



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:03 PM UTC

PDB ID : 3FBY / pdb_00003fby
Title : The crystal structure of the signature domain of cartilage oligomeric matrix protein.
Authors : Tan, K.; Lawler, J.
Deposited on : 2008-11-20
Resolution : 3.15 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

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

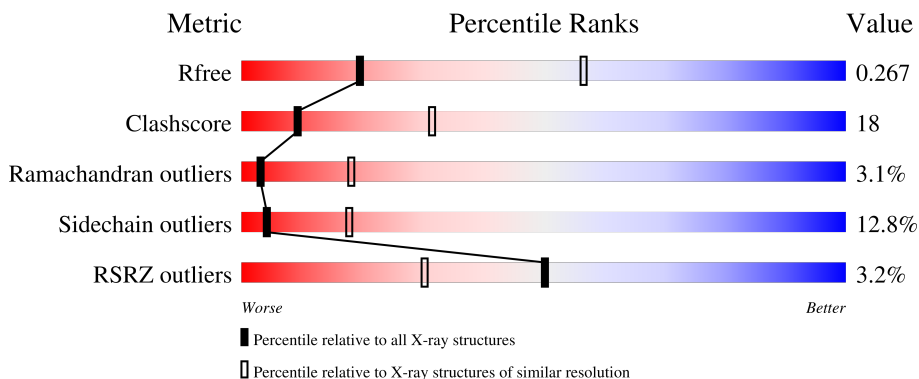
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

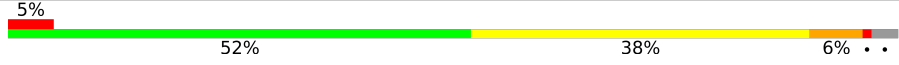


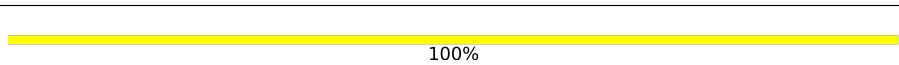
The reported resolution of this entry is 3.15 Å.

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.



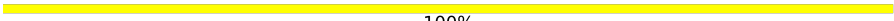
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	551	 61% 29% 7% .
1	B	551	 52% 38% 6% . .
1	C	551	 60% 30% 7% .
2	D	4	 50% 50%
3	E	3	 100%

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Mol	Chain	Length	Quality of chain
4	F	5	 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	-	-	-
3	NAG	E	1	X	-	-	-
3	MAN	E	3	X	-	-	-
4	MAN	F	3	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12777 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 Cartilage oligomeric matrix protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	535	4161	2495	749	888	29	0	0	0
1	B	535	4161	2495	749	888	29	0	0	0
1	C	535	4161	2495	749	888	29	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	ARG	-	expression tag	UNP P49747
A	210	SER	-	expression tag	UNP P49747
A	211	PRO	-	expression tag	UNP P49747
A	212	TRP	-	expression tag	UNP P49747
A	213	PRO	-	expression tag	UNP P49747
A	214	GLY	-	expression tag	UNP P49747
A	215	VAL	-	expression tag	UNP P49747
A	216	PRO	-	expression tag	UNP P49747
A	217	THR	-	expression tag	UNP P49747
A	218	SER	-	expression tag	UNP P49747
A	219	PRO	-	expression tag	UNP P49747
A	220	VAL	-	expression tag	UNP P49747
A	221	TRP	-	expression tag	UNP P49747
A	222	TRP	-	expression tag	UNP P49747
A	223	ASN	-	expression tag	UNP P49747
A	224	SER	-	expression tag	UNP P49747
A	758	GLY	-	expression tag	UNP P49747
A	759	THR	-	expression tag	UNP P49747
B	209	ARG	-	expression tag	UNP P49747
B	210	SER	-	expression tag	UNP P49747
B	211	PRO	-	expression tag	UNP P49747
B	212	TRP	-	expression tag	UNP P49747
B	213	PRO	-	expression tag	UNP P49747

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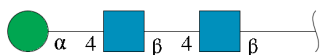
Chain	Residue	Modelled	Actual	Comment	Reference
B	214	GLY	-	expression tag	UNP P49747
B	215	VAL	-	expression tag	UNP P49747
B	216	PRO	-	expression tag	UNP P49747
B	217	THR	-	expression tag	UNP P49747
B	218	SER	-	expression tag	UNP P49747
B	219	PRO	-	expression tag	UNP P49747
B	220	VAL	-	expression tag	UNP P49747
B	221	TRP	-	expression tag	UNP P49747
B	222	TRP	-	expression tag	UNP P49747
B	223	ASN	-	expression tag	UNP P49747
B	224	SER	-	expression tag	UNP P49747
B	758	GLY	-	expression tag	UNP P49747
B	759	THR	-	expression tag	UNP P49747
C	209	ARG	-	expression tag	UNP P49747
C	210	SER	-	expression tag	UNP P49747
C	211	PRO	-	expression tag	UNP P49747
C	212	TRP	-	expression tag	UNP P49747
C	213	PRO	-	expression tag	UNP P49747
C	214	GLY	-	expression tag	UNP P49747
C	215	VAL	-	expression tag	UNP P49747
C	216	PRO	-	expression tag	UNP P49747
C	217	THR	-	expression tag	UNP P49747
C	218	SER	-	expression tag	UNP P49747
C	219	PRO	-	expression tag	UNP P49747
C	220	VAL	-	expression tag	UNP P49747
C	221	TRP	-	expression tag	UNP P49747
C	222	TRP	-	expression tag	UNP P49747
C	223	ASN	-	expression tag	UNP P49747
C	224	SER	-	expression tag	UNP P49747
C	758	GLY	-	expression tag	UNP P49747
C	759	THR	-	expression tag	UNP P49747

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



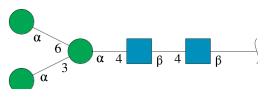
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	4	50	28	2	20	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	3	39	22	2	15	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	5	61	34	2	25	0	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	Ca	0	0
			30	30		
5	B	29	Total	Ca	0	0
			29	29		
5	C	29	Total	Ca	0	0
			29	29		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	B	3	Total O 3 3	0	0

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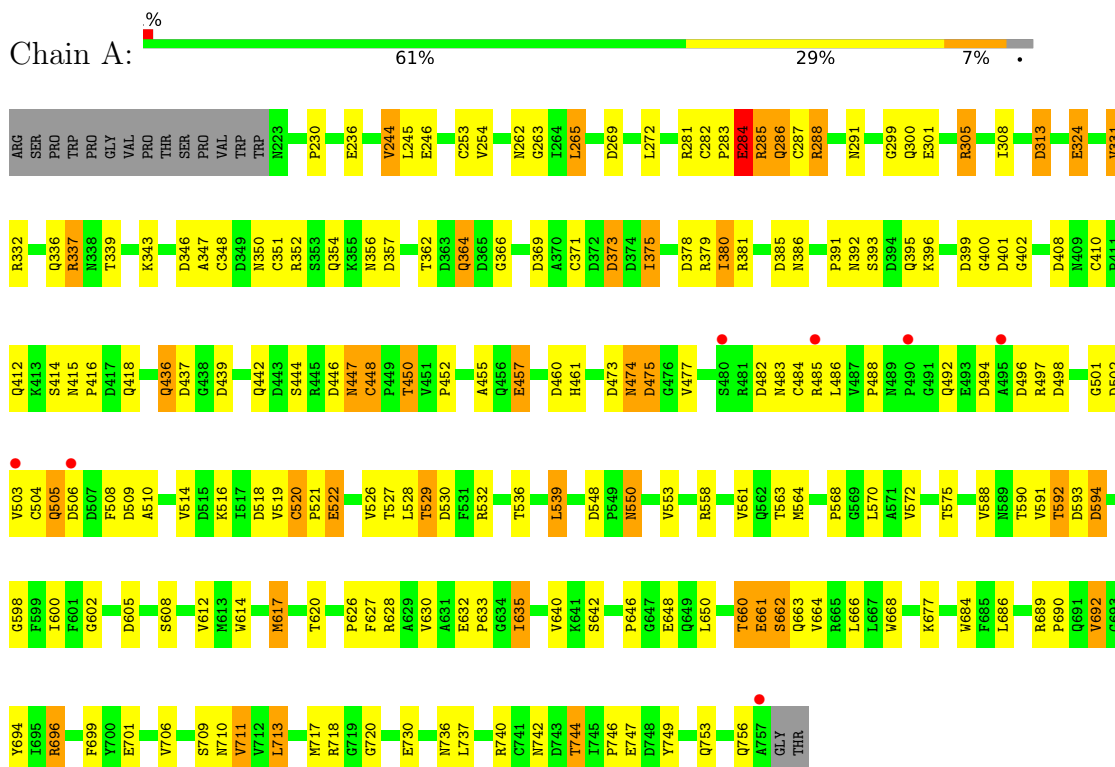
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	2	Total O 2 2	0	0

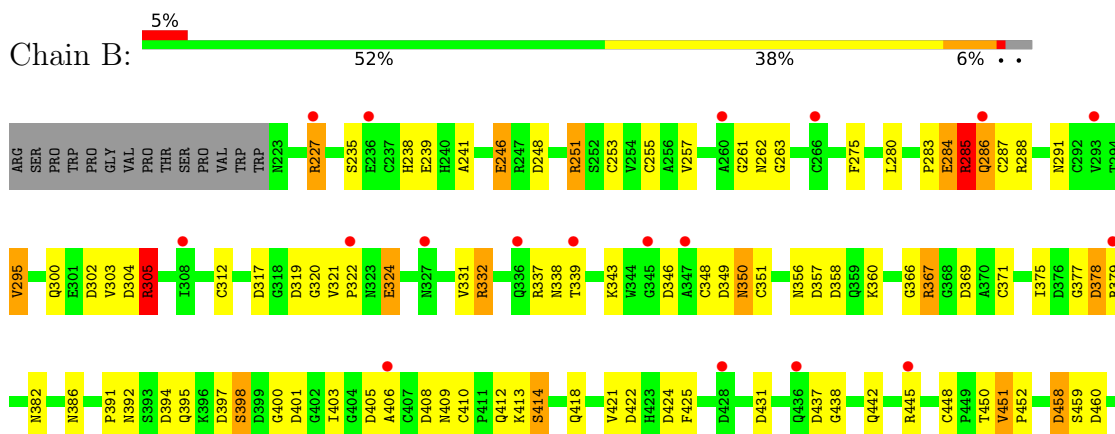
3 Residue-property plots [i](#)

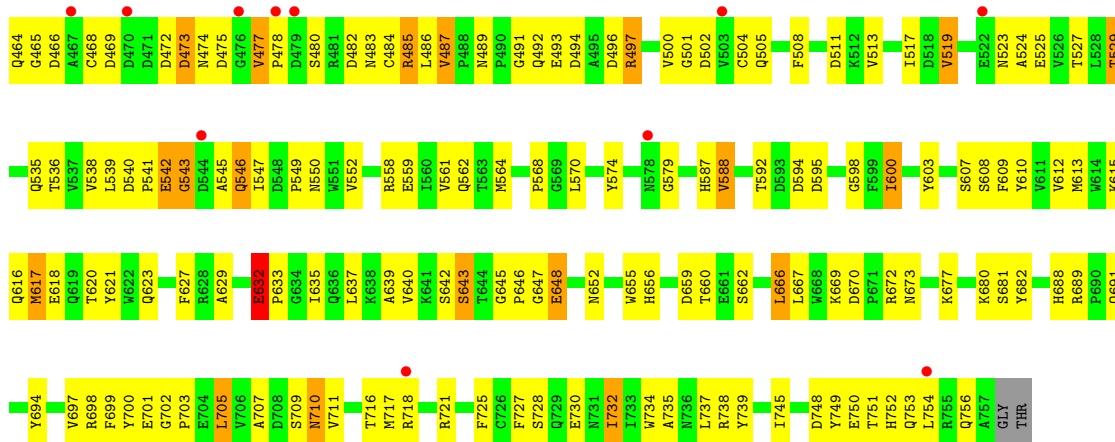
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cartilage oligomeric matrix protein

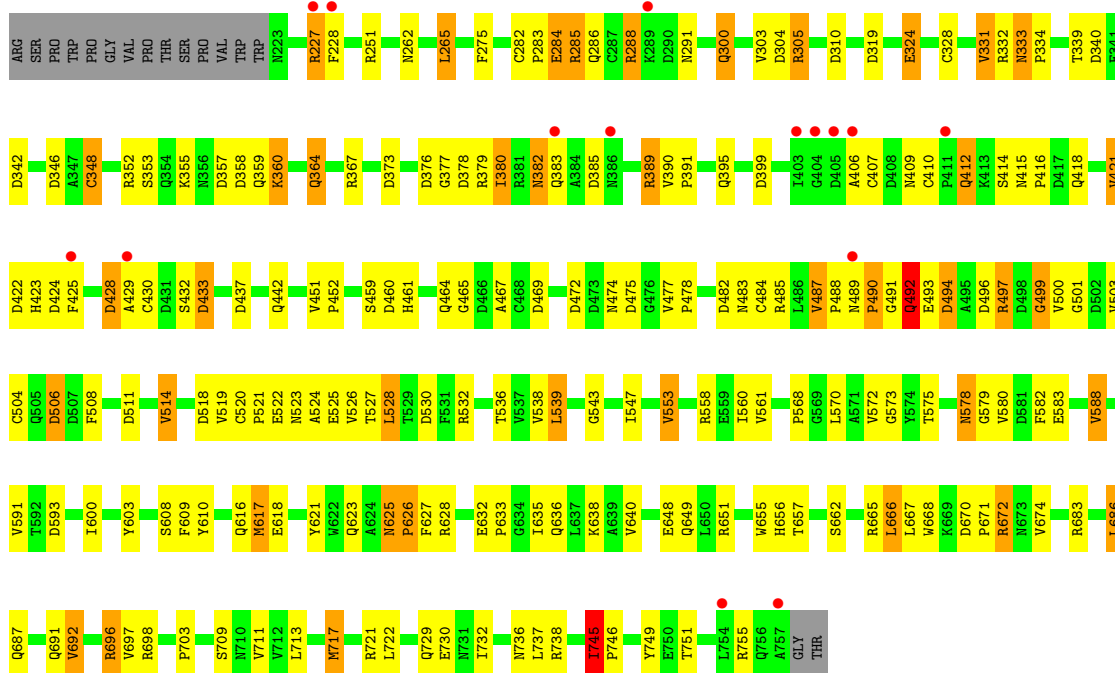


- Molecule 1: Cartilage oligomeric matrix protein





• Molecule 1: Cartilage oligomeric matrix protein



• Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



MAG1
MAG2
MAN3

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

100%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.24Å 192.24Å 145.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.00 – 3.15 39.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.00-3.15) 99.6 (39.00-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 3.12Å)	Xtrriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.202 , 0.266 0.204 , 0.267	Depositor DCC
R_{free} test set	2735 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12777	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: CA, NAG, SO4, 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	0.86	1/4245 (0.0%)	1.12	15/5770 (0.3%)
1	B	0.82	2/4245 (0.0%)	1.09	13/5770 (0.2%)
1	C	0.82	3/4245 (0.1%)	1.07	8/5770 (0.1%)
All	All	0.84	6/12735 (0.0%)	1.09	36/17310 (0.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	ARG	C-N	-6.47	1.24	1.33
1	A	285	ARG	C-N	-5.85	1.25	1.33
1	C	275	PHE	CA-C	-5.69	1.48	1.52
1	C	703	PRO	N-CA	-5.20	1.44	1.47
1	C	588	VAL	CA-CB	5.06	1.59	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	VAL	CB-CA-C	-8.28	101.27	111.04
1	A	520	CYS	CA-C-N	8.16	127.88	119.56
1	A	520	CYS	C-N-CA	8.16	127.88	119.56
1	C	410	CYS	CA-C-N	7.40	129.09	119.84
1	C	410	CYS	C-N-CA	7.40	129.09	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4161	0	3698	131	0
1	B	4161	0	3698	178	0
1	C	4161	0	3698	127	0
2	D	50	0	43	3	0
3	E	39	0	34	0	0
4	F	61	0	52	0	0
5	A	30	0	0	0	0
5	B	29	0	0	0	0
5	C	29	0	0	0	0
6	A	25	0	0	0	0
6	B	10	0	0	0	0
6	C	15	0	0	1	0
7	A	1	0	0	0	0
7	B	3	0	0	0	0
7	C	2	0	0	0	0
All	All	12777	0	11223	435	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 18.

The worst 5 of 435 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:B:251:ARG:HG3	1:B:251:ARG:HH11	1.04	1.17
1:A:617:MET:HE3	1:A:617:MET:HA	1.36	1.02
1:A:253:CYS:HB2	1:A:263:GLY:HA3	1.39	1.01
1:B:749:TYR:O	1:B:753:GLN:HG2	1.69	0.93
1:B:570:LEU:HD22	1:B:600:ILE:CD1	1.99	0.92

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	533/551 (97%)	443 (83%)	74 (14%)	16 (3%)	3	19
1	B	533/551 (97%)	435 (82%)	82 (15%)	16 (3%)	3	19
1	C	533/551 (97%)	443 (83%)	72 (14%)	18 (3%)	3	16
All	All	1599/1653 (97%)	1321 (83%)	228 (14%)	50 (3%)	3	18

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	B	474	ASN
1	B	543	GLY
1	C	352	ARG
1	C	379	ARG

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	459/473 (97%)	398 (87%)	61 (13%)	4	17
1	B	459/473 (97%)	408 (89%)	51 (11%)	6	22
1	C	459/473 (97%)	395 (86%)	64 (14%)	3	15
All	All	1377/1419 (97%)	1201 (87%)	176 (13%)	4	18

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	282	CYS
1	C	514	VAL
1	C	303	VAL
1	C	412	GLN
1	C	547	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	240	HIS
1	C	474	ASN
1	C	300	GLN
1	C	418	GLN
1	C	589	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](#)

12 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	1,2	14,14,15	0.60	0	17,19,21	1.99	6 (35%)
2	NAG	D	2	2	14,14,15	0.76	0	17,19,21	1.42	2 (11%)
2	MAN	D	3	2	11,11,12	0.97	0	15,15,17	1.28	1 (6%)
2	MAN	D	4	2	11,11,12	0.77	0	15,15,17	1.33	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.85	0	17,19,21	1.56	3 (17%)
3	NAG	E	2	3	14,14,15	0.81	1 (7%)	17,19,21	2.29	5 (29%)
3	MAN	E	3	3	11,11,12	0.64	0	15,15,17	1.55	2 (13%)
4	NAG	F	1	1,4	14,14,15	0.61	0	17,19,21	1.58	3 (17%)
4	NAG	F	2	4	14,14,15	0.93	1 (7%)	17,19,21	1.79	4 (23%)
4	MAN	F	3	4	11,11,12	0.60	0	15,15,17	1.45	3 (20%)
4	MAN	F	4	4	11,11,12	0.79	0	15,15,17	1.82	4 (26%)
4	MAN	F	5	4	11,11,12	0.51	0	15,15,17	1.40	1 (6%)

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	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	1/1/4/5	1/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	MAN	E	3	3	1/1/4/5	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	MAN	F	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O5-C1	-2.13	1.40	1.43
4	F	2	NAG	O5-C5	-2.06	1.39	1.43

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	O5-C1-C2	-5.73	102.42	111.29
4	F	2	NAG	C2-N2-C7	-5.05	116.13	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	O5-C1-C2	-4.84	103.80	111.29
2	D	1	NAG	C1-O5-C5	4.49	118.20	112.19
4	F	5	MAN	C1-O5-C5	4.27	117.91	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	3	MAN	C1
3	E	1	NAG	C1
3	E	3	MAN	C1
4	F	3	MAN	C1

5 of 20 torsion outliers are listed below:

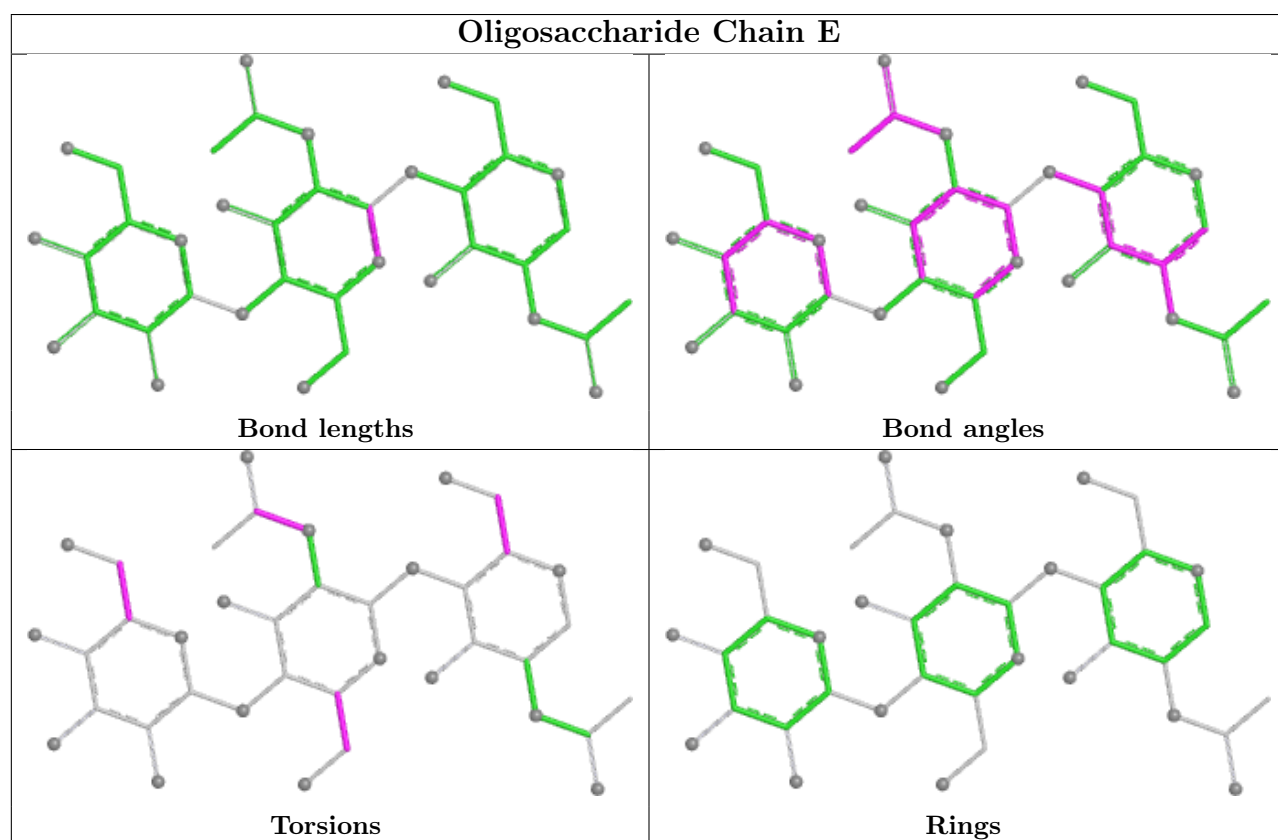
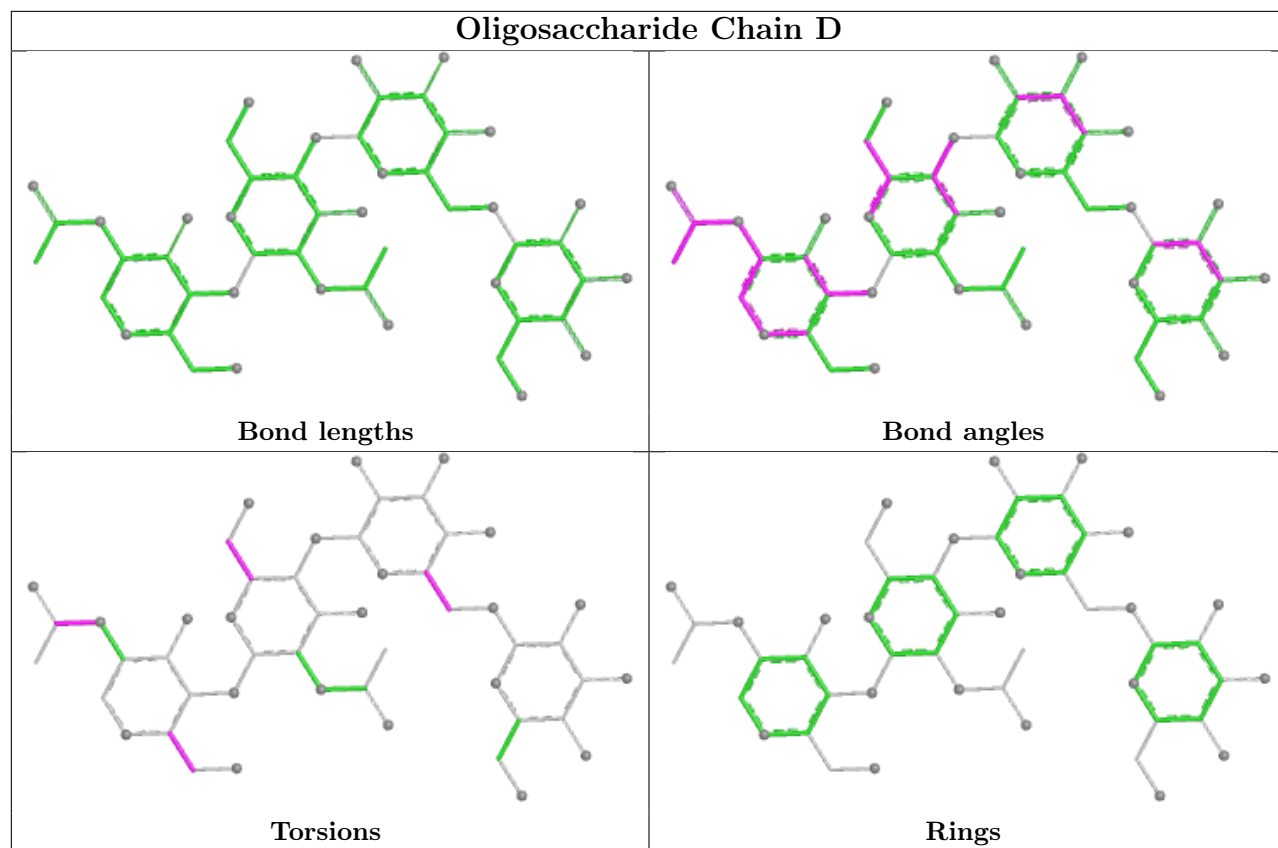
Mol	Chain	Res	Type	Atoms
3	E	3	MAN	O5-C5-C6-O6
3	E	3	MAN	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

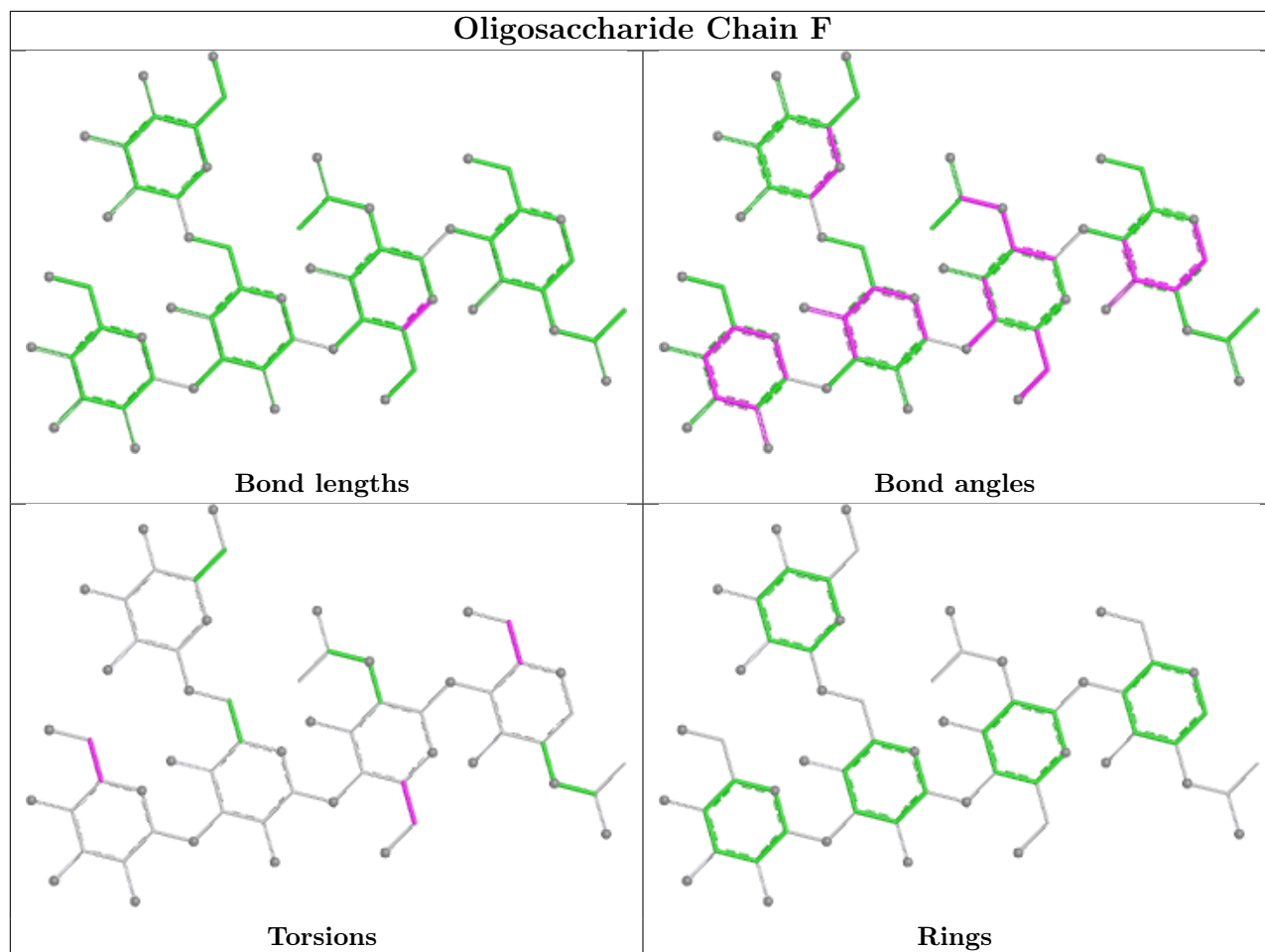
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	D	1	NAG	2	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 [i](#)

Of 98 ligands modelled in this entry, 88 are monoatomic - leaving 10 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	SO4	A	1002	-	4,4,4	0.25	0	6,6,6	0.51	0
6	SO4	B	1001	-	4,4,4	0.31	0	6,6,6	0.45	0
6	SO4	C	1002	-	4,4,4	0.28	0	6,6,6	0.16	0
6	SO4	C	1003	-	4,4,4	0.26	0	6,6,6	0.37	0
6	SO4	A	1001	-	4,4,4	0.20	0	6,6,6	0.32	0
6	SO4	B	1002	-	4,4,4	0.19	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	C	1001	-	4,4,4	0.27	0	6,6,6	0.23	0
6	SO4	A	1004	-	4,4,4	0.29	0	6,6,6	0.19	0
6	SO4	A	1005	-	4,4,4	0.36	0	6,6,6	0.13	0
6	SO4	A	1003	-	4,4,4	0.27	0	6,6,6	0.18	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1003	SO4	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 [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	535/551 (97%)	-0.09	7 (1%) 75 55	33, 49, 76, 90	0
1	B	535/551 (97%)	0.55	29 (5%) 31 18	24, 54, 70, 82	0
1	C	535/551 (97%)	0.23	15 (2%) 55 34	38, 54, 77, 85	0
All	All	1605/1653 (97%)	0.23	51 (3%) 50 30	24, 52, 75, 90	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	757	ALA	4.4
1	B	578	ASN	4.3
1	C	429	ALA	3.7
1	C	406	ALA	3.6
1	B	293	VAL	3.6

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.

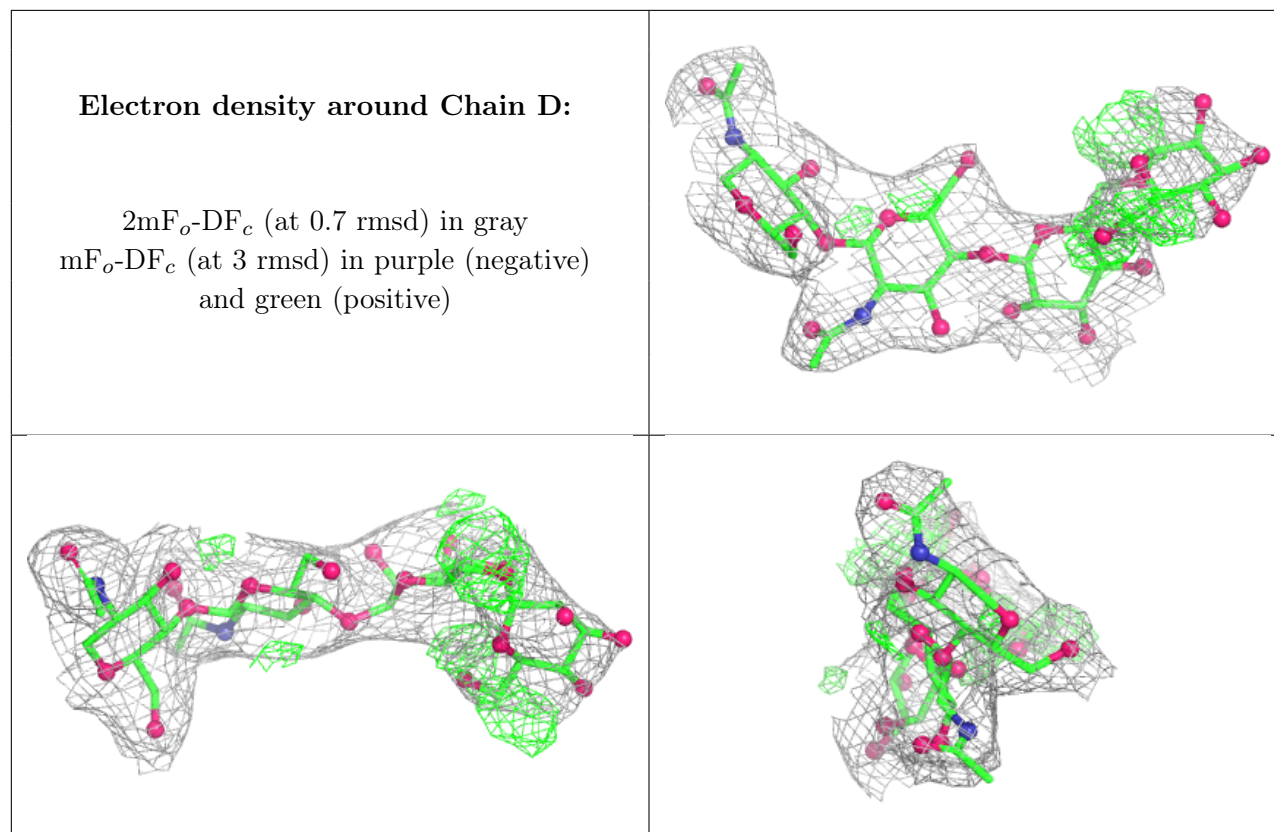
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	D	4	11/12	0.67	0.30	97,99,100,100	11
3	MAN	E	3	11/12	0.69	0.23	85,89,90,90	11
4	MAN	F	5	11/12	0.69	0.22	84,88,90,90	11

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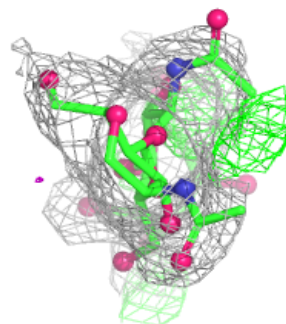
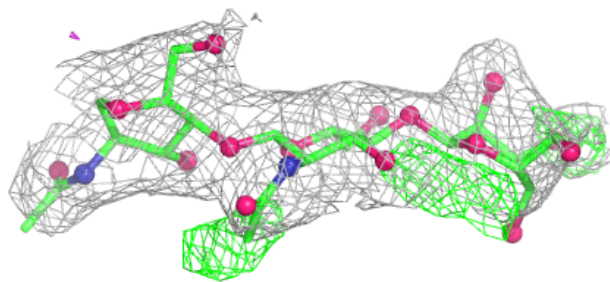
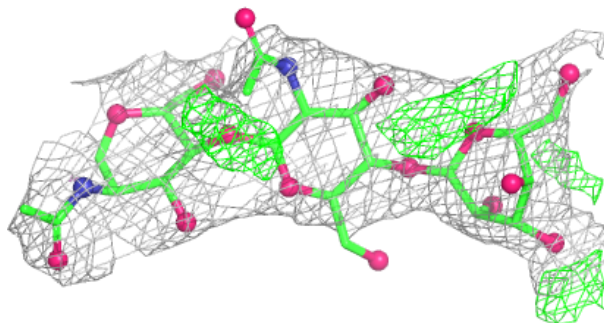
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	D	3	11/12	0.70	0.16	96,98,101,101	11
4	MAN	F	4	11/12	0.75	0.35	87,91,93,95	11
3	NAG	E	2	14/15	0.76	0.25	84,86,90,93	14
4	MAN	F	3	11/12	0.78	0.12	91,93,95,95	11
3	NAG	E	1	14/15	0.87	0.15	78,84,86,87	0
4	NAG	F	2	14/15	0.89	0.12	79,82,85,90	0
2	NAG	D	2	14/15	0.91	0.12	70,81,90,91	0
2	NAG	D	1	14/15	0.93	0.10	61,67,71,74	0
4	NAG	F	1	14/15	0.94	0.17	64,69,72,77	0

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

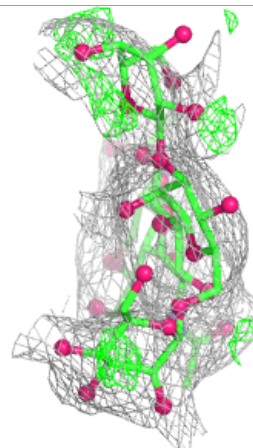
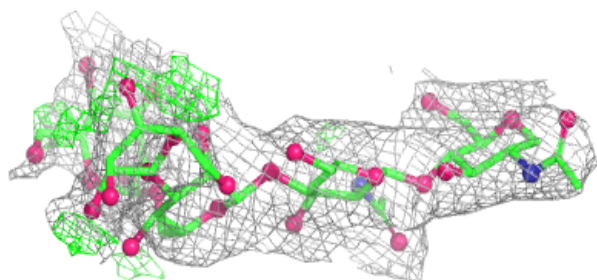
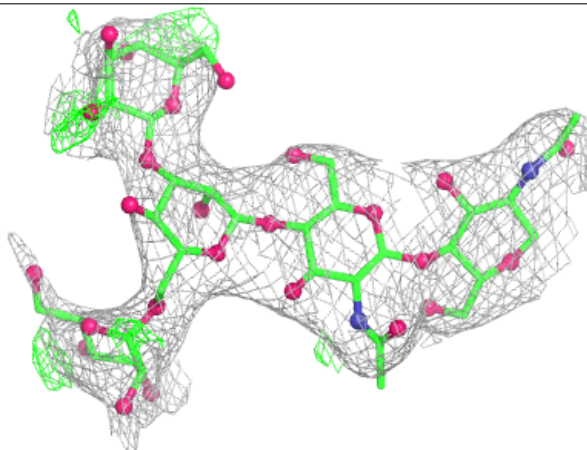


Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain F:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	SO4	A	1004	5/5	0.49	0.14	105,106,106,106	5
5	CA	C	810	1/1	0.57	0.16	174,174,174,174	0
5	CA	B	822	1/1	0.71	0.14	114,114,114,114	0
6	SO4	B	1002	5/5	0.73	0.17	94,94,95,97	5
6	SO4	C	1003	5/5	0.74	0.16	97,97,98,98	5
5	CA	B	811	1/1	0.76	0.14	123,123,123,123	0
6	SO4	A	1005	5/5	0.76	0.16	108,108,108,108	5
6	SO4	A	1003	5/5	0.77	0.15	106,107,107,107	5
6	SO4	A	1001	5/5	0.80	0.11	104,105,106,106	5
5	CA	C	809	1/1	0.81	0.12	108,108,108,108	0
6	SO4	C	1001	5/5	0.81	0.12	88,89,89,89	5
5	CA	A	824	1/1	0.81	0.09	160,160,160,160	0
6	SO4	C	1002	5/5	0.82	0.16	96,96,97,97	5
5	CA	B	816	1/1	0.84	0.15	111,111,111,111	0
5	CA	B	819	1/1	0.86	0.10	114,114,114,114	0
6	SO4	A	1002	5/5	0.86	0.20	94,94,97,97	5
5	CA	B	824	1/1	0.86	0.09	140,140,140,140	0
5	CA	A	816	1/1	0.87	0.12	114,114,114,114	0
5	CA	B	815	1/1	0.87	0.16	103,103,103,103	0
5	CA	C	822	1/1	0.87	0.11	118,118,118,118	0
5	CA	C	811	1/1	0.88	0.11	117,117,117,117	0
5	CA	C	816	1/1	0.88	0.09	123,123,123,123	0
5	CA	B	820	1/1	0.88	0.17	118,118,118,118	0
5	CA	C	819	1/1	0.89	0.10	118,118,118,118	0
5	CA	B	821	1/1	0.90	0.10	125,125,125,125	0
5	CA	B	817	1/1	0.90	0.11	127,127,127,127	0
5	CA	B	823	1/1	0.91	0.10	131,131,131,131	0
5	CA	A	820	1/1	0.92	0.09	119,119,119,119	0
5	CA	C	821	1/1	0.92	0.11	95,95,95,95	0
5	CA	A	821	1/1	0.92	0.12	104,104,104,104	0
5	CA	A	822	1/1	0.92	0.11	107,107,107,107	0
6	SO4	B	1001	5/5	0.93	0.08	82,82,85,85	0
5	CA	B	825	1/1	0.93	0.10	111,111,111,111	0
5	CA	C	813	1/1	0.93	0.07	119,119,119,119	0
5	CA	C	815	1/1	0.93	0.06	125,125,125,125	0
5	CA	B	829	1/1	0.93	0.08	89,89,89,89	0
5	CA	A	829	1/1	0.95	0.06	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	C	829	1/1	0.95	0.08	109,109,109,109	0
5	CA	B	818	1/1	0.95	0.07	106,106,106,106	0
5	CA	A	800	1/1	0.95	0.06	65,65,65,65	0
5	CA	C	820	1/1	0.96	0.09	125,125,125,125	0
5	CA	B	810	1/1	0.96	0.07	109,109,109,109	0
5	CA	A	819	1/1	0.96	0.07	119,119,119,119	0
5	CA	C	804	1/1	0.96	0.06	74,74,74,74	0
5	CA	A	805	1/1	0.96	0.05	60,60,60,60	0
5	CA	C	818	1/1	0.96	0.05	94,94,94,94	0
5	CA	B	804	1/1	0.96	0.06	83,83,83,83	0
5	CA	B	801	1/1	0.97	0.04	70,70,70,70	0
5	CA	C	824	1/1	0.97	0.09	115,115,115,115	0
5	CA	C	825	1/1	0.97	0.04	85,85,85,85	0
5	CA	A	801	1/1	0.97	0.04	56,56,56,56	0
5	CA	A	815	1/1	0.97	0.04	115,115,115,115	0
5	CA	C	812	1/1	0.97	0.07	117,117,117,117	0
5	CA	A	828	1/1	0.97	0.05	54,54,54,54	0
5	CA	B	814	1/1	0.97	0.05	121,121,121,121	0
5	CA	C	801	1/1	0.97	0.06	52,52,52,52	0
5	CA	C	817	1/1	0.97	0.07	105,105,105,105	0
5	CA	C	803	1/1	0.97	0.04	71,71,71,71	0
5	CA	A	804	1/1	0.97	0.04	78,78,78,78	0
5	CA	C	805	1/1	0.97	0.08	75,75,75,75	0
5	CA	C	807	1/1	0.97	0.09	65,65,65,65	0
5	CA	A	810	1/1	0.98	0.05	104,104,104,104	0
5	CA	A	811	1/1	0.98	0.05	75,75,75,75	0
5	CA	A	803	1/1	0.98	0.07	76,76,76,76	0
5	CA	A	807	1/1	0.98	0.04	61,61,61,61	0
5	CA	C	827	1/1	0.98	0.04	47,47,47,47	0
5	CA	C	828	1/1	0.98	0.04	58,58,58,58	0
5	CA	B	805	1/1	0.98	0.03	55,55,55,55	0
5	CA	B	806	1/1	0.98	0.05	54,54,54,54	0
5	CA	B	809	1/1	0.98	0.04	85,85,85,85	0
5	CA	A	823	1/1	0.98	0.05	103,103,103,103	0
5	CA	C	814	1/1	0.98	0.04	119,119,119,119	0
5	CA	A	817	1/1	0.98	0.06	81,81,81,81	0
5	CA	B	812	1/1	0.98	0.05	87,87,87,87	0
5	CA	B	828	1/1	0.98	0.05	69,69,69,69	0
5	CA	B	813	1/1	0.98	0.04	111,111,111,111	0
5	CA	A	825	1/1	0.98	0.04	93,93,93,93	0
5	CA	A	827	1/1	0.98	0.03	64,64,64,64	0
5	CA	C	823	1/1	0.99	0.02	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	C	808	1/1	0.99	0.03	64,64,64,64	0
5	CA	A	809	1/1	0.99	0.04	65,65,65,65	0
5	CA	C	826	1/1	0.99	0.03	85,85,85,85	0
5	CA	A	812	1/1	0.99	0.02	70,70,70,70	0
5	CA	B	802	1/1	0.99	0.04	53,53,53,53	0
5	CA	B	803	1/1	0.99	0.03	65,65,65,65	0
5	CA	B	826	1/1	0.99	0.04	86,86,86,86	0
5	CA	B	827	1/1	0.99	0.02	62,62,62,62	0
5	CA	A	818	1/1	0.99	0.03	85,85,85,85	0
5	CA	A	813	1/1	0.99	0.04	81,81,81,81	0
5	CA	A	826	1/1	0.99	0.03	86,86,86,86	0
5	CA	B	807	1/1	0.99	0.03	56,56,56,56	0
5	CA	B	808	1/1	0.99	0.05	56,56,56,56	0
5	CA	A	814	1/1	0.99	0.03	101,101,101,101	0
5	CA	C	806	1/1	0.99	0.03	72,72,72,72	0
5	CA	A	808	1/1	0.99	0.04	56,56,56,56	0
5	CA	A	802	1/1	1.00	0.01	58,58,58,58	0
5	CA	C	802	1/1	1.00	0.03	50,50,50,50	0
5	CA	A	806	1/1	1.00	0.03	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.