

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

Jan 21, 2024 – 12:10 am GMT

PDB ID : 7PRS

Title : Crystal Structure of the B subunit of heat labile enterotoxin LT-IIc from Es-

cherichia coli in complex with Sialyl-lacto-N-neotetraose d

Authors : Varrot, A. Deposited on : 2021-09-22

Resolution : 2.00 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:

MolProbity: 4.02b-467

Mogul : 1.8.4, 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)

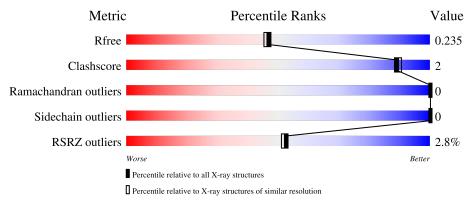
Validation Pipeline (wwPDB-VP) : 2.36

## 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 2.00 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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	DDD	104		
1	DDD	104	92%	• 5%
			5%	
1	EEE	104	91%	5%
			7%	
1	FFF	104	92%	• 5%
			2%	
1	GGG	104	90%	% 5%
			<u>%</u>	
1	ННН	104	91%	5%



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Mol	Chain	Length	Quality of chain		
1	III	104	5% 91%	•	5%
1	JJJ	104	88%	7%	5%
1	KKK	104	91%	•	5%
1	LLL	104	89%	6%	5%
1	MMM	104	93%		5%
2	DaD	5	100%		
3	GaG	4	100%		
3	JaJ	4	100%		
4	НаН	3	100%		



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8462 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 Heat-labile enterotoxin IIA, B chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	DDD	99	Total	С	N	О	S	0	0	0
1	מממ	99	750	474	127	145	4	U	U	U
1	EEE	EEE 99	Total	С	N	О	S	0	0	0
1		33	748	473	126	145	4	0	U	U
1	FFF	99	Total	$\mathbf{C}$	N	Ο	S	0	1	0
1	I. I. I.	33	745	470	125	146	4	O	1	U
1	GGG	99	Total	$\mathbf{C}$	N	O	S	0	1	0
1	aaa	33	749	475	126	144	4	O	1	U
1	ННН	99	Total	$\mathbf{C}$	N	Ο	S	0	0	0
1	111111	33	748	473	126	145	4	O	O .	U
1	III	99	Total	С	N	O	S	0	1	0
1	111	33	752	477	127	144	4	O		U
1	JJJ	99	Total	С	N	O	S	0	0	0
1	333	33	758	480	129	145	4	0	0	U
1	KKK	99	Total	$\mathbf{C}$	N	О	S	0	0	0
1	IXIXIX	33	748	473	126	145	4	0	0	U
1	LLL	99	Total	$\mathbf{C}$	N	O	S	0	0	0
1	LUL	33	748	473	126	145	4		U	U
1	MMM	99	Total	$\mathbf{C}$	N	O	S	0	0	0
1	141141141	33	750	474	127	145	4			U

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	99	HIS	-	expression tag	UNP H6W8F2
DDD	100	HIS	-	expression tag	UNP H6W8F2
DDD	101	HIS	-	expression tag	UNP H6W8F2
DDD	102	HIS	-	expression tag	UNP H6W8F2
DDD	103	HIS	-	expression tag	UNP H6W8F2
DDD	104	HIS	-	expression tag	UNP H6W8F2
EEE	99	HIS	-	expression tag	UNP H6W8F2
EEE	100	HIS	-	expression tag	UNP H6W8F2
EEE	101	HIS	-	expression tag	UNP H6W8F2



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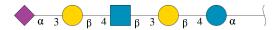
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	102	HIS	-	expression tag	UNP H6W8F2
EEE	103	HIS	_	expression tag	UNP H6W8F2
EEE	104	HIS	-	expression tag	UNP H6W8F2
FFF	99	HIS	-	expression tag	UNP H6W8F2
FFF	100	HIS	-	expression tag	UNP H6W8F2
FFF	101	HIS	-	expression tag	UNP H6W8F2
FFF	102	HIS	-	expression tag	UNP H6W8F2
FFF	103	HIS	-	expression tag	UNP H6W8F2
FFF	104	HIS	-	expression tag	UNP H6W8F2
GGG	99	HIS	-	expression tag	UNP H6W8F2
GGG	100	HIS	-	expression tag	UNP H6W8F2
GGG	101	HIS	-	expression tag	UNP H6W8F2
GGG	102	HIS	-	expression tag	UNP H6W8F2
GGG	103	HIS	-	expression tag	UNP H6W8F2
GGG	104	HIS	-	expression tag	UNP H6W8F2
ННН	99	HIS	-	expression tag	UNP H6W8F2
ННН	100	HIS	-	expression tag	UNP H6W8F2
ННН	101	HIS	-	expression tag	UNP H6W8F2
ННН	102	HIS	-	expression tag	UNP H6W8F2
ННН	103	HIS	-	expression tag	UNP H6W8F2
ННН	104	HIS	-	expression tag	UNP H6W8F2
III	99	HIS	-	expression tag	UNP H6W8F2
III	100	HIS	-	expression tag	UNP H6W8F2
III	101	HIS	-	expression tag	UNP H6W8F2
III	102	HIS	-	expression tag	UNP H6W8F2
III	103	HIS	-	expression tag	UNP H6W8F2
III	104	HIS	-	expression tag	UNP H6W8F2
JJJ	99	HIS	-	expression tag	UNP H6W8F2
JJJ	100	HIS	-	expression tag	UNP H6W8F2
JJJ	101	HIS	-	expression tag	UNP H6W8F2
JJJ	102	HIS	-	expression tag	UNP H6W8F2
JJJ	103	HIS	-	expression tag	UNP H6W8F2
JJJ	104	HIS	-	expression tag	UNP H6W8F2
KKK	99	HIS	-	expression tag	UNP H6W8F2
KKK	100	HIS	-	expression tag	UNP H6W8F2
KKK	101	HIS	-	expression tag	UNP H6W8F2
KKK	102	HIS	-	expression tag	UNP H6W8F2
KKK	103	HIS	-	expression tag	UNP H6W8F2
KKK	104	HIS	-	expression tag	UNP H6W8F2
LLL	99	HIS	-	expression tag	UNP H6W8F2
LLL	100	HIS	-	expression tag	UNP H6W8F2
LLL	101	HIS	-	expression tag	UNP H6W8F2



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Continued	trom	nremous	naae.

Chain	Residue	Modelled	Actual	Comment	Reference
LLL	102	HIS	-	expression tag	UNP H6W8F2
LLL	103	HIS	-	expression tag	UNP H6W8F2
LLL	104	HIS	-	expression tag	UNP H6W8F2
MMM	99	HIS	-	expression tag	UNP H6W8F2
MMM	100	HIS	-	expression tag	UNP H6W8F2
MMM	101	HIS	-	expression tag	UNP H6W8F2
MMM	102	HIS	-	expression tag	UNP H6W8F2
MMM	103	HIS	-	expression tag	UNP H6W8F2
MMM	104	HIS	-	expression tag	UNP H6W8F2

• Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose.



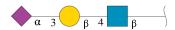
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	DaD	5	Total C N O 68 37 2 29	0	0	0

• Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	GaG	4	Total 57				0	0	0
3	JaJ	4	Total 57	C 31		O 24	0	0	0

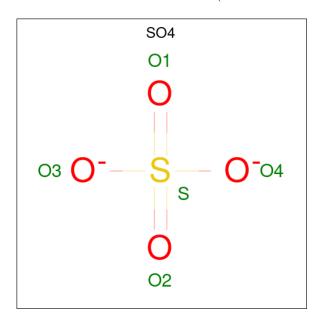
• Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
4	НаН	3	Total 45	C 25	N 2	O 18	0	0	0

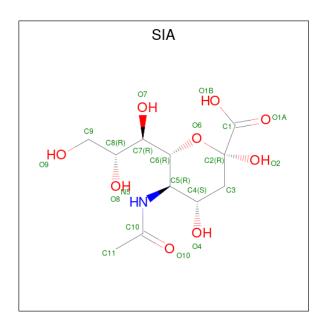
 $\bullet$  Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	DDD	1	Total O S 5 4 1	0	0
5	EEE	1	Total O S 5 4 1	0	0
5	FFF	1	Total O S 5 4 1	0	0
5	ННН	1	Total O S 5 4 1	0	0

• Molecule 6 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
6	III	1	Total C N O	0	0		
	111	1	21 11 1 9				
6	JJJ	1	Total C N O	0	0		
0	999	333	000	1	21 11 1 9	U	U
6	KKK	1	Total C N O	0	0		
0	MMM	1	21 11 1 9	U	0		
6	TTT	1	Total C N O	0	0		
0	LLL	1	20 11 1 8	U	0		

#### • Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	DDD	71	Total O 73 73	0	2
7	EEE	61	Total O 64 64	0	3
7	FFF	45	Total O 46 46	0	1
7	GGG	56	Total O 58 58	0	2
7	ННН	73	Total O 75 75	0	2
7	III	57	Total O 59 59	0	2
7	JJJ	68	Total O 69 69	0	1
7	KKK	69	Total O 70 70	0	1



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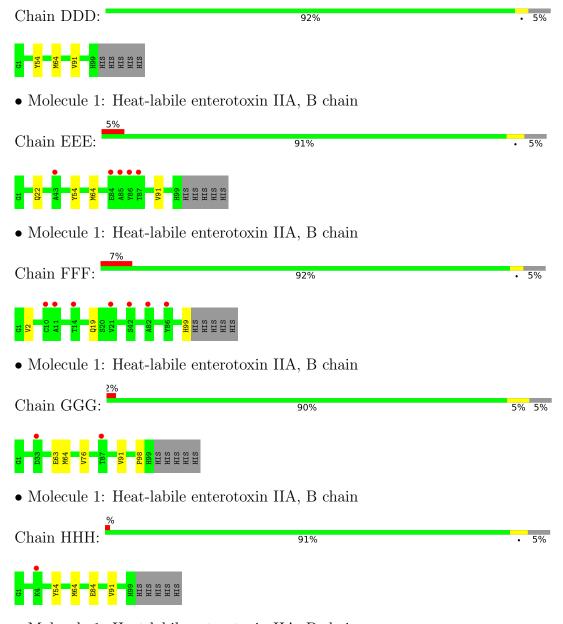
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	LLL	54	Total O 56 56	0	2
7	MMM	62	Total O 66 66	0	4



## 3 Residue-property plots (i)

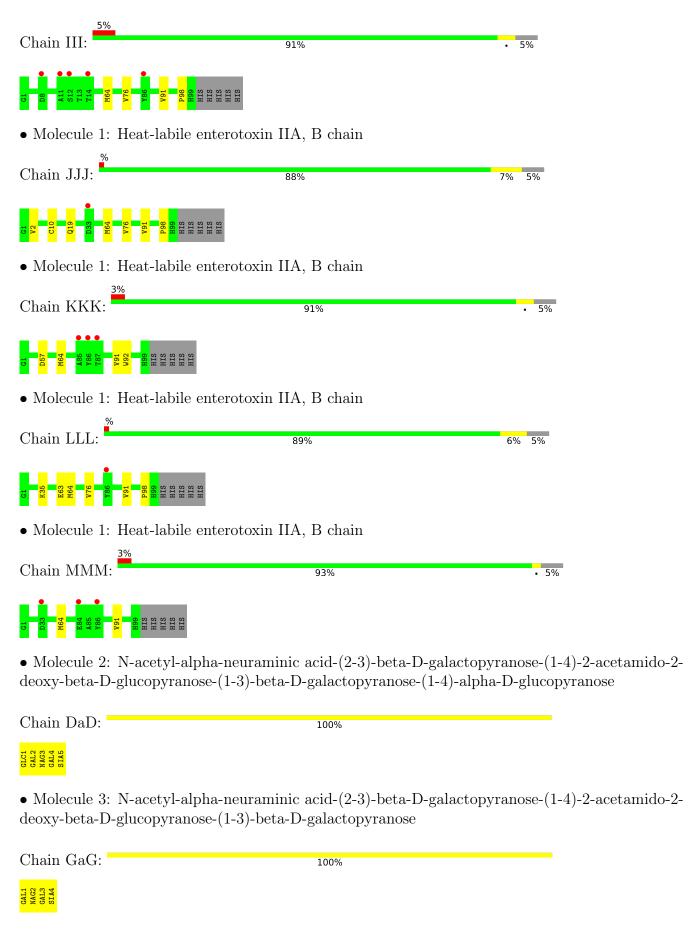
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Heat-labile enterotoxin IIA, B chain







v	alpha-neuraminic acid-(2-3)-beta-D-galactor mose-(1-3)-beta-D-galactopyranose	pyranose-(1-4)-2-acetamido-2-
Chain JaJ:	100%	
GAL1 NAG2 GAL3 SIA4		
• Molecule 4: N-acetyl-adeoxy-beta-D-glucopyra	alpha-neuraminic acid-(2-3)-beta-D-galactor nose	pyranose-(1-4)-2-acetamido-2-
Chain HaH:	100%	

NAG1 GAL2 SIA3



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	73.09Å 121.27Å 126.73Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	38.54 - 2.00	Depositor
Resolution (A)	38.51 - 2.00	EDS
% Data completeness	99.9 (38.54-2.00)	Depositor
(in resolution range)	100.0 (38.51-2.00)	EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.33  (at  2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
$R, R_{free}$	0.188 , $0.230$	Depositor
it, it free	0.196 , $0.235$	DCC
$R_{free}$ test set	4010  reflections  (5.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, 49.5	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8462	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 46.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1140e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: SIA, GLC, SO4, GAL, NAG

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).

Mal	Mol Chain		Bond lengths		ond angles
IVIOI	Moi Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	DDD	0.90	0/766	0.93	1/1043 (0.1%)
1	EEE	0.87	0/764	0.90	1/1041 (0.1%)
1	FFF	0.84	0/761	0.93	1/1041 (0.1%)
1	GGG	0.90	1/765~(0.1%)	0.91	0/1044
1	ННН	0.92	1/764 (0.1%)	0.93	1/1041 (0.1%)
1	III	0.88	0/768	0.90	0/1047
1	JJJ	0.87	0/774	0.92	0/1051
1	KKK	0.86	0/764	0.91	0/1041
1	LLL	0.90	1/764~(0.1%)	0.91	0/1041
1	MMM	0.92	0/766	0.96	0/1043
All	All	0.89	$3/7656 \ (0.0\%)$	0.92	$4/10433 \ (0.0\%)$

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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	GGG	63	GLU	CD-OE1	-8.51	1.16	1.25
1	ННН	84	GLU	CD-OE1	-6.88	1.18	1.25
1	LLL	63	GLU	CD-OE1	-5.11	1.20	1.25

#### All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	EEE	54	TYR	CB-CG-CD1	-5.84	117.49	121.00
1	DDD	54	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	ННН	54	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	FFF	99	HIS	CA-C-O	5.25	131.13	120.10

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	DDD	750	0	734	2	0
1	EEE	748	0	727	3	0
1	FFF	745	0	710	1	0
1	GGG	749	0	724	3	0
1	ННН	748	0	727	2	0
1	III	752	0	733	3	0
1	JJJ	758	0	756	5	0
1	KKK	748	0	727	4	0
1	LLL	748	0	727	4	0
1	MMM	750	0	734	2	0
2	DaD	68	0	58	0	0
3	GaG	57	0	49	0	0
3	JaJ	57	0	49	0	0
4	НаН	45	0	38	0	0
5	DDD	5	0	0	0	0
5	EEE	5	0	0	0	0
5	FFF	5	0	0	0	0
5	ННН	5	0	0	0	0
6	III	21	0	18	0	0
6	JJJ	21	0	18	0	0
6	KKK	21	0	18	1	0
6	LLL	20	0	17	0	0
7	DDD	73	0	0	0	0
7	EEE	64	0	0	1	0
7	FFF	46	0	0	0	0
7	GGG	58	0	0	0	0
7	ННН	75	0	0	0	0
7	III	59	0	0	0	0
7	JJJ	69	0	0	1	0
7	KKK	70	0	0	0	0
7	LLL	56	0	0	0	0
7	MMM	66	0	0	0	0
All	All	8462	0	7564	28	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 (28) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:KKK:57:ASP:OD1	1:LLL:35:LYS:HE3	1.84	0.76
1:JJJ:76:VAL:HG13	1:JJJ:98:PRO:HA	1.76	0.67
1:GGG:64:MET:HE1	1:GGG:91:VAL:HG12	1.76	0.66
1:EEE:64:MET:CE	1:EEE:91:VAL:HG12	2.27	0.64
1:KKK:64:MET:CE	1:KKK:91:VAL:HG12	2.28	0.62
1:GGG:64:MET:CE	1:GGG:91:VAL:HG12	2.30	0.62
1:HHH:64:MET:CE	1:HHH:91:VAL:HG12	2.30	0.60
1:JJJ:64:MET:CE	1:JJJ:91:VAL:HG12	2.31	0.60
1:GGG:76[B]:VAL:HG13	1:GGG:98:PRO:HA	1.84	0.59
1:MMM:64:MET:CE	1:MMM:91:VAL:HG12	2.31	0.59
1:DDD:64:MET:CE	1:DDD:91:VAL:HG12	2.32	0.59
1:III:64:MET:CE	1:III:91:VAL:HG12	2.32	0.59
1:LLL:64:MET:CE	1:LLL:91:VAL:HG12	2.33	0.59
1:KKK:64:MET:HE1	1:KKK:91:VAL:HG12	1.85	0.58
1:EEE:64:MET:HE1	1:EEE:91:VAL:HG12	1.84	0.58
1:III:64:MET:HE1	1:III:91:VAL:HG12	1.86	0.57
1:JJJ:64:MET:HE1	1:JJJ:91:VAL:HG12	1.87	0.55
1:HHH:64:MET:HE1	1:HHH:91:VAL:HG12	1.87	0.55
1:LLL:64:MET:HE1	1:LLL:91:VAL:HG12	1.89	0.54
1:III:76[B]:VAL:HG13	1:III:98:PRO:HA	1.92	0.52
1:MMM:64:MET:HE1	1:MMM:91:VAL:HG12	1.92	0.52
1:DDD:64:MET:HE1	1:DDD:91:VAL:HG12	1.93	0.51
1:EEE:22:GLN:HG2	7:EEE:353[B]:HOH:O	2.15	0.46
1:FFF:2:VAL:HG21	1:FFF:19:GLN:HG2	1.99	0.43
1:JJJ:2:VAL:HG21	1:JJJ:19:GLN:HG2	2.00	0.43
1:KKK:92:TRP:CH2	6:KKK:201:SIA:H6	2.53	0.43
1:JJJ:10:CYS:HB3	7:JJJ:323:HOH:O	2.21	0.41
1:LLL:76:VAL:HG13	1:LLL:98:PRO:HA	2.03	0.41

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	DDD	97/104 (93%)	97 (100%)	0	0	100	100
1	EEE	97/104 (93%)	97 (100%)	0	0	100	100
1	FFF	98/104 (94%)	98 (100%)	0	0	100	100
1	GGG	98/104 (94%)	98 (100%)	0	0	100	100
1	ННН	97/104 (93%)	97 (100%)	0	0	100	100
1	III	98/104 (94%)	98 (100%)	0	0	100	100
1	JJJ	97/104 (93%)	97 (100%)	0	0	100	100
1	KKK	97/104 (93%)	97 (100%)	0	0	100	100
1	LLL	97/104 (93%)	97 (100%)	0	0	100	100
1	MMM	97/104 (93%)	97 (100%)	0	0	100	100
All	All	973/1040 (94%)	973 (100%)	0	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	Perce	ntiles
1	DDD	82/89 (92%)	82 (100%)	0	100	100
1	EEE	81/89 (91%)	81 (100%)	0	100	100
1	FFF	79/89 (89%)	79 (100%)	0	100	100
1	GGG	80/89 (90%)	80 (100%)	0	100	100
1	ННН	81/89 (91%)	81 (100%)	0	100	100
1	III	81/89 (91%)	81 (100%)	0	100	100
1	JJJ	84/89 (94%)	84 (100%)	0	100	100
1	KKK	81/89 (91%)	81 (100%)	0	100	100
1	LLL	81/89 (91%)	81 (100%)	0	100	100
1	MMM	82/89 (92%)	82 (100%)	0	100	100
All	All	812/890 (91%)	812 (100%)	0	100	100



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

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

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

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).

N / L 1	<b>D</b>	Cl :-	D	T ! 1-	Вс	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	DaD	1	2	12,12,12	0.44	0	17,17,17	1.32	2 (11%)
2	GAL	DaD	2	2	11,11,12	0.47	0	15,15,17	1.18	1 (6%)
2	NAG	DaD	3	2	14,14,15	1.14	1 (7%)	17,19,21	1.35	3 (17%)
2	GAL	DaD	4	2	11,11,12	1.01	0	15,15,17	1.85	5 (33%)
2	SIA	DaD	5	2	20,20,21	0.77	1 (5%)	24,28,31	1.26	3 (12%)
3	GAL	GaG	1	3	12,12,12	0.82	0	17,17,17	1.37	4 (23%)
3	NAG	GaG	2	3	14,14,15	0.95	0	17,19,21	1.40	2 (11%)
3	GAL	GaG	3	3	11,11,12	0.93	0	15,15,17	1.75	4 (26%)
3	SIA	GaG	4	3	20,20,21	0.62	1 (5%)	24,28,31	1.16	2 (8%)
4	NAG	НаН	1	4	14,14,15	1.42	1 (7%)	17,19,21	1.90	4 (23%)
4	GAL	НаН	2	4	11,11,12	0.85	0	15,15,17	1.95	3 (20%)
4	SIA	НаН	3	4	20,20,21	0.72	1 (5%)	24,28,31	1.30	4 (16%)
3	GAL	JaJ	1	3	12,12,12	0.61	0	17,17,17	1.29	3 (17%)
3	NAG	JaJ	2	3	14,14,15	1.22	1 (7%)	17,19,21	1.70	4 (23%)



Mal	Mol Type		Dag	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	GAL	JaJ	3	3	11,11,12	0.96	1 (9%)	15,15,17	1.29	2 (13%)
3	SIA	JaJ	4	3	20,20,21	1.15	2 (10%)	24,28,31	0.93	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	GLC	DaD	1	2	-	0/2/22/22	0/1/1/1
2	GAL	DaD	2	2	-	1/2/19/22	0/1/1/1
2	NAG	DaD	3	2	-	0/6/23/26	0/1/1/1
2	GAL	DaD	4	2	-	2/2/19/22	0/1/1/1
2	SIA	DaD	5	2	-	5/18/34/38	0/1/1/1
3	GAL	GaG	1	3	-	1/2/22/22	0/1/1/1
3	NAG	GaG	2	3	-	0/6/23/26	0/1/1/1
3	GAL	GaG	3	3	-	2/2/19/22	0/1/1/1
3	SIA	GaG	4	3	-	0/18/34/38	0/1/1/1
4	NAG	НаН	1	4	-	0/6/23/26	0/1/1/1
4	GAL	НаН	2	4	-	2/2/19/22	0/1/1/1
4	SIA	НаН	3	4	-	4/18/34/38	0/1/1/1
3	GAL	JaJ	1	3	-	2/2/22/22	0/1/1/1
3	NAG	JaJ	2	3	-	0/6/23/26	0/1/1/1
3	GAL	JaJ	3	3	-	0/2/19/22	0/1/1/1
3	SIA	JaJ	4	3	_	3/18/34/38	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
3	$_{ m JaJ}$	4	SIA	O1B-C1	-3.73	1.18	1.30
2	DaD	3	NAG	C1-C2	3.15	1.57	1.52
3	JaJ	4	SIA	C2-C1	2.92	1.55	1.52
4	НаН	1	NAG	C1-C2	2.59	1.56	1.52
3	GaG	4	SIA	O1B-C1	-2.20	1.23	1.30
2	DaD	5	SIA	C2-C1	2.18	1.54	1.52
4	НаН	3	SIA	O1B-C1	-2.15	1.23	1.30
3	JaJ	3	GAL	C1-C2	2.06	1.56	1.52
3	JaJ	2	NAG	C4-C3	2.00	1.57	1.52

All (46) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
4	НаН	2	GAL	C1-O5-C5	5.87	120.14	112.19
4	НаН	1	NAG	O5-C1-C2	-4.54	104.11	111.29
2	DaD	1	GLC	C4-C3-C2	-3.97	103.90	110.82
4	НаН	1	NAG	O5-C5-C6	3.60	112.84	107.20
3	JaJ	2	NAG	O5-C5-C6	3.53	112.73	107.20
4	НаН	1	NAG	C1-O5-C5	3.49	116.92	112.19
2	DaD	5	SIA	O1B-C1-C2	3.32	122.51	113.03
3	JaJ	2	NAG	O4-C4-C5	-3.29	101.13	109.30
2	DaD	4	GAL	C2-C3-C4	-3.26	105.26	110.89
3	GaG	3	GAL	O3-C3-C2	-3.26	103.76	109.99
3	GaG	1	GAL	C3-C4-C5	3.10	115.77	110.24
4	НаН	2	GAL	O5-C5-C6	3.05	111.99	107.20
4	НаН	3	SIA	O1B-C1-C2	3.04	121.72	113.03
3	GaG	2	NAG	C2-N2-C7	-3.04	118.57	122.90
2	DaD	4	GAL	O5-C1-C2	-3.04	106.08	110.77
2	DaD	4	GAL	O4-C4-C3	-2.88	103.69	110.35
3	JaJ	1	GAL	C1-O5-C5	2.86	119.05	113.66
2	DaD	3	NAG	C1-O5-C5	2.85	116.06	112.19
3	GaG	4	SIA	C3-C4-C5	-2.83	108.04	111.46
2	DaD	3	NAG	O4-C4-C5	-2.81	102.32	109.30
3	GaG	3	GAL	C3-C4-C5	2.72	115.09	110.24
4	НаН	1	NAG	C6-C5-C4	-2.70	106.67	113.00
2	DaD	4	GAL	C1-C2-C3	2.68	112.96	109.67
2	DaD	5	SIA	C3-C4-C5	-2.57	108.35	111.46
4	НаН	3	SIA	O6-C2-C1	2.56	112.72	107.70
3	JaJ	3	GAL	O5-C1-C2	-2.50	106.91	110.77
3	GaG	2	NAG	C1-C2-N2	2.50	114.75	110.49
3	GaG	1	GAL	O1-C1-C2	2.44	115.91	109.03
3	GaG	3	GAL	O2-C2-C1	2.38	114.02	109.15
3	GaG	3	GAL	O5-C5-C6	2.34	110.88	107.20
3	GaG	4	SIA	C8-C7-C6	-2.24	108.78	113.03
3	JaJ	1	GAL	O5-C5-C6	2.24	112.02	106.44
2	DaD	1	GLC	C6-C5-C4	-2.23	107.78	113.00
3	JaJ	2	NAG	C8-C7-N2	2.23	119.87	116.10
4	НаН	3	SIA	C3-C4-C5	-2.22	108.78	111.46
2	DaD	5	SIA	O1A-C1-C2	-2.19	117.39	122.57
3	JaJ	1	GAL	O5-C1-C2	2.18	114.17	110.28
4	НаН	3	SIA	O1A-C1-C2	-2.17	117.43	122.57
2	DaD	4	GAL	O3-C3-C2	-2.15	105.88	109.99
2	DaD	2	GAL	O5-C1-C2	-2.14	107.46	110.77
3	GaG	1	GAL	O5-C1-C2	-2.13	106.48	110.28
3	GaG	1	GAL	O2-C2-C1	2.11	114.05	109.16
3	JaJ	3	GAL	C6-C5-C4	2.11	117.94	113.00



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	JaJ	2	NAG	O3-C3-C2	2.09	113.80	109.47
2	DaD	3	NAG	C1-C2-N2	-2.00	107.06	110.49
4	НаН	2	GAL	O3-C3-C2	-2.00	106.16	109.99

There are no chirality outliers.

All (22) torsion outliers are listed below:

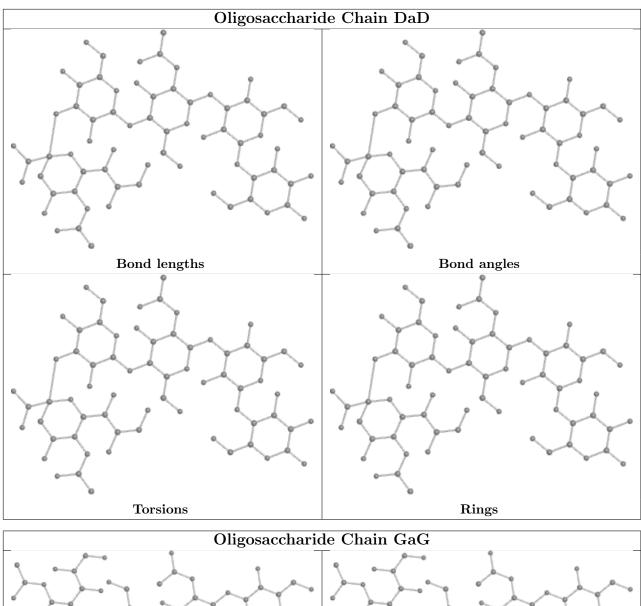
Mol	Chain	Res	Type	Atoms
4	НаН	2	GAL	O5-C5-C6-O6
4	НаН	2	GAL	C4-C5-C6-O6
3	JaJ	1	GAL	O5-C5-C6-O6
2	DaD	4	GAL	O5-C5-C6-O6
3	GaG	3	GAL	O5-C5-C6-O6
4	НаН	3	SIA	O7-C7-C8-C9
4	НаН	3	SIA	C6-C7-C8-C9
2	DaD	4	GAL	C4-C5-C6-O6
3	JaJ	1	GAL	C4-C5-C6-O6
4	НаН	3	SIA	C6-C7-C8-O8
3	GaG	3	GAL	C4-C5-C6-O6
4	НаН	3	SIA	O7-C7-C8-O8
2	DaD	5	SIA	C6-C7-C8-O8
3	JaJ	4	SIA	C6-C7-C8-O8
2	DaD	5	SIA	C6-C7-C8-C9
2	DaD	5	SIA	O7-C7-C8-C9
3	GaG	1	GAL	C4-C5-C6-O6
3	JaJ	4	SIA	C6-C7-C8-C9
2	DaD	5	SIA	O7-C7-C8-O8
2	DaD	5	SIA	O1B-C1-C2-O6
3	JaJ	4	SIA	O7-C7-C8-C9
2	DaD	2	GAL	C4-C5-C6-O6

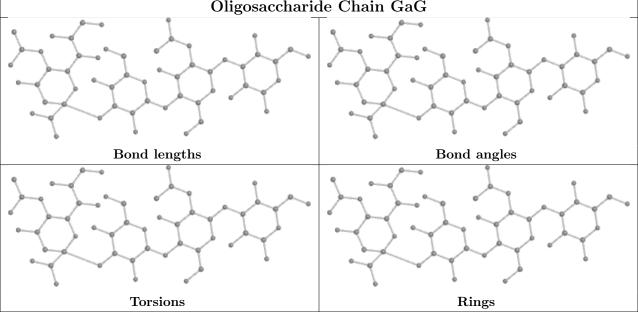
There are no ring outliers.

No monomer is involved in short contacts.

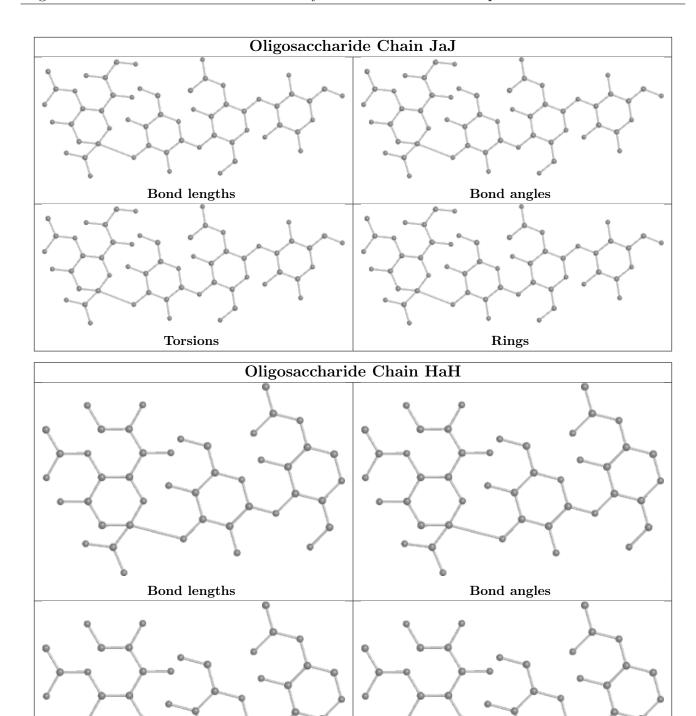
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry (i)

Torsions

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

Rings



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	ths	В	ond ang	les
IVIOI	Type	Chain	rtes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SIA	III	201	-	21,21,21	0.59	0	25,31,31	1.01	1 (4%)
5	SO4	FFF	201	-	4,4,4	0.32	0	6,6,6	0.49	0
5	SO4	DDD	201	-	4,4,4	0.46	0	6,6,6	0.22	0
6	SIA	LLL	201	-	20,20,21	0.81	1 (5%)	24,28,31	0.85	1 (4%)
5	SO4	ННН	201	-	4,4,4	0.52	0	6,6,6	0.27	0
6	SIA	JJJ	201	-	21,21,21	0.71	1 (4%)	25,31,31	0.96	2 (8%)
6	SIA	KKK	201	-	21,21,21	0.73	1 (4%)	25,31,31	0.97	1 (4%)
5	SO4	EEE	201	-	4,4,4	0.45	0	6,6,6	0.12	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
6	SIA	III	201	-	-	7/20/38/38	0/1/1/1
6	SIA	KKK	201	-	-	6/20/38/38	0/1/1/1
6	SIA	LLL	201	-	-	8/18/34/38	0/1/1/1
6	SIA	JJJ	201	-	-	8/20/38/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
6	LLL	201	SIA	O1B-C1	-2.65	1.21	1.30
6	JJJ	201	SIA	O1B-C1	-2.24	1.21	1.30
6	KKK	201	SIA	O1B-C1	-2.18	1.22	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
6	III	201	SIA	O1A-C1-C2	-4.05	117.46	123.59
6	KKK	201	SIA	O1A-C1-C2	-3.12	118.87	123.59
6	JJJ	201	SIA	O1A-C1-C2	-2.58	119.69	123.59



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
6	JJJ	201	SIA	O2-C2-O6	-2.36	103.42	109.42
6	LLL	201	SIA	O1B-C1-C2	2.27	119.50	113.03

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	III	201	SIA	C6-C7-C8-O8
6	III	201	SIA	O7-C7-C8-C9
6	III	201	SIA	O7-C7-C8-O8
6	III	201	SIA	C7-C8-C9-O9
6	III	201	SIA	O8-C8-C9-O9
6	KKK	201	SIA	C6-C7-C8-C9
6	KKK	201	SIA	O7-C7-C8-C9
6	LLL	201	SIA	C6-C7-C8-C9
6	LLL	201	SIA	C6-C7-C8-O8
6	LLL	201	SIA	O7-C7-C8-C9
6	LLL	201	SIA	O7-C7-C8-O8
6	KKK	201	SIA	O7-C7-C8-O8
6	KKK	201	SIA	C6-C7-C8-O8
6	LLL	201	SIA	C11-C10-N5-C5
6	LLL	201	SIA	O10-C10-N5-C5
6	III	201	SIA	C6-C7-C8-C9
6	LLL	201	SIA	C7-C8-C9-O9
6	JJJ	201	SIA	C6-C7-C8-O8
6	LLL	201	SIA	O8-C8-C9-O9
6	JJJ	201	SIA	C7-C8-C9-O9
6	JJJ	201	SIA	O8-C8-C9-O9
6	JJJ	201	SIA	C6-C7-C8-C9
6	JJJ	201	SIA	O1A-C1-C2-C3
6	III	201	SIA	O1A-C1-C2-O6
6	JJJ	201	SIA	O7-C7-C8-O8
6	KKK	201	SIA	O1B-C1-C2-C3
6	JJJ	201	SIA	O7-C7-C8-C9
6	JJJ	201	SIA	O1A-C1-C2-O6
6	KKK	201	SIA	O1A-C1-C2-O2

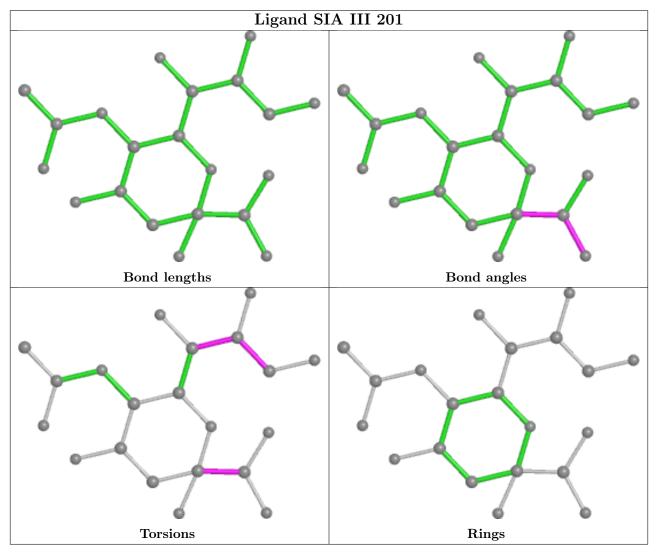
There are no ring outliers.

1 monomer is involved in 1 short contact:

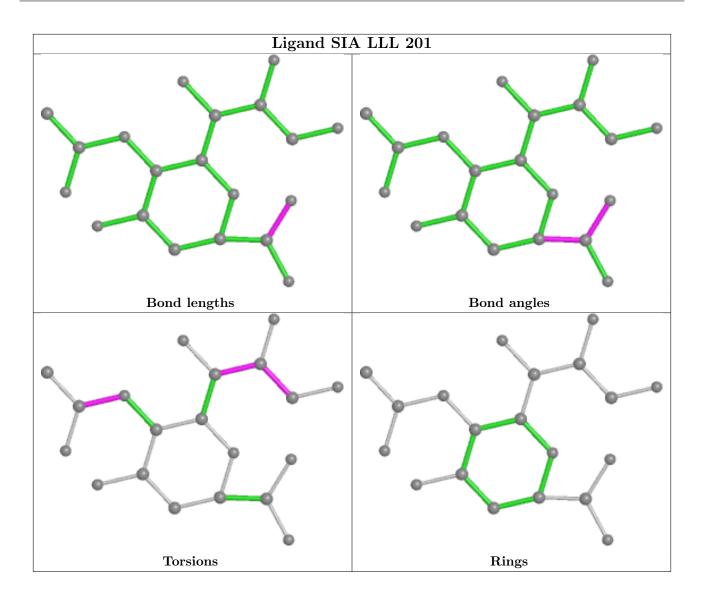


Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	KKK	201	SIA	1	0

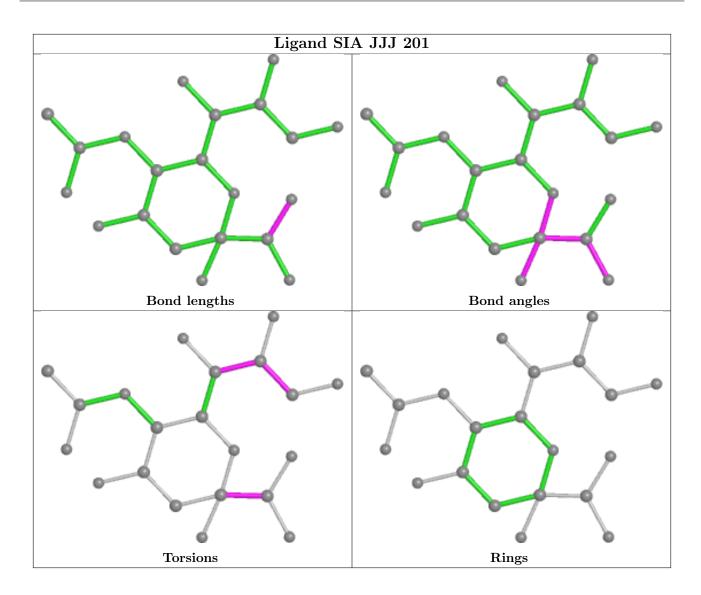
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



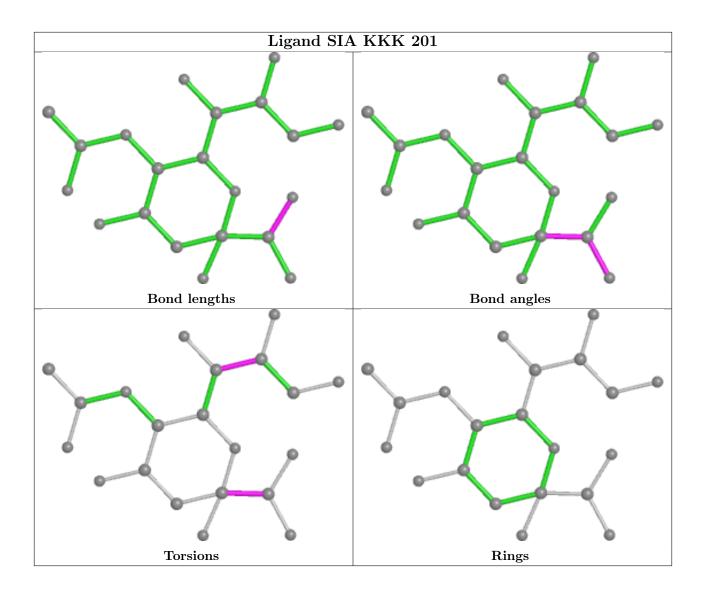












## 5.7 Other polymers (i)

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	$OWAB(Å^2)$	Q < 0.9
1	DDD	99/104 (95%)	-0.07	0 100 100	22, 33, 47, 53	0
1	EEE	99/104 (95%)	0.24	5 (5%) 28 27	24, 37, 56, 60	2 (2%)
1	FFF	99/104 (95%)	0.49	7 (7%) 16 15	28, 42, 59, 71	0
1	GGG	99/104 (95%)	0.15	2 (2%) 65 63	26, 40, 57, 63	0
1	ННН	99/104 (95%)	-0.01	1 (1%) 82 81	23, 34, 48, 56	0
1	III	99/104 (95%)	0.36	5 (5%) 28 27	25, 38, 58, 64	0
1	JJJ	99/104 (95%)	0.09	1 (1%) 82 81	25, 36, 52, 67	0
1	KKK	99/104 (95%)	0.13	3 (3%) 50 49	25, 36, 53, 59	0
1	LLL	99/104 (95%)	0.04	1 (1%) 82 81	23, 35, 54, 61	0
1	MMM	99/104 (95%)	0.06	3 (3%) 50 49	23, 34, 49, 60	0
All	All	990/1040 (95%)	0.15	28 (2%) 53 51	22, 37, 55, 71	2 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	11	ALA	4.0
1	MMM	86	TYR	3.3
1	EEE	86	TYR	3.2
1	EEE	84	GLU	3.1
1	FFF	86	TYR	3.0
1	EEE	87	THR	3.0
1	III	11	ALA	3.0
1	GGG	87	THR	3.0
1	KKK	85	ALA	2.8
1	III	86	TYR	2.7
1	JJJ	33	ASP	2.6
1	GGG	33	ASP	2.5
1	FFF	10	CYS	2.5



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Mol	Chain	Res	Type	RSRZ
1	FFF	21	VAL	2.4
1	III	12	SER	2.4
1	MMM	84	GLU	2.4
1	KKK	87	THR	2.3
1	FFF	14	THR	2.3
1	FFF	42	SER	2.2
1	FFF	82	ALA	2.2
1	III	8	ASP	2.2
1	LLL	86	TYR	2.1
1	MMM	33	ASP	2.1
1	ННН	4	LYS	2.1
1	EEE	85	ALA	2.1
1	III	14	THR	2.1
1	KKK	86	TYR	2.1
1	EEE	43	ALA	2.0

## 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.

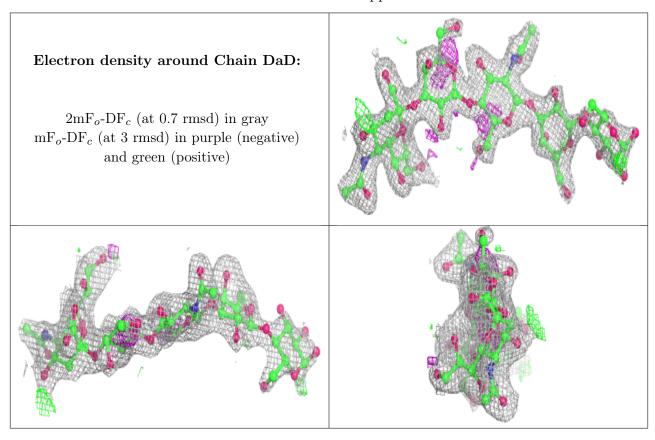
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	NAG	НаН	1	14/15	0.71	0.27	46,52,58,64	0
4	GAL	НаН	2	11/12	0.77	0.25	42,50,62,63	0
3	GAL	GaG	3	11/12	0.79	0.34	49,55,69,71	0
2	GLC	DaD	1	12/12	0.80	0.23	49,52,55,57	12
3	GAL	JaJ	1	12/12	0.81	0.18	40,54,64,67	12
2	GAL	DaD	2	11/12	0.85	0.13	42,54,61,61	11
3	GAL	GaG	1	12/12	0.86	0.20	44,69,80,81	0
2	GAL	DaD	4	11/12	0.87	0.32	39,50,59,61	0
3	GAL	JaJ	3	11/12	0.88	0.19	39,43,47,47	0
3	SIA	JaJ	4	20/21	0.88	0.13	33,42,45,48	0
2	NAG	DaD	3	14/15	0.89	0.21	35,42,47,51	0
4	SIA	НаН	3	20/21	0.89	0.15	39,46,52,52	0
3	SIA	GaG	4	20/21	0.91	0.17	39,44,50,55	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	NAG	JaJ	2	14/15	0.92	0.17	33,38,44,47	0
3	NAG	GaG	2	14/15	0.92	0.27	34,44,49,50	0
2	SIA	DaD	5	20/21	0.92	0.17	35,42,49,50	0

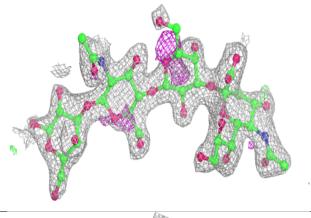
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

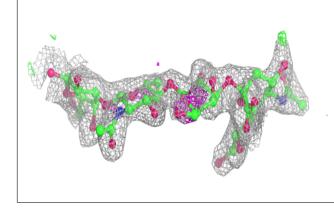


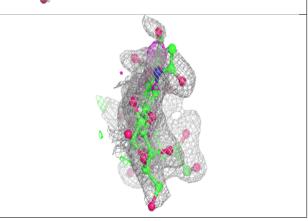


#### Electron density around Chain GaG:

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

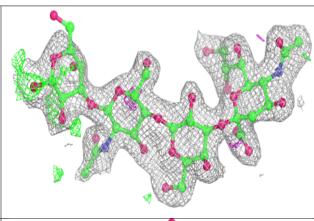


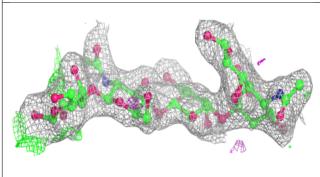


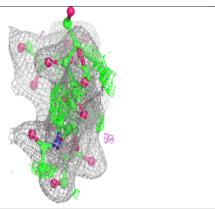


#### Electron density around Chain JaJ:

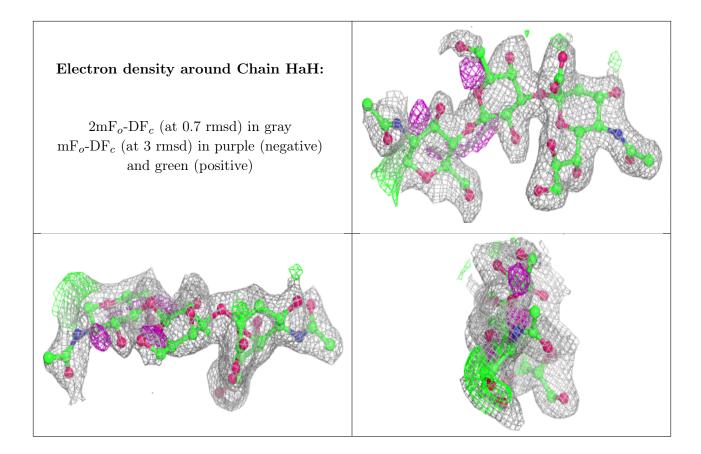
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)











## 6.4 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.

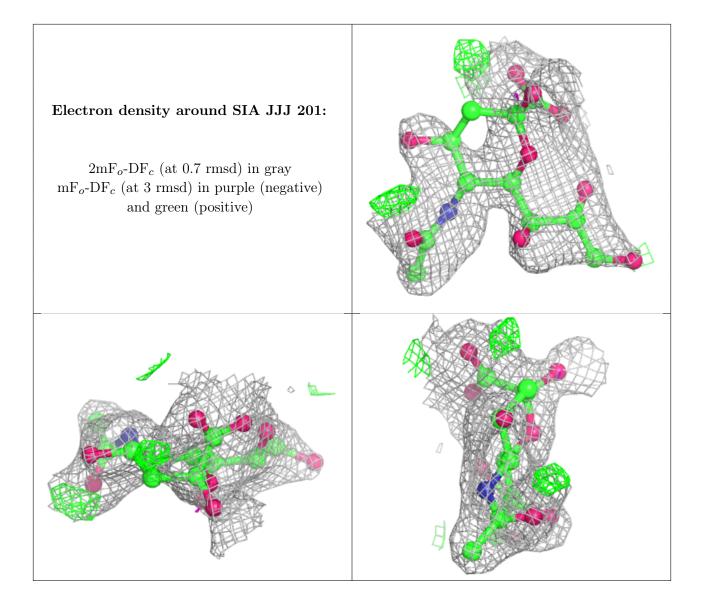
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
6	SIA	III	201	21/21	0.58	0.34	45,57,62,69	21
6	SIA	JJJ	201	21/21	0.65	0.28	51,63,67,69	20
5	SO4	FFF	201	5/5	0.69	0.32	31,35,46,48	5
6	SIA	LLL	201	20/21	0.78	0.31	47,58,62,68	20
6	SIA	KKK	201	21/21	0.79	0.29	56,63,70,95	0
5	SO4	EEE	201	5/5	0.92	0.36	43,44,48,58	5
5	SO4	DDD	201	5/5	0.95	0.33	27,31,39,44	5
5	SO4	ННН	201	5/5	0.97	0.13	27,29,42,55	5

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.

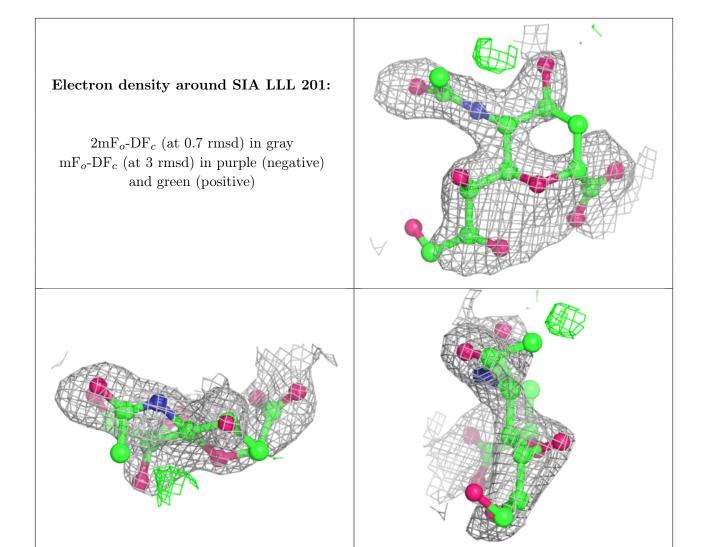


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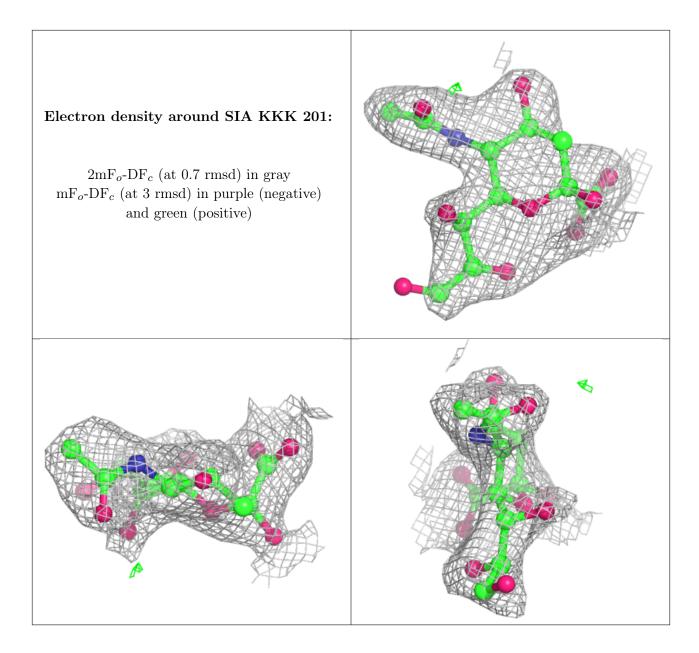












# 6.5 Other polymers (i)

There are no such residues in this entry.

