



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 03:32 PM EDT

PDB ID : 4NYT  
Title : L-Ficolin Complexed to Phosphocholine  
Authors : Laffly, E.; Gaboriaud, C.; Martin, L.; Thielens, N.  
Deposited on : 2013-12-11  
Resolution : 2.25 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	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)	:	2.37.1

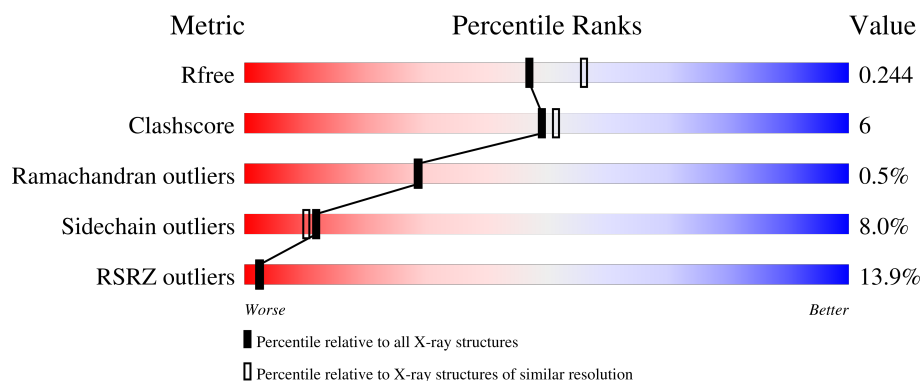
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	217	<div> <div>3%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	B	217	<div> <div>36%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	C	217	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>
2	D	4	<div> <div>100%</div> </div>

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
2	MAN	D	3	X	-	-	-
7	PC	A	303	-	X	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5347 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.

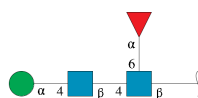
- Molecule 1 is a protein called Ficolin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	216	Total	C	N	O	S	0	3	0
			1757	1106	310	331	10			
1	A	212	Total	C	N	O	S	0	3	0
			1727	1085	306	328	8			
1	B	212	Total	C	N	O	S	0	0	0
			1702	1071	300	323	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	168	THR	VAL	SEE REMARK 999	UNP Q15485
C	247	THR	VAL	SEE REMARK 999	UNP Q15485
A	168	THR	VAL	SEE REMARK 999	UNP Q15485
A	247	THR	VAL	SEE REMARK 999	UNP Q15485
B	168	THR	VAL	SEE REMARK 999	UNP Q15485
B	247	THR	VAL	SEE REMARK 999	UNP Q15485

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

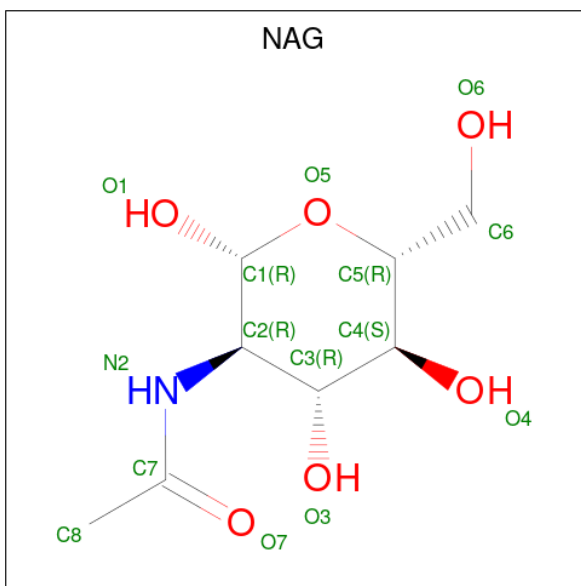
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		
4	A	2	Total	Ca	0	0
			2	2		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



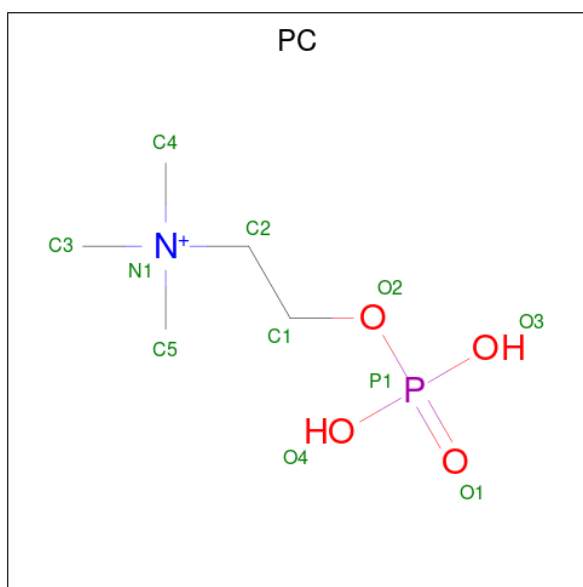
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is PHOSPHOCHOLINE (three-letter code: PC) (formula:  $C_5H_{15}NO_4P$ ).



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

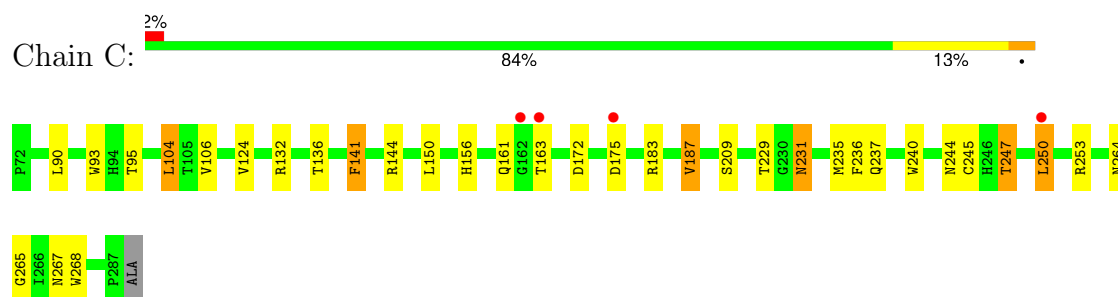
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	33	Total	O	0	0
			33	33		
8	A	34	Total	O	0	0
			34	34		
8	B	3	Total	O	0	0
			3	3		

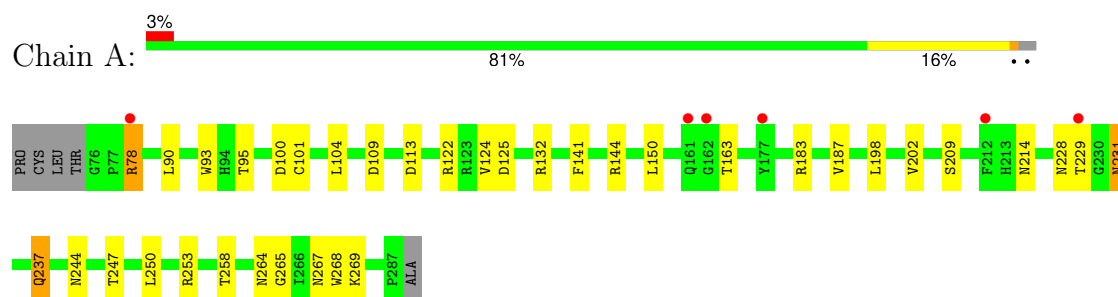
### 3 Residue-property plots

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.

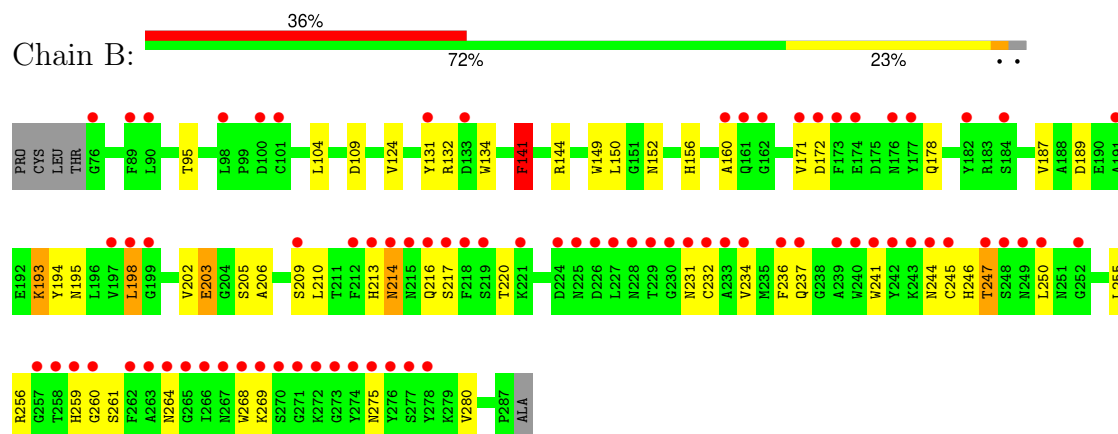
#### • Molecule 1: Ficolin-2



#### • Molecule 1: Ficolin-2




#### • Molecule 1: Ficolin-2



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



Chain D:  100%

MAG1  
MAG2  
MAN3  
FUC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.13Å 96.13Å 139.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.25 19.95 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.95-2.25) 99.6 (19.95-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.62 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.213 , 0.243 0.214 , 0.244	Depositor DCC
$R_{free}$ test set	1795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, FUC, ACT, CA, PC, PO4

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	0.95	3/1774 (0.2%)	0.97	5/2400 (0.2%)
1	B	0.76	7/1749 (0.4%)	0.85	6/2366 (0.3%)
1	C	1.08	4/1805 (0.2%)	1.04	5/2441 (0.2%)
All	All	0.94	14/5328 (0.3%)	0.96	16/7207 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	PHE	CG-CD2	-14.68	1.16	1.38
1	C	141	PHE	CG-CD1	-12.70	1.19	1.38
1	B	141	PHE	CG-CD2	-9.61	1.24	1.38
1	C	141	PHE	CE1-CZ	-9.48	1.19	1.37
1	A	141	PHE	CG-CD2	-9.02	1.25	1.38
1	C	141	PHE	CE2-CZ	-8.70	1.20	1.37
1	B	141	PHE	CG-CD1	-8.48	1.26	1.38
1	B	203	GLU	CD-OE1	7.54	1.33	1.25
1	B	203	GLU	CD-OE2	7.24	1.33	1.25
1	A	141	PHE	CG-CD1	-6.93	1.28	1.38
1	B	141	PHE	CE1-CZ	-6.46	1.25	1.37
1	A	141	PHE	CE1-CZ	-6.21	1.25	1.37
1	B	141	PHE	CE2-CZ	-5.33	1.27	1.37
1	B	206	ALA	C-O	5.10	1.33	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	C	132	ARG	NE-CZ-NH2	-12.05	114.28	120.30
1	A	132	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	B	132	ARG	NE-CZ-NH2	-8.52	116.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	ARG	CG-CD-NE	-7.82	95.37	111.80
1	B	132	ARG	CG-CD-NE	-6.68	97.77	111.80
1	B	109	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	132	ARG	CG-CD-NE	-6.30	98.57	111.80
1	C	132	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	132	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	C	172	ASP	CB-CG-OD2	-5.61	113.26	118.30
1	A	109	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	141	PHE	CE1-CZ-CE2	-5.09	110.84	120.00
1	B	172	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	113	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	144	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	1727	0	1596	15	0
1	B	1702	0	1573	28	0
1	C	1757	0	1631	17	0
2	D	49	0	43	0	0
3	A	4	0	3	0	0
3	C	4	0	3	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	C	5	0	0	0	0
6	A	14	0	13	0	0
7	A	11	0	13	0	0
8	A	34	0	0	0	0
8	B	3	0	0	0	0
8	C	33	0	0	0	0
All	All	5347	0	4875	60	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 6.

All (60) 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:237:GLN:HE22	1:A:264:ASN:HD22	1.37	0.72
1:B:259:HIS:O	1:B:261:SER:N	2.23	0.72
1:A:237:GLN:NE2	1:A:264:ASN:HD22	1.88	0.72
1:C:237:GLN:NE2	1:C:264:ASN:HD22	1.94	0.65
1:B:141:PHE:CE1	1:B:149:TRP:HB3	2.35	0.62
1:C:235[B]:MET:HE2	1:C:236:PHE:CE2	2.34	0.62
1:B:134:TRP:HA	1:B:220:THR:HG21	1.83	0.61
1:C:237:GLN:HE21	1:C:264:ASN:HD22	1.49	0.59
1:C:265:GLY:H	1:C:267:ASN:HD21	1.49	0.58
1:B:198:LEU:N	1:B:214:ASN:HD21	2.01	0.58
1:B:156:HIS:CD2	1:B:187:VAL:O	2.57	0.57
1:B:198:LEU:H	1:B:214:ASN:HD21	1.50	0.57
1:A:247[A]:THR:HG23	1:A:269:LYS:HB3	1.88	0.56
1:A:265:GLY:H	1:A:267:ASN:HD21	1.54	0.55
1:B:244:ASN:N	1:B:245:CYS:HA	2.21	0.55
1:C:156:HIS:HD2	1:C:187:VAL:O	1.90	0.55
1:A:78:ARG:CZ	1:A:78:ARG:HB3	2.37	0.55
1:B:209:SER:HB2	1:B:268:TRP:CE2	2.42	0.54
1:B:171:VAL:HB	1:B:280:VAL:HB	1.89	0.54
1:B:156:HIS:HD2	1:B:187:VAL:O	1.90	0.53
1:B:259:HIS:O	1:B:259:HIS:ND1	2.42	0.52
1:A:209:SER:HB3	1:A:247[A]:THR:HG22	1.93	0.50
1:A:100:ASP:O	1:A:101:CYS:HB2	2.10	0.50
1:C:265:GLY:H	1:C:267:ASN:ND2	2.11	0.49
1:B:259:HIS:CE1	1:B:275:ASN:HA	2.49	0.48
1:C:209:SER:HB2	1:C:268:TRP:CE2	2.49	0.48
1:A:209:SER:HB2	1:A:268:TRP:CE2	2.49	0.47
1:B:131:TYR:CE1	1:B:237:GLN:HA	2.49	0.47
1:B:187:VAL:HA	1:B:195:ASN:O	2.15	0.47
1:C:104[A]:LEU:HD13	1:C:106:VAL:HG12	1.98	0.46
1:B:217:SER:O	1:B:241:TRP:HA	2.15	0.46
1:C:136:THR:HG22	1:C:141:PHE:HD2	1.81	0.46
1:C:104[A]:LEU:HD13	1:C:106:VAL:CG1	2.46	0.46
1:B:195:ASN:HA	1:B:216:GLN:O	2.15	0.46
1:C:253[B]:ARG:HG2	1:C:253[B]:ARG:HH11	1.82	0.45
1:B:189:ASP:O	1:B:193:LYS:O	2.35	0.44
1:A:237:GLN:HE21	1:A:253:ARG:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASN:HD22	1:A:231:ASN:C	2.19	0.44
1:A:265:GLY:H	1:A:267:ASN:ND2	2.14	0.44
1:B:198:LEU:HD13	1:B:210:LEU:HD23	2.00	0.43
1:B:231:ASN:OD1	1:B:234:VAL:HG23	2.17	0.43
1:B:210:LEU:O	1:B:213:HIS:N	2.48	0.43
1:C:209:SER:HB3	1:C:247:THR:HG23	2.00	0.43
1:B:237:GLN:NE2	1:B:264:ASN:HD22	2.15	0.43
1:B:247:THR:O	1:B:269:LYS:HB2	2.19	0.42
1:B:255:LEU:O	1:B:256:ARG:HB2	2.19	0.42
1:C:93:TRP:CZ2	1:C:144:ARG:HA	2.54	0.42
1:C:240:TRP:CH2	1:C:250:LEU:HB2	2.55	0.42
1:C:244:ASN:N	1:C:245:CYS:HA	2.33	0.42
1:C:136:THR:HG22	1:C:141:PHE:CD2	2.54	0.42
1:A:198:LEU:H	1:A:214:ASN:ND2	2.17	0.42
1:A:237:GLN:HE21	1:A:253:ARG:HH11	1.67	0.42
1:B:178:GLN:HA	1:B:205:SER:OG	2.20	0.42
1:A:228:ASN:ND2	1:A:244:ASN:OD1	2.51	0.42
1:B:194:TYR:O	1:B:195:ASN:C	2.58	0.42
1:C:231:ASN:C	1:C:231:ASN:HD22	2.23	0.42
1:B:232:CYS:O	1:B:236:PHE:N	2.54	0.41
1:B:213:HIS:ND1	1:B:241:TRP:O	2.50	0.41
1:A:93:TRP:CZ2	1:A:144:ARG:HA	2.56	0.40
1:B:152:ASN:HB3	1:B:194:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/217 (98%)	199 (93%)	13 (6%)	1 (0%)	29	29
1	B	210/217 (97%)	188 (90%)	20 (10%)	2 (1%)	15	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	217/217 (100%)	207 (95%)	10 (5%)	0	100	100
All	All	640/651 (98%)	594 (93%)	43 (7%)	3 (0%)	29	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	GLY
1	B	160	ALA
1	A	125	ASP

### 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	181/182 (100%)	164 (91%)	17 (9%)	8	6
1	B	178/182 (98%)	165 (93%)	13 (7%)	14	12
1	C	185/182 (102%)	170 (92%)	15 (8%)	11	10
All	All	544/546 (100%)	499 (92%)	45 (8%)	12	9

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	90	LEU
1	C	95	THR
1	C	104[A]	LEU
1	C	104[B]	LEU
1	C	124	VAL
1	C	150	LEU
1	C	161	GLN
1	C	163	THR
1	C	175	ASP
1	C	183	ARG
1	C	187	VAL
1	C	229	THR

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Mol	Chain	Res	Type
1	C	231	ASN
1	C	247	THR
1	C	250	LEU
1	A	78	ARG
1	A	90	LEU
1	A	95	THR
1	A	104	LEU
1	A	122	ARG
1	A	124	VAL
1	A	150	LEU
1	A	163	THR
1	A	183	ARG
1	A	187	VAL
1	A	202	VAL
1	A	229	THR
1	A	231	ASN
1	A	237	GLN
1	A	250	LEU
1	A	258[A]	THR
1	A	258[B]	THR
1	B	95	THR
1	B	104	LEU
1	B	124	VAL
1	B	141	PHE
1	B	150	LEU
1	B	193	LYS
1	B	198	LEU
1	B	202	VAL
1	B	203	GLU
1	B	214	ASN
1	B	246	HIS
1	B	247	THR
1	B	250	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	139	GLN
1	C	156	HIS
1	C	161	GLN
1	C	214	ASN
1	C	216	GLN

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Mol	Chain	Res	Type
1	C	231	ASN
1	C	237	GLN
1	C	267	ASN
1	A	139	GLN
1	A	156	HIS
1	A	195	ASN
1	A	214	ASN
1	A	231	ASN
1	A	237	GLN
1	A	267	ASN
1	B	139	GLN
1	B	156	HIS
1	B	214	ASN
1	B	225	ASN
1	B	237	GLN
1	B	267	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](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	D	1	2,1	14,14,15	0.81	0	17,19,21	2.09	6 (35%)
2	NAG	D	2	2	14,14,15	0.85	0	17,19,21	2.09	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	D	3	2	11,11,12	0.70	0	15,15,17	1.83	5 (33%)
2	FUC	D	4	2	10,10,11	1.38	1 (10%)	14,14,16	2.30	4 (28%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	MAN	D	3	2	1/1/4/5	1/2/19/22	1/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	FUC	C2-C3	2.08	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	FUC	C1-C2-C3	-5.26	101.98	109.64
2	D	2	NAG	C1-O5-C5	-4.24	106.50	112.19
2	D	1	NAG	O5-C1-C2	-4.01	105.09	111.29
2	D	3	MAN	C1-O5-C5	3.65	117.08	112.19
2	D	2	NAG	C4-C3-C2	-3.42	106.00	111.02
2	D	3	MAN	O2-C2-C1	3.42	117.06	109.22
2	D	4	FUC	O3-C3-C2	3.40	116.98	110.05
2	D	1	NAG	C3-C4-C5	-3.24	104.35	110.23
2	D	1	NAG	C1-O5-C5	-3.17	107.94	112.19
2	D	4	FUC	C2-C3-C4	-3.16	105.31	110.86
2	D	2	NAG	O4-C4-C5	-3.11	101.67	109.32
2	D	1	NAG	O5-C5-C6	-3.04	101.75	107.66
2	D	3	MAN	O2-C2-C3	-2.98	103.98	110.15
2	D	4	FUC	C1-O5-C5	-2.96	105.98	112.97
2	D	2	NAG	C2-N2-C7	2.92	126.81	122.90
2	D	1	NAG	C6-C5-C4	-2.84	106.05	113.02
2	D	2	NAG	C6-C5-C4	-2.43	107.06	113.02
2	D	3	MAN	O3-C3-C2	-2.13	105.70	110.05
2	D	2	NAG	O5-C5-C6	2.10	111.75	107.66
2	D	1	NAG	O6-C6-C5	-2.01	104.47	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	MAN	O5-C1-C2	2.01	115.58	110.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	3	MAN	C1

All (1) torsion outliers are listed below:

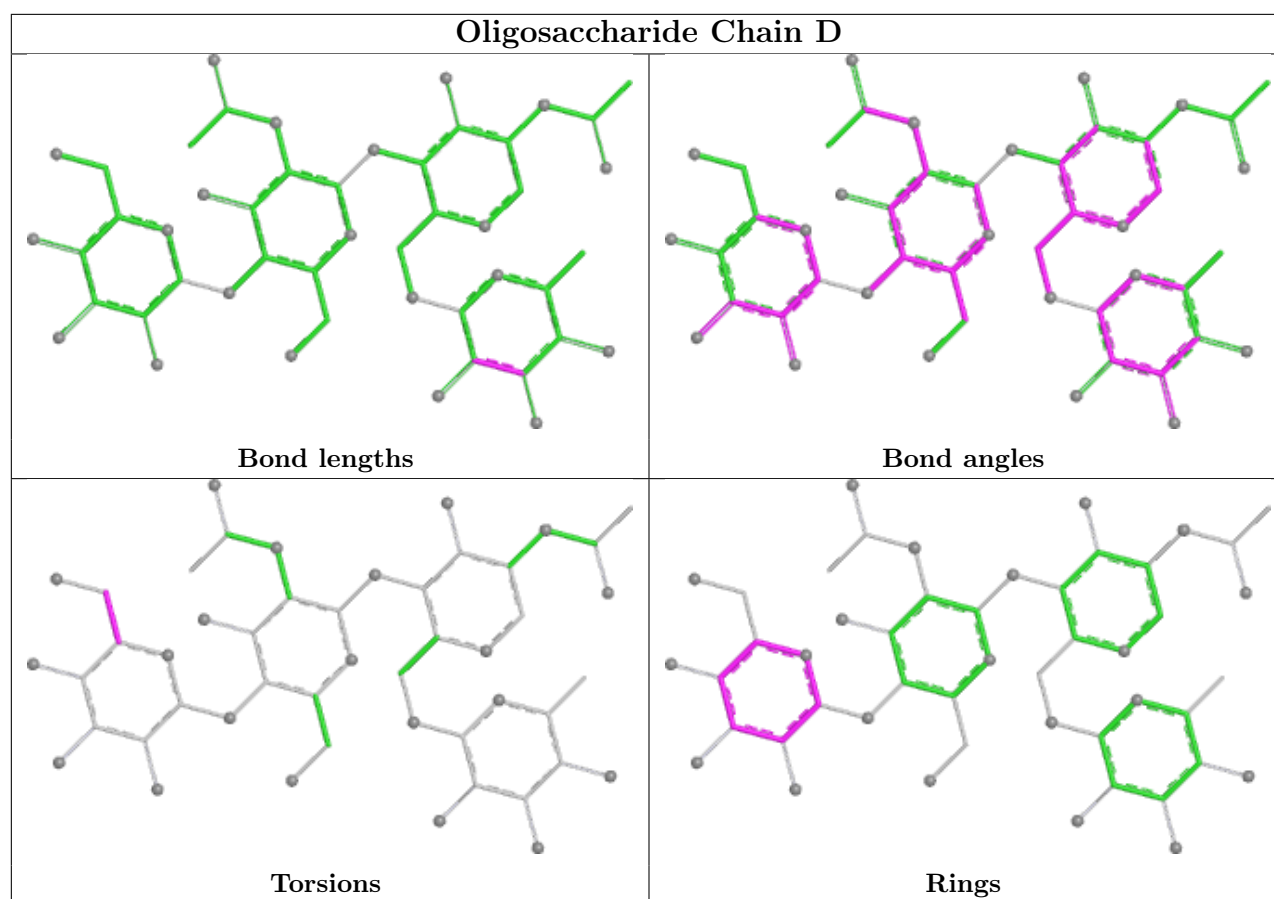
Mol	Chain	Res	Type	Atoms
2	D	3	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	MAN	C1-C2-C3-C4-C5-O5

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z  > 2$
6	NAG	A	302	1	14,14,15	1.08	1 (7%)	17,19,21	1.75	5 (29%)
3	ACT	A	301	-	3,3,3	1.16	0	3,3,3	0.09	0
3	ACT	C	301	-	3,3,3	0.79	0	3,3,3	1.31	0
7	PC	A	303	-	10,10,10	0.86	0	15,15,15	3.49	10 (66%)
5	PO4	C	307	-	4,4,4	1.36	0	6,6,6	1.38	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
7	PC	A	303	-	-	4/8/8/8	-
6	NAG	A	302	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	302	NAG	C4-C5	2.27	1.57	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	303	PC	C5-N1-C3	-6.21	92.67	108.98
7	A	303	PC	C5-N1-C4	-6.11	92.93	108.98
7	A	303	PC	C5-N1-C2	-5.60	87.63	109.91
7	A	303	PC	O4-P1-O1	3.92	126.11	110.83
6	A	302	NAG	C4-C3-C2	3.62	116.32	111.02
7	A	303	PC	C4-N1-C3	3.52	118.22	108.98
7	A	303	PC	C3-N1-C2	3.47	123.69	109.91
7	A	303	PC	C1-C2-N1	-2.91	106.49	115.82
7	A	303	PC	P1-O2-C1	-2.89	110.35	118.21
7	A	303	PC	O2-P1-O1	-2.83	98.80	106.44
6	A	302	NAG	O4-C4-C5	2.77	116.14	109.32
6	A	302	NAG	O4-C4-C3	-2.76	103.87	110.38
6	A	302	NAG	C2-N2-C7	2.63	126.42	122.90
6	A	302	NAG	C6-C5-C4	2.15	118.29	113.02
7	A	303	PC	C4-N1-C2	2.03	117.99	109.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	303	PC	C1-O2-P1-O1
7	A	303	PC	C1-O2-P1-O4
7	A	303	PC	C1-C2-N1-C4
7	A	303	PC	C1-O2-P1-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	212/217 (97%)	-0.20	6 (2%) 53 55	17, 34, 64, 89	5 (2%)
1	B	212/217 (97%)	1.85	79 (37%) 0 0	37, 109, 205, 253	4 (1%)
1	C	216/217 (99%)	-0.28	4 (1%) 66 69	16, 30, 56, 73	4 (1%)
All	All	640/651 (98%)	0.45	89 (13%) 2 2	16, 42, 179, 253	13 (2%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	THR	13.4
1	B	268	TRP	8.7
1	B	250	LEU	6.8
1	B	242	TYR	6.4
1	B	191	ALA	6.3
1	B	161	GLN	6.0
1	B	260	GLY	5.9
1	B	274	TYR	5.9
1	B	218	PHE	5.7
1	B	197	VAL	5.6
1	B	262	PHE	5.3
1	B	248	SER	5.3
1	B	227	LEU	5.2
1	B	176	ASN	5.0
1	B	101	CYS	5.0
1	A	161	GLN	4.9
1	B	263	ALA	4.9
1	B	241	TRP	4.8
1	B	219	SER	4.8
1	B	240	TRP	4.7
1	B	174	GLU	4.7
1	B	100	ASP	4.7
1	B	273	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	172	ASP	4.6
1	B	239	ALA	4.4
1	B	231	ASN	4.3
1	B	171	VAL	4.3
1	B	243	LYS	4.3
1	B	224	ASP	4.0
1	B	257	GLY	3.9
1	B	173	PHE	3.9
1	B	199	GLY	3.9
1	B	236	PHE	3.8
1	B	249	ASN	3.8
1	B	275	ASN	3.8
1	B	76	GLY	3.8
1	B	98	LEU	3.7
1	B	245	CYS	3.7
1	B	277	SER	3.7
1	A	162	GLY	3.7
1	B	160	ALA	3.6
1	B	271	GLY	3.6
1	B	177	TYR	3.6
1	B	264	ASN	3.5
1	B	265	GLY	3.5
1	B	216	GLN	3.4
1	B	276	TYR	3.4
1	B	230	GLY	3.3
1	B	90	LEU	3.3
1	B	252	GLY	3.2
1	B	209	SER	3.1
1	B	272	LYS	3.1
1	B	182	TYR	3.0
1	B	258	THR	3.0
1	B	215	ASN	3.0
1	B	267	ASN	3.0
1	B	212	PHE	3.0
1	B	226	ASP	2.9
1	A	212	PHE	2.9
1	B	89	PHE	2.8
1	B	269	LYS	2.8
1	C	250	LEU	2.8
1	B	217	SER	2.7
1	B	198	LEU	2.7
1	B	266	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	270	SER	2.6
1	B	233	ALA	2.6
1	B	221	LYS	2.5
1	B	162	GLY	2.5
1	A	229	THR	2.5
1	B	228	ASN	2.5
1	B	133	ASP	2.4
1	B	247	THR	2.4
1	B	244	ASN	2.3
1	B	225	ASN	2.3
1	A	78	ARG	2.3
1	B	184	SER	2.3
1	B	234	VAL	2.2
1	C	175	ASP	2.2
1	B	214	ASN	2.2
1	B	237	GLN	2.1
1	B	213	HIS	2.1
1	B	259	HIS	2.1
1	A	177	TYR	2.1
1	B	232	CYS	2.1
1	C	162	GLY	2.1
1	B	278	TYR	2.1
1	B	131	TYR	2.0
1	C	163	THR	2.0

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

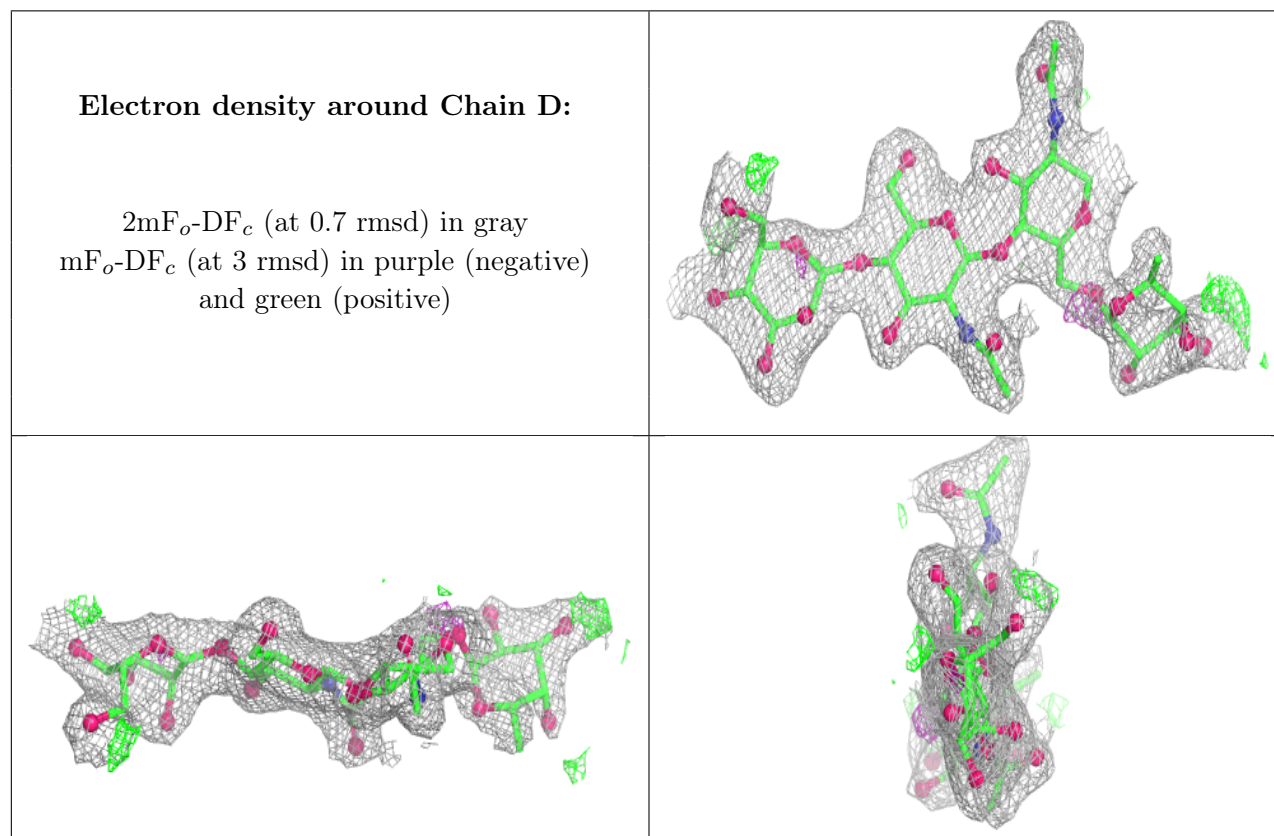
There are no non-standard protein/DNA/RNA residues in this entry.

## 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
2	FUC	D	4	10/11	0.76	0.27	37,40,42,47	10
2	MAN	D	3	11/12	0.80	0.27	46,54,61,64	0
2	NAG	D	1	14/15	0.94	0.17	19,26,33,34	0
2	NAG	D	2	14/15	0.96	0.22	28,35,39,40	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 ⓘ

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<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	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	A	302	14/15	0.85	0.43	39,49,57,59	0
5	PO4	C	307	5/5	0.91	0.26	30,37,45,46	0
3	ACT	C	301	4/4	0.92	0.14	29,31,32,33	0
3	ACT	A	301	4/4	0.95	0.13	37,38,38,39	0
4	CA	B	301	1/1	0.95	0.20	67,67,67,67	0
7	PC	A	303	11/11	0.95	0.22	32,43,58,58	0
4	CA	A	304	1/1	0.97	0.06	38,38,38,38	0
4	CA	A	305	1/1	0.97	0.18	46,46,46,46	0
4	CA	C	306	1/1	0.99	0.03	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.