



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:50 AM UTC

PDB ID : 1LOG / pdb_00001log
Title : X-RAY STRUCTURE OF A (ALPHA-MAN(1-3)BETA-MAN(1-4)GLCNAC
)-LECTIN COMPLEX AT 2.1 ANGSTROMS RESOLUTION
Authors : Bourne, Y.; Cambillau, C.
Deposited on : 1994-01-27
Resolution : 2.10 Å(reported)

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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

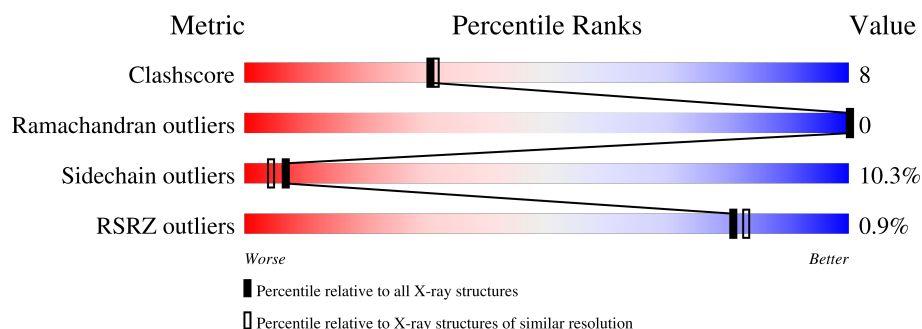
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	181	
1	C	181	
2	B	52	
2	D	52	
3	E	3	
3	F	3	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3993 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 LEGUME ISOLECTIN I (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	C	181	Total	C	N	O	0	0	0
			1406	894	232	280			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	LYS	conflict	UNP P04122
C	153	ALA	LYS	conflict	UNP P04122

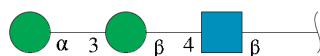
- Molecule 2 is a protein called LEGUME ISOLECTIN I (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	46	Total	C	N	O	0	0	0
			372	246	57	69			
2	D	51	Total	C	N	O	0	0	0
			402	262	62	78			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	TYR	PHE	conflict	UNP P12306
D	41	TYR	PHE	conflict	UNP P12306

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			37	20	1	16			
3	F	3	Total	C	N	O	0	0	0
			37	20	1	16			

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

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

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		

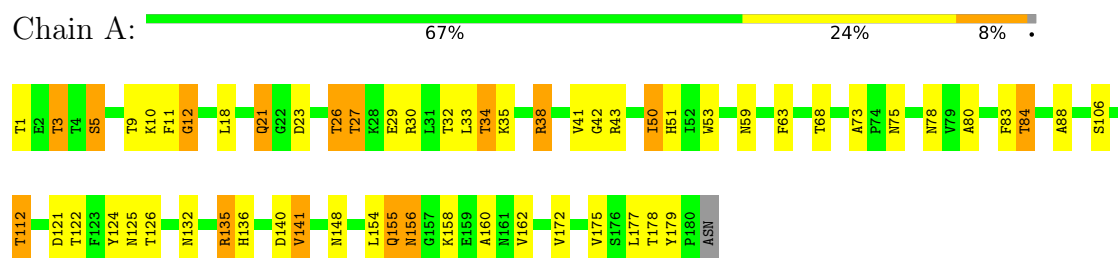
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	146	Total	O	0	0
			146	146		
6	B	32	Total	O	0	0
			32	32		
6	C	135	Total	O	0	0
			135	135		
6	D	25	Total	O	0	0
			25	25		

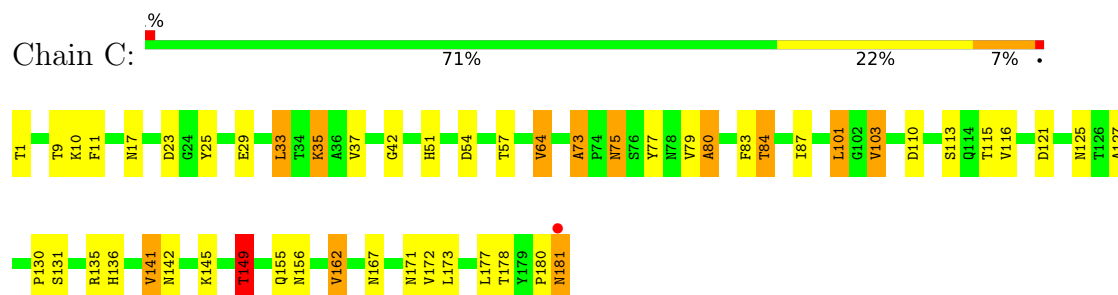
3 Residue-property plots

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.

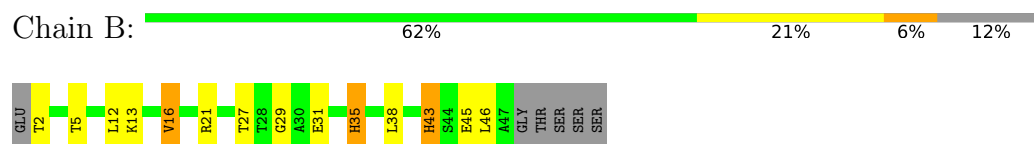
• Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



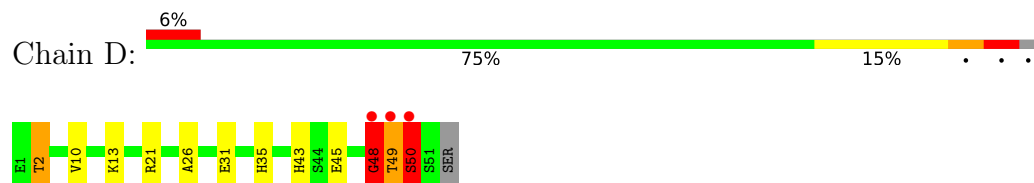
• Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  67% 33%



- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.10Å 63.30Å 54.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 8.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.10) 82.6 (8.00-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.26 (at 2.12Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.175 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3993	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, NAG, CA, BMA, MAN

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	1.00	4/1431 (0.3%)	1.82	32/1954 (1.6%)
1	C	1.00	6/1440 (0.4%)	1.77	34/1965 (1.7%)
2	B	1.04	2/385 (0.5%)	1.71	5/527 (0.9%)
2	D	1.09	3/415 (0.7%)	1.94	12/567 (2.1%)
All	All	1.01	15/3671 (0.4%)	1.80	83/5013 (1.7%)

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
2	D	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	PRO	CA-CB	-7.66	1.48	1.53
1	C	141	VAL	CA-CB	7.29	1.64	1.54
1	C	51	HIS	CD2-NE2	-7.22	1.29	1.37
1	A	136	HIS	CG-ND1	-6.91	1.30	1.38
1	A	51	HIS	CD2-NE2	-6.87	1.30	1.37
2	D	43	HIS	CD2-NE2	-6.58	1.30	1.37
2	B	43	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	141	VAL	CA-CB	6.40	1.62	1.54
1	C	180	PRO	N-CA	-6.30	1.42	1.47
2	D	35	HIS	CD2-NE2	-5.99	1.31	1.37
2	B	35	HIS	CD2-NE2	-5.82	1.31	1.37
1	C	162	VAL	CA-CB	5.76	1.63	1.55
1	C	136	HIS	CG-ND1	-5.30	1.32	1.38
1	A	50	ILE	CA-CB	5.20	1.62	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	43	HIS	CG-ND1	-5.20	1.32	1.38

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	49	THR	N-CA-C	16.96	141.02	107.62
1	C	171	ASN	OD1-CG-ND2	-9.63	112.97	122.60
1	A	38	ARG	CB-CG-CD	-8.74	91.19	111.30
2	B	16	VAL	N-CA-CB	-8.31	99.58	111.21
1	C	103	VAL	N-CA-CB	-7.99	101.34	112.12
1	C	103	VAL	CB-CA-C	7.87	118.36	110.65
2	D	21	ARG	CA-CB-CG	-7.43	99.25	114.10
1	C	51	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	A	63	PHE	CA-CB-CG	6.93	120.73	113.80
2	B	21	ARG	CA-CB-CG	-6.87	100.36	114.10
1	A	21	GLN	OE1-CD-NE2	-6.80	115.80	122.60
2	D	49	THR	N-CA-CB	-6.74	99.08	110.46
1	A	156	ASN	OD1-CG-ND2	-6.63	115.97	122.60
2	B	43	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	C	121	ASP	CA-CB-CG	6.39	118.99	112.60
2	D	50	SER	N-CA-C	-6.37	98.81	109.07
1	A	9	THR	CA-CB-OG1	-6.35	100.07	109.60
1	C	181	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	C	155	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	A	148	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	C	127	ALA	N-CA-C	6.19	118.83	111.71
1	C	149	THR	N-CA-CB	-6.16	100.07	111.53
1	A	21	GLN	CG-CD-NE2	6.14	125.61	116.40
1	C	80	ALA	O-C-N	-6.09	117.43	123.46
1	A	140	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	83	PHE	CA-CB-CG	5.98	119.78	113.80
1	C	75	ASN	O-C-N	-5.97	117.32	123.29
1	C	23	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	125	ASN	N-CA-C	-5.93	98.74	108.41
2	D	13	LYS	CB-CG-CD	-5.92	97.68	111.30
1	C	167	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	C	142	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	26	THR	N-CA-CB	-5.79	100.52	111.00
1	C	101	LEU	N-CA-CB	-5.74	103.39	112.63
1	A	12	GLY	CA-C-N	5.73	125.41	119.56
1	A	12	GLY	C-N-CA	5.73	125.41	119.56
1	C	135	ARG	N-CA-C	-5.69	102.48	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ASN	CB-CG-ND2	5.66	124.89	116.40
1	A	155	GLN	OE1-CD-NE2	-5.62	116.98	122.60
2	D	48	GLY	CA-C-N	-5.55	114.92	123.14
2	D	48	GLY	C-N-CA	-5.55	114.92	123.14
1	C	171	ASN	CB-CG-ND2	5.52	124.69	116.40
1	A	132	ASN	OD1-CG-ND2	-5.49	117.11	122.60
2	D	45	GLU	N-CA-CB	-5.48	102.32	110.71
1	C	136	HIS	CA-CB-CG	-5.46	108.34	113.80
2	D	2	THR	CB-CA-C	5.46	119.22	110.16
1	A	179	TYR	N-CA-C	-5.46	98.87	108.69
1	C	180	PRO	CA-C-O	-5.45	117.28	121.31
1	A	27	THR	CA-CB-OG1	-5.42	101.47	109.60
1	C	87	ILE	N-CA-C	-5.42	99.75	107.77
1	A	23	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	9	THR	CA-CB-CG2	5.41	119.69	110.50
1	A	3	THR	N-CA-CB	-5.40	101.47	111.13
2	B	35	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	A	84	THR	N-CA-CB	-5.37	101.52	111.13
1	A	88	ALA	CA-C-N	5.37	125.37	119.89
1	A	88	ALA	C-N-CA	5.37	125.37	119.89
1	C	35	LYS	N-CA-C	-5.36	102.05	110.36
1	A	121	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	26	THR	CB-CA-C	5.31	119.86	109.35
1	C	131	SER	N-CA-C	5.30	117.81	111.71
1	C	156	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	C	64	VAL	CB-CA-C	-5.27	101.59	110.71
2	B	43	HIS	CB-CG-ND1	5.26	130.59	122.70
1	C	84	THR	N-CA-CB	-5.23	101.67	111.13
2	D	35	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	C	83	PHE	N-CA-CB	-5.22	101.80	111.52
1	A	112	THR	N-CA-CB	-5.22	101.72	110.39
1	A	32	THR	OG1-CB-CG2	-5.22	98.87	109.30
1	A	136	HIS	N-CA-C	5.20	116.98	108.76
1	A	178	THR	CA-CB-OG1	-5.19	101.81	109.60
1	C	73	ALA	CA-C-N	5.16	124.83	119.56
1	C	73	ALA	C-N-CA	5.16	124.83	119.56
1	C	51	HIS	CB-CG-ND1	5.13	130.39	122.70
1	C	172	VAL	CG1-CB-CG2	-5.13	99.52	110.80
1	C	37	VAL	N-CA-CB	-5.11	102.37	111.92
2	D	45	GLU	CA-CB-CG	5.10	124.31	114.10
1	C	1	THR	CA-CB-OG1	-5.10	101.95	109.60
2	D	43	HIS	CB-CG-CD2	-5.10	124.57	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	ASN	N-CA-C	-5.09	98.98	107.99
1	A	10	LYS	N-CA-C	-5.08	99.33	108.48
1	A	59	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	C	17	ASN	CA-CB-CG	5.05	117.65	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	48	GLY	Peptide

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	1397	0	1346	32	0
1	C	1406	0	1352	14	0
2	B	372	0	348	12	0
2	D	402	0	373	9	0
3	E	37	0	33	1	0
3	F	37	0	33	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	146	0	0	6	0
6	B	32	0	0	0	0
6	C	135	0	0	2	0
6	D	25	0	0	0	0
All	All	3993	0	3485	51	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 8.

All (51) 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:C:130:PRO:HG3	1:C:149:THR:HG21	1.50	0.89
1:A:122:THR:HA	1:A:135:ARG:HG3	1.63	0.80
1:A:73:ALA:H	1:A:156:ASN:HD21	1.31	0.79
1:A:21:GLN:HE22	1:A:43:ARG:HH21	1.29	0.78
6:A:889:HOH:O	2:B:38:LEU:HA	1.92	0.67
1:A:30:ARG:HA	6:A:889:HOH:O	1.95	0.67
1:A:11:PHE:O	1:A:29:GLU:HA	1.94	0.66
1:A:160:ALA:HB1	1:A:177:LEU:HD21	1.78	0.66
1:A:73:ALA:H	1:A:156:ASN:ND2	1.93	0.66
1:A:155:GLN:HE21	1:A:158:LYS:HG3	1.61	0.66
6:C:921:HOH:O	3:F:1:NAG:H2	1.97	0.64
1:A:34:THR:HG21	2:B:35:HIS:HD2	1.67	0.60
1:A:162:VAL:HG22	1:A:177:LEU:HD23	1.83	0.60
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.49	0.59
1:C:75:ASN:HD22	1:C:77:TYR:H	1.50	0.59
1:A:5:SER:OG	2:B:43:HIS:HD2	1.87	0.57
1:A:34:THR:CG2	2:B:35:HIS:HD2	2.18	0.56
1:A:12:GLY:HA3	2:D:50:SER:HB3	1.87	0.56
1:A:73:ALA:N	1:A:156:ASN:HD21	2.02	0.56
1:A:80:ALA:HB3	2:B:31:GLU:HB3	1.87	0.56
1:A:80:ALA:CB	2:B:31:GLU:HB3	2.37	0.55
1:A:21:GLN:NE2	1:A:43:ARG:HE	2.05	0.54
1:A:1:THR:HA	2:B:46:LEU:O	2.08	0.54
1:A:12:GLY:CA	2:D:50:SER:HB3	2.39	0.53
1:C:80:ALA:HB3	2:D:31:GLU:HB2	1.91	0.53
1:A:122:THR:O	1:A:135:ARG:HD2	2.08	0.53
1:A:12:GLY:N	2:D:50:SER:HB3	2.26	0.50
1:C:33:LEU:O	1:C:42:GLY:HA3	2.12	0.49
6:A:726:HOH:O	2:D:48:GLY:HA3	2.11	0.49
1:A:38:ARG:HB2	2:B:29:GLY:O	2.12	0.49
1:C:80:ALA:CB	2:D:31:GLU:HB2	2.44	0.48
1:A:75:ASN:HD21	1:A:78:ASN:ND2	2.12	0.48
1:C:73:ALA:HB2	1:C:79:VAL:HG13	1.96	0.47
1:A:106:SER:HB2	6:A:843:HOH:O	2.14	0.47
1:A:124:TYR:CE2	1:A:126:THR:HG22	2.50	0.47
1:C:75:ASN:ND2	1:C:77:TYR:H	2.11	0.47
1:C:110:ASP:O	1:C:113:SER:HB3	2.15	0.46
1:C:54:ASP:OD2	2:D:49:THR:HB	2.15	0.46
1:C:11:PHE:O	1:C:29:GLU:HA	2.15	0.46
1:C:57:THR:HG21	2:D:49:THR:HG21	1.97	0.45
1:C:25:TYR:OH	1:C:35:LYS:HE2	2.18	0.44
1:A:41:VAL:HG22	2:B:27:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:THR:HG23	6:C:686:HOH:O	2.19	0.43
1:C:33:LEU:HB3	2:D:26:ALA:HB3	2.00	0.43
1:A:11:PHE:HD1	6:A:889:HOH:O	2.03	0.42
1:A:33:LEU:O	1:A:42:GLY:HA3	2.19	0.41
1:A:34:THR:HG21	2:B:35:HIS:CD2	2.51	0.41
1:A:53:TRP:CE3	2:B:13:LYS:HD2	2.55	0.41
3:E:2:BMA:H2	3:E:3:MAN:H5	2.03	0.41
1:A:21:GLN:NE2	1:A:43:ARG:HH21	2.08	0.41
6:A:735:HOH:O	2:B:35:HIS:HE1	2.03	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	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
1	C	179/181 (99%)	176 (98%)	3 (2%)	0	100	100
2	B	44/52 (85%)	42 (96%)	2 (4%)	0	100	100
2	D	49/52 (94%)	45 (92%)	4 (8%)	0	100	100
All	All	450/466 (97%)	437 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	154/155 (99%)	138 (90%)	16 (10%)	7	4
1	C	155/155 (100%)	139 (90%)	16 (10%)	7	4
2	B	39/44 (89%)	34 (87%)	5 (13%)	4	2
2	D	42/44 (96%)	39 (93%)	3 (7%)	13	11
All	All	390/398 (98%)	350 (90%)	40 (10%)	7	4

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	5	SER
1	A	18	LEU
1	A	26	THR
1	A	27	THR
1	A	34	THR
1	A	35	LYS
1	A	50	ILE
1	A	68	THR
1	A	84	THR
1	A	112	THR
1	A	135	ARG
1	A	141	VAL
1	A	154	LEU
1	A	172	VAL
1	A	175	VAL
2	B	2	THR
2	B	5	THR
2	B	12	LEU
2	B	16	VAL
2	B	45	GLU
1	C	9	THR
1	C	10	LYS
1	C	33	LEU
1	C	64	VAL
1	C	84	THR
1	C	101	LEU
1	C	103	VAL
1	C	115	THR
1	C	116	VAL
1	C	141	VAL
1	C	145	LYS
1	C	149	THR

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Mol	Chain	Res	Type
1	C	162	VAL
1	C	173	LEU
1	C	177	LEU
1	C	181	ASN
2	D	2	THR
2	D	10	VAL
2	D	50	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	21	GLN
1	A	59	ASN
1	A	78	ASN
1	A	95	GLN
1	A	105	ASN
1	A	155	GLN
1	A	156	ASN
1	A	171	ASN
2	B	7	ASN
2	B	35	HIS
2	B	43	HIS
1	C	39	ASN
1	C	75	ASN
1	C	78	ASN
1	C	95	GLN
1	C	105	ASN
1	C	142	ASN
1	C	161	ASN
1	C	181	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

6 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
3	NAG	E	1	3	15,15,15	0.80	0	21,21,21	1.81	2 (9%)
3	BMA	E	2	3	11,11,12	0.72	0	15,15,17	1.09	0
3	MAN	E	3	3	11,11,12	0.79	0	15,15,17	0.77	1 (6%)
3	NAG	F	1	3	15,15,15	0.79	1 (6%)	21,21,21	1.63	4 (19%)
3	BMA	F	2	3	11,11,12	0.81	0	15,15,17	0.79	0
3	MAN	F	3	3	11,11,12	0.96	0	15,15,17	0.95	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
3	NAG	E	1	3	-	4/6/26/26	0/1/1/1
3	BMA	E	2	3	-	0/2/19/22	0/1/1/1
3	MAN	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3	-	2/6/26/26	0/1/1/1
3	BMA	F	2	3	-	2/2/19/22	0/1/1/1
3	MAN	F	3	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C4-C5	2.22	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-C2-N2	-6.43	103.28	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-C2-N2	-4.98	104.96	110.73
3	F	1	NAG	O4-C4-C3	-3.35	102.48	110.38
3	E	1	NAG	C3-C4-C5	3.13	115.92	110.23
3	F	1	NAG	C3-C4-C5	2.67	115.07	110.23
3	F	1	NAG	C6-C5-C4	2.44	119.01	113.02
3	E	3	MAN	C1-O5-C5	2.39	115.38	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

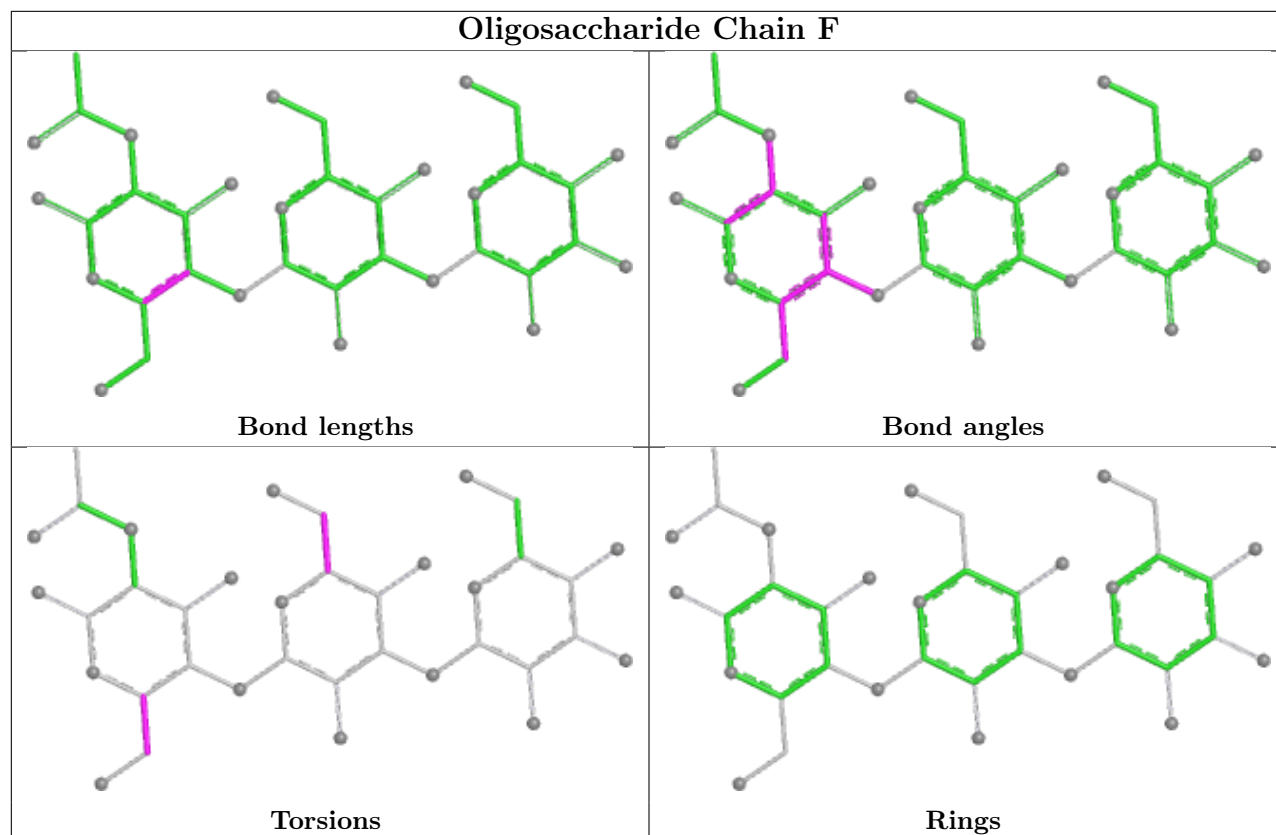
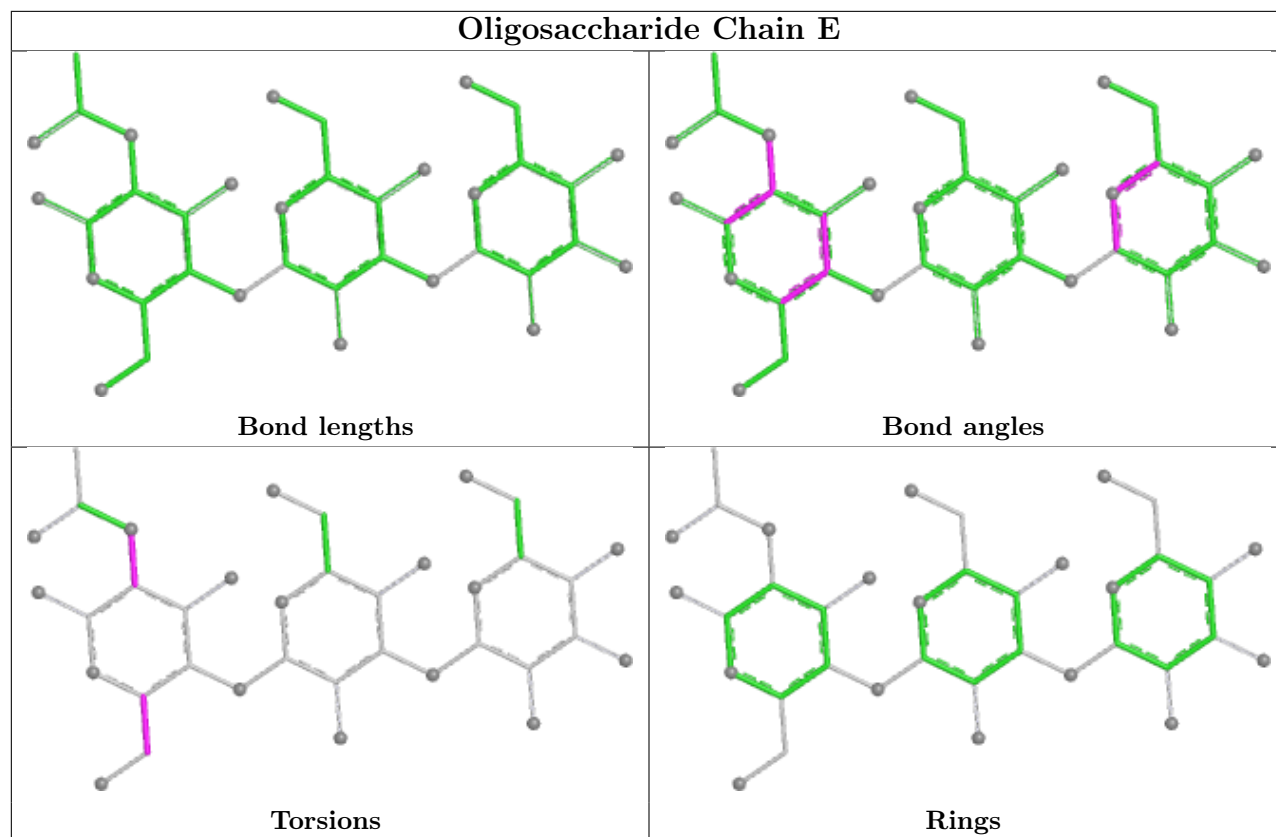
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7
3	F	2	BMA	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	2	BMA	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	E	3	MAN	1	0
3	E	2	BMA	1	0

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



5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	180/181 (99%)	-0.77	0 100 100	3, 12, 27, 40	0
1	C	181/181 (100%)	-0.76	1 (0%) 85 87	4, 12, 24, 53	0
2	B	46/52 (88%)	-0.78	0 100 100	3, 12, 25, 34	0
2	D	51/52 (98%)	-0.49	3 (5%) 28 30	4, 13, 42, 59	0
All	All	458/466 (98%)	-0.74	4 (0%) 81 83	3, 12, 27, 59	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	49	THR	3.5
2	D	48	GLY	3.4
2	D	50	SER	2.6
1	C	181	ASN	2.1

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.

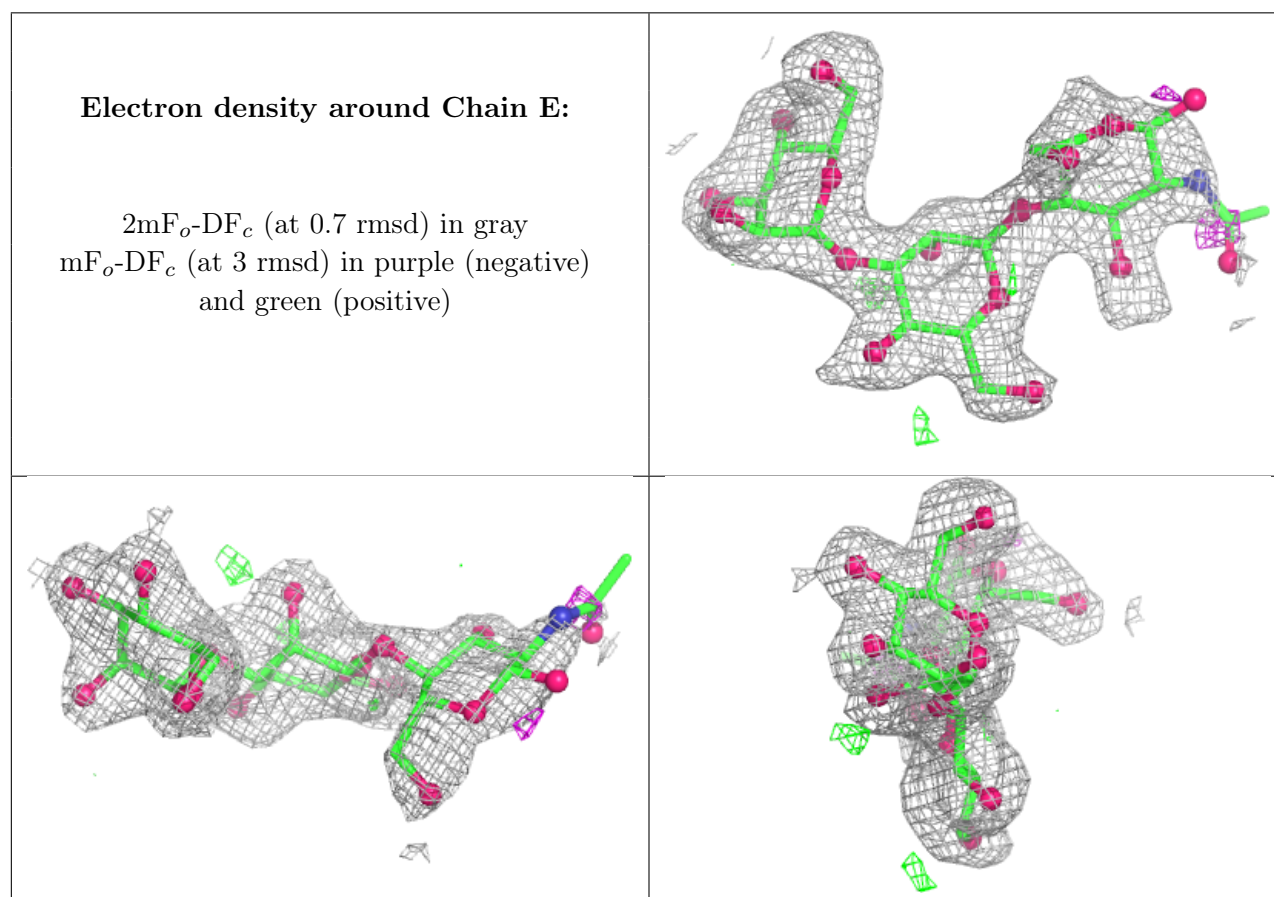
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	1	15/15	0.67	0.12	40,47,55,56	0
3	NAG	E	1	15/15	0.74	0.10	42,50,60,61	0
3	BMA	F	2	11/12	0.86	0.09	18,28,36,40	0

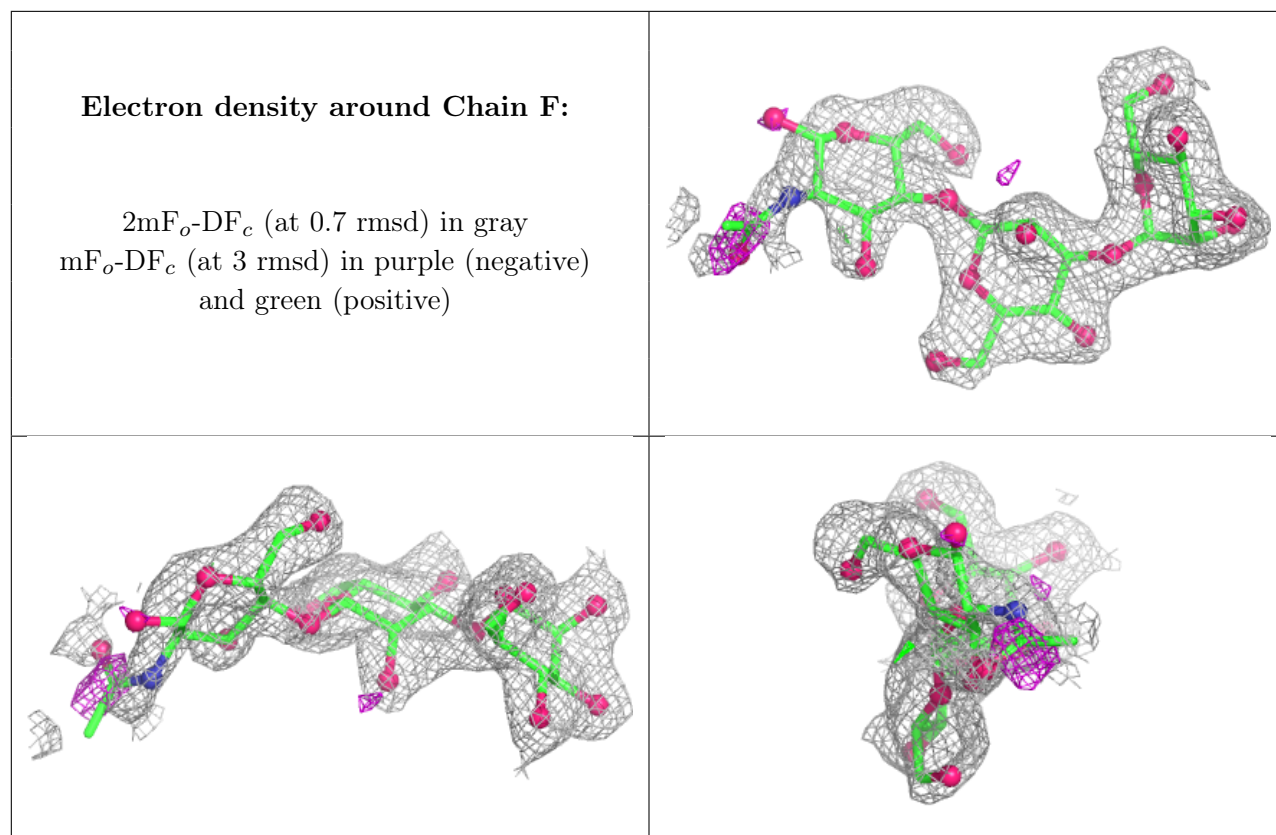
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	E	2	11/12	0.91	0.07	27,33,38,41	0
3	MAN	E	3	11/12	0.91	0.07	14,19,24,27	0
3	MAN	F	3	11/12	0.95	0.05	12,15,17,20	0

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(Å ²)	Q<0.9
4	CA	C	571	1/1	0.80	0.10	6,6,6,6	0
4	CA	A	561	1/1	0.81	0.08	16,16,16,16	0
5	MN	C	572	1/1	0.93	0.04	17,17,17,17	0
5	MN	A	562	1/1	0.96	0.03	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.