	5.6
1	С	113	LEU	4.6
1	А	110	ILE	4.2
1	С	111	THR	3.7
1	С	377	HIS	3.6

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.

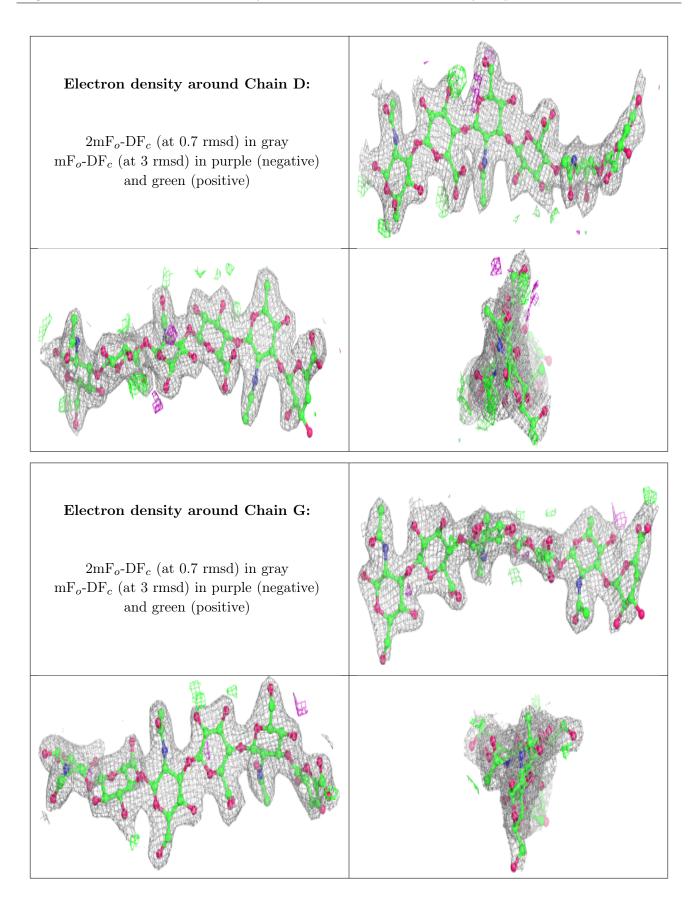
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q < 0.9
2	GCD	D	6	11/12	0.80	0.23	74,91,99,102	0
2	GCD	G	6	11/12	0.80	0.26	84,90,95,96	0
4	GCD	Н	4	11/12	0.84	0.26	66,78,86,86	0



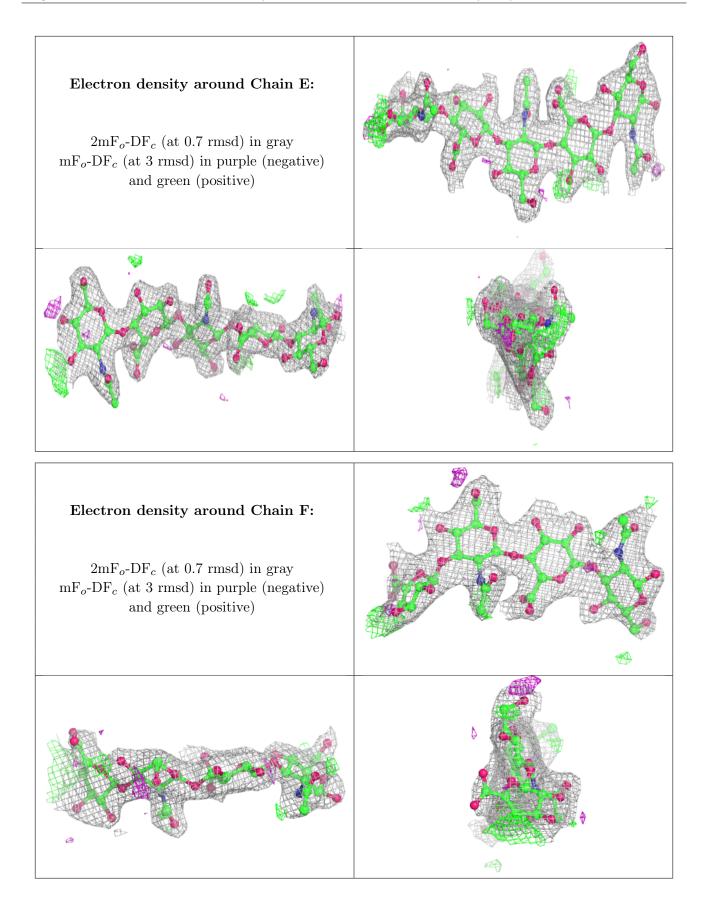
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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	$\operatorname{B-factors}(\operatorname{\AA}^2)$	$Q{<}0.9$		
4	NAG	Н	1	15/15	0.85	0.12	$46,\!66,\!72,\!73$	0		
4	GCD	F	4	11/12	0.85	0.19	66,71,83,84	0		
3	NAG	Е	5	14/15	0.86	0.14	46,55,64,64	0		
4	NAG	F	1	15/15	0.89	0.14	52,63,69,69	0		
2	NAG	G	1	15/15	0.89	0.21	50,57,64,66	0		
2	BDP	D	2	12/13	0.91	0.13	40,44,48,48	0		
4	BDP	F	2	12/13	0.92	0.11	47,49,59,61	0		
4	NAG	Н	3	14/15	0.92	0.11	39,51,61,61	0		
3	BDP	Е	4	12/13	0.92	0.10	49,53,56,61	0		
2	NAG	D	5	14/15	0.93	0.12	47,53,64,68	0		
4	NAG	F	3	14/15	0.93	0.12	41,48,54,56	0		
2	NAG	G	5	14/15	0.93	0.14	46,54,64,65	0		
2	BDP	G	4	12/13	0.94	0.17	44,53,61,65	0		
3	NAG	Е	1	15/15	0.94	0.14	44,53,63,63	0		
4	BDP	Н	2	12/13	0.94	0.11	54,61,62,64	0		
3	BDP	Е	2	12/13	0.94	0.11	41,47,49,50	0		
2	BDP	G	2	12/13	0.94	0.12	47,54,59,64	0		
2	NAG	G	3	14/15	0.95	0.14	42,47,49,50	0		
2	NAG	D	1	15/15	0.95	0.12	42,51,59,59	0		
3	NAG	Е	3	14/15	0.96	0.11	37,44,47,49	0		
2	BDP	D	4	12/13	0.97	0.13	35,40,57,58	0		
2	NAG	D	3	14/15	0.97	0.15	32,38,40,43	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.

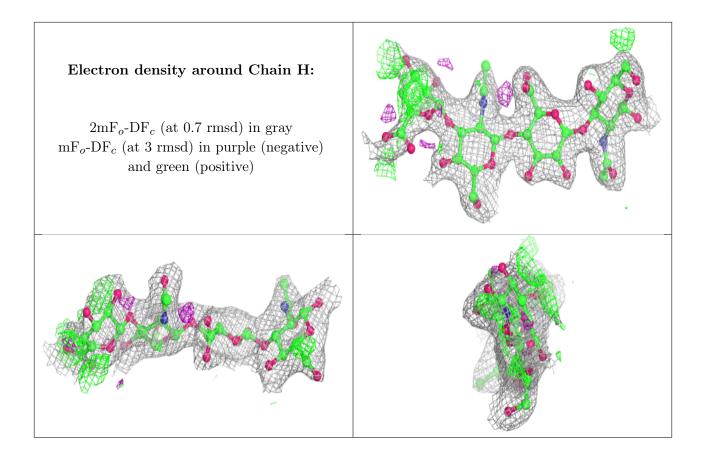












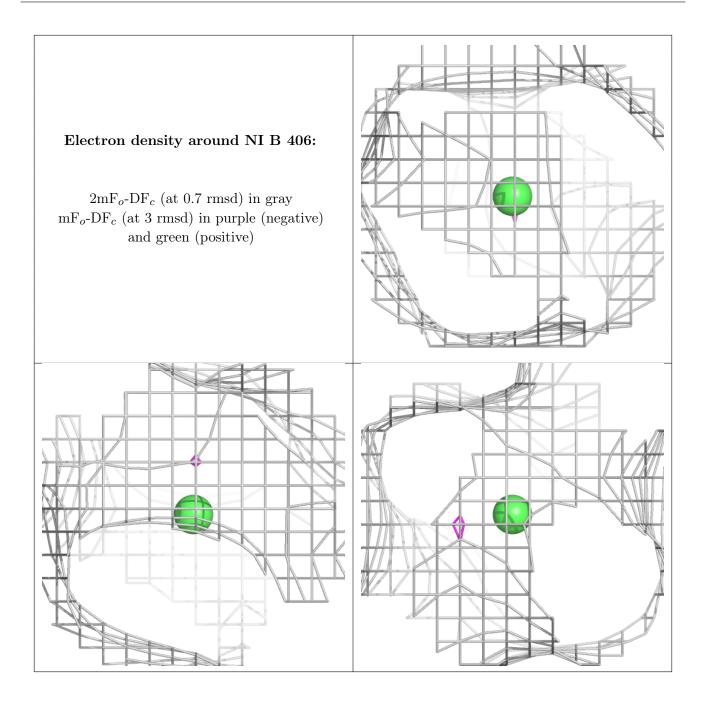
6.4 Ligands (i)

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	$B-factors(Å^2)$	Q<0.9
5	NI	В	406	1/1	0.90	0.04	80,80,80,80	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.





6.5 Other polymers (i)

There are no such residues in this entry.

