



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:54 PM UTC

PDB ID : 1DWF / pdb_00001dwf
Title : Study on radiation damage on a cryocooled crystal. Part 2: Structure after irradiation with 9.1×10^{15} photons/mm²
Authors : Burmeister, W.P.
Deposited on : 1999-12-05
Resolution : 2.00 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

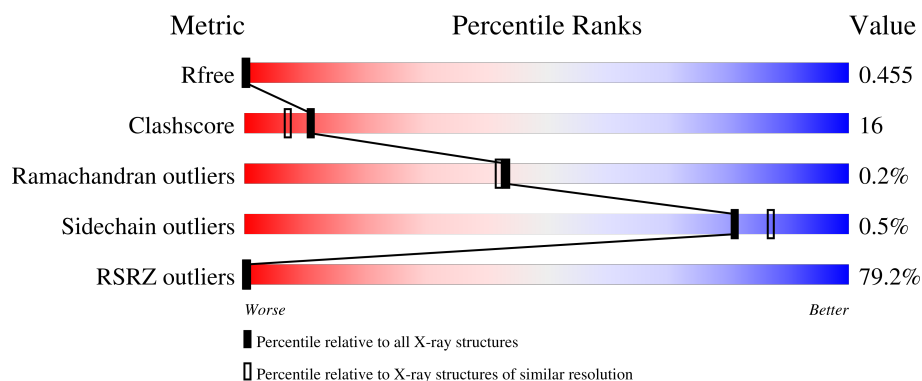
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	M	499	79% 80%18%.
2	A	2	50%50%
2	D	2	50%50%
3	B	5	100%
4	C	7	71%29%

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
4	BMA	C	3	-	-	X	-
4	MAN	C	6	X	X	X	-
5	NAG	M	1506	-	-	X	-
5	NAG	M	1519	X	-	-	-
7	SO4	M	1526	-	-	X	-
7	SO4	M	1527	-	-	X	-
7	SO4	M	1529	-	X	-	-
7	SO4	M	1532	-	X	X	X
8	GOL	M	1533	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5220 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 MYROSINASE MA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	21	0
			4083	2619	660	788	16			

There is a discrepancy between the modelled and reference sequences:

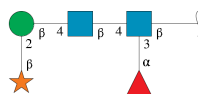
Chain	Residue	Modelled	Actual	Comment	Reference
M	497	THR	SER	SEE REMARK 999	UNP P29736

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



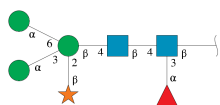
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



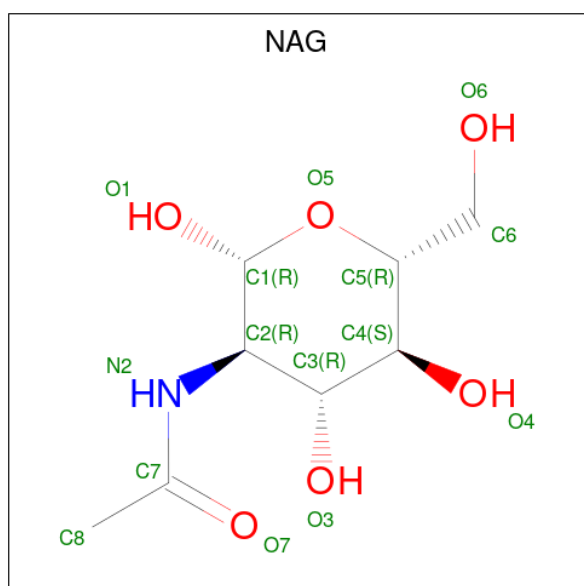
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	5	Total	C	N	O	0	0	0
			58	33	2	23			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	7	Total	C	N	O	0	0	0
			80	45	2	33			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

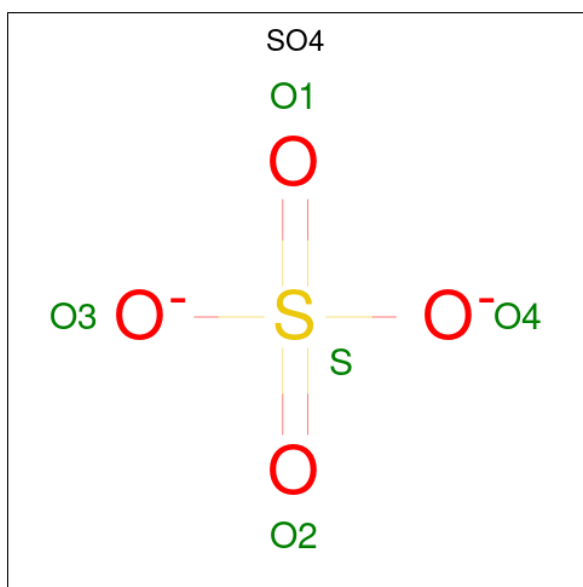
Continued from previous page...

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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Zn	0	0
			1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			6	3	3		
8	M	1	Total	C	O	0	0
			6	3	3		
8	M	1	Total	C	O	0	0
			6	3	3		
8	M	1	Total	C	O	0	0
			6	3	3		
8	M	1	Total	C	O	0	0
			6	3	3		

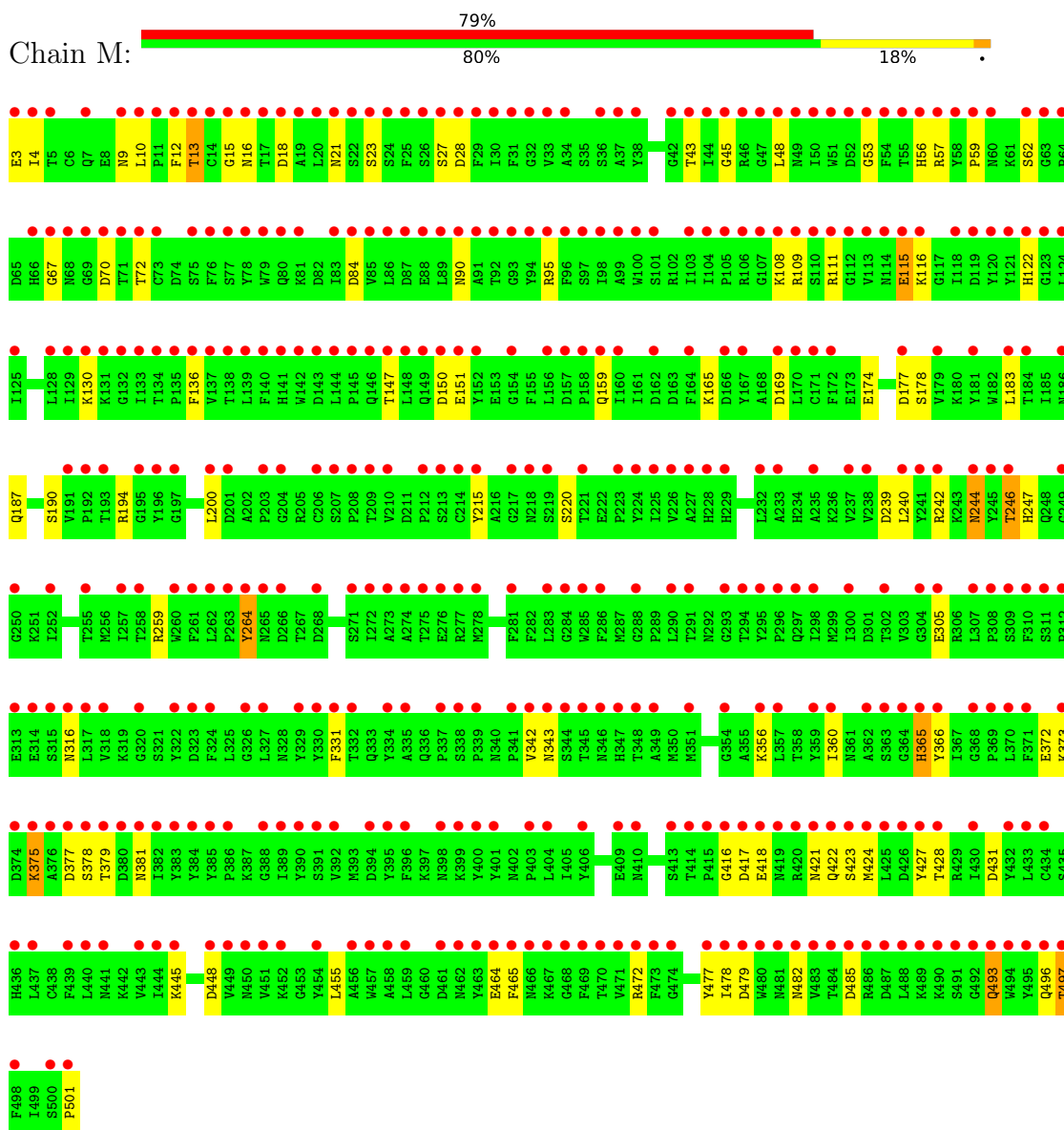
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	788	Total	O	0	0
			788	788		

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: MYROSINASE MA1



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

Chain A:  50% 50%

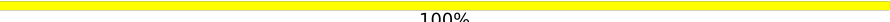
NAG1
NAG2

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

Chain D:  50% 50%

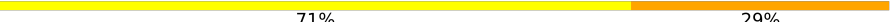
NAG1
NAG2

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

Chain B:  100%

NAG1
NAG2
BMA3
XYP4
FUC5

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

Chain C:  71% 29%

NAG1
NAG2
BMA3
XYP4
MAN5
MAN6
FUC7

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	134.30Å 136.40Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.40 – 2.00 17.40 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (17.40-2.00) 98.3 (17.40-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.70 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.169 , 0.180 0.441 , 0.455	Depositor DCC
R_{free} test set	2570 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: SO4, FUC, XYP, ZN, GOL, MAN, NAG, BMA

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	M	1.25	16/4291 (0.4%)	1.34	41/5835 (0.7%)

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
1	M	0	1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	264	TYR	CZ-OH	16.26	1.72	1.38
1	M	16	ASN	CG-ND2	14.88	1.64	1.33
1	M	13	THR	C-O	-12.91	1.04	1.24
1	M	264	TYR	CE1-CZ	-11.67	1.10	1.38
1	M	356	LYS	CE-NZ	-9.33	1.21	1.49

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	482	ASN	CA-CB-CG	-12.47	100.13	112.60
1	M	482	ASN	OD1-CG-ND2	-10.79	111.81	122.60
1	M	264	TYR	CE1-CZ-CE2	9.03	138.36	120.30
1	M	16	ASN	CA-CB-CG	-8.60	104.00	112.60
1	M	115	GLU	OE1-CD-OE2	-7.46	105.00	122.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	13	THR	Mainchain

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	M	4083	0	3835	106	4
2	A	28	0	24	3	0
2	D	28	0	25	1	0
3	B	58	0	42	0	0
4	C	80	0	58	9	0
5	M	84	0	77	17	0
6	M	1	0	0	0	1
7	M	40	0	0	9	0
8	M	30	0	39	4	0
9	M	788	0	0	78	17
All	All	5220	0	4100	136	21

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 16.

The worst 5 of 136 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:M:244:ASN:HD21	5:M:1506:NAG:C1	0.96	1.56
1:M:21:ASN:HD21	5:M:1502:NAG:C1	0.90	1.52
1:M:264:TYR:OH	1:M:264:TYR:CZ	1.72	1.42
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CZ	1.57	1.37
8:M:1533:GOL:C1	9:M:3026:HOH:O	1.71	1.34

The worst 5 of 21 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1524:ZN:ZN	6:M:1524:ZN:ZN[3_656]	1.10	1.10
9:M:2279:HOH:O	9:M:2279:HOH:O[3_656]	1.10	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:2009:HOH:O	9:M:2520:HOH:O[4_576]	1.36	0.84
9:M:2248:HOH:O	9:M:2534:HOH:O[4_576]	1.37	0.83
9:M:2247:HOH:O	9:M:2247:HOH:O[4_576]	1.42	0.78

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	M	518/499 (104%)	504 (97%)	13 (2%)	1 (0%)	43 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

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	M	456/435 (105%)	454 (100%)	2 (0%)	84 89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLU
1	M	375	LYS

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

Mol	Chain	Res	Type
1	M	365	HIS
1	M	402	ASN
1	M	410	ASN
1	M	230	GLN
1	M	122	HIS

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 ⓘ

16 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	A	1	2,1	14,14,15	5.90	7 (50%)	17,19,21	3.46	9 (52%)
2	NAG	A	2	2	14,14,15	2.98	4 (28%)	17,19,21	4.02	9 (52%)
3	NAG	B	1	3,1	14,14,15	0.59	0	17,19,21	2.03	5 (29%)
3	NAG	B	2	3	14,14,15	1.06	1 (7%)	17,19,21	1.36	2 (11%)
3	BMA	B	3	3	11,11,12	1.83	2 (18%)	15,15,17	1.74	6 (40%)
3	XYP	B	4	3	9,9,10	1.30	1 (11%)	10,12,14	2.51	4 (40%)
3	FUC	B	5	3	10,10,11	1.65	3 (30%)	14,14,16	1.97	4 (28%)
4	NAG	C	1	4,1	14,14,15	1.93	3 (21%)	17,19,21	2.47	4 (23%)
4	NAG	C	2	4	14,14,15	1.53	3 (21%)	17,19,21	1.65	5 (29%)
4	BMA	C	3	4	11,11,12	2.41	2 (18%)	15,15,17	4.55	9 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	XYP	C	4	4	9,9,10	1.87	4 (44%)	10,12,14	2.15	4 (40%)
4	MAN	C	5	4	11,11,12	1.97	2 (18%)	15,15,17	2.53	8 (53%)
4	MAN	C	6	4	11,11,12	3.13	7 (63%)	15,15,17	7.21	12 (80%)
4	FUC	C	7	4	10,10,11	2.66	5 (50%)	14,14,16	1.65	2 (14%)
2	NAG	D	1	2,1	14,14,15	2.41	3 (21%)	17,19,21	2.56	3 (17%)
2	NAG	D	2	2	14,14,15	1.46	3 (21%)	17,19,21	2.62	10 (58%)

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	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	XYP	B	4	3	-	-	0/1/1/1
3	FUC	B	5	3	-	-	0/1/1/1
4	NAG	C	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	1/2/19/22	0/1/1/1
4	XYP	C	4	4	-	-	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	MAN	C	6	4	1/1/4/5	1/2/19/22	0/1/1/1
4	FUC	C	7	4	-	-	0/1/1/1
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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	O3-C3	18.86	1.89	1.43
4	C	6	MAN	O5-C5	8.17	1.59	1.43
2	A	1	NAG	O7-C7	7.59	1.40	1.23
2	A	2	NAG	O5-C5	7.39	1.57	1.43
2	D	1	NAG	O7-C7	-6.60	1.08	1.23

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	C	6	MAN	C1-O5-C5	-16.05	90.67	112.19
4	C	6	MAN	C6-C5-C4	12.27	143.14	113.02
4	C	3	BMA	O4-C4-C5	10.08	134.15	109.32
4	C	6	MAN	O5-C5-C6	-9.98	88.23	107.66
2	A	2	NAG	C3-C4-C5	8.86	126.30	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	6	MAN	C5

All (2) torsion outliers are listed below:

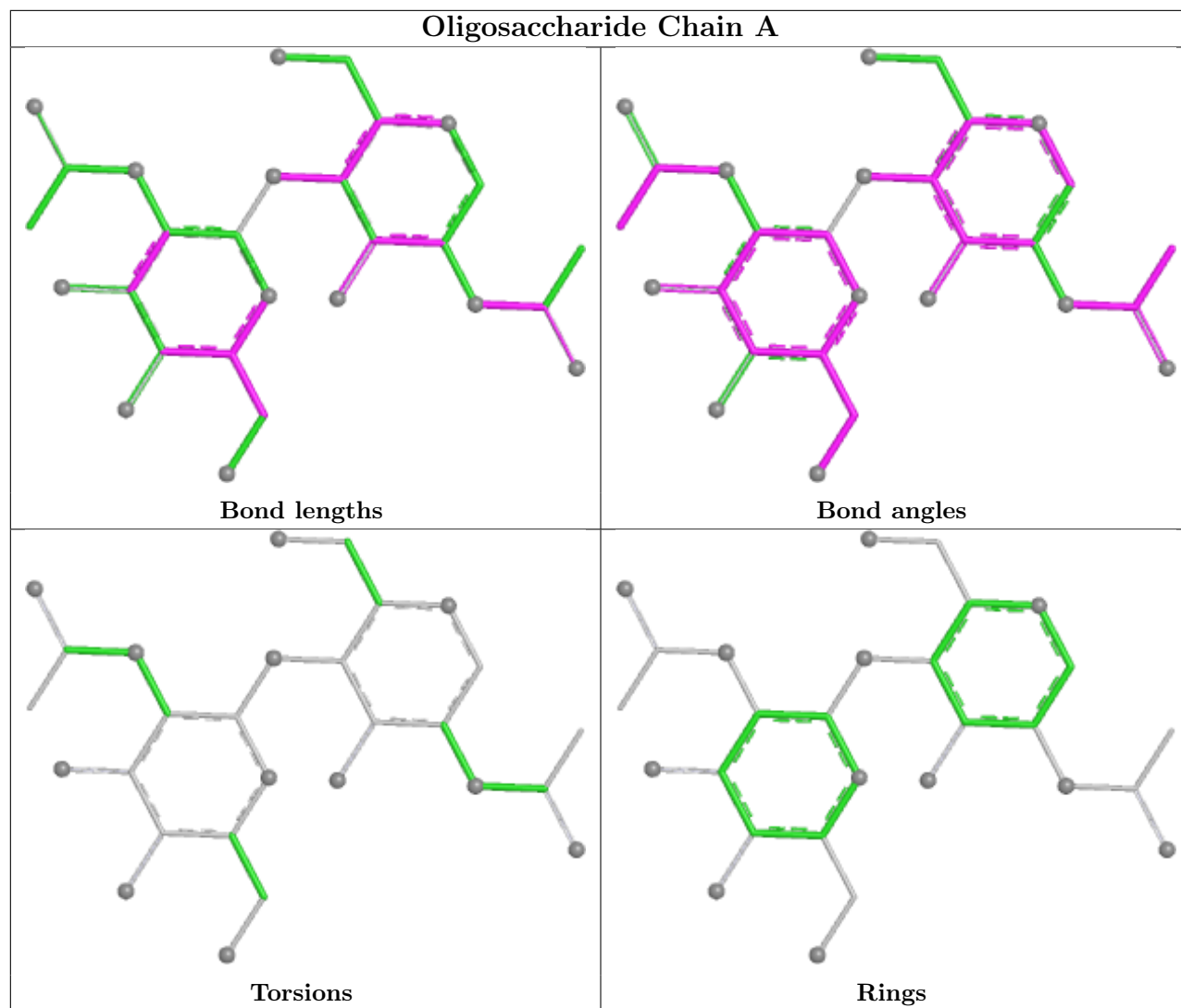
Mol	Chain	Res	Type	Atoms
4	C	6	MAN	O5-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6

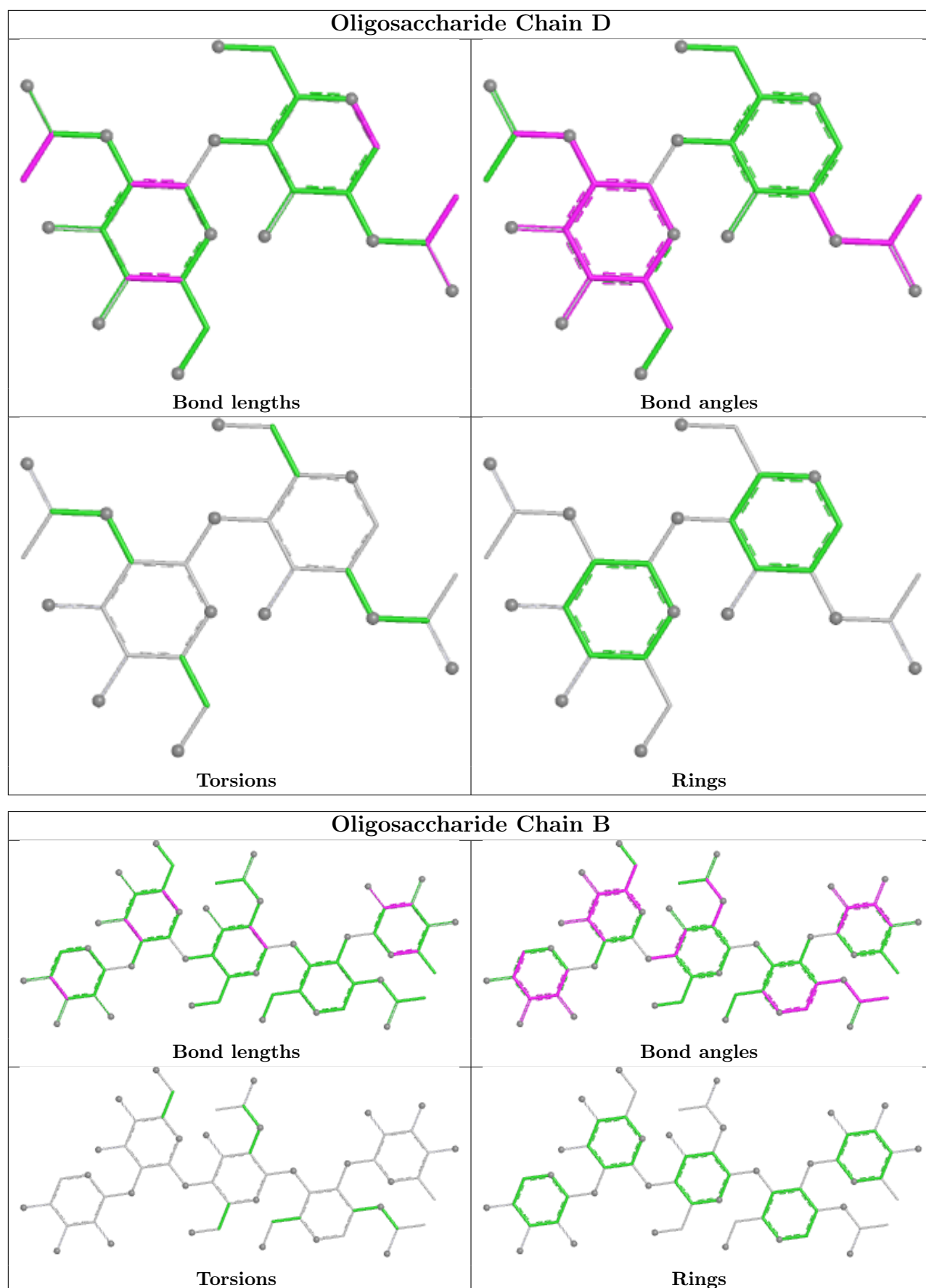
There are no ring outliers.

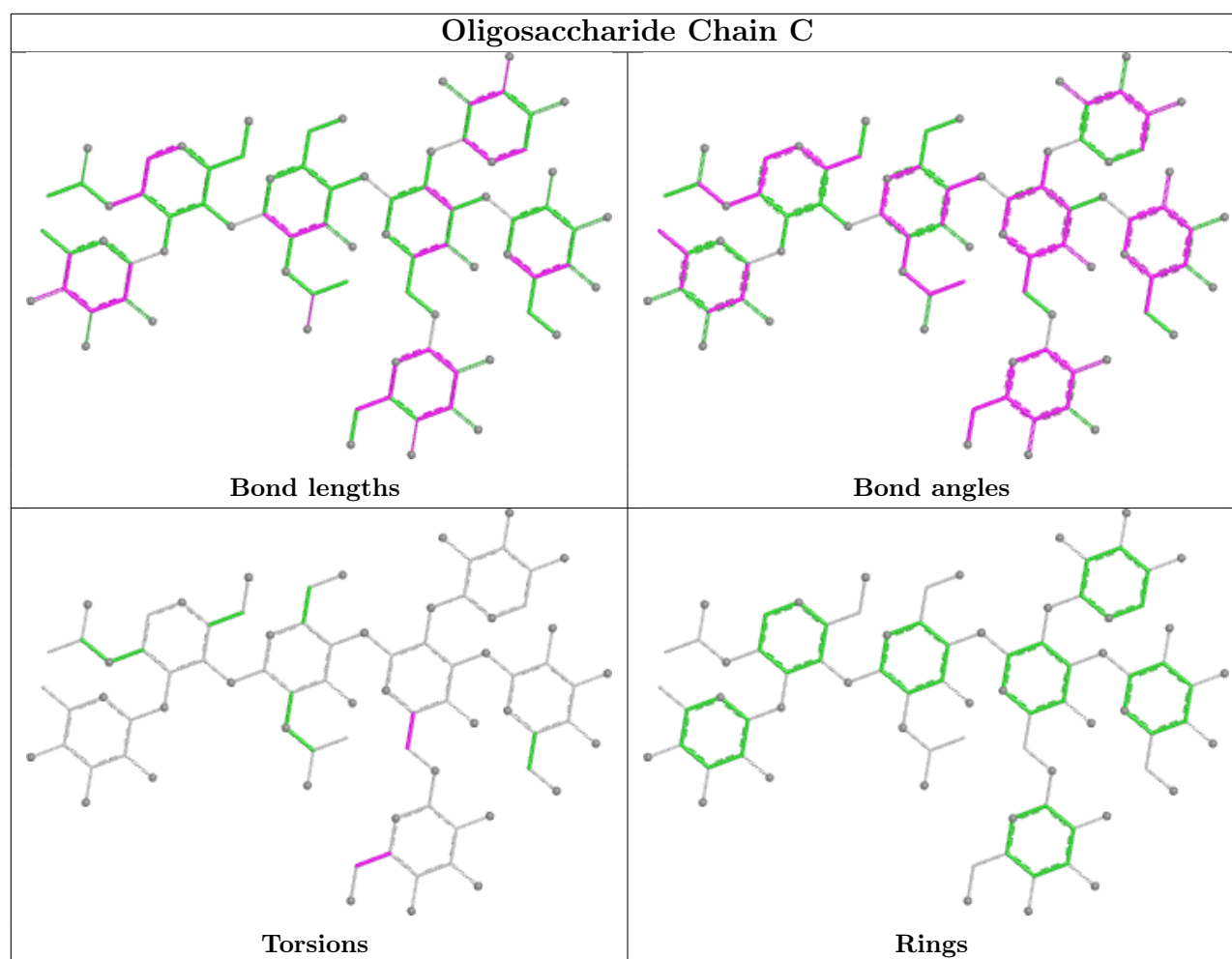
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
4	C	6	MAN	8	0
4	C	3	BMA	7	0
2	A	1	NAG	3	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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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$
5	NAG	M	1506	1	14,14,15	2.01	5 (35%)	17,19,21	8.34	13 (76%)
5	NAG	M	1503	1	14,14,15	1.72	2 (14%)	17,19,21	2.16	5 (29%)
5	NAG	M	1520	1	14,14,15	1.36	1 (7%)	17,19,21	2.50	8 (47%)
7	SO4	M	1527	7	4,4,4	1.42	1 (25%)	6,6,6	1.31	1 (16%)
8	GOL	M	1535	-	5,5,5	0.94	0	5,5,5	1.15	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	1502	1	14,14,15	1.21	1 (7%)	17,19,21	2.06	5 (29%)
5	NAG	M	1523	1	14,14,15	1.26	1 (7%)	17,19,21	1.97	5 (29%)
7	SO4	M	1525	-	4,4,4	0.88	0	6,6,6	1.39	1 (16%)
7	SO4	M	1528	-	4,4,4	0.27	0	6,6,6	0.32	0
7	SO4	M	1530	-	4,4,4	1.10	0	6,6,6	1.36	1 (16%)
8	GOL	M	1537	-	5,5,5	0.87	0	5,5,5	1.37	1 (20%)
7	SO4	M	1532	7	4,4,4	1.53	1 (25%)	6,6,6	2.76	5 (83%)
8	GOL	M	1534	-	5,5,5	1.28	1 (20%)	5,5,5	1.12	0
7	SO4	M	1531	-	4,4,4	0.81	0	6,6,6	0.35	0
7	SO4	M	1526	-	4,4,4	0.57	0	6,6,6	0.51	0
5	NAG	M	1519	1	14,14,15	1.40	2 (14%)	17,19,21	2.84	4 (23%)
8	GOL	M	1536	-	5,5,5	0.66	0	5,5,5	1.19	1 (20%)
8	GOL	M	1533	-	5,5,5	0.68	0	5,5,5	1.21	1 (20%)
7	SO4	M	1529	-	4,4,4	1.88	1 (25%)	6,6,6	2.46	3 (50%)

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
5	NAG	M	1506	1	-	2/6/23/26	0/1/1/1
5	NAG	M	1503	1	-	0/6/23/26	0/1/1/1
5	NAG	M	1520	1	-	4/6/23/26	0/1/1/1
8	GOL	M	1536	-	-	0/4/4/4	-
8	GOL	M	1535	-	-	0/4/4/4	-
5	NAG	M	1502	1	-	0/6/23/26	0/1/1/1
5	NAG	M	1523	1	-	0/6/23/26	0/1/1/1
8	GOL	M	1537	-	-	0/4/4/4	-
5	NAG	M	1519	1	1/1/5/7	0/6/23/26	0/1/1/1
8	GOL	M	1533	-	-	4/4/4/4	-
8	GOL	M	1534	-	-	0/4/4/4	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1503	NAG	O5-C5	4.36	1.51	1.43
5	M	1520	NAG	O7-C7	-4.20	1.13	1.23
5	M	1506	NAG	O7-C7	-3.99	1.14	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1523	NAG	O7-C7	-3.84	1.14	1.23
7	M	1529	SO4	O2-S	3.57	1.66	1.44

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1506	NAG	C2-N2-C7	22.97	153.68	122.90
5	M	1506	NAG	O5-C1-C2	15.06	134.59	111.29
5	M	1506	NAG	C8-C7-N2	14.70	140.50	116.12
5	M	1506	NAG	O7-C7-N2	-8.72	106.58	121.98
5	M	1519	NAG	C1-O5-C5	8.53	123.61	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1519	NAG	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1506	NAG	C8-C7-N2-C2
8	M	1533	GOL	O1-C1-C2-O2
8	M	1533	GOL	O1-C1-C2-C3
5	M	1506	NAG	O7-C7-N2-C2
5	M	1520	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1506	NAG	7	0
5	M	1503	NAG	3	0
7	M	1527	SO4	5	0
5	M	1502	NAG	5	0
7	M	1532	SO4	7	0
7	M	1526	SO4	2	0
5	M	1519	NAG	2	0
8	M	1533	GOL	4	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	M	499/499 (100%)	2.77	395 (79%) 0 0	8, 13, 26, 54	23 (4%)

The worst 5 of 395 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	378	SER	6.8
1	M	376	ALA	6.4
1	M	212	PRO	6.4
1	M	345	THR	6.2
1	M	23	SER	6.0

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.

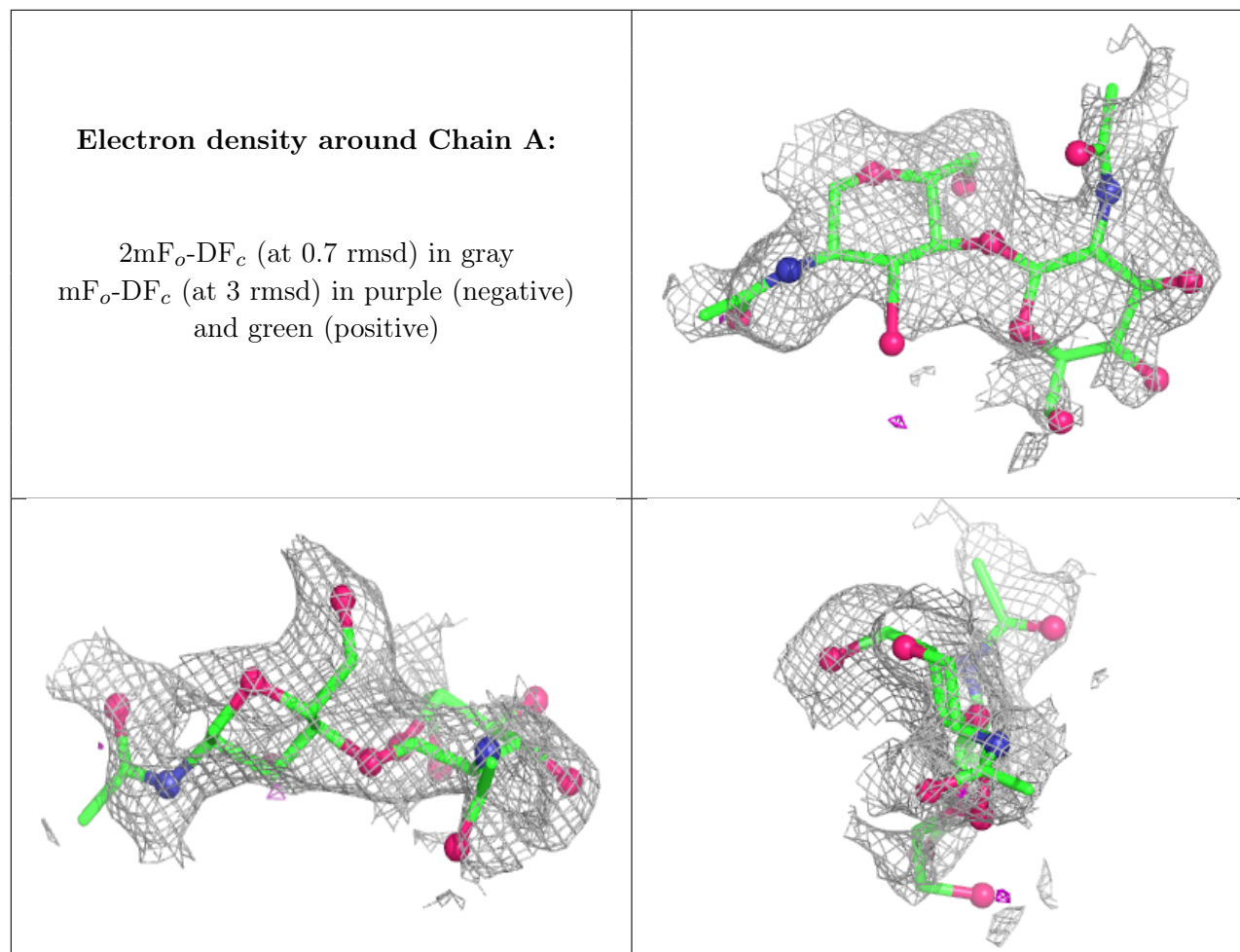
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	17,21,30,35	0
2	NAG	A	2	14/15	-	-	35,43,55,57	0
4	BMA	C	3	11/12	0.34	0.27	23,28,33,45	0
4	XYP	C	4	9/10	0.41	0.21	30,36,41,61	0
3	NAG	B	2	14/15	0.45	0.22	19,25,31,36	0
3	NAG	B	1	14/15	0.58	0.19	13,20,25,25	0
3	BMA	B	3	11/12	-	-	36,41,46,51	0

Continued on next page...

Continued from previous page...

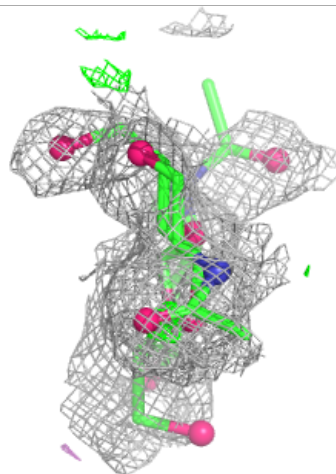
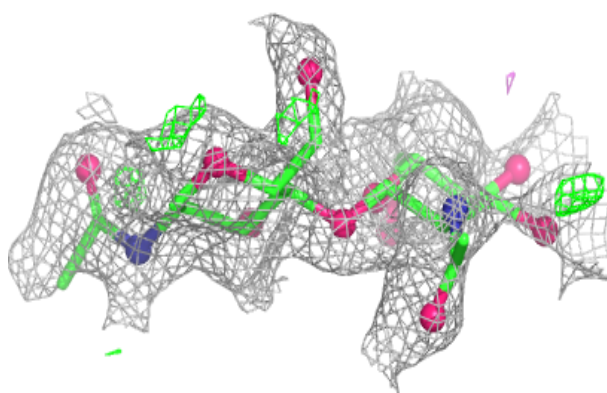
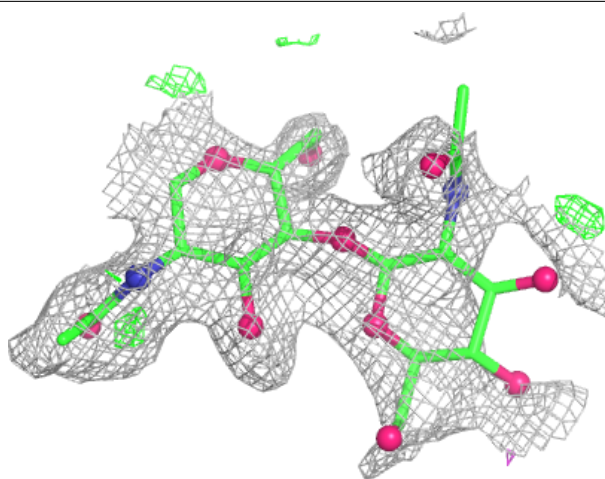
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	XYP	B	4	9/10	-	-	39,46,50,52	0
3	FUC	B	5	10/11	-	-	22,30,37,46	0
4	NAG	C	1	14/15	0.60	0.23	15,18,24,27	0
2	NAG	D	1	14/15	0.64	0.19	7,14,19,21	0
4	NAG	C	2	14/15	0.68	0.17	18,21,26,30	0
2	NAG	D	2	14/15	0.69	0.15	24,29,47,54	0
4	MAN	C	5	11/12	-	-	23,37,49,54	0
4	MAN	C	6	11/12	-	-	31,41,52,53	0
4	FUC	C	7	10/11	-	-	17,19,31,31	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.



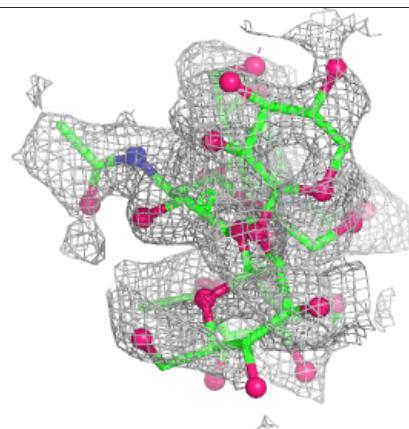
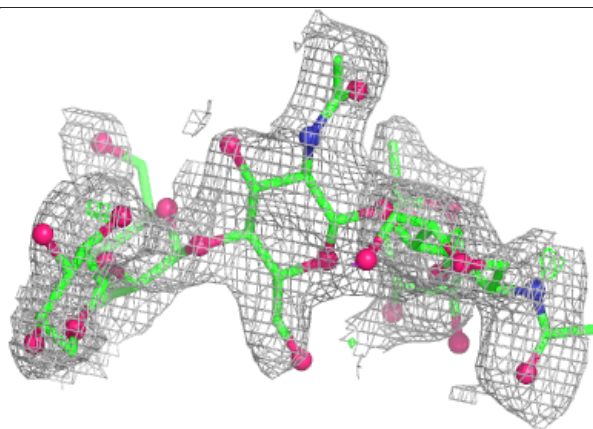
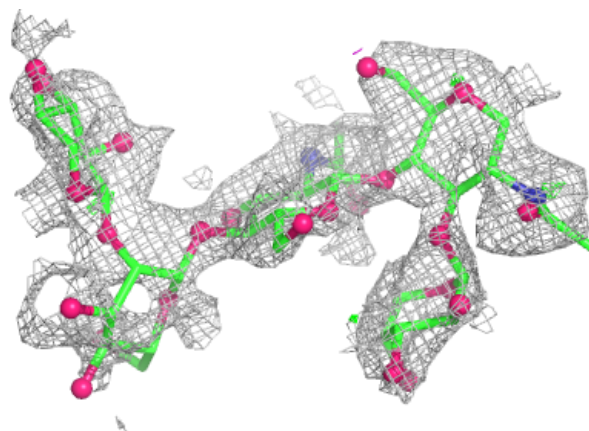
Electron density around Chain D:

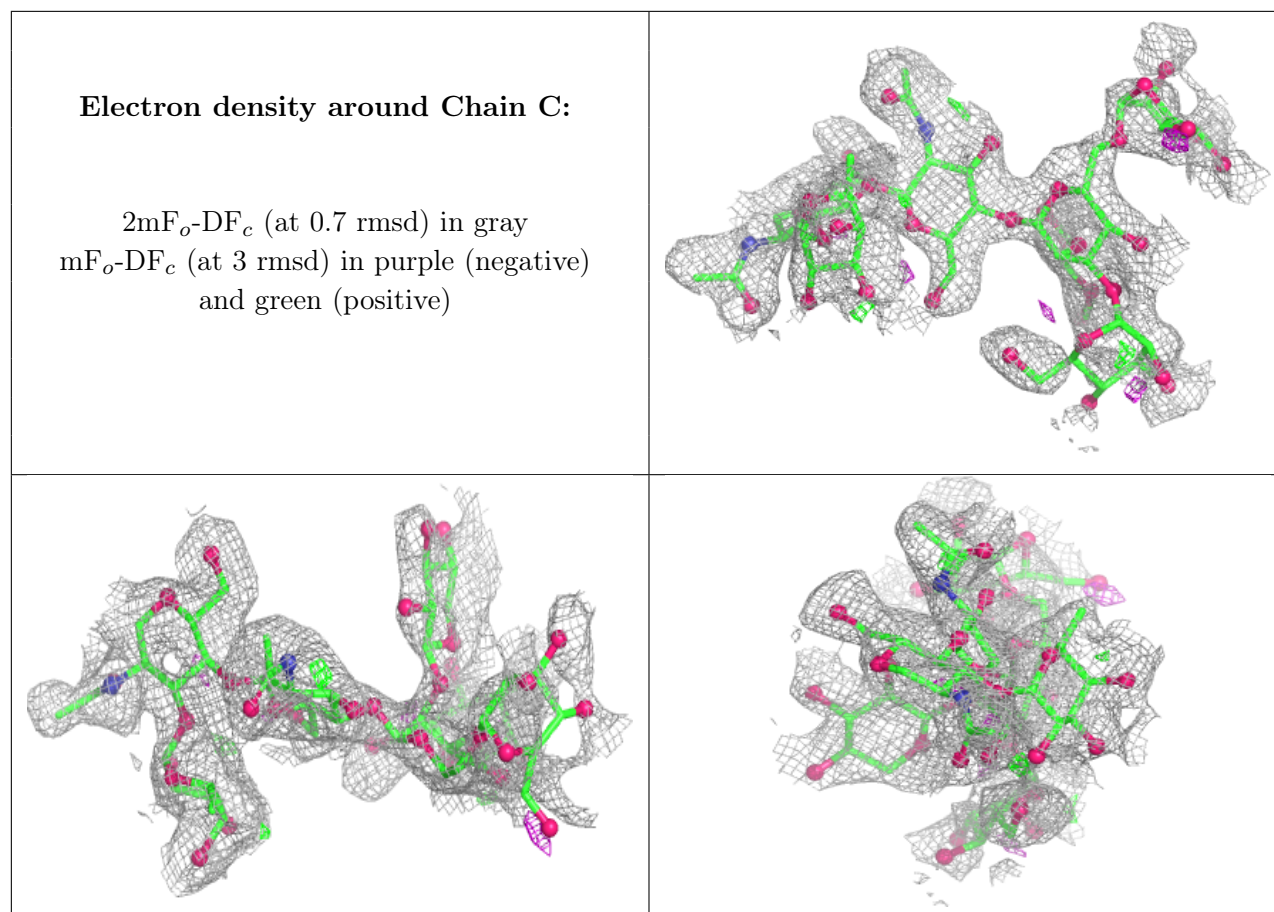
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain B:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
8	GOL	M	1533	6/6	0.32	0.33	34,40,42,49	6
5	NAG	M	1523	14/15	0.47	0.25	32,38,51,54	0
5	NAG	M	1502	14/15	0.48	0.24	23,32,44,46	0
5	NAG	M	1519	14/15	0.49	0.24	41,48,60,66	0
5	NAG	M	1520	14/15	0.49	0.32	54,62,68,68	0
7	SO4	M	1526	5/5	0.53	0.26	23,26,33,34	5
7	SO4	M	1532	5/5	0.53	0.43	36,38,44,57	1
5	NAG	M	1506	14/15	0.53	0.21	33,40,46,47	0
8	GOL	M	1534	6/6	0.56	0.21	3,12,16,16	1
5	NAG	M	1503	14/15	0.57	0.19	22,25,34,43	0
8	GOL	M	1536	6/6	0.59	0.33	29,29,41,43	6
7	SO4	M	1531	5/5	0.64	0.28	31,33,36,37	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	M	1537	6/6	0.64	0.14	13,14,20,20	0
7	SO4	M	1528	5/5	0.69	0.20	15,19,24,27	0
8	GOL	M	1535	6/6	0.70	0.14	9,19,24,29	6
7	SO4	M	1527	5/5	0.71	0.16	12,26,28,32	5
7	SO4	M	1525	5/5	0.78	0.24	24,27,30,35	5
7	SO4	M	1530	5/5	0.79	0.17	11,31,32,35	5
6	ZN	M	1524	1/1	0.80	0.15	34,34,34,34	0
7	SO4	M	1529	5/5	0.81	0.27	24,28,32,33	5

6.5 Other polymers [i](#)

There are no such residues in this entry.