



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:49 AM UTC

PDB ID : 2W59 / pdb_00002w59
Title : STRUCTURE OF AN AVIAN IGY-FC 3-4 FRAGMENT
Authors : Fabiane, S.M.; Taylor, A.I.; Sutton, B.J.; Calvert, R.A.
Deposited on : 2008-12-08
Resolution : 1.75 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

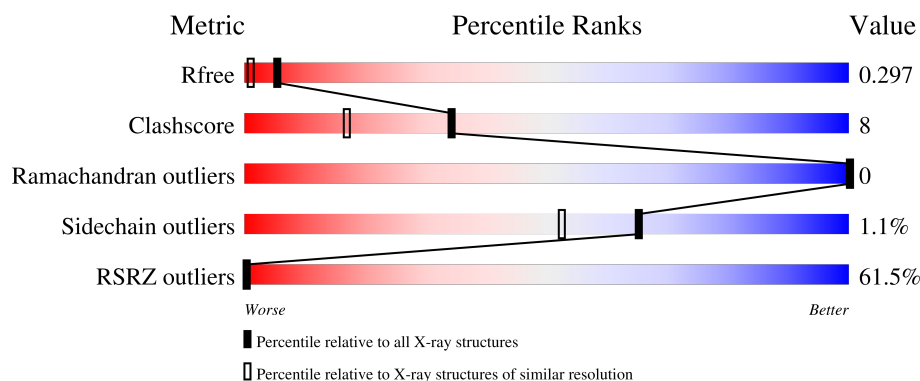
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	231	55% 81% 11% 7%
1	B	231	60% 78% 14% 7%
2	C	3	100%
2	D	3	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	NAG	C	1	X	-	-	-
2	MAN	C	3	X	-	-	-
2	MAN	D	3	X	-	-	-

2 Entry composition [i](#)

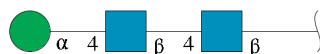
There are 4 unique types of molecules in this entry. The entry contains 4072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 IGY FCU3-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	4	0
			1701	1082	293	315	11			
1	B	214	Total	C	N	O	S	0	5	0
			1701	1082	292	315	12			

- Molecule 2 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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

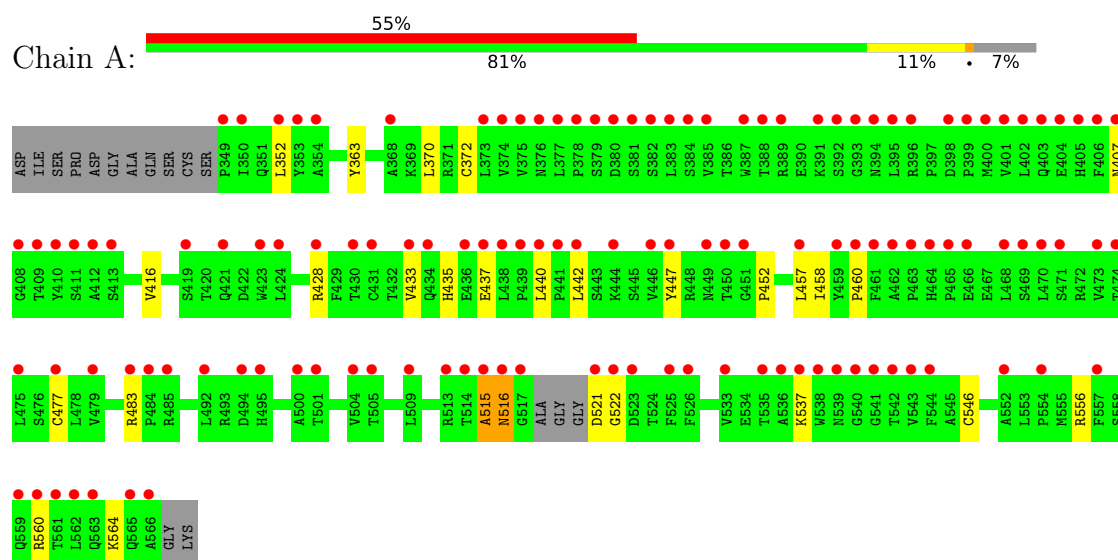
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	271	Total	O	0	0
			271	271		
4	B	285	Total	O	0	0
			285	285		

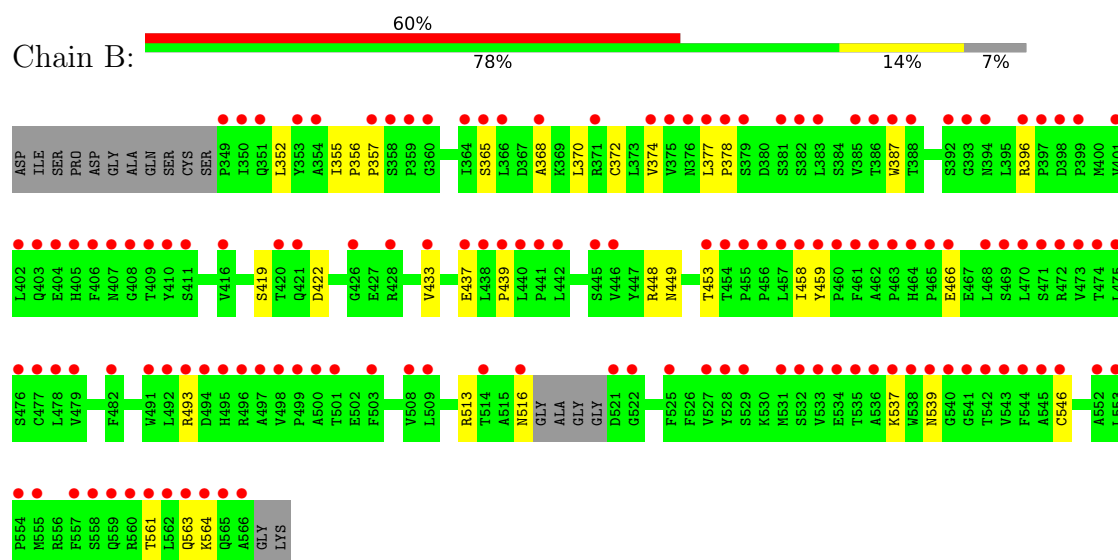
3 Residue-property plots

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: IGY FCU3-4



• Molecule 1: IGY FCU3-4



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

Chain C:  100%

MAG1
MAG2
MAN3

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

Chain D:  100%

MAG1
MAG2
MAN3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.48Å 80.14Å 99.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 1.75 49.57 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.57-1.75) 99.5 (49.57-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.68Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.169 , 0.196 (Not available) , 0.297	Depositor DCC
R_{free} test set	3101 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4072	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: MAN, GOL, NAG

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	0.35	0/1759	0.71	1/2400 (0.0%)
1	B	0.38	0/1762	0.71	0/2404
All	All	0.37	0/3521	0.71	1/4804 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ALA	N-CA-C	6.40	119.07	111.33

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	1701	0	1684	20	0
1	B	1701	0	1682	32	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	A	6	0	8	2	0
3	B	30	0	40	8	0
4	A	271	0	0	4	1
4	B	285	0	0	7	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4072	0	3482	53	1

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 (53) 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:419:SER:H	3:B:605:GOL:H32	1.20	1.02
1:B:563:GLN:OE1	4:B:701:HOH:O	1.88	0.89
1:A:564:LYS:NZ	4:A:701:HOH:O	2.09	0.85
1:A:352:LEU:HD11	1:A:372:CYS:SG	2.24	0.78
1:B:422:ASP:OD1	3:B:605:GOL:H31	1.87	0.74
1:A:515:ALA:N	1:A:516:ASN:HA	2.06	0.70
1:B:419:SER:N	3:B:605:GOL:H32	2.02	0.70
1:B:513:ARG:HD3	4:B:896:HOH:O	1.90	0.70
1:B:352:LEU:HD11	1:B:372[A]:CYS:SG	2.33	0.68
1:B:459:TYR:CE1	3:B:606:GOL:H31	2.31	0.64
1:A:363:TYR:CD1	1:A:556:ARG:HD2	2.33	0.64
1:B:352:LEU:HD11	1:B:372[B]:CYS:SG	2.38	0.63
1:B:365:SER:HB3	4:B:926:HOH:O	1.98	0.63
1:A:435:HIS:CE1	1:A:437:GLU:HG2	2.35	0.61
1:A:440:LEU:HG	4:A:880:HOH:O	2.01	0.60
1:B:372[B]:CYS:HB2	1:B:387:TRP:CZ2	2.36	0.60
1:B:563:GLN:CD	4:B:701:HOH:O	2.37	0.59
3:A:604:GOL:H31	1:B:466:GLU:OE1	2.04	0.57
1:B:437:GLU:O	1:B:439:PRO:HD3	2.06	0.55
1:A:521:ASP:CG	1:A:522:GLY:H	2.14	0.55
1:A:516:ASN:C	1:A:516:ASN:ND2	2.66	0.54
1:B:357:PRO:HB3	1:B:368:ALA:HB1	1.89	0.54
1:A:483:ARG:CZ	1:A:521:ASP:HB3	2.39	0.53
1:B:372[A]:CYS:HB2	1:B:387:TRP:CZ2	2.44	0.53
4:A:808:HOH:O	3:B:608:GOL:H32	2.09	0.53
1:B:449:ASN:ND2	1:B:453:THR:HG22	2.23	0.53
1:A:516:ASN:C	1:A:516:ASN:HD22	2.18	0.52
1:A:433:VAL:CG1	1:A:442:LEU:HB3	2.40	0.52
1:B:561:THR:O	3:B:608:GOL:H31	2.09	0.52
1:A:452:PRO:HG2	1:A:521:ASP:OD1	2.09	0.51
1:B:448:ARG:HD3	4:B:725:HOH:O	2.10	0.51
1:B:449:ASN:HB2	3:B:607:GOL:O2	2.11	0.51
1:A:435:HIS:HE1	1:A:437:GLU:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ARG:HD2	1:B:537:LYS:HE2	1.93	0.51
1:A:537:LYS:HD2	4:A:795:HOH:O	2.11	0.50
1:A:460:PRO:HG3	1:A:560:ARG:HB3	1.92	0.49
1:B:396:ARG:HG3	4:B:760:HOH:O	2.14	0.48
1:B:539:ASN:HA	1:B:564:LYS:HD2	1.95	0.48
1:A:352:LEU:HB3	1:A:442:LEU:HD22	1.96	0.47
1:B:352:LEU:HD13	1:B:433:VAL:HG21	1.96	0.47
1:B:448:ARG:HD2	1:B:449:ASN:O	2.15	0.47
1:B:458:ILE:O	3:B:606:GOL:H2	2.17	0.45
1:A:428:ARG:HA	1:A:447:TYR:HB3	1.98	0.45
1:B:352:LEU:HD13	1:B:433:VAL:CG2	2.49	0.43
1:B:377:LEU:HA	1:B:378:PRO:HD3	1.88	0.42
1:B:352:LEU:HD13	1:B:374:VAL:HG22	2.02	0.42
1:B:355:ILE:HA	1:B:356:PRO:HD3	1.88	0.42
1:A:370:LEU:HB2	1:A:416:VAL:CG1	2.50	0.41
1:B:516:ASN:ND2	4:B:709:HOH:O	2.52	0.41
1:A:458:ILE:HG23	1:A:477[A]:CYS:SG	2.61	0.41
1:B:357:PRO:HG3	1:B:370:LEU:HD23	2.02	0.41
1:B:374:VAL:HG22	1:B:433:VAL:HG21	2.03	0.41
1:A:457:LEU:HD22	3:A:604:GOL:H11	2.04	0.40

All (1) 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)
4:A:789:HOH:O	4:B:748:HOH:O[3_455]	1.41	0.79

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	215/231 (93%)	214 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	215/231 (93%)	211 (98%)	4 (2%)	0	100	100
All	All	430/462 (93%)	425 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/201 (96%)	190 (98%)	4 (2%)	47	27
1	B	195/201 (97%)	193 (99%)	2 (1%)	68	56
All	All	389/402 (97%)	383 (98%)	6 (2%)	65	41

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
1	A	516	ASN
1	A	546[A]	CYS
1	A	546[B]	CYS
1	B	546[A]	CYS
1	B	546[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	516	ASN
1	B	449	ASN
1	B	559	GLN

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	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.49	0	17,19,21	1.09	1 (5%)
2	NAG	C	2	2	14,14,15	0.47	0	17,19,21	1.18	1 (5%)
2	MAN	C	3	2	11,11,12	0.72	0	15,15,17	1.15	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.46	0	17,19,21	1.31	1 (5%)
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	1.21	2 (11%)
2	MAN	D	3	2	11,11,12	0.71	0	15,15,17	1.44	2 (13%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	MAN	C1-C2-C3	4.16	115.70	109.64
2	D	1	NAG	C1-O5-C5	3.94	117.47	112.19
2	C	2	NAG	C4-C3-C2	-3.69	105.60	111.02
2	C	3	MAN	C1-C2-C3	3.42	114.62	109.64
2	D	2	NAG	C1-O5-C5	3.34	116.66	112.19
2	C	1	NAG	C1-O5-C5	2.69	115.78	112.19
2	D	3	MAN	C2-C3-C4	2.41	115.11	110.86
2	D	2	NAG	C2-N2-C7	-2.31	119.81	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	NAG	C1
2	C	3	MAN	C1
2	D	3	MAN	C1

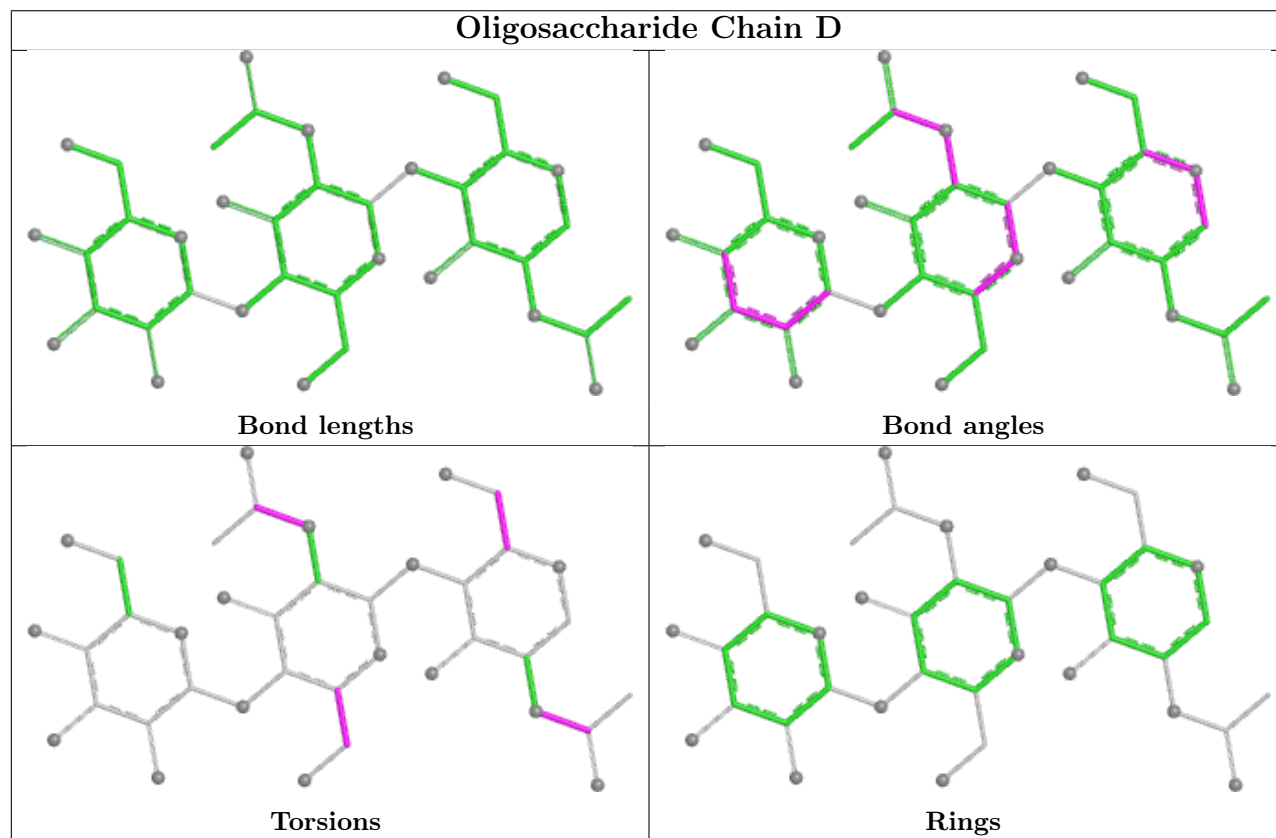
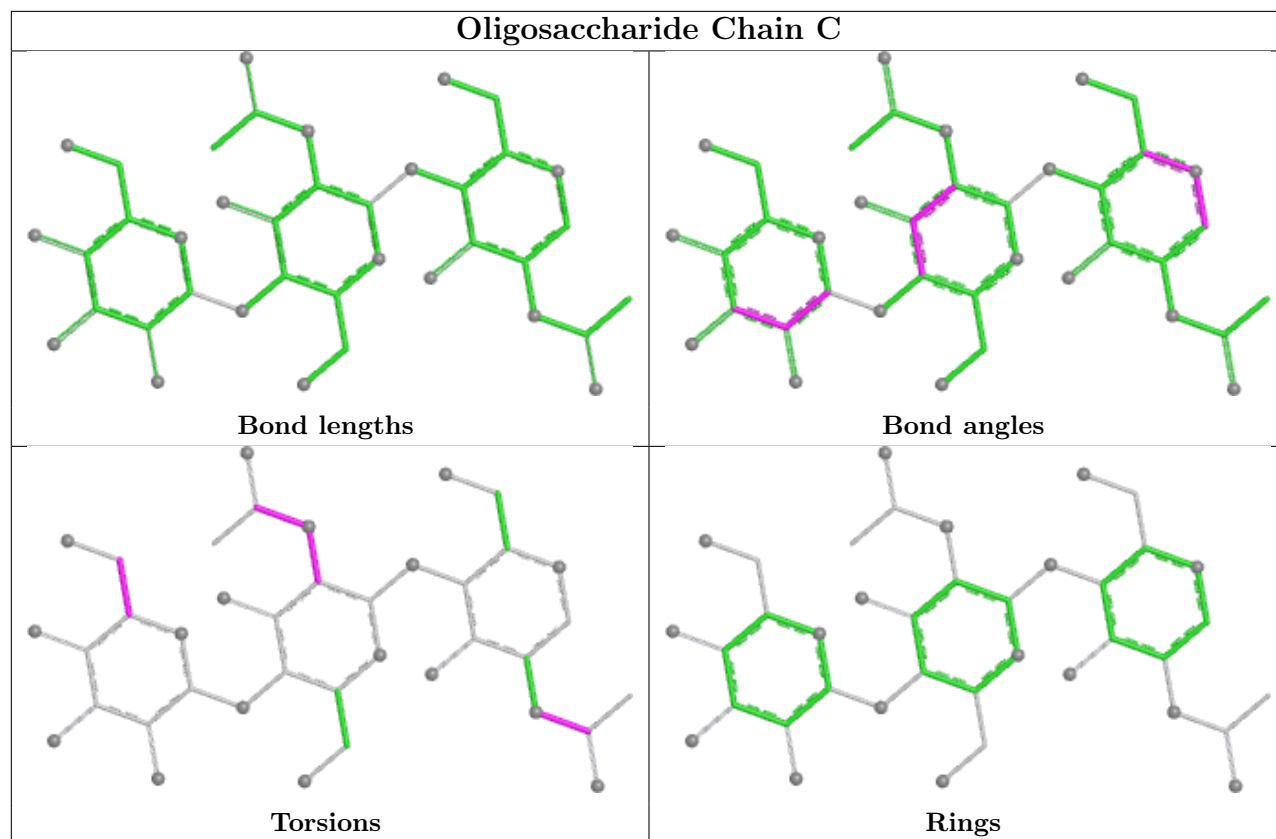
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	D	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

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

6 ligands 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	GOL	B	606	-	5,5,5	0.35	0	5,5,5	0.58	0
3	GOL	A	604	-	5,5,5	0.33	0	5,5,5	0.39	0
3	GOL	B	605	-	5,5,5	0.45	0	5,5,5	0.55	0
3	GOL	B	604	-	5,5,5	0.40	0	5,5,5	0.65	0
3	GOL	B	608	-	5,5,5	0.36	0	5,5,5	0.25	0
3	GOL	B	607	-	5,5,5	0.28	0	5,5,5	0.34	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	GOL	B	606	-	-	2/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	B	605	-	-	2/4/4/4	-
3	GOL	B	604	-	-	4/4/4/4	-
3	GOL	B	608	-	-	2/4/4/4	-
3	GOL	B	607	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	GOL	C1-C2-C3-O3
3	A	604	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	604	GOL	C1-C2-C3-O3
3	B	607	GOL	C1-C2-C3-O3
3	B	607	GOL	O2-C2-C3-O3
3	B	608	GOL	C1-C2-C3-O3
3	B	608	GOL	O2-C2-C3-O3
3	B	604	GOL	O2-C2-C3-O3
3	B	604	GOL	O1-C1-C2-C3
3	B	605	GOL	C1-C2-C3-O3
3	B	606	GOL	C1-C2-C3-O3
3	B	606	GOL	O2-C2-C3-O3
3	B	604	GOL	O1-C1-C2-O2
3	B	605	GOL	O2-C2-C3-O3
3	B	607	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	606	GOL	2	0
3	A	604	GOL	2	0
3	B	605	GOL	3	0
3	B	608	GOL	2	0
3	B	607	GOL	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

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	215/231 (93%)	2.49	126 (58%) 0 0	11, 32, 76, 95	4 (1%)
1	B	214/231 (92%)	2.65	138 (64%) 0 0	12, 26, 69, 103	5 (2%)
All	All	429/462 (92%)	2.57	264 (61%) 0 0	11, 29, 76, 103	9 (2%)

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	406	PHE	6.4
1	A	408	GLY	6.4
1	B	538	TRP	6.3
1	A	401	VAL	6.2
1	A	440	LEU	6.1
1	B	541	GLY	6.1
1	B	406	PHE	6.0
1	B	382	SER	5.8
1	B	469	SER	5.8
1	B	494	ASP	5.8
1	B	564	LYS	5.8
1	A	410	TYR	5.8
1	A	566	ALA	5.5
1	A	383	LEU	5.5
1	A	438	LEU	5.5
1	A	441	PRO	5.5
1	B	378	PRO	5.4
1	A	515	ALA	5.4
1	A	409	THR	5.2
1	B	404	GLU	5.2
1	A	450	THR	5.2
1	B	540	GLY	5.1
1	A	516	ASN	5.1
1	B	465	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	375	VAL	5.0
1	B	440	LEU	4.9
1	A	396	ARG	4.9
1	A	382	SER	4.9
1	A	517	GLY	4.9
1	B	562	LEU	4.8
1	A	468	LEU	4.7
1	A	521	ASP	4.7
1	A	442	LEU	4.7
1	A	394	ASN	4.6
1	B	405	HIS	4.6
1	B	437	GLU	4.6
1	B	495	HIS	4.5
1	B	409	THR	4.5
1	A	433	VAL	4.4
1	A	395	LEU	4.4
1	B	535	THR	4.4
1	A	439	PRO	4.4
1	B	410	TYR	4.4
1	A	381	SER	4.4
1	B	565	GLN	4.4
1	B	554	PRO	4.4
1	B	557	PHE	4.4
1	B	468	LEU	4.4
1	A	536	ALA	4.4
1	B	503	PHE	4.3
1	A	378	PRO	4.3
1	B	544	PHE	4.3
1	A	380	ASP	4.3
1	B	349	PRO	4.3
1	B	403	GLN	4.3
1	B	539	ASN	4.2
1	B	460	PRO	4.2
1	B	408	GLY	4.2
1	B	543	VAL	4.1
1	A	379	SER	4.1
1	B	536	ALA	4.1
1	A	349	PRO	4.1
1	A	465	PRO	4.1
1	A	522	GLY	4.0
1	A	392	SER	3.9
1	B	555	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	461	PHE	3.9
1	B	377	LEU	3.9
1	A	405	HIS	3.9
1	A	513	ARG	3.8
1	A	377	LEU	3.8
1	B	553	LEU	3.8
1	A	461	PHE	3.8
1	A	421	GLN	3.8
1	B	393	GLY	3.8
1	B	439	PRO	3.8
1	B	496	ARG	3.8
1	A	424	LEU	3.8
1	B	438	LEU	3.8
1	A	412	ALA	3.7
1	B	473	VAL	3.7
1	A	561	THR	3.7
1	B	402	LEU	3.7
1	A	393	GLY	3.7
1	A	463	PRO	3.6
1	B	521	ASP	3.6
1	B	477[A]	CYS	3.6
1	B	394	ASN	3.6
1	B	462	ALA	3.6
1	A	387	TRP	3.5
1	B	381	SER	3.5
1	B	559	GLN	3.5
1	B	385	VAL	3.5
1	B	542	THR	3.5
1	B	472	ARG	3.5
1	A	538	TRP	3.5
1	B	566	ALA	3.4
1	A	449	ASN	3.4
1	B	534	GLU	3.4
1	A	543	VAL	3.4
1	B	464	HIS	3.4
1	A	391	LYS	3.4
1	A	407	ASN	3.4
1	A	451	GLY	3.4
1	B	453	THR	3.4
1	B	456	PRO	3.4
1	B	475	LEU	3.3
1	B	516	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	514	THR	3.3
1	A	470	LEU	3.3
1	B	499	PRO	3.3
1	B	497	ALA	3.3
1	B	350	ILE	3.3
1	A	514	THR	3.2
1	A	350	ILE	3.2
1	B	441	PRO	3.2
1	B	463	PRO	3.2
1	B	470	LEU	3.2
1	B	533	VAL	3.2
1	A	384	SER	3.2
1	B	383	LEU	3.2
1	B	560	ARG	3.2
1	B	537	LYS	3.2
1	A	389	ARG	3.1
1	B	368	ALA	3.1
1	B	558	SER	3.1
1	B	492	LEU	3.1
1	B	471	SER	3.1
1	B	416	VAL	3.0
1	A	400	MET	3.0
1	B	552	ALA	3.0
1	B	561	THR	3.0
1	B	397	PRO	3.0
1	B	401	VAL	3.0
1	A	466	GLU	3.0
1	B	563	GLN	3.0
1	A	460	PRO	3.0
1	A	540	GLY	3.0
1	B	428	ARG	3.0
1	A	431[A]	CYS	3.0
1	B	498	VAL	2.9
1	A	474	THR	2.9
1	A	501	THR	2.9
1	A	552	ALA	2.9
1	A	436	GLU	2.9
1	B	491	TRP	2.9
1	A	403	GLN	2.9
1	B	375	VAL	2.9
1	B	474	THR	2.9
1	B	396	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	354	ALA	2.9
1	B	500	ALA	2.9
1	A	459	TYR	2.9
1	B	546[A]	CYS	2.9
1	A	563	GLN	2.8
1	B	358	SER	2.8
1	B	455	PRO	2.8
1	A	437	GLU	2.8
1	B	466	GLU	2.8
1	A	504	VAL	2.8
1	A	539	ASN	2.8
1	B	458	ILE	2.8
1	B	501	THR	2.8
1	B	407	ASN	2.8
1	A	565	GLN	2.8
1	A	457	LEU	2.8
1	A	398	ASP	2.8
1	A	523	ASP	2.7
1	A	430	THR	2.7
1	B	532	SER	2.7
1	A	434	GLN	2.7
1	A	353	TYR	2.7
1	A	484	PRO	2.7
1	B	482	PHE	2.7
1	B	433	VAL	2.7
1	A	554	PRO	2.6
1	A	559	GLN	2.6
1	A	525	PHE	2.6
1	B	446	VAL	2.6
1	B	411	SER	2.6
1	A	537	LYS	2.6
1	B	360	GLY	2.6
1	B	426	GLY	2.6
1	B	421	GLN	2.6
1	A	444	LYS	2.6
1	A	352	LEU	2.6
1	A	471	SER	2.6
1	B	364	ILE	2.6
1	B	531	MET	2.6
1	B	420	THR	2.5
1	A	560	ARG	2.5
1	A	462	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	479	VAL	2.5
1	B	522	GLY	2.5
1	A	388	THR	2.5
1	B	392	SER	2.5
1	B	529	SER	2.5
1	A	373	LEU	2.4
1	A	492	LEU	2.4
1	B	457	LEU	2.4
1	B	478	LEU	2.4
1	A	533	VAL	2.4
1	B	386	THR	2.4
1	A	402	LEU	2.4
1	A	419	SER	2.4
1	A	469	SER	2.4
1	B	545	ALA	2.4
1	A	535	THR	2.4
1	A	446	VAL	2.4
1	A	473	VAL	2.4
1	A	541	GLY	2.4
1	B	359	PRO	2.4
1	B	379	SER	2.4
1	B	374	VAL	2.4
1	A	464	HIS	2.4
1	A	477[A]	CYS	2.3
1	A	368	ALA	2.3
1	B	442	LEU	2.3
1	A	544	PHE	2.3
1	B	525	PHE	2.3
1	B	387	TRP	2.3
1	B	376	ASN	2.3
1	A	557	PHE	2.3
1	B	445	SER	2.3
1	B	527	VAL	2.3
1	A	374	VAL	2.3
1	A	385	VAL	2.3
1	A	411	SER	2.2
1	A	494	ASP	2.2
1	B	528	TYR	2.2
1	A	404	GLU	2.2
1	B	508	VAL	2.2
1	A	542	THR	2.2
1	A	413	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	398	ASP	2.2
1	B	366	LEU	2.2
1	B	353	TYR	2.2
1	B	459	TYR	2.2
1	A	399	PRO	2.2
1	B	454	THR	2.2
1	B	476	SER	2.2
1	A	354	ALA	2.2
1	B	351	GLN	2.2
1	A	526	PHE	2.2
1	A	447	TYR	2.2
1	A	505	THR	2.2
1	B	399	PRO	2.2
1	A	428	ARG	2.1
1	A	376	ASN	2.1
1	A	495	HIS	2.1
1	A	562	LEU	2.1
1	B	509	LEU	2.1
1	A	423	TRP	2.1
1	A	485	ARG	2.1
1	B	388	THR	2.1
1	B	493	ARG	2.1
1	A	500	ALA	2.1
1	A	483	ARG	2.1
1	A	509	LEU	2.1
1	A	479	VAL	2.0
1	B	371	ARG	2.0
1	A	475	LEU	2.0
1	B	357	PRO	2.0
1	B	365	SER	2.0

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

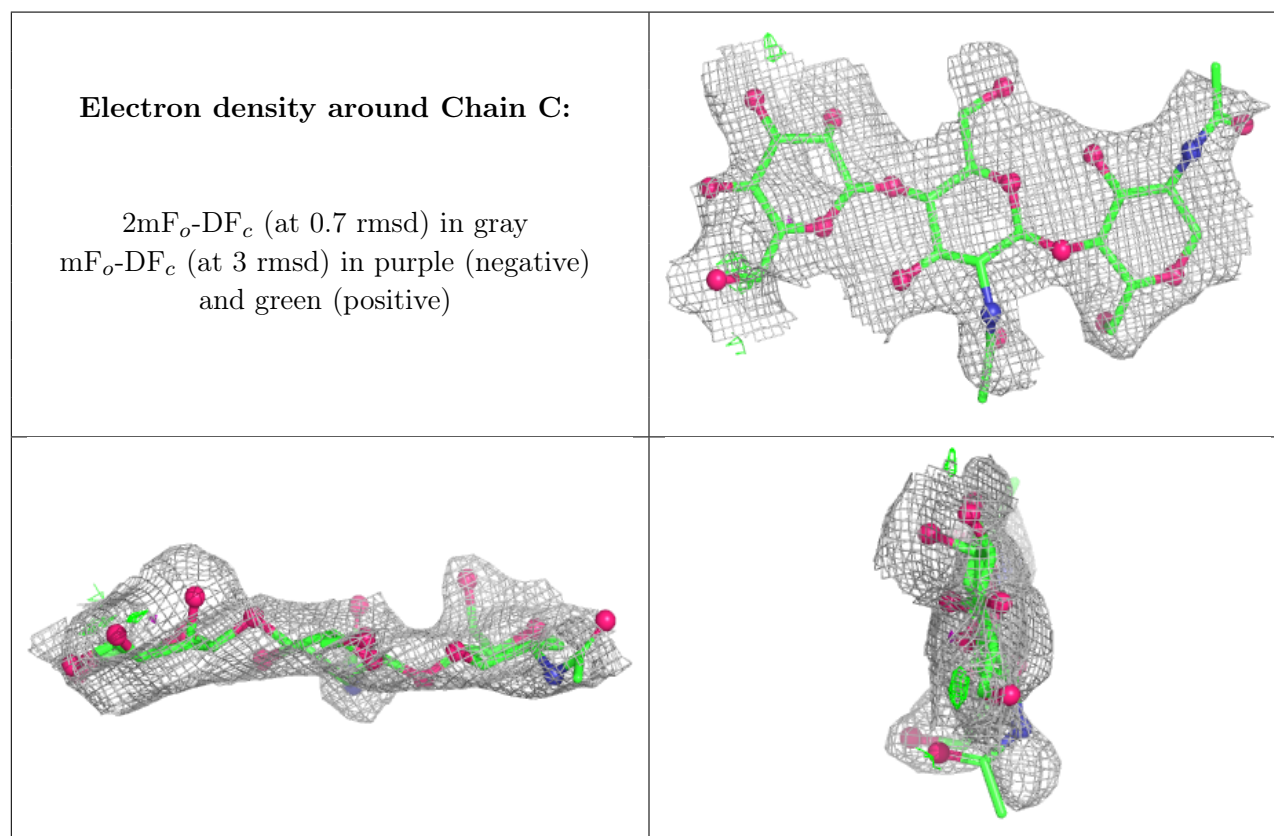
There are no non-standard protein/DNA/RNA residues in this entry.

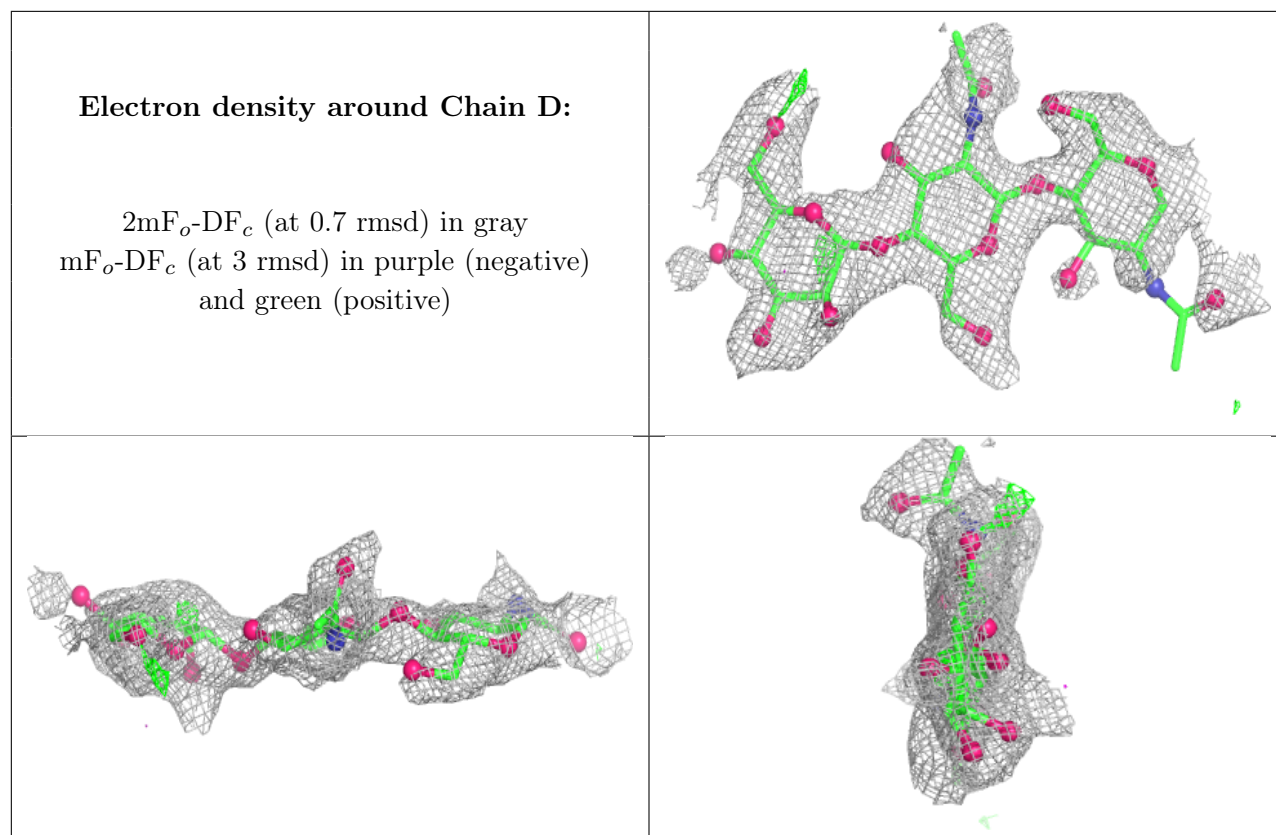
6.3 Carbohydrates ⓘ

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
2	MAN	C	3	11/12	0.52	0.25	71,77,81,82	11
2	MAN	D	3	11/12	0.72	0.24	77,79,81,82	11
2	NAG	D	1	14/15	0.75	0.23	66,73,81,85	0
2	NAG	C	2	14/15	0.75	0.26	71,74,90,93	0
2	NAG	D	2	14/15	0.81	0.16	61,67,76,80	0
2	NAG	C	1	14/15	0.83	0.15	70,75,78,81	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
3	GOL	B	608	6/6	0.58	0.20	32,59,64,69	0
3	GOL	B	606	6/6	0.61	0.23	34,43,48,58	0
3	GOL	A	604	6/6	0.73	0.18	39,56,65,71	0
3	GOL	B	605	6/6	0.80	0.23	20,38,46,48	0
3	GOL	B	604	6/6	0.81	0.24	24,45,51,62	0
3	GOL	B	607	6/6	0.82	0.22	23,57,58,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.