



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2017 – 01:15 AM EDT

PDB ID : 5ELB  
Title : Cholera toxin classical B-pentamer in complex with Lewis-y  
Authors : Heggelund, J.E.; Burschowsky, D.; Krengel, U.  
Deposited on : unknown  
Resolution : 1.08 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

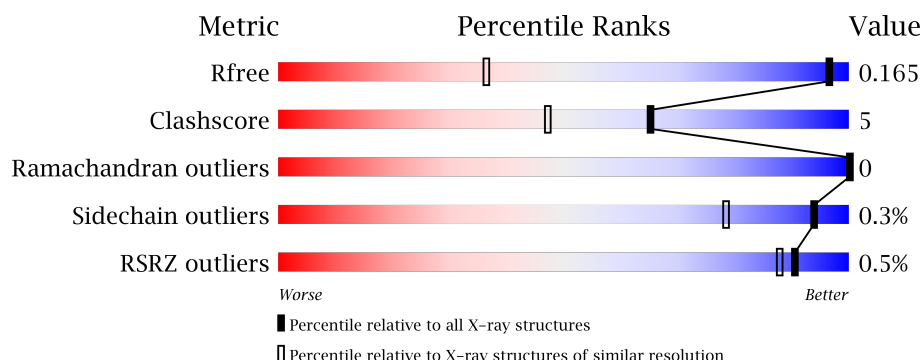
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.08 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.



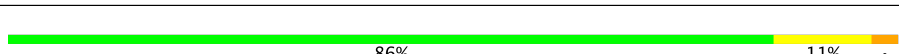
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1006 (1.12-1.04)
Clashscore	112137	1051 (1.12-1.04)
Ramachandran outliers	110173	1008 (1.12-1.04)
Sidechain outliers	110143	1006 (1.12-1.04)
RSRZ outliers	101464	1009 (1.12-1.04)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	103	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	B	103	<div> <div>86%</div> <div>14%</div> </div>
1	C	103	<div> <div>%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	D	103	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	E	103	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	103	
1	G	103	
1	H	103	
1	I	103	
1	J	103	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GAL	A	202[A]	-	-	-	X
3	GAL	B	203[A]	-	-	-	X
3	GAL	D	204[A]	-	-	-	X
3	GAL	J	1201[A]	-	-	-	X
4	GLA	A	203[B]	-	-	-	X
4	GLA	B	204[B]	-	-	-	X
4	GLA	D	205[B]	-	-	-	X
4	GLA	J	1202[B]	-	-	-	X
6	NDG	C	208[B]	-	-	-	X
6	NDG	D	208[A]	-	-	-	X
6	NDG	D	208[B]	-	-	X	X
6	NDG	H	1204	-	-	-	X
7	FUC	D	209[A]	-	-	-	X
7	FUC	D	209[B]	-	-	-	X
7	FUC	D	210[A]	-	-	-	X
7	FUC	D	210[B]	-	-	-	X
7	FUC	I	1205[A]	-	-	-	X
7	FUC	I	1205[B]	-	-	-	X
8	PEG	G	201	-	-	X	X
9	NAG	I	1204[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11575 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 Cholera enterotoxin B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	9	0
			874	553	148	167	6			
1	B	103	Total	C	N	O	S	0	11	0
			893	566	152	169	6			
1	C	103	Total	C	N	O	S	0	11	0
			900	570	155	169	6			
1	D	103	Total	C	N	O	S	0	11	0
			892	566	152	168	6			
1	E	103	Total	C	N	O	S	0	10	0
			881	561	151	163	6			
1	F	103	Total	C	N	O	S	0	10	0
			882	561	150	164	7			
1	G	103	Total	C	N	O	S	0	12	0
			894	570	153	165	6			
1	H	103	Total	C	N	O	S	0	11	0
			892	567	152	167	6			
1	I	103	Total	C	N	O	S	0	6	0
			855	542	146	161	6			
1	J	103	Total	C	N	O	S	0	9	0
			878	556	150	166	6			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

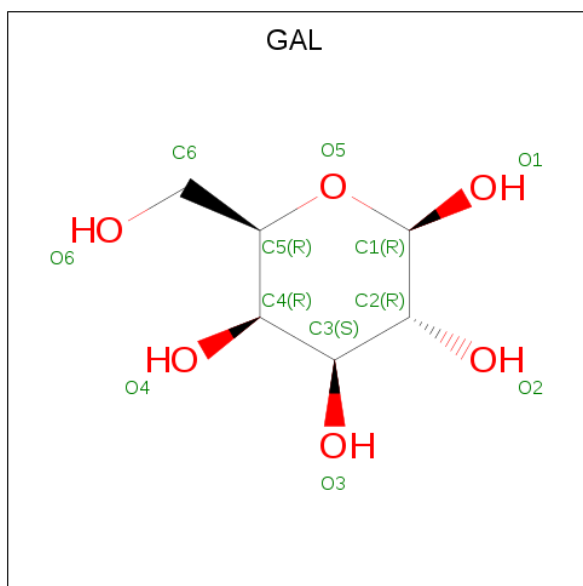
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Ca	0	0
			2	2		

- Molecule 3 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



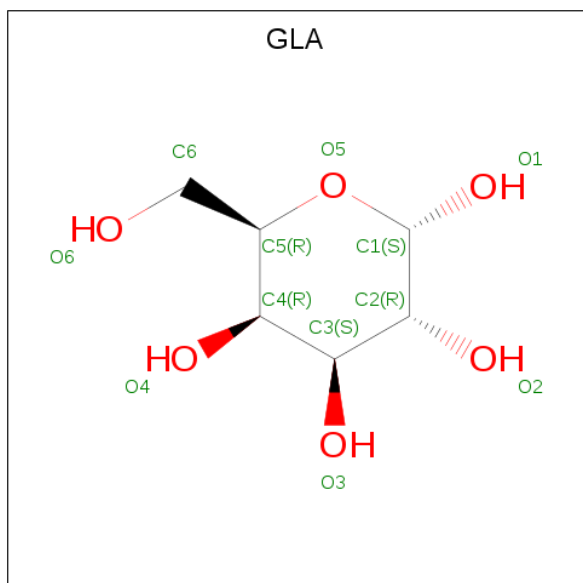
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	1
			22	12	10		
3	B	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	1
			22	12	10		
3	C	1	Total	C	O	0	1
			12	6	6		
3	C	1	Total	C	O	0	1
			22	12	10		
3	D	1	Total	C	O	0	1
			12	6	6		
3	D	1	Total	C	O	0	1
			22	12	10		
3	E	1	Total	C	O	0	1
			12	6	6		
3	E	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	1
			12	6	6		
3	F	1	Total	C	O	0	0
			11	6	5		
3	G	1	Total	C	O	0	1
			12	6	6		
3	G	1	Total	C	O	0	1
			22	12	10		
3	H	1	Total	C	O	0	1
			12	6	6		
3	H	1	Total	C	O	0	0
			11	6	5		
3	I	1	Total	C	O	0	1
			12	6	6		
3	I	1	Total	C	O	0	1
			22	12	10		
3	J	1	Total	C	O	0	1
			12	6	6		
3	J	1	Total	C	O	0	1
			22	12	10		

- Molecule 4 is ALPHA D-GALACTOSE (three-letter code: GLA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



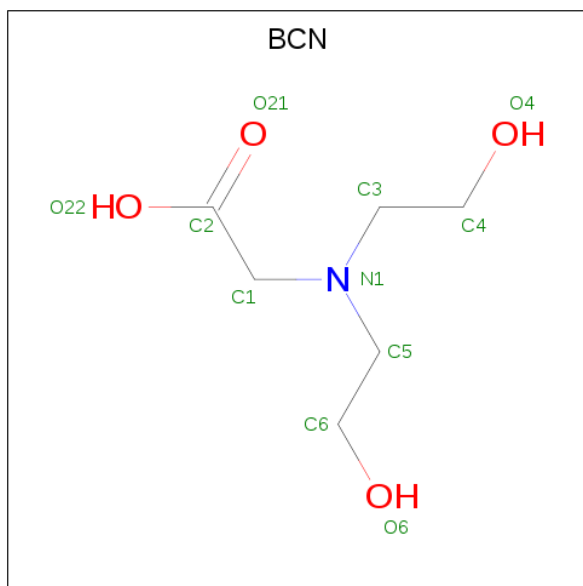
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			12	6	6		
4	C	1	Total	C	O	0	1
			12	6	6		
4	D	1	Total	C	O	0	1
			12	6	6		
4	E	1	Total	C	O	0	1
			12	6	6		
4	F	1	Total	C	O	0	1
			12	6	6		
4	G	1	Total	C	O	0	1
			12	6	6		
4	H	1	Total	C	O	0	1
			12	6	6		
4	I	1	Total	C	O	0	1
			12	6	6		
4	J	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is BICINE (three-letter code: BCN) (formula:  $C_6H_{13}NO_4$ ).



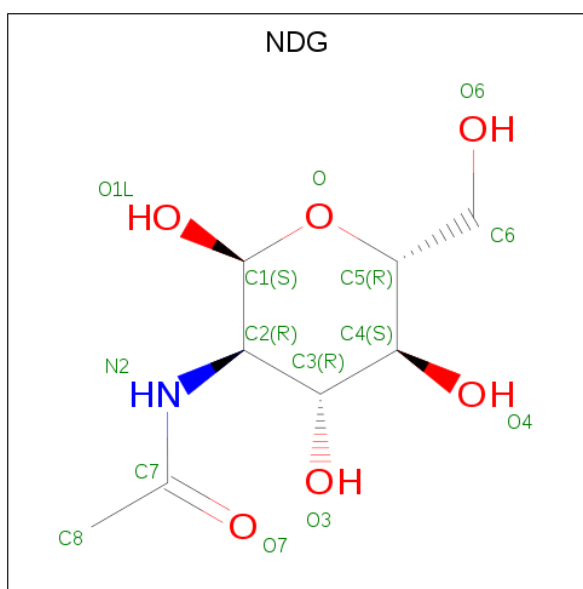
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	6	1	4		
5	A	1	Total	C	N	O	0	0
			11	6	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			11	6	1	4		
5	B	1	Total	C	N	O	0	0
			11	6	1	4		
5	C	1	Total	C	N	O	0	0
			11	6	1	4		
5	C	1	Total	C	N	O	0	0
			11	6	1	4		
5	D	1	Total	C	N	O	0	0
			11	6	1	4		
5	D	1	Total	C	N	O	0	0
			11	6	1	4		
5	E	1	Total	C	N	O	0	0
			11	6	1	4		
5	E	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 6 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	1
			30	16	2	12		
6	B	1	Total	C	N	O	0	1
			30	16	2	12		
6	C	1	Total	C	N	O	0	1
			30	16	2	12		

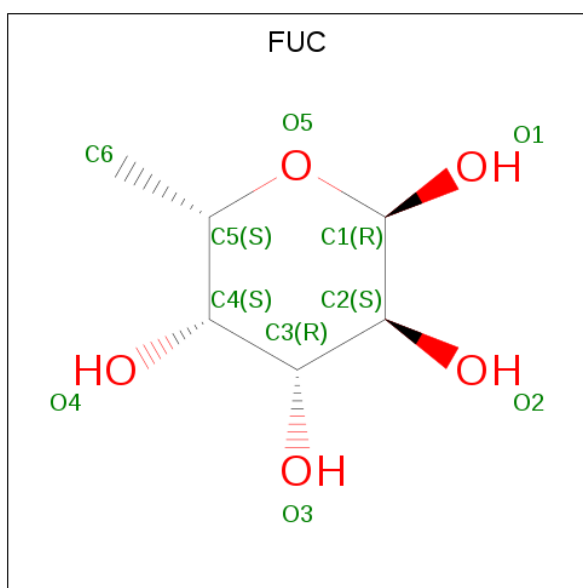
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	1
			30	16	2	12		
6	E	1	Total	C	N	O	0	0
			15	8	1	6		
6	F	1	Total	C	N	O	0	0
			15	8	1	6		
6	G	1	Total	C	N	O	0	1
			30	16	2	12		
6	H	1	Total	C	N	O	0	0
			15	8	1	6		
6	I	1	Total	C	N	O	0	1
			15	8	1	6		
6	J	1	Total	C	N	O	0	1
			15	8	1	6		

- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



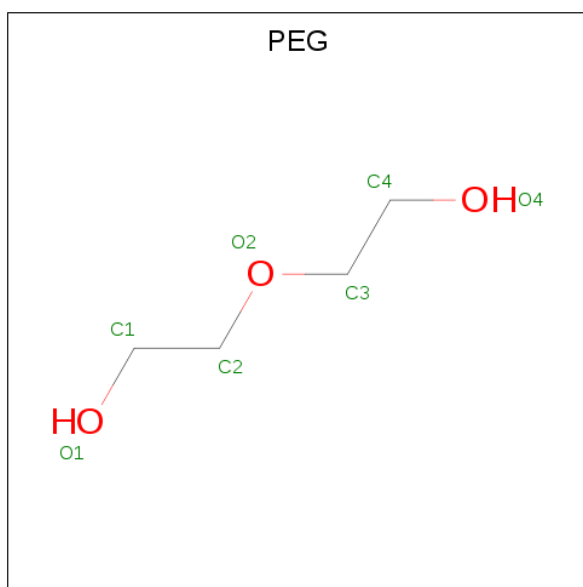
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	1
			20	12	8		
7	A	1	Total	C	O	0	1
			20	12	8		
7	B	1	Total	C	O	0	1
			20	12	8		
7	B	1	Total	C	O	0	1
			20	12	8		

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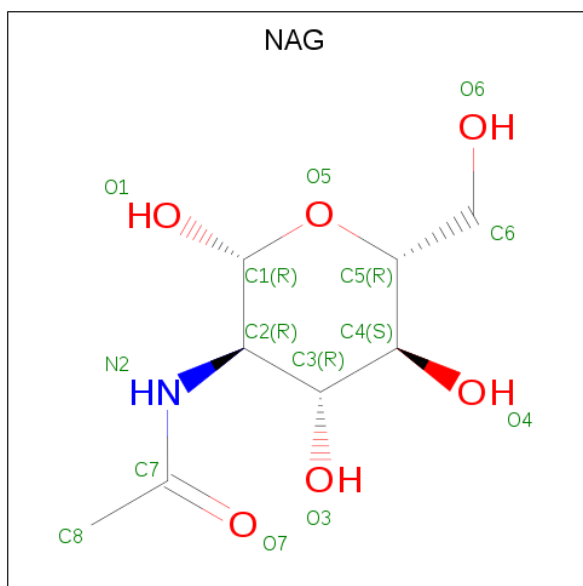
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	1
			20	12	8		
7	C	1	Total	C	O	0	1
			20	12	8		
7	D	1	Total	C	O	0	1
			20	12	8		
7	D	1	Total	C	O	0	1
			20	12	8		
7	E	1	Total	C	O	0	0
			10	6	4		
7	E	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	1
			20	12	8		
7	G	1	Total	C	O	0	1
			20	12	8		
7	H	1	Total	C	O	0	0
			10	6	4		
7	H	1	Total	C	O	0	0
			10	6	4		
7	I	1	Total	C	O	0	1
			20	12	8		
7	I	1	Total	C	O	0	1
			20	12	8		
7	J	1	Total	C	O	0	1
			20	12	8		
7	J	1	Total	C	O	0	1
			20	12	8		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	I	1	Total	C	N	O	0	1
			15	8	1	6		
9	J	1	Total	C	N	O	0	1
			15	8	1	6		


- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	161	Total 163	O 163	0	2
10	B	164	Total 169	O 169	0	5
10	C	166	Total 173	O 173	0	7
10	D	150	Total 154	O 154	0	5
10	E	140	Total 143	O 143	0	4
10	F	145	Total 147	O 147	0	2
10	G	154	Total 157	O 157	0	3
10	H	154	Total 157	O 157	0	3
10	I	156	Total 159	O 159	0	3
10	J	160	Total 163	O 163	0	3

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

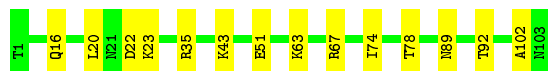
- Molecule 1: Cholera enterotoxin B subunit

Chain A: 




- Molecule 1: Cholera enterotoxin B subunit

Chain B: 



- Molecule 1: Cholera enterotoxin B subunit

Chain C: 



- Molecule 1: Cholera enterotoxin B subunit

Chain D: 

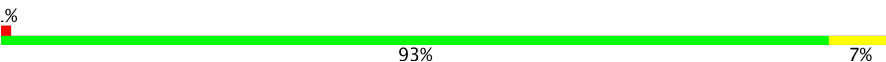


- Molecule 1: Cholera enterotoxin B subunit

Chain E: 

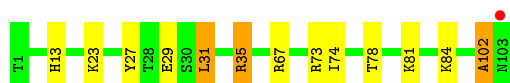
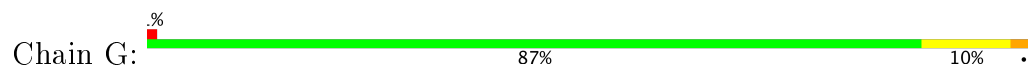


- Molecule 1: Cholera enterotoxin B subunit

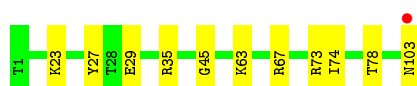
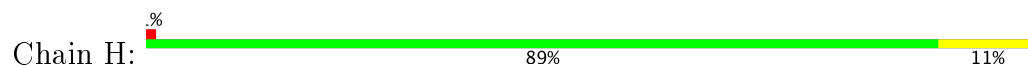
Chain F: 



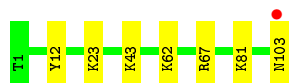
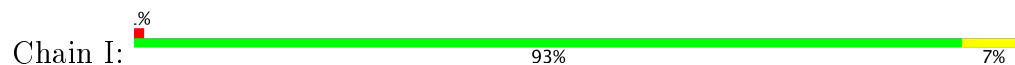
- Molecule 1: Cholera enterotoxin B subunit



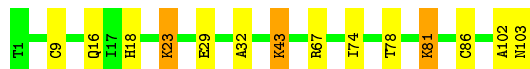
- Molecule 1: Cholera enterotoxin B subunit



- Molecule 1: Cholera enterotoxin B subunit



- Molecule 1: Cholera enterotoxin B subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.33Å 98.98Å 152.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 1.08 49.49 – 1.08	Depositor EDS
% Data completeness (in resolution range)	79.0 (49.49-1.08) 78.9 (49.49-1.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 1.08Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.120 , 0.155 0.135 , 0.165	Depositor DCC
$R_{free}$ test set	18331 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.5	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	11575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: BCN, NAG, GLA, CA, NDG, GAL, FUC, PEG

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	A	0.86	0/904	1.04	6/1219 (0.5%)
1	B	0.93	1/923 (0.1%)	0.99	6/1244 (0.5%)
1	C	0.92	0/927	1.03	5/1246 (0.4%)
1	D	0.95	0/931	1.18	4/1254 (0.3%)
1	E	0.88	1/918 (0.1%)	1.08	6/1236 (0.5%)
1	F	0.94	1/915 (0.1%)	0.98	4/1231 (0.3%)
1	G	0.92	0/937	1.02	6/1262 (0.5%)
1	H	0.91	0/925	0.88	4/1244 (0.3%)
1	I	0.95	0/882	0.96	2/1189 (0.2%)
1	J	0.95	0/909	1.13	7/1226 (0.6%)
All	All	0.92	3/9171 (0.0%)	1.03	50/12351 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	11	GLU	CD-OE1	-6.79	1.18	1.25
1	B	51	GLU	CD-OE1	-5.62	1.19	1.25
1	F	83	GLU	CD-OE2	-5.11	1.20	1.25

The worst 5 of 50 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	67[A]	ARG	NE-CZ-NH2	14.46	127.53	120.30
1	D	67[B]	ARG	NE-CZ-NH2	14.46	127.53	120.30
1	D	67[A]	ARG	NE-CZ-NH1	-12.26	114.17	120.30
1	D	67[B]	ARG	NE-CZ-NH1	-12.26	114.17	120.30
1	A	67	ARG	NE-CZ-NH1	11.11	125.86	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	ALA	Peptide
1	G	102	ALA	Peptide

## 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	874	0	888	8	0
1	B	893	0	915	8	0
1	C	900	0	920	7	0
1	D	892	0	921	18	0
1	E	881	0	911	10	0
1	F	882	0	910	6	0
1	G	894	0	928	13	0
1	H	892	0	921	8	0
1	I	855	0	872	10	0
1	J	878	0	890	9	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	34	0	29	0	0
3	B	34	0	30	0	0
3	C	34	0	30	2	0
3	D	34	0	30	3	0
3	E	23	0	21	1	0
3	F	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	34	0	30	0	0
3	H	23	0	21	0	0
3	I	34	0	30	0	0
3	J	34	0	30	1	0
4	A	12	0	12	0	0
4	B	12	0	12	0	0
4	C	12	0	12	0	0
4	D	12	0	12	0	0
4	E	12	0	12	0	0
4	F	12	0	12	0	0
4	G	12	0	12	0	0
4	H	12	0	12	0	0
4	I	12	0	12	0	0
4	J	12	0	12	0	0
5	A	22	0	20	0	0
5	B	22	0	20	0	0
5	C	22	0	20	0	0
5	D	22	0	20	0	0
5	E	22	0	20	0	0
6	A	30	0	25	0	0
6	B	30	0	26	0	0
6	C	30	0	26	1	0
6	D	30	0	26	8	0
6	E	15	0	13	0	0
6	F	15	0	13	0	0
6	G	30	0	26	0	0
6	H	15	0	13	3	0
6	I	15	0	13	0	0
6	J	15	0	13	0	0
7	A	40	0	40	2	0
7	B	40	0	40	0	0
7	C	40	0	40	1	0
7	D	40	0	40	6	0
7	E	20	0	20	0	0
7	F	20	0	20	0	0
7	G	40	0	40	0	0
7	H	20	0	20	1	0
7	I	40	0	40	0	0
7	J	40	0	40	0	0
8	G	7	0	10	4	0
9	I	15	0	13	0	0
9	J	15	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	163	0	0	4	0
10	B	169	0	0	3	1
10	C	173	0	0	2	0
10	D	154	0	0	3	0
10	E	143	0	0	6	0
10	F	147	0	0	1	0
10	G	157	0	0	3	0
10	H	157	0	0	3	0
10	I	159	0	0	3	0
10	J	163	0	0	1	1
All	All	11575	0	10138	94	1

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 5.

The worst 5 of 94 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:27[B]:TYR:OH	1:A:29[B]:GLU:OE2	1.78	1.02
1:H:27[B]:TYR:OH	1:H:29[B]:GLU:OE2	1.80	0.99
1:G:27[B]:TYR:OH	1:G:29[B]:GLU:OE2	1.81	0.98
6:D:208[B]:NDG:H6C2	7:D:210[B]:FUC:H3	1.46	0.94
1:D:103:ASN:ND2	10:D:301:HOH:O	2.06	0.87

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
10:B:310:HOH:O	10:J:1408:HOH:O[3_545]	2.03	0.17

## 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	110/103 (107%)	109 (99%)	1 (1%)	0	100	100
1	B	112/103 (109%)	111 (99%)	1 (1%)	0	100	100
1	C	112/103 (109%)	111 (99%)	1 (1%)	0	100	100
1	D	113/103 (110%)	111 (98%)	2 (2%)	0	100	100
1	E	111/103 (108%)	110 (99%)	1 (1%)	0	100	100
1	F	111/103 (108%)	110 (99%)	1 (1%)	0	100	100
1	G	113/103 (110%)	112 (99%)	1 (1%)	0	100	100
1	H	112/103 (109%)	111 (99%)	1 (1%)	0	100	100
1	I	107/103 (104%)	106 (99%)	1 (1%)	0	100	100
1	J	110/103 (107%)	109 (99%)	1 (1%)	0	100	100
All	All	1111/1030 (108%)	1100 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	98/89 (110%)	96 (98%)	2 (2%)	60	19
1	B	100/89 (112%)	100 (100%)	0	100	100
1	C	100/89 (112%)	100 (100%)	0	100	100
1	D	101/89 (114%)	101 (100%)	0	100	100
1	E	99/89 (111%)	99 (100%)	0	100	100
1	F	99/89 (111%)	99 (100%)	0	100	100
1	G	101/89 (114%)	99 (98%)	2 (2%)	60	19
1	H	100/89 (112%)	100 (100%)	0	100	100
1	I	95/89 (107%)	95 (100%)	0	100	100
1	J	98/89 (110%)	97 (99%)	1 (1%)	80	46
All	All	991/890 (111%)	986 (100%)	5 (0%)	94	66

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23[A]	LYS
1	A	23[B]	LYS
1	G	31[A]	LEU
1	G	31[B]	LEU
1	J	43	LYS

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

Mol	Chain	Res	Type
1	D	103	ASN
1	J	103	ASN
1	F	103	ASN
1	B	16	GLN
1	I	103	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 10 are monoatomic - leaving 99 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GAL	A	202[A]	-	12,12,12	1.74	3 (25%)	17,17,17	1.23	3 (17%)
4	GLA	A	203[B]	-	12,12,12	1.70	3 (25%)	17,17,17	1.16	1 (5%)
5	BCN	A	204	2	7,10,10	1.44	1 (14%)	8,11,11	2.29	1 (12%)
5	BCN	A	206	2	7,10,10	0.63	0	8,11,11	1.27	1 (12%)
3	GAL	A	207[A]	7,6	11,11,12	2.91	5 (45%)	13,15,17	2.30	7 (53%)
3	GAL	A	207[B]	7,6	11,11,12	1.49	2 (18%)	13,15,17	1.44	1 (7%)
6	NDG	A	208[A]	3,7	15,15,15	1.09	2 (13%)	21,21,21	1.24	2 (9%)
6	NDG	A	208[B]	3,7	15,15,15	0.58	0	21,21,21	1.92	5 (23%)
7	FUC	A	209[A]	6	9,10,11	1.03	0	13,14,16	0.93	1 (7%)
7	FUC	A	209[B]	6	9,10,11	0.89	1 (11%)	13,14,16	0.85	0
7	FUC	A	210[A]	3	9,10,11	1.50	2 (22%)	13,14,16	1.38	2 (15%)
7	FUC	A	210[B]	3	9,10,11	1.21	0	13,14,16	1.66	2 (15%)
5	BCN	B	202	2	7,10,10	1.24	2 (28%)	8,11,11	1.62	2 (25%)
3	GAL	B	203[A]	-	12,12,12	1.12	1 (8%)	17,17,17	1.26	1 (5%)
4	GLA	B	204[B]	-	12,12,12	1.55	2 (16%)	17,17,17	1.53	3 (17%)
5	BCN	B	206	2	7,10,10	1.22	1 (14%)	8,11,11	1.33	1 (12%)
3	GAL	B	207[A]	7,6	11,11,12	2.02	4 (36%)	13,15,17	1.73	2 (15%)
3	GAL	B	207[B]	7,6	11,11,12	1.95	4 (36%)	13,15,17	1.66	2 (15%)
6	NDG	B	208[A]	3,7	15,15,15	1.13	1 (6%)	21,21,21	1.46	3 (14%)
6	NDG	B	208[B]	3,7	15,15,15	0.90	1 (6%)	21,21,21	1.60	6 (28%)
7	FUC	B	209[A]	6	9,10,11	1.15	1 (11%)	13,14,16	1.43	3 (23%)
7	FUC	B	209[B]	6	9,10,11	1.01	0	13,14,16	1.19	1 (7%)
7	FUC	B	210[A]	3	9,10,11	1.54	2 (22%)	13,14,16	1.81	3 (23%)
7	FUC	B	210[B]	3	9,10,11	1.40	1 (11%)	13,14,16	1.52	3 (23%)
3	GAL	C	202[A]	-	12,12,12	0.87	0	17,17,17	0.77	0
4	GLA	C	203[B]	-	12,12,12	0.47	0	17,17,17	0.84	0
5	BCN	C	205	2	7,10,10	1.20	1 (14%)	8,11,11	2.32	3 (37%)
5	BCN	C	206	2	7,10,10	1.47	1 (14%)	8,11,11	1.41	1 (12%)
3	GAL	C	207[A]	7,6	11,11,12	1.88	4 (36%)	13,15,17	1.71	5 (38%)
3	GAL	C	207[B]	7,6	11,11,12	2.65	5 (45%)	13,15,17	3.22	5 (38%)
6	NDG	C	208[A]	3,7	15,15,15	1.39	3 (20%)	21,21,21	1.85	5 (23%)
6	NDG	C	208[B]	3,7	15,15,15	0.87	1 (6%)	21,21,21	2.07	7 (33%)
7	FUC	C	209[A]	6	9,10,11	1.48	2 (22%)	13,14,16	1.56	3 (23%)
7	FUC	C	209[B]	6	9,10,11	1.18	1 (11%)	13,14,16	1.13	1 (7%)
7	FUC	C	210[A]	3	9,10,11	2.64	5 (55%)	13,14,16	1.81	5 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	FUC	C	210[B]	3	9,10,11	1.39	2 (22%)	13,14,16	2.62	7 (53%)
5	BCN	D	201	2	7,10,10	1.67	2 (28%)	8,11,11	1.09	1 (12%)
5	BCN	D	203	2	7,10,10	1.03	1 (14%)	8,11,11	1.91	3 (37%)
3	GAL	D	204[A]	-	12,12,12	0.98	0	17,17,17	0.67	0
4	GLA	D	205[B]	-	12,12,12	0.77	0	17,17,17	0.83	0
3	GAL	D	207[A]	7,6	11,11,12	2.33	5 (45%)	13,15,17	2.12	5 (38%)
3	GAL	D	207[B]	7,6	11,11,12	2.73	2 (18%)	13,15,17	2.77	9 (69%)
6	NDG	D	208[A]	3,7	15,15,15	1.25	2 (13%)	21,21,21	2.23	4 (19%)
6	NDG	D	208[B]	3,7	15,15,15	1.35	1 (6%)	21,21,21	2.00	4 (19%)
7	FUC	D	209[A]	6	9,10,11	1.13	1 (11%)	13,14,16	1.15	1 (7%)
7	FUC	D	209[B]	6	9,10,11	1.22	1 (11%)	13,14,16	1.16	1 (7%)
7	FUC	D	210[A]	3	9,10,11	1.34	1 (11%)	13,14,16	1.24	2 (15%)
7	FUC	D	210[B]	3	9,10,11	2.88	5 (55%)	13,14,16	2.87	8 (61%)
5	BCN	E	201	2	7,10,10	0.65	0	8,11,11	1.91	2 (25%)
5	BCN	E	203	2	7,10,10	1.04	0	8,11,11	1.24	1 (12%)
3	GAL	E	204[A]	-	12,12,12	0.67	0	17,17,17	0.61	0
4	GLA	E	205[B]	-	12,12,12	0.82	0	17,17,17	0.73	0
3	GAL	E	207	7,6	11,11,12	1.99	4 (36%)	13,15,17	3.07	6 (46%)
6	NDG	E	208	3,7	15,15,15	1.28	2 (13%)	21,21,21	1.71	5 (23%)
7	FUC	E	209	6	9,10,11	1.13	1 (11%)	13,14,16	0.62	0
7	FUC	E	210	3	9,10,11	1.87	3 (33%)	13,14,16	1.13	0
4	GLA	F	1201[A]	-	12,12,12	0.98	1 (8%)	17,17,17	0.97	0
3	GAL	F	1202[B]	-	12,12,12	0.49	0	17,17,17	1.03	0
3	GAL	F	1203	7,6	11,11,12	2.59	5 (45%)	13,15,17	2.25	4 (30%)
6	NDG	F	1204	3,7	15,15,15	1.64	3 (20%)	21,21,21	1.40	3 (14%)
7	FUC	F	1205	6	9,10,11	0.96	0	13,14,16	1.36	2 (15%)
7	FUC	F	1206	3	9,10,11	1.79	3 (33%)	13,14,16	1.16	1 (7%)
8	PEG	G	201	-	6,6,6	0.71	0	5,5,5	2.67	3 (60%)
4	GLA	G	202[A]	-	12,12,12	0.95	0	17,17,17	1.19	3 (17%)
3	GAL	G	203[B]	-	12,12,12	1.04	0	17,17,17	1.28	1 (5%)
3	GAL	G	204[A]	7,6	11,11,12	1.15	1 (9%)	13,15,17	2.69	2 (15%)
3	GAL	G	204[B]	7,6	11,11,12	2.07	4 (36%)	13,15,17	1.88	6 (46%)
6	NDG	G	205[A]	3,7	15,15,15	0.78	0	21,21,21	1.04	2 (9%)
6	NDG	G	205[B]	3,7	15,15,15	1.07	2 (13%)	21,21,21	1.39	2 (9%)
7	FUC	G	206[A]	6	9,10,11	1.12	1 (11%)	13,14,16	0.60	0
7	FUC	G	206[B]	6	9,10,11	1.40	2 (22%)	13,14,16	1.19	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	FUC	G	207[A]	3	9,10,11	1.31	1 (11%)	13,14,16	0.97	0
7	FUC	G	207[B]	3	9,10,11	2.41	2 (22%)	13,14,16	2.11	5 (38%)
3	GAL	H	1201[A]	-	12,12,12	1.05	0	17,17,17	0.86	0
4	GLA	H	1202[B]	-	12,12,12	0.90	0	17,17,17	0.96	0
3	GAL	H	1203	7,6	11,11,12	2.71	5 (45%)	13,15,17	2.39	5 (38%)
6	NDG	H	1204	3,7	15,15,15	2.44	6 (40%)	21,21,21	3.37	12 (57%)
7	FUC	H	1205	6	9,10,11	1.99	3 (33%)	13,14,16	0.92	0
7	FUC	H	1206	3	9,10,11	1.27	1 (11%)	13,14,16	1.36	2 (15%)
3	GAL	I	1201[A]	-	12,12,12	0.98	2 (16%)	17,17,17	0.78	0
4	GLA	I	1202[B]	-	12,12,12	0.95	1 (8%)	17,17,17	0.95	1 (5%)
3	GAL	I	1203[A]	7,6	11,11,12	0.86	1 (9%)	13,15,17	1.28	2 (15%)
3	GAL	I	1203[B]	9,7	11,11,12	1.17	2 (18%)	13,15,17	1.15	1 (7%)
9	NAG	I	1204[B]	3,7	15,15,15	1.04	1 (6%)	21,21,21	1.30	5 (23%)
7	FUC	I	1205[A]	6	9,10,11	1.15	0	13,14,16	1.14	0
7	FUC	I	1205[B]	9	9,10,11	0.36	0	13,14,16	1.13	2 (15%)
7	FUC	I	1206[A]	3	9,10,11	1.10	0	13,14,16	1.33	1 (7%)
7	FUC	I	1206[B]	3	9,10,11	1.24	1 (11%)	13,14,16	1.25	1 (7%)
6	NDG	I	1207[A]	3,7	15,15,15	1.33	2 (13%)	21,21,21	0.99	1 (4%)
3	GAL	J	1201[A]	-	12,12,12	0.89	1 (8%)	17,17,17	0.93	0
4	GLA	J	1202[B]	-	12,12,12	1.02	1 (8%)	17,17,17	0.89	0
3	GAL	J	1203[A]	7,6	11,11,12	1.41	2 (18%)	13,15,17	1.99	4 (30%)
3	GAL	J	1203[B]	9,7	11,11,12	1.00	1 (9%)	13,15,17	1.88	2 (15%)
9	NAG	J	1204[B]	3,7	15,15,15	0.90	1 (6%)	21,21,21	1.16	2 (9%)
7	FUC	J	1205[A]	6	9,10,11	1.04	0	13,14,16	1.01	0
7	FUC	J	1205[B]	9	9,10,11	0.99	0	13,14,16	0.75	0
7	FUC	J	1206[A]	3	9,10,11	1.12	1 (11%)	13,14,16	0.81	0
7	FUC	J	1206[B]	3	9,10,11	0.56	0	13,14,16	0.72	0
6	NDG	J	1207[A]	3,7	15,15,15	0.99	0	21,21,21	1.19	1 (4%)

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
3	GAL	A	202[A]	-	-	0/2/22/22	0/1/1/1
4	GLA	A	203[B]	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCN	A	204	2	-	0/8/10/10	0/0/0/0
5	BCN	A	206	2	-	0/8/10/10	0/0/0/0
3	GAL	A	207[A]	7,6	-	0/2/19/22	0/1/1/1
3	GAL	A	207[B]	7,6	-	0/2/19/22	0/1/1/1
6	NDG	A	208[A]	3,7	-	0/6/26/26	0/1/1/1
6	NDG	A	208[B]	3,7	-	0/6/26/26	0/1/1/1
7	FUC	A	209[A]	6	-	0/0/17/20	0/1/1/1
7	FUC	A	209[B]	6	-	0/0/17/20	0/1/1/1
7	FUC	A	210[A]	3	-	0/0/17/20	0/1/1/1
7	FUC	A	210[B]	3	-	0/0/17/20	0/1/1/1
5	BCN	B	202	2	-	0/8/10/10	0/0/0/0
3	GAL	B	203[A]	-	-	0/2/22/22	0/1/1/1
4	GLA	B	204[B]	-	-	0/2/22/22	0/1/1/1
5	BCN	B	206	2	-	0/8/10/10	0/0/0/0
3	GAL	B	207[A]	7,6	-	0/2/19/22	0/1/1/1
3	GAL	B	207[B]	7,6	-	0/2/19/22	0/1/1/1
6	NDG	B	208[A]	3,7	-	0/6/26/26	0/1/1/1
6	NDG	B	208[B]	3,7	-	0/6/26/26	0/1/1/1
7	FUC	B	209[A]	6	-	0/0/17/20	0/1/1/1
7	FUC	B	209[B]	6	-	0/0/17/20	0/1/1/1
7	FUC	B	210[A]	3	-	0/0/17/20	0/1/1/1
7	FUC	B	210[B]	3	-	0/0/17/20	0/1/1/1
3	GAL	C	202[A]	-	-	0/2/22/22	0/1/1/1
4	GLA	C	203[B]	-	-	0/2/22/22	0/1/1/1
5	BCN	C	205	2	-	0/8/10/10	0/0/0/0
5	BCN	C	206	2	-	0/8/10/10	0/0/0/0
3	GAL	C	207[A]	7,6	-	0/2/19/22	0/1/1/1
3	GAL	C	207[B]	7,6	-	0/2/19/22	0/1/1/1
6	NDG	C	208[A]	3,7	-	0/6/26/26	0/1/1/1
6	NDG	C	208[B]	3,7	-	0/6/26/26	0/1/1/1
7	FUC	C	209[A]	6	-	0/0/17/20	0/1/1/1
7	FUC	C	209[B]	6	-	0/0/17/20	0/1/1/1
7	FUC	C	210[A]	3	-	0/0/17/20	0/1/1/1
7	FUC	C	210[B]	3	-	0/0/17/20	0/1/1/1
5	BCN	D	201	2	-	0/8/10/10	0/0/0/0
5	BCN	D	203	2	-	0/8/10/10	0/0/0/0
3	GAL	D	204[A]	-	-	0/2/22/22	0/1/1/1
4	GLA	D	205[B]	-	-	0/2/22/22	0/1/1/1
3	GAL	D	207[A]	7,6	-	0/2/19/22	0/1/1/1
3	GAL	D	207[B]	7,6	-	0/2/19/22	0/1/1/1
6	NDG	D	208[A]	3,7	-	0/6/26/26	0/1/1/1
6	NDG	D	208[B]	3,7	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUC	D	209[A]	6	-	0/0/17/20	0/1/1/1
7	FUC	D	209[B]	6	-	0/0/17/20	0/1/1/1
7	FUC	D	210[A]	3	-	0/0/17/20	0/1/1/1
7	FUC	D	210[B]	3	-	0/0/17/20	0/1/1/1
5	BCN	E	201	2	-	0/8/10/10	0/0/0/0
5	BCN	E	203	2	-	0/8/10/10	0/0/0/0
3	GAL	E	204[A]	-	-	0/2/22/22	0/1/1/1
4	GLA	E	205[B]	-	-	0/2/22/22	0/1/1/1
3	GAL	E	207	7,6	-	0/2/19/22	0/1/1/1
6	NDG	E	208	3,7	-	0/6/26/26	0/1/1/1
7	FUC	E	209	6	-	0/0/17/20	0/1/1/1
7	FUC	E	210	3	-	0/0/17/20	0/1/1/1
4	GLA	F	1201[A]	-	-	0/2/22/22	0/1/1/1
3	GAL	F	1202[B]	-	-	0/2/22/22	0/1/1/1
3	GAL	F	1203	7,6	-	0/2/19/22	0/1/1/1
6	NDG	F	1204	3,7	-	0/6/26/26	0/1/1/1
7	FUC	F	1205	6	-	0/0/17/20	0/1/1/1
7	FUC	F	1206	3	-	0/0/17/20	0/1/1/1
8	PEG	G	201	-	-	0/4/4/4	0/0/0/0
4	GLA	G	202[A]	-	-	0/2/22/22	0/1/1/1
3	GAL	G	203[B]	-	-	0/2/22/22	0/1/1/1
3	GAL	G	204[A]	7,6	-	0/2/19/22	0/1/1/1
3	GAL	G	204[B]	7,6	-	0/2/19/22	0/1/1/1
6	NDG	G	205[A]	3,7	-	0/6/26/26	0/1/1/1
6	NDG	G	205[B]	3,7	-	0/6/26/26	0/1/1/1
7	FUC	G	206[A]	6	-	0/0/17/20	0/1/1/1
7	FUC	G	206[B]	6	-	0/0/17/20	0/1/1/1
7	FUC	G	207[A]	3	-	0/0/17/20	0/1/1/1
7	FUC	G	207[B]	3	-	0/0/17/20	0/1/1/1
3	GAL	H	1201[A]	-	-	0/2/22/22	0/1/1/1
4	GLA	H	1202[B]	-	-	0/2/22/22	0/1/1/1
3	GAL	H	1203	7,6	-	0/2/19/22	0/1/1/1
6	NDG	H	1204	3,7	-	0/6/26/26	0/1/1/1
7	FUC	H	1205	6	-	0/0/17/20	0/1/1/1
7	FUC	H	1206	3	-	0/0/17/20	0/1/1/1
3	GAL	I	1201[A]	-	-	0/2/22/22	0/1/1/1
4	GLA	I	1202[B]	-	-	0/2/22/22	0/1/1/1
3	GAL	I	1203[A]	7,6	-	0/2/19/22	0/1/1/1
3	GAL	I	1203[B]	9,7	-	0/2/19/22	0/1/1/1
9	NAG	I	1204[B]	3,7	-	0/6/26/26	0/1/1/1
7	FUC	I	1205[A]	6	-	0/0/17/20	0/1/1/1
7	FUC	I	1205[B]	9	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUC	I	1206[A]	3	-	0/0/17/20	0/1/1/1
7	FUC	I	1206[B]	3	-	0/0/17/20	0/1/1/1
6	NDG	I	1207[A]	3,7	-	0/6/26/26	0/1/1/1
3	GAL	J	1201[A]	-	-	0/2/22/22	0/1/1/1
4	GLA	J	1202[B]	-	-	0/2/22/22	0/1/1/1
3	GAL	J	1203[A]	7,6	-	0/2/19/22	0/1/1/1
3	GAL	J	1203[B]	9,7	-	0/2/19/22	0/1/1/1
9	NAG	J	1204[B]	3,7	-	0/6/26/26	0/1/1/1
7	FUC	J	1205[A]	6	-	0/0/17/20	0/1/1/1
7	FUC	J	1205[B]	9	-	0/0/17/20	0/1/1/1
7	FUC	J	1206[A]	3	-	0/0/17/20	0/1/1/1
7	FUC	J	1206[B]	3	-	0/0/17/20	0/1/1/1
6	NDG	J	1207[A]	3,7	-	0/6/26/26	0/1/1/1

The worst 5 of 152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	207[B]	GAL	C2-C3	-8.08	1.41	1.52
3	A	207[A]	GAL	C1-C2	-5.99	1.38	1.52
3	A	207[A]	GAL	C4-C5	-4.83	1.42	1.53
3	C	207[B]	GAL	C2-C3	-4.31	1.46	1.52
7	H	1205	FUC	O5-C1	-4.27	1.36	1.43

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	207	GAL	C1-O5-C5	-8.13	100.96	112.17
3	C	207[B]	GAL	C1-O5-C5	-8.00	101.14	112.17
3	G	204[A]	GAL	C1-O5-C5	-7.84	101.36	112.17
6	H	1204	NDG	C1-C2-N2	-7.62	101.90	110.73
6	D	208[A]	NDG	O-C1-C2	-6.43	103.05	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	210[A]	FUC	1	0
7	A	210[B]	FUC	1	0
3	C	207[B]	GAL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	208[B]	NDG	1	0
7	C	210[B]	FUC	1	0
3	D	207[B]	GAL	3	0
6	D	208[A]	NDG	1	0
6	D	208[B]	NDG	7	0
7	D	210[A]	FUC	1	0
7	D	210[B]	FUC	5	0
3	E	207	GAL	1	0
8	G	201	PEG	4	0
6	H	1204	NDG	3	0
7	H	1206	FUC	1	0
3	J	1201[A]	GAL	1	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	103/103 (100%)	-0.57	0 100 100	8, 13, 21, 37	0
1	B	103/103 (100%)	-0.57	0 100 100	7, 11, 18, 35	0
1	C	103/103 (100%)	-0.60	1 (0%) 82 77	7, 10, 16, 38	0
1	D	103/103 (100%)	-0.56	0 100 100	7, 11, 18, 31	0
1	E	103/103 (100%)	-0.53	0 100 100	8, 14, 21, 43	0
1	F	103/103 (100%)	-0.49	1 (0%) 82 77	8, 12, 18, 36	0
1	G	103/103 (100%)	-0.45	1 (0%) 82 77	7, 10, 19, 37	0
1	H	103/103 (100%)	-0.51	1 (0%) 82 77	8, 12, 18, 51	0
1	I	103/103 (100%)	-0.54	1 (0%) 82 77	8, 12, 21, 51	0
1	J	103/103 (100%)	-0.52	0 100 100	8, 13, 20, 35	0
All	All	1030/1030 (100%)	-0.53	5 (0%) 90 88	7, 12, 20, 51	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	103	ASN	4.4
1	C	103	ASN	3.4
1	I	103	ASN	3.3
1	F	103	ASN	3.3
1	G	103	ASN	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	FUC	D	210[A]	10/11	0.80	0.25	49.80	20,26,34,36	10
7	FUC	D	210[B]	10/11	0.80	0.25	43.85	27,35,39,41	10
6	NDG	H	1204	15/15	0.91	0.15	13.91	18,24,36,38	0
6	NDG	D	208[B]	15/15	0.96	0.13	13.52	18,25,32,36	15
6	NDG	D	208[A]	15/15	0.96	0.13	13.52	15,23,31,35	15
3	GAL	B	203[A]	12/12	0.96	0.13	8.59	13,15,17,22	12
8	PEG	G	201	7/7	0.91	0.16	8.55	22,26,30,33	7
4	GLA	B	204[B]	12/12	0.95	0.13	8.34	15,16,20,23	12
6	NDG	C	208[B]	15/15	0.97	0.12	7.60	16,19,23,25	15
3	GAL	A	202[A]	12/12	0.96	0.10	7.57	15,17,18,23	12
4	GLA	A	203[B]	12/12	0.96	0.10	7.30	15,17,19,23	12
4	GLA	D	205[B]	12/12	0.97	0.07	7.03	13,15,16,21	12
3	GAL	D	204[A]	12/12	0.97	0.07	6.30	13,14,15,16	12
4	GLA	J	1202[B]	12/12	0.98	0.07	3.07	13,14,18,20	12
9	NAG	I	1204[B]	15/15	0.98	0.06	2.84	13,15,18,19	15
7	FUC	I	1205[A]	10/11	0.99	0.06	2.50	11,12,15,16	10
7	FUC	I	1205[B]	10/11	0.99	0.06	2.50	12,14,16,18	10
7	FUC	D	209[A]	10/11	0.98	0.05	2.37	11,14,20,23	10
7	FUC	D	209[B]	10/11	0.98	0.05	2.37	14,16,19,23	10
3	GAL	J	1201[A]	12/12	0.98	0.07	2.29	12,13,16,16	12
6	NDG	I	1207[A]	15/15	0.98	0.06	1.95	11,13,18,22	15
4	GLA	G	202[A]	12/12	0.98	0.07	1.88	11,13,17,19	12
3	GAL	G	203[B]	12/12	0.98	0.07	1.88	11,13,18,20	12
7	FUC	C	209[A]	10/11	0.98	0.06	1.62	9,11,16,17	10
7	FUC	C	209[B]	10/11	0.98	0.06	1.61	13,18,23,24	10
4	GLA	H	1202[B]	12/12	0.98	0.07	1.58	12,15,18,21	12
6	NDG	J	1207[A]	15/15	0.98	0.05	1.53	11,12,15,15	15
7	FUC	I	1206[B]	10/11	0.98	0.06	1.52	12,12,14,15	10
7	FUC	I	1206[A]	10/11	0.98	0.06	1.52	13,14,17,19	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	FUC	A	209[B]	10/11	0.98	0.05	1.33	17,18,19,21	10
9	NAG	J	1204[B]	15/15	0.99	0.06	1.31	13,15,18,18	15
3	GAL	H	1201[A]	12/12	0.98	0.06	1.19	12,14,17,19	12
6	NDG	A	208[A]	15/15	0.98	0.06	1.09	14,16,24,27	15
6	NDG	A	208[B]	15/15	0.98	0.06	1.09	15,19,21,25	15
7	FUC	A	209[A]	10/11	0.98	0.05	1.03	15,18,20,24	10
7	FUC	E	209	10/11	0.97	0.06	0.68	16,19,24,26	0
4	GLA	E	205[B]	12/12	0.98	0.06	0.63	14,16,19,21	12
3	GAL	E	204[A]	12/12	0.98	0.06	0.57	14,15,18,20	12
6	NDG	G	205[A]	15/15	0.99	0.06	0.33	10,11,17,20	15
4	GLA	I	1202[B]	12/12	0.99	0.05	0.31	12,14,17,19	12
6	NDG	G	205[B]	15/15	0.99	0.06	0.24	10,10,13,13	15
6	NDG	B	208[B]	15/15	0.98	0.05	0.19	12,15,21,28	15
6	NDG	B	208[A]	15/15	0.98	0.05	0.18	10,13,17,17	15
3	GAL	I	1201[A]	12/12	0.99	0.05	0.06	12,14,17,19	12
7	FUC	J	1206[B]	10/11	0.98	0.05	-0.09	12,14,14,16	10
7	FUC	J	1206[A]	10/11	0.98	0.05	-0.09	10,11,12,15	10
7	FUC	H	1205	10/11	0.98	0.04	-0.19	12,15,23,24	0
5	BCN	E	203	11/11	0.97	0.06	-0.39	12,15,24,25	0
3	GAL	F	1202[B]	12/12	0.99	0.06	-0.40	12,15,16,18	12
7	FUC	F	1205	10/11	0.98	0.05	-0.41	14,17,27,29	0
5	BCN	D	201	11/11	0.97	0.06	-0.47	10,17,22,27	0
7	FUC	B	209[B]	10/11	0.98	0.04	-0.47	13,18,22,23	10
7	FUC	B	209[A]	10/11	0.98	0.04	-0.47	10,11,14,14	10
4	GLA	F	1201[A]	12/12	0.99	0.06	-0.49	11,13,15,16	12
5	BCN	B	202	11/11	0.98	0.06	-0.53	12,18,27,29	0
5	BCN	C	205	11/11	0.97	0.06	-0.67	11,16,23,23	0
5	BCN	B	206	11/11	0.97	0.05	-0.68	12,17,23,26	0
7	FUC	J	1205[B]	10/11	0.99	0.04	-0.70	13,14,17,18	10
5	BCN	A	204	11/11	0.97	0.06	-0.70	11,19,22,25	0
7	FUC	J	1205[A]	10/11	0.99	0.04	-0.70	10,11,14,15	10
5	BCN	D	203	11/11	0.98	0.05	-0.79	11,19,26,26	0
4	GLA	C	203[B]	12/12	0.99	0.04	-0.94	10,11,13,14	12
5	BCN	C	206	11/11	0.98	0.05	-0.95	11,19,25,27	0
5	BCN	E	201	11/11	0.98	0.05	-1.03	12,17,23,26	0
7	FUC	G	206[A]	10/11	0.99	0.04	-1.10	10,11,13,13	10
5	BCN	A	206	11/11	0.98	0.04	-1.15	12,17,23,26	0
7	FUC	G	206[B]	10/11	0.99	0.04	-1.20	9,10,13,13	10
3	GAL	C	202[A]	12/12	0.99	0.04	-1.97	9,11,13,14	12
3	GAL	A	207[B]	11/12	0.97	0.09	-	17,20,23,24	11
7	FUC	B	210[A]	10/11	0.95	0.08	-	18,26,34,36	10
3	GAL	E	207	11/12	0.89	0.12	-	29,39,48,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	FUC	C	210[B]	10/11	0.85	0.20	-	16,26,33,34	10
6	NDG	C	208[A]	15/15	0.97	0.12	-	11,17,21,23	15
6	NDG	E	208	15/15	0.95	0.10	-	21,28,37,44	0
2	CA	E	202	1/1	1.00	0.03	-	11,11,11,11	0
3	GAL	C	207[B]	11/12	0.92	0.12	-	18,22,33,38	11
2	CA	B	201	1/1	1.00	0.04	-	11,11,11,11	0
2	CA	D	206	1/1	1.00	0.03	-	11,11,11,11	0
7	FUC	F	1206	10/11	0.92	0.22	-	28,31,42,45	0
3	GAL	D	207[A]	11/12	0.94	0.16	-	23,26,32,34	11
2	CA	E	206	1/1	1.00	0.03	-	12,12,12,12	0
2	CA	D	202	1/1	1.00	0.03	-	11,11,11,11	0
2	CA	A	205	1/1	1.00	0.03	-	12,12,12,12	0
3	GAL	F	1203	11/12	0.89	0.18	-	24,30,39,49	0
7	FUC	A	210[A]	10/11	0.93	0.11	-	28,33,43,47	10
2	CA	B	205	1/1	1.00	0.03	-	12,12,12,12	0
7	FUC	G	207[A]	10/11	0.90	0.14	-	15,18,20,25	10
3	GAL	J	1203[A]	11/12	0.98	0.05	-	11,12,19,20	11
3	GAL	J	1203[B]	11/12	0.98	0.05	-	14,15,19,19	11
3	GAL	C	207[A]	11/12	0.92	0.12	-	24,28,34,35	11
3	GAL	D	207[B]	11/12	0.94	0.16	-	21,26,33,39	11
3	GAL	G	204[B]	11/12	0.98	0.12	-	15,20,24,30	11
7	FUC	H	1206	10/11	0.89	0.29	-	24,31,45,52	0
3	GAL	B	207[B]	11/12	0.97	0.11	-	11,12,15,22	11
2	CA	C	201	1/1	1.00	0.04	-	11,11,11,11	0
3	GAL	H	1203	11/12	0.91	0.14	-	19,27,35,42	0
7	FUC	A	210[B]	10/11	0.93	0.11	-	16,19,21,22	10
3	GAL	I	1203[B]	11/12	0.98	0.07	-	14,16,18,20	11
6	NDG	F	1204	15/15	0.93	0.13	-	18,24,38,45	0
2	CA	C	204	1/1	1.00	0.03	-	11,11,11,11	0
3	GAL	A	207[A]	11/12	0.97	0.09	-	23,24,27,30	11
3	GAL	G	204[A]	11/12	0.98	0.12	-	17,20,32,32	11
3	GAL	I	1203[A]	11/12	0.98	0.07	-	11,13,20,21	11
2	CA	A	201	1/1	1.00	0.03	-	11,11,11,11	0
7	FUC	E	210	10/11	0.78	0.21	-	34,40,47,48	0
3	GAL	B	207[A]	11/12	0.97	0.11	-	15,18,26,28	11
7	FUC	G	207[B]	10/11	0.90	0.14	-	16,25,37,39	10
7	FUC	B	210[B]	10/11	0.95	0.08	-	13,15,17,18	10
7	FUC	C	210[A]	10/11	0.85	0.20	-	26,28,34,34	10

## 6.5 Other polymers ⓘ

There are no such residues in this entry.