



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:44 AM UTC

PDB ID : 4NYT / pdb_00004nyt
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

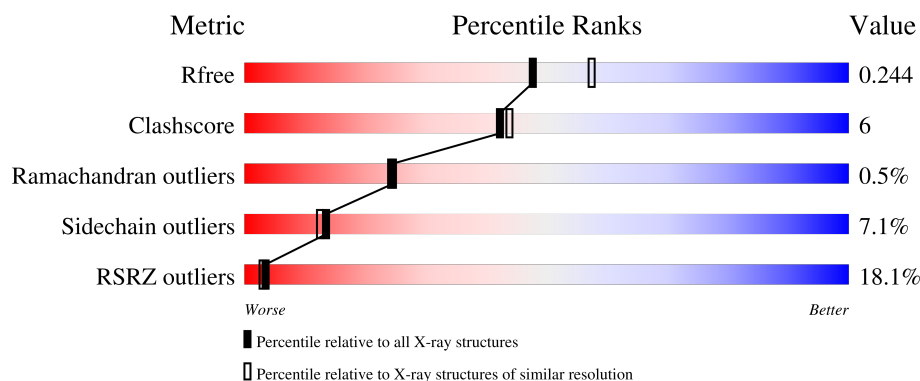
1 Overall quality at a glance

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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 ≥ 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	2% 80% 16% ..
1	B	217	49% 73% 21% ..
1	C	217	2% 83% 13% .
2	D	4	100%

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.

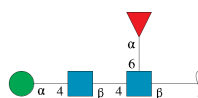
- Molecule 1 is a protein called Ficolin-2.

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:

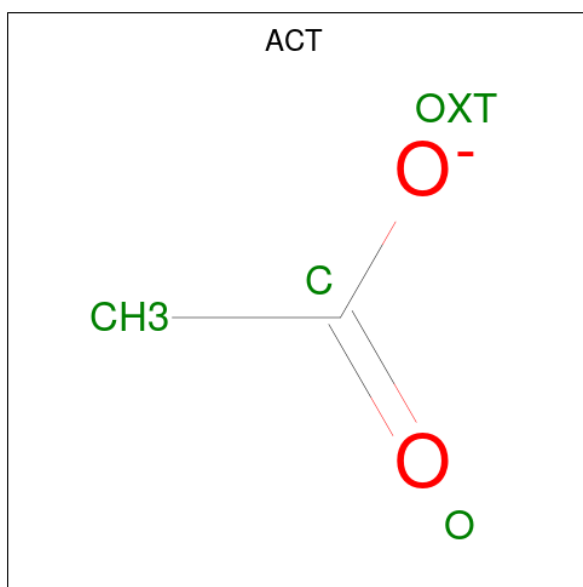
Chain	Residue	Modelled	Actual	Comment	Reference
C	168	THR	VAL	SEE REMARK 999	UNP Q15485
C	247	THR	VAL	SEE REMARK 999	UNP Q15485
A	168	THR	VAL	SEE REMARK 999	UNP Q15485
A	247	THR	VAL	SEE REMARK 999	UNP Q15485
B	168	THR	VAL	SEE REMARK 999	UNP Q15485
B	247	THR	VAL	SEE REMARK 999	UNP Q15485

- 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 (CCD ID: ACT) (formula: C₂H₃O₂).

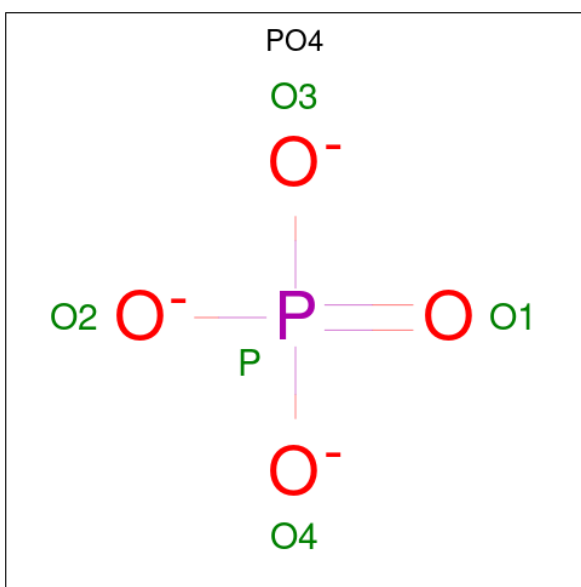


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

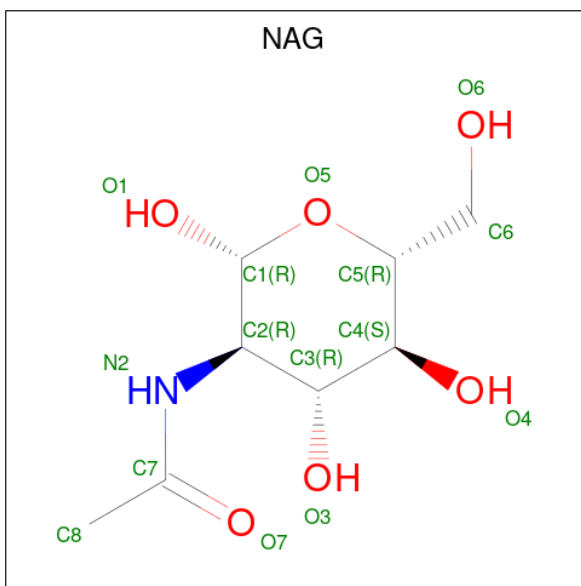
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		
4	A	2	Total	Ca	0	0
			2	2		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



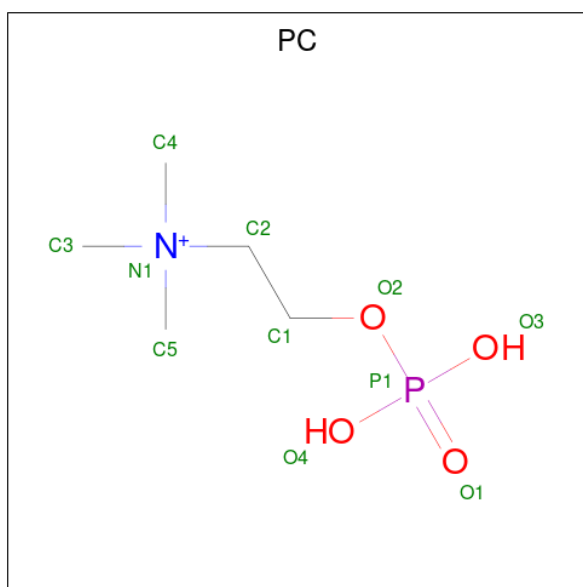
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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 (CCD ID: 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		

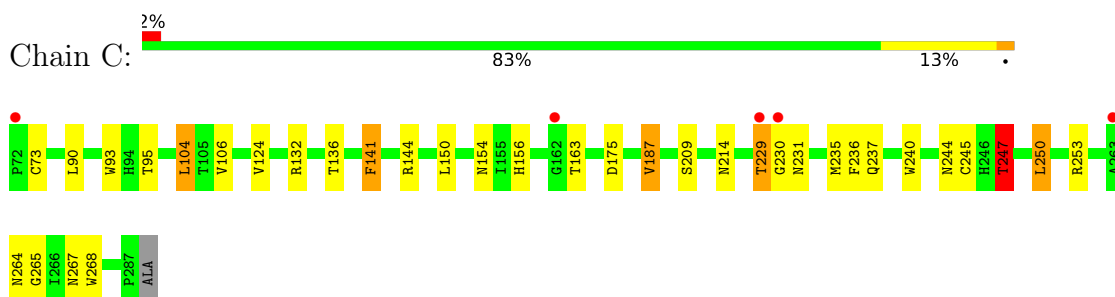
- Molecule 8 is water.

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		

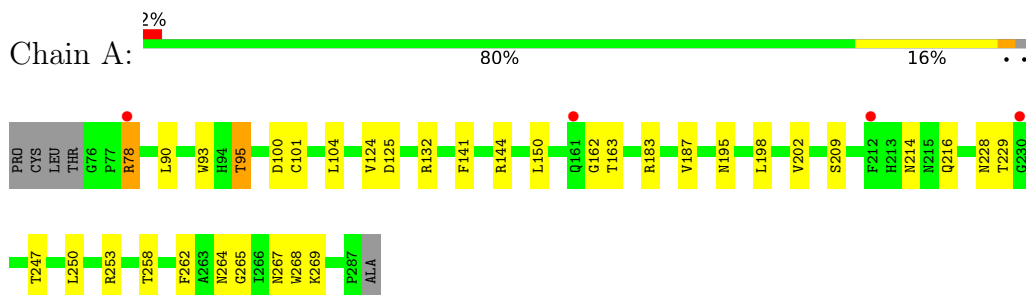
3 Residue-property plots

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.

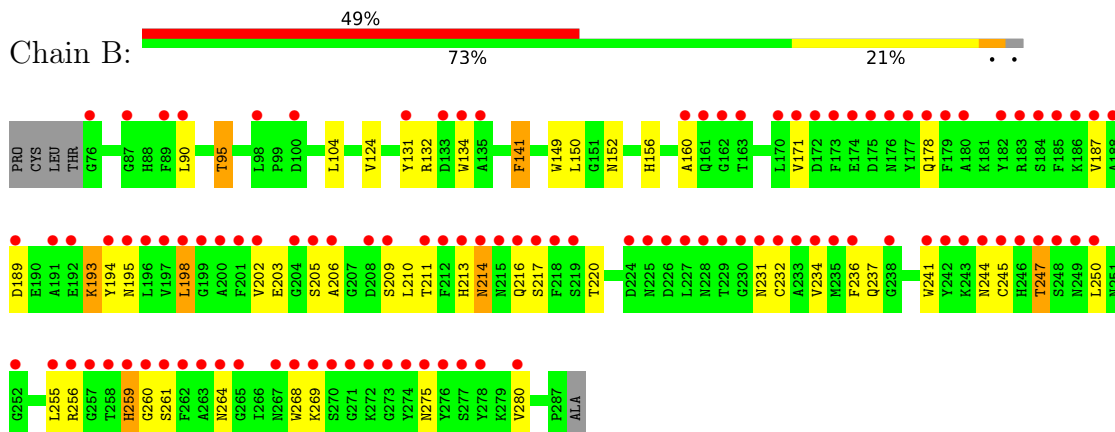
- Molecule 1: Ficolin-2



- 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, α , β , γ	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) 99.4 (19.95-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	32.3	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5347	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, PC, MAN, ACT, FUC, 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	1.15	1/1774 (0.1%)	1.04	5/2400 (0.2%)
1	B	0.89	3/1749 (0.2%)	0.93	3/2366 (0.1%)
1	C	1.26	6/1805 (0.3%)	1.16	8/2441 (0.3%)
All	All	1.11	10/5328 (0.2%)	1.05	16/7207 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	PHE	CG-CD2	-10.53	1.16	1.38
1	C	141	PHE	CG-CD1	-9.12	1.19	1.38
1	B	206	ALA	C-O	7.00	1.33	1.24
1	B	141	PHE	CG-CD2	-6.91	1.24	1.38
1	C	154	ASN	C-O	-6.69	1.16	1.24
1	A	141	PHE	CG-CD2	-6.49	1.25	1.38
1	C	141	PHE	CE1-CZ	-6.44	1.19	1.38
1	B	141	PHE	CG-CD1	-6.11	1.26	1.38
1	C	141	PHE	CE2-CZ	-5.95	1.20	1.38
1	C	214	ASN	C-O	-5.91	1.16	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	ARG	CG-CD-NE	-7.56	95.37	112.00
1	B	132	ARG	CG-CD-NE	-6.47	97.77	112.00
1	A	262	PHE	N-CA-C	6.39	118.57	108.67
1	A	132	ARG	CG-CD-NE	-6.10	98.57	112.00
1	C	230	GLY	N-CA-C	6.06	121.26	112.60
1	B	259	HIS	N-CA-C	5.88	118.94	109.83
1	C	73	CYS	N-CA-C	5.77	118.31	111.33
1	B	95	THR	CB-CA-C	5.72	119.18	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	THR	N-CA-CB	-5.71	103.30	110.90
1	A	132	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	C	247	THR	CB-CA-C	5.56	118.36	109.02
1	A	162	GLY	N-CA-C	5.55	118.28	111.45
1	C	132	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	C	229	THR	N-CA-CB	-5.35	101.51	110.39
1	C	141	PHE	CE1-CZ-CE2	-5.09	110.84	120.00
1	A	95	THR	CB-CA-C	5.08	118.13	109.75

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	16	0
1	B	1702	0	1573	29	0
1	C	1757	0	1631	19	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	64	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 (64) 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	2.35	0.61
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:A:231:ASN:HD22	1:A:231:ASN:C	2.19	0.49
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:B:194:TYR:O	1:B:195:ASN:C	2.58	0.46
1:C:231:ASN:C	1:C:231:ASN:HD22	2.23	0.46
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:210:LEU:O	1:B:211:THR:C	2.62	0.42
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:232:CYS:O	1:B:236:PHE:N	2.54	0.41
1:C:235[B]:MET:HE3	1:C:235[B]:MET:HB3	1.95	0.41
1:C:141:PHE:CD1	1:C:141:PHE:C	2.98	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:A:195:ASN:HD22	1:A:216:GLN:C	2.29	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%)	24	24
1	B	210/217 (97%)	188 (90%)	20 (10%)	2 (1%)	12	10
1	C	217/217 (100%)	207 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	640/651 (98%)	594 (93%)	43 (7%)	3 (0%)	24 24

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	181/182 (100%)	165 (91%)	16 (9%)	9 7
1	B	178/182 (98%)	166 (93%)	12 (7%)	15 14
1	C	185/182 (102%)	173 (94%)	12 (6%)	15 14
All	All	544/546 (100%)	504 (93%)	40 (7%)	13 11

All (40) 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	163	THR
1	C	175	ASP
1	C	187	VAL
1	C	229	THR
1	C	247	THR
1	C	250	LEU
1	A	78	ARG

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Mol	Chain	Res	Type
1	A	90	LEU
1	A	95	THR
1	A	104	LEU
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	90	LEU
1	B	95	THR
1	B	104	LEU
1	B	124	VAL
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	247	THR
1	B	250	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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
1	C	231	ASN
1	C	237	GLN
1	C	267	ASN
1	A	94	HIS
1	A	139	GLN
1	A	156	HIS

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Mol	Chain	Res	Type
1	A	195	ASN
1	A	214	ASN
1	A	225	ASN
1	A	231	ASN
1	A	237	GLN
1	A	267	ASN
1	B	94	HIS
1	B	139	GLN
1	B	156	HIS
1	B	214	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%)
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
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:

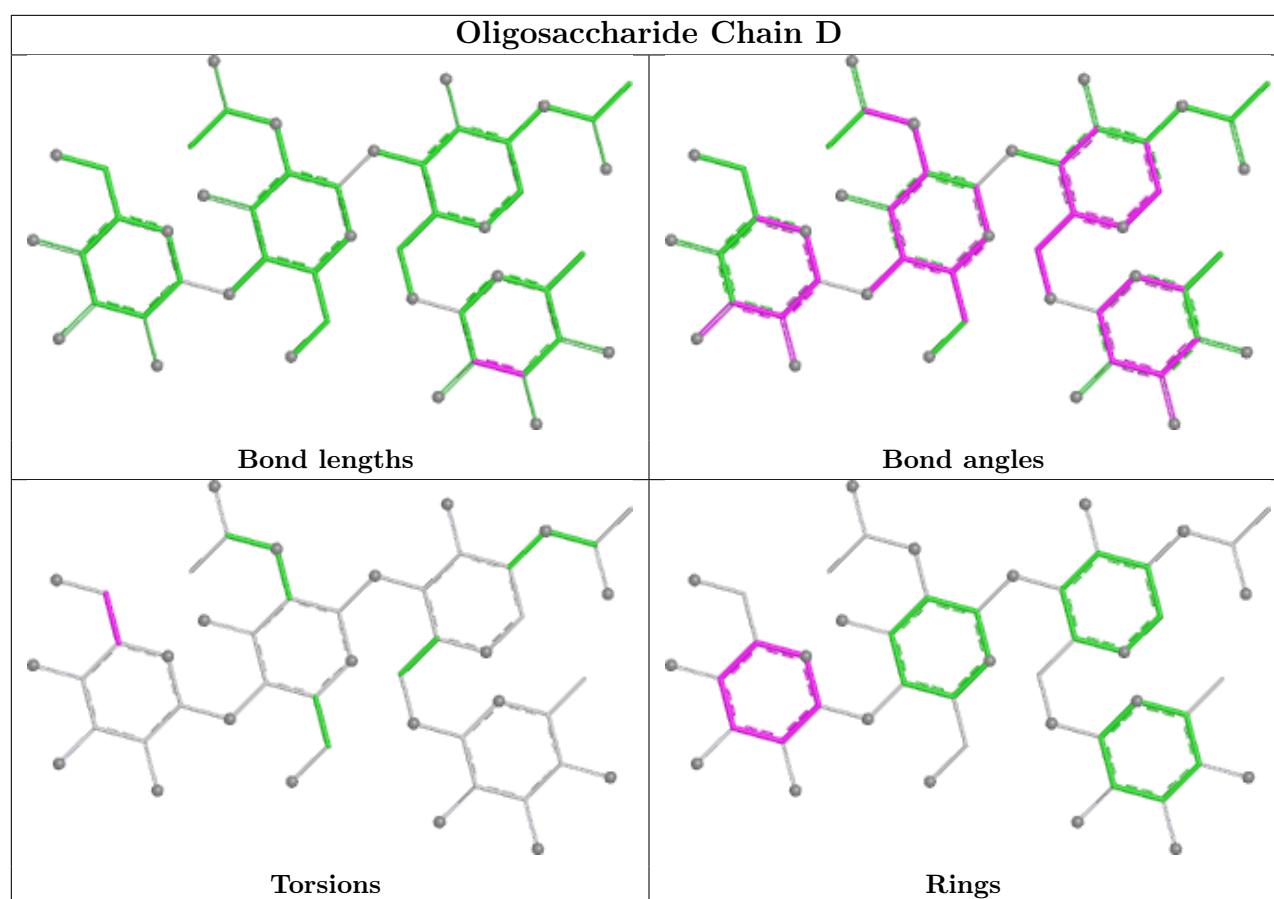
Mol	Chain	Res	Type	Atoms
2	D	3	MAN	O5-C5-C6-O6

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
7	PC	A	303	-	10,10,10	0.86	0	15,15,15	3.49	10 (66%)
3	ACT	C	301	-	3,3,3	0.79	0	3,3,3	1.31	0
5	PO4	C	307	-	4,4,4	1.36	0	6,6,6	1.38	0
3	ACT	A	301	-	3,3,3	1.16	0	3,3,3	0.09	0
6	NAG	A	302	1	14,14,15	1.08	1 (7%)	17,19,21	1.75	5 (29%)

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	NAG	A	302	1	-	0/6/23/26	0/1/1/1
7	PC	A	303	-	-	4/8/8/8	-

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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, 95th 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 ²)	Q<0.9
1	A	212/217 (97%)	-0.23	4 (1%) 66 67	14, 34, 64, 89	8 (3%)
1	B	212/217 (97%)	2.21	107 (50%) 0 0	37, 109, 205, 234	4 (1%)
1	C	216/217 (99%)	-0.21	5 (2%) 61 61	12, 30, 56, 73	7 (3%)
All	All	640/651 (98%)	0.59	116 (18%) 3 3	12, 42, 178, 234	19 (2%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	GLY	7.6
1	A	212	PHE	7.5
1	B	268	TRP	7.4
1	B	242	TYR	6.8
1	B	229	THR	6.6
1	B	274	TYR	6.2
1	B	199	GLY	6.1
1	B	227	LEU	5.4
1	B	276	TYR	5.4
1	B	226	ASP	5.2
1	B	191	ALA	5.0
1	B	173	PHE	4.8
1	B	257	GLY	4.8
1	B	219	SER	4.8
1	B	215	ASN	4.7
1	B	216	GLN	4.7
1	B	197	VAL	4.6
1	B	236	PHE	4.5
1	B	263	ALA	4.4
1	B	76	GLY	4.4
1	B	224	ASP	4.4
1	B	271	GLY	4.4
1	B	273	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	231	ASN	4.3
1	B	177	TYR	4.2
1	B	258	THR	4.2
1	B	214	ASN	4.2
1	B	262	PHE	4.2
1	B	269	LYS	4.2
1	B	178	GLN	4.1
1	B	270	SER	4.1
1	B	255	LEU	4.1
1	B	278	TYR	4.0
1	B	200	ALA	4.0
1	B	172	ASP	3.9
1	B	198	LEU	3.9
1	B	248	SER	3.9
1	B	182	TYR	3.8
1	B	212	PHE	3.8
1	B	217	SER	3.8
1	B	275	ASN	3.8
1	B	211	THR	3.7
1	B	228	ASN	3.7
1	B	267	ASN	3.7
1	B	225	ASN	3.6
1	B	209	SER	3.6
1	B	90	LEU	3.6
1	B	206	ALA	3.6
1	B	245	CYS	3.6
1	B	272	LYS	3.6
1	B	265	GLY	3.5
1	C	229	THR	3.4
1	B	171	VAL	3.4
1	B	179	PHE	3.3
1	B	277	SER	3.3
1	B	174	GLU	3.3
1	B	260	GLY	3.3
1	B	244	ASN	3.2
1	B	249	ASN	3.2
1	B	89	PHE	3.2
1	B	180	ALA	3.2
1	B	188	ALA	3.2
1	B	235	MET	3.1
1	B	232	CYS	3.1
1	C	72	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	233	ALA	3.1
1	B	194	TYR	3.0
1	B	192	GLU	3.0
1	B	205	SER	3.0
1	B	161	GLN	3.0
1	B	247	THR	3.0
1	B	256	ARG	3.0
1	B	243	LYS	2.9
1	B	234	VAL	2.9
1	B	176	ASN	2.9
1	B	195	ASN	2.9
1	B	131	TYR	2.9
1	B	170	LEU	2.8
1	B	134	TRP	2.8
1	B	241	TRP	2.8
1	B	202	VAL	2.8
1	B	218	PHE	2.8
1	B	204	GLY	2.8
1	B	189	ASP	2.7
1	B	184	SER	2.7
1	B	98	LEU	2.7
1	B	280	VAL	2.7
1	B	252	GLY	2.7
1	B	201	PHE	2.6
1	B	250	LEU	2.5
1	C	263	ALA	2.5
1	B	208	ASP	2.5
1	B	163	THR	2.5
1	B	186	LYS	2.4
1	B	187	VAL	2.4
1	A	230	GLY	2.4
1	B	246	HIS	2.4
1	B	133	ASP	2.4
1	B	264	ASN	2.4
1	B	213	HIS	2.4
1	B	261	SER	2.3
1	B	175	ASP	2.3
1	B	238	GLY	2.3
1	A	161	GLN	2.2
1	B	100	ASP	2.2
1	C	230	GLY	2.2
1	B	87	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	160	ALA	2.2
1	C	162	GLY	2.2
1	B	183	ARG	2.1
1	B	185	PHE	2.1
1	B	162	GLY	2.1
1	B	196	LEU	2.1
1	B	135	ALA	2.0
1	A	78	ARG	2.0
1	B	259	HIS	2.0

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

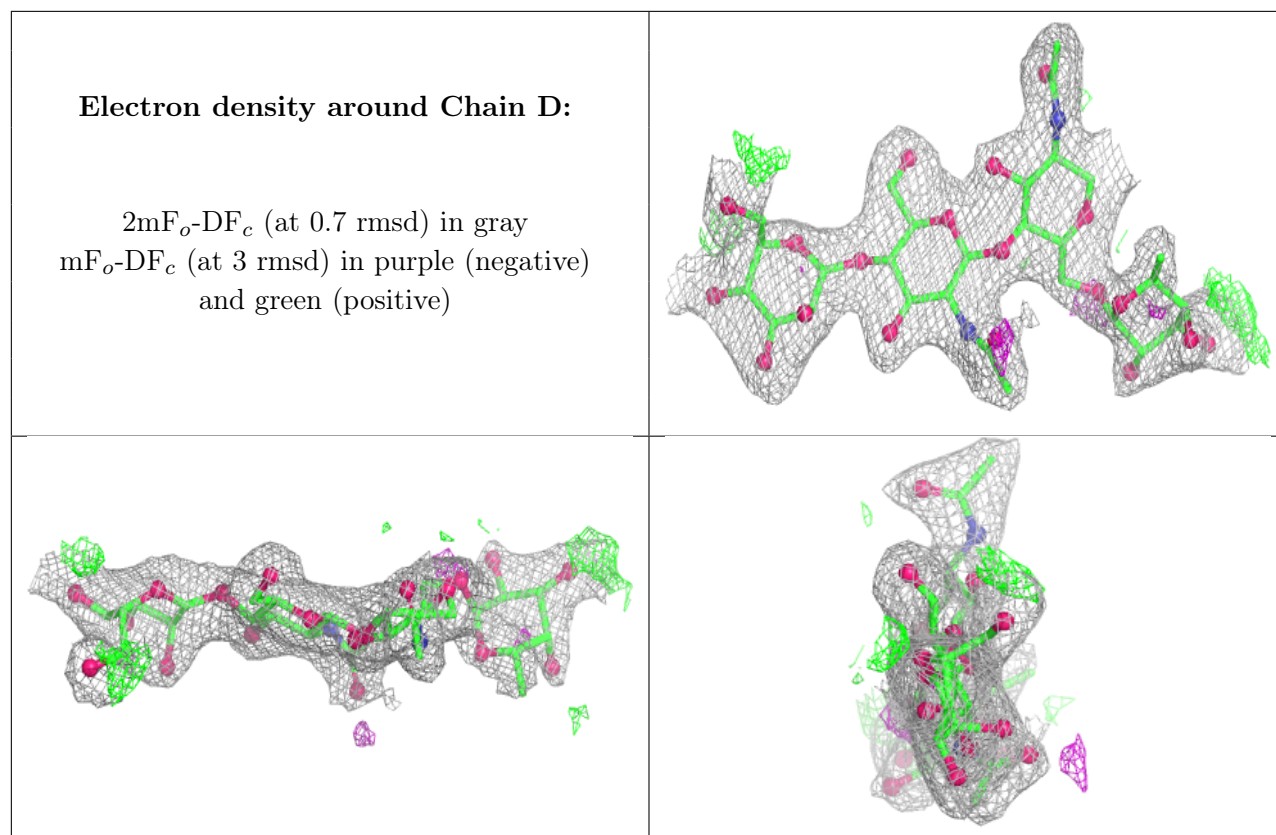
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUC	D	4	10/11	0.66	0.15	37,40,42,47	10
2	MAN	D	3	11/12	0.71	0.11	46,54,61,64	0
2	NAG	D	2	14/15	0.92	0.07	28,35,39,40	0
2	NAG	D	1	14/15	0.94	0.07	19,26,33,34	0

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



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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($\text{\AA}^2$)	Q<0.9
6	NAG	A	302	14/15	0.73	0.13	39,49,57,59	0
4	CA	B	301	1/1	0.83	0.10	67,67,67,67	0
7	PC	A	303	11/11	0.90	0.14	32,43,58,58	0
5	PO4	C	307	5/5	0.92	0.15	30,37,45,46	0
3	ACT	C	301	4/4	0.93	0.10	29,31,32,33	0
4	CA	A	305	1/1	0.94	0.10	46,46,46,46	0
3	ACT	A	301	4/4	0.95	0.12	37,38,38,39	0
4	CA	A	304	1/1	0.97	0.05	38,38,38,38	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.