



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 08:46 PM EDT

PDB ID : 5FNO
Title : Manganese Lipxygenase
Authors : Wennman, A.; Karkehabadi, S.; Oliw, E.H.; Chen, Y.
Deposited on : 2015-11-16
Resolution : 2.04 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

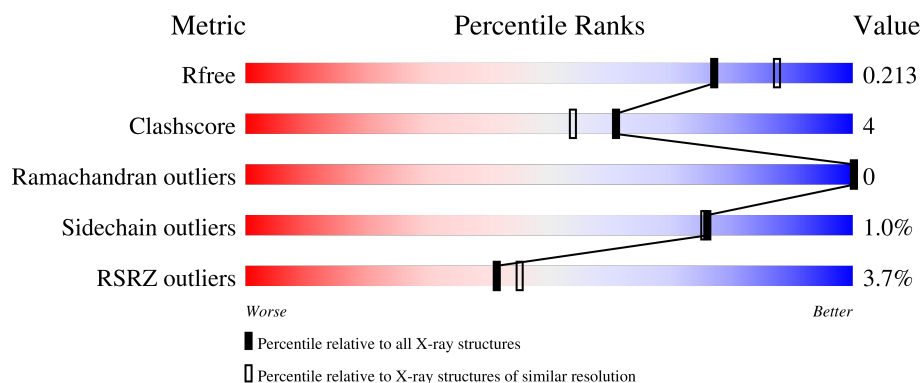
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	605	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	B	605	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9741 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 MANGANESE LIPOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4472	2845	788	824	15			
1	B	568	Total	C	N	O	S	0	0	0
			4472	2845	788	824	15			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP G4NAP4
A	2	PHE	-	expression tag	UNP G4NAP4
A	575	ALA	-	expression tag	UNP G4NAP4
A	576	ARG	-	expression tag	UNP G4NAP4
A	577	ARG	-	expression tag	UNP G4NAP4
A	578	PHE	-	expression tag	UNP G4NAP4
A	579	ASP	-	expression tag	UNP G4NAP4
A	580	ASP	-	expression tag	UNP G4NAP4
A	581	ARG	-	expression tag	UNP G4NAP4
A	582	GLY	-	expression tag	UNP G4NAP4
A	583	LEU	-	expression tag	UNP G4NAP4
A	584	SER	-	expression tag	UNP G4NAP4
A	585	GLN	-	expression tag	UNP G4NAP4
A	586	GLY	-	expression tag	UNP G4NAP4
A	587	MET	-	expression tag	UNP G4NAP4
A	588	PRO	-	expression tag	UNP G4NAP4
A	589	PHE	-	expression tag	UNP G4NAP4
A	590	ILE	-	expression tag	UNP G4NAP4
A	591	TRP	-	expression tag	UNP G4NAP4
A	592	GLN	-	expression tag	UNP G4NAP4
A	593	ALA	-	expression tag	UNP G4NAP4
A	594	LEU	-	expression tag	UNP G4NAP4
A	595	ASP	-	expression tag	UNP G4NAP4
A	596	PRO	-	expression tag	UNP G4NAP4
A	597	GLY	-	expression tag	UNP G4NAP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ASN	-	expression tag	UNP G4NAP4
A	599	ILE	-	expression tag	UNP G4NAP4
A	600	PRO	-	expression tag	UNP G4NAP4
A	601	PHE	-	expression tag	UNP G4NAP4
A	602	TYR	-	expression tag	UNP G4NAP4
A	603	LEU	-	expression tag	UNP G4NAP4
A	604	SER	-	expression tag	UNP G4NAP4
A	605	VAL	-	expression tag	UNP G4NAP4
B	1	GLU	-	expression tag	UNP G4NAP4
B	2	PHE	-	expression tag	UNP G4NAP4
B	575	ALA	-	expression tag	UNP G4NAP4
B	576	ARG	-	expression tag	UNP G4NAP4
B	577	ARG	-	expression tag	UNP G4NAP4
B	578	PHE	-	expression tag	UNP G4NAP4
B	579	ASP	-	expression tag	UNP G4NAP4
B	580	ASP	-	expression tag	UNP G4NAP4
B	581	ARG	-	expression tag	UNP G4NAP4
B	582	GLY	-	expression tag	UNP G4NAP4
B	583	LEU	-	expression tag	UNP G4NAP4
B	584	SER	-	expression tag	UNP G4NAP4
B	585	GLN	-	expression tag	UNP G4NAP4
B	586	GLY	-	expression tag	UNP G4NAP4
B	587	MET	-	expression tag	UNP G4NAP4
B	588	PRO	-	expression tag	UNP G4NAP4
B	589	PHE	-	expression tag	UNP G4NAP4
B	590	ILE	-	expression tag	UNP G4NAP4
B	591	TRP	-	expression tag	UNP G4NAP4
B	592	GLN	-	expression tag	UNP G4NAP4
B	593	ALA	-	expression tag	UNP G4NAP4
B	594	LEU	-	expression tag	UNP G4NAP4
B	595	ASP	-	expression tag	UNP G4NAP4
B	596	PRO	-	expression tag	UNP G4NAP4
B	597	GLY	-	expression tag	UNP G4NAP4
B	598	ASN	-	expression tag	UNP G4NAP4
B	599	ILE	-	expression tag	UNP G4NAP4
B	600	PRO	-	expression tag	UNP G4NAP4
B	601	PHE	-	expression tag	UNP G4NAP4
B	602	TYR	-	expression tag	UNP G4NAP4
B	603	LEU	-	expression tag	UNP G4NAP4
B	604	SER	-	expression tag	UNP G4NAP4
B	605	VAL	-	expression tag	UNP G4NAP4

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

cetamido-2-deoxy-beta-D-glucopyranose.

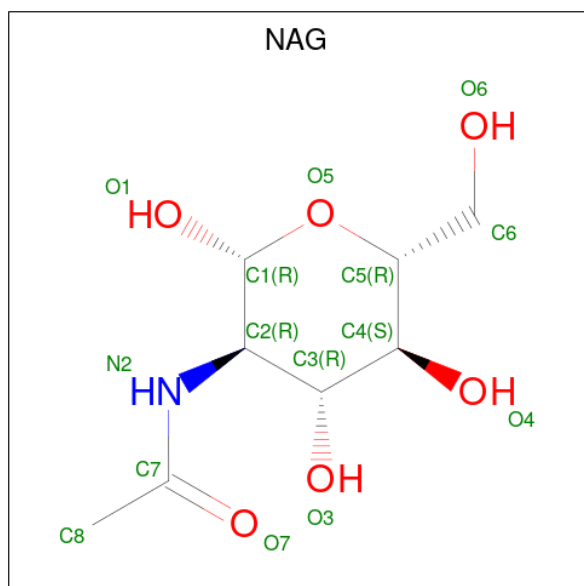


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

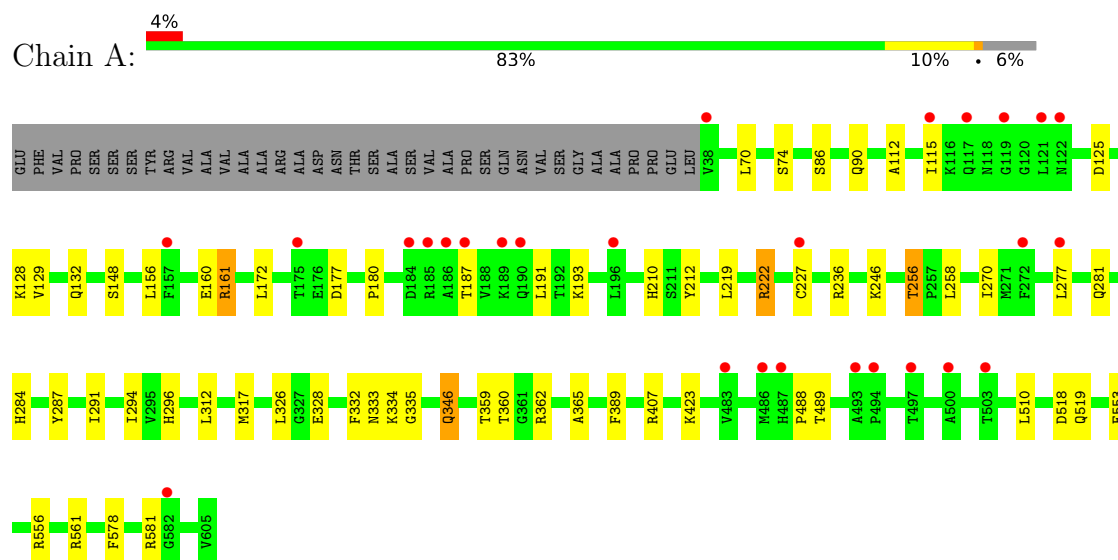
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	364	Total	O	0	0
			364	364		
5	B	319	Total	O	0	0
			319	319		

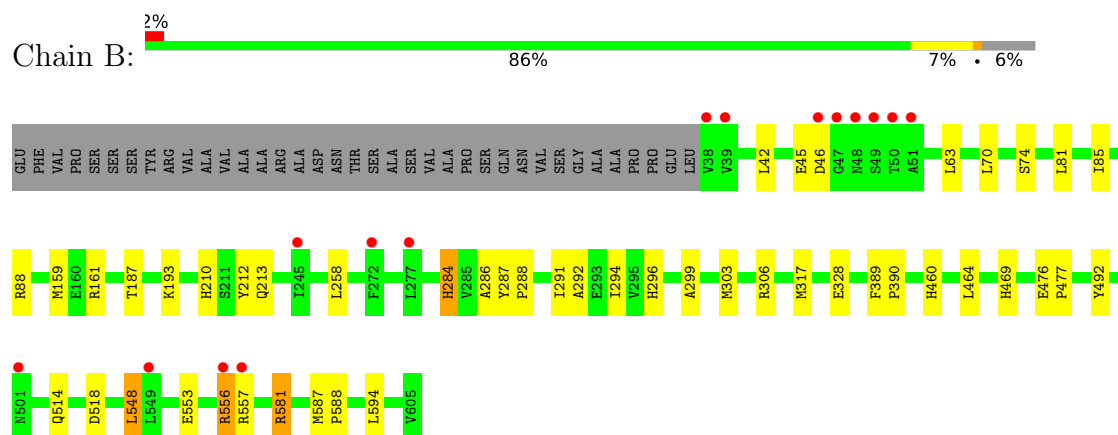
3 Residue-property plots

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: MANGANESE LIPOXYGENASE



• Molecule 1: MANGANESE LIPOXYGENASE



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



MAG1
MAG2

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

Chain D: 

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.72Å 111.37Å 171.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.04 29.71 – 2.04	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.70-2.04) 96.8 (29.71-2.04)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.04Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.168 , 0.213 0.168 , 0.213	Depositor DCC
R_{free} test set	4185 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9741	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

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	0.37	0/4585	0.56	1/6243 (0.0%)
1	B	0.41	1/4585 (0.0%)	0.58	5/6243 (0.1%)
All	All	0.39	1/9170 (0.0%)	0.57	6/12486 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	556	ARG	CB-CG	-8.14	1.30	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	581	ARG	NE-CZ-NH1	-8.41	116.10	120.30
1	B	556	ARG	CG-CD-NE	-7.82	95.38	111.80
1	A	312	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	556	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	548	LEU	CB-CG-CD2	5.25	119.93	111.00
1	B	581	ARG	NE-CZ-NH2	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4472	0	4385	44	0
1	B	4472	0	4384	38	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	26	0	0
4	B	28	0	25	0	0
5	A	364	0	0	5	0
5	B	319	0	0	2	0
All	All	9741	0	8870	80	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 4.

All (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HA	1:A:132:GLN:HG2	1.60	0.84
1:A:581:ARG:NH1	1:B:581:ARG:HH12	1.75	0.84
1:B:556:ARG:N	1:B:556:ARG:HD2	1.93	0.82
1:B:548:LEU:O	1:B:556:ARG:NH2	2.15	0.79
1:A:128:LYS:HD3	1:A:148:SER:HB3	1.67	0.77
1:B:548:LEU:O	1:B:556:ARG:NH1	2.20	0.73
1:A:187:THR:HG23	1:A:258:LEU:HD12	1.68	0.73
1:B:296:HIS:CG	1:B:317:MET:HG3	2.27	0.69
1:B:548:LEU:C	1:B:556:ARG:HH22	1.98	0.66
1:B:556:ARG:N	1:B:556:ARG:CD	2.61	0.62
1:B:514:GLN:NE2	1:B:518:ASP:OD1	2.33	0.62
1:A:553:GLU:OE1	1:A:556:ARG:NH1	2.33	0.61
1:A:407:ARG:NH1	5:A:2261:HOH:O	2.23	0.61
1:A:219:LEU:HB2	1:A:222:ARG:HG3	1.84	0.60
1:A:128:LYS:CD	1:A:148:SER:HB3	2.33	0.58
1:A:129:VAL:HA	1:A:132:GLN:CG	2.33	0.57
1:A:561:ARG:NH2	5:A:2330:HOH:O	2.37	0.56
1:A:256:THR:HG22	1:A:258:LEU:H	1.70	0.56
1:B:284:HIS:HA	1:B:287:TYR:O	2.05	0.56
1:B:548:LEU:O	1:B:556:ARG:CZ	2.53	0.56
1:B:390:PRO:HG2	1:B:587:MET:SD	2.46	0.56
1:A:581:ARG:HH11	1:B:581:ARG:HH12	1.49	0.56
1:B:161:ARG:HD3	5:B:2073:HOH:O	2.08	0.54
1:A:333:ASN:O	1:A:335:GLY:HA2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ALA:HB1	1:B:317:MET:HE3	1.90	0.53
1:A:210:HIS:HA	1:A:212:TYR:CE2	2.44	0.52
1:B:210:HIS:HA	1:B:212:TYR:CE2	2.44	0.52
1:A:281:GLN:O	1:A:284:HIS:ND1	2.40	0.52
1:A:284:HIS:HA	1:A:287:TYR:O	2.10	0.52
1:A:193:LYS:HG2	1:A:236:ARG:HH11	1.75	0.51
1:A:112:ALA:O	1:A:115:ILE:HG13	2.11	0.50
1:A:332:PHE:O	1:A:346:GLN:NE2	2.43	0.50
1:B:286:ALA:O	1:B:291:ILE:HG13	2.12	0.50
1:A:222:ARG:NH1	5:A:2150:HOH:O	2.40	0.49
1:A:74:SER:HB2	1:A:294:ILE:HB	1.94	0.49
1:B:212:TYR:CE1	1:B:213:GLN:HG3	2.48	0.49
1:A:291:ILE:HD11	1:A:360:THR:O	2.14	0.48
1:B:548:LEU:C	1:B:556:ARG:NH2	2.63	0.48
1:A:270:ILE:HD13	1:A:510:LEU:HD21	1.96	0.48
1:B:588:PRO:HB3	2:D:1:NAG:H82	1.96	0.48
1:B:492:TYR:OH	5:B:2176:HOH:O	2.20	0.47
1:B:46:ASP:OD2	1:B:306:ARG:NH1	2.45	0.47
1:A:172:LEU:HD11	1:A:180:PRO:HD3	1.96	0.47
1:B:42:LEU:HB2	1:B:45:GLU:HG3	1.97	0.47
1:B:193:LYS:HD3	1:B:193:LYS:HA	1.59	0.46
1:A:578:PHE:CE2	2:C:1:NAG:H5	2.50	0.46
1:A:86:SER:O	1:A:90:GLN:HG3	2.15	0.46
1:A:256:THR:CG2	1:A:258:LEU:H	2.29	0.46
1:B:553:GLU:O	1:B:557:ARG:HG3	2.15	0.46
1:A:359:THR:O	1:A:362:ARG:HG3	2.16	0.45
1:A:161:ARG:HA	1:A:161:ARG:HD3	1.77	0.45
1:B:187:THR:HG23	1:B:258:LEU:HD12	1.99	0.45
1:B:159:MET:HB3	1:B:587:MET:HG2	1.97	0.45
1:B:74:SER:HB2	1:B:294:ILE:HB	1.99	0.45
1:A:129:VAL:HG13	1:A:132:GLN:NE2	2.32	0.45
1:A:172:LEU:HD22	1:A:177:ASP:HB3	1.99	0.45
1:A:70:LEU:HD23	1:A:328:GLU:HG2	1.98	0.44
1:A:191:LEU:HD11	1:A:256:THR:HG23	1.98	0.44
1:A:334:LYS:NZ	5:A:2194:HOH:O	2.41	0.44
1:B:288:PRO:HG3	1:B:469:HIS:HB2	1.99	0.44
1:B:460:HIS:O	1:B:464:LEU:HG	2.18	0.44
1:B:556:ARG:CD	1:B:556:ARG:H	2.28	0.44
1:B:299:ALA:HB1	1:B:303:MET:HE1	1.99	0.43
1:B:70:LEU:HD23	1:B:328:GLU:HG2	2.00	0.43
1:A:423:LYS:HD3	1:A:423:LYS:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:HB2	1:B:81:LEU:HD23	2.01	0.43
1:B:594:LEU:HD23	1:B:594:LEU:HA	1.89	0.43
1:B:476:GLU:HB3	1:B:477:PRO:HD3	2.01	0.42
1:A:296:HIS:CG	1:A:317:MET:HG3	2.54	0.42
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.83	0.42
1:A:227:CYS:HA	1:A:246:LYS:O	2.20	0.42
1:B:299:ALA:HB1	1:B:303:MET:CE	2.49	0.42
1:A:193:LYS:N	1:A:193:LYS:HD3	2.35	0.42
1:A:362:ARG:HB2	1:A:365:ALA:HB3	2.02	0.41
1:A:156:LEU:O	1:A:160:GLU:HG3	2.20	0.41
1:A:222:ARG:HD2	5:A:2150:HOH:O	2.20	0.41
1:A:277:LEU:HD21	1:A:489:THR:HG22	2.02	0.41
1:B:85:ILE:HG23	1:B:88:ARG:NH2	2.37	0.40
1:A:488:PRO:HA	1:A:519:GLN:HE22	1.86	0.40
1:B:303:MET:HB2	1:B:303:MET:HE2	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	566/605 (94%)	547 (97%)	19 (3%)	0	100	100
1	B	566/605 (94%)	547 (97%)	19 (3%)	0	100	100
All	All	1132/1210 (94%)	1094 (97%)	38 (3%)	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	468/496 (94%)	461 (98%)	7 (2%)	65	62
1	B	468/496 (94%)	466 (100%)	2 (0%)	91	91
All	All	936/992 (94%)	927 (99%)	9 (1%)	76	75

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ASP
1	A	161	ARG
1	A	222	ARG
1	A	256	THR
1	A	346	GLN
1	A	389	PHE
1	A	518	ASP
1	B	284	HIS
1	B	389	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	100	GLN
1	A	132	GLN
1	A	519	GLN
1	B	190	GLN
1	B	213	GLN
1	B	514	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

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.36	0	17,19,21	0.76	0
2	NAG	C	2	2	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.63	0	17,19,21	0.70	1 (5%)
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	0.52	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	2.32	115.33	112.19
2	D	1	NAG	C1-O5-C5	2.25	115.24	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

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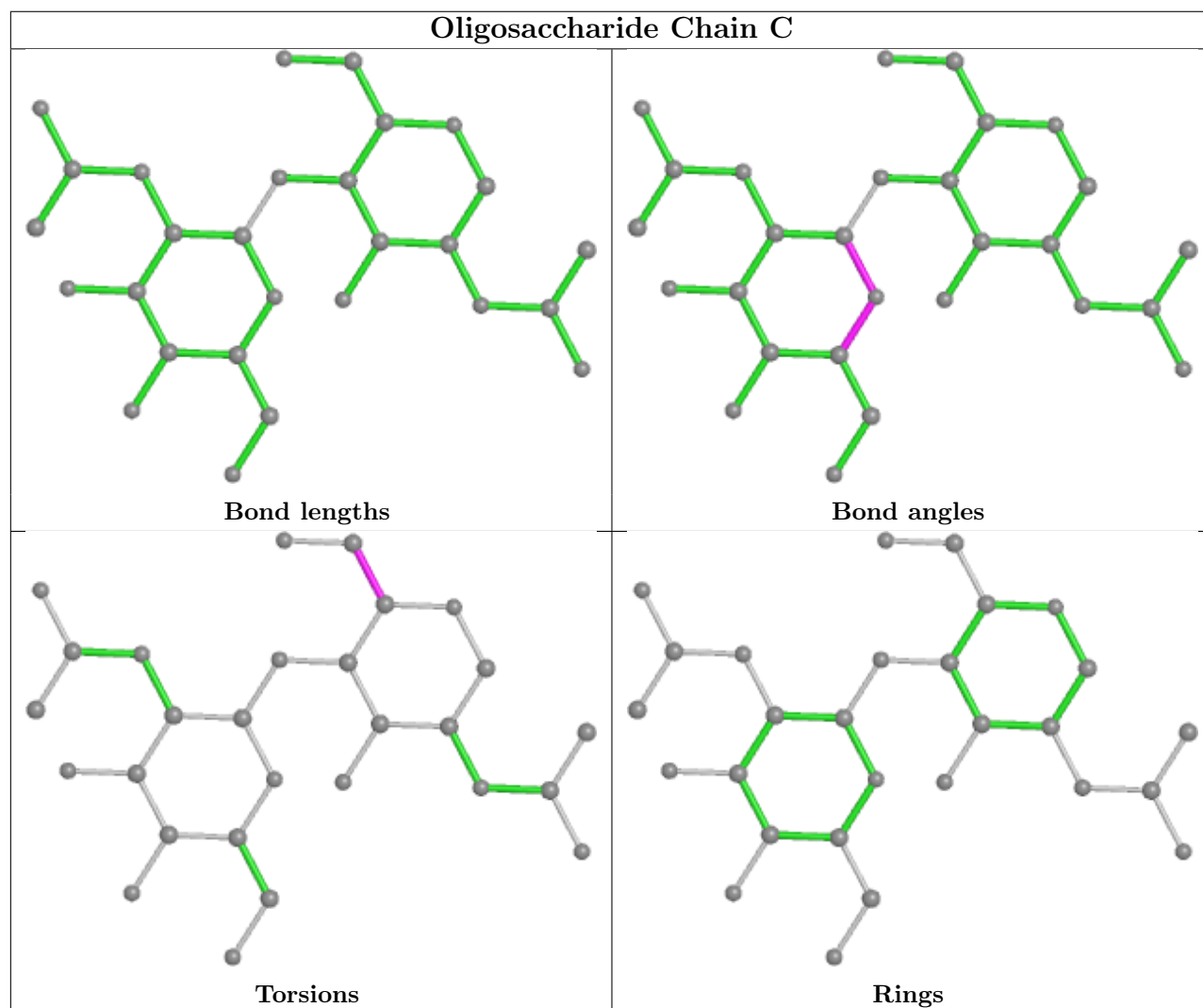
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

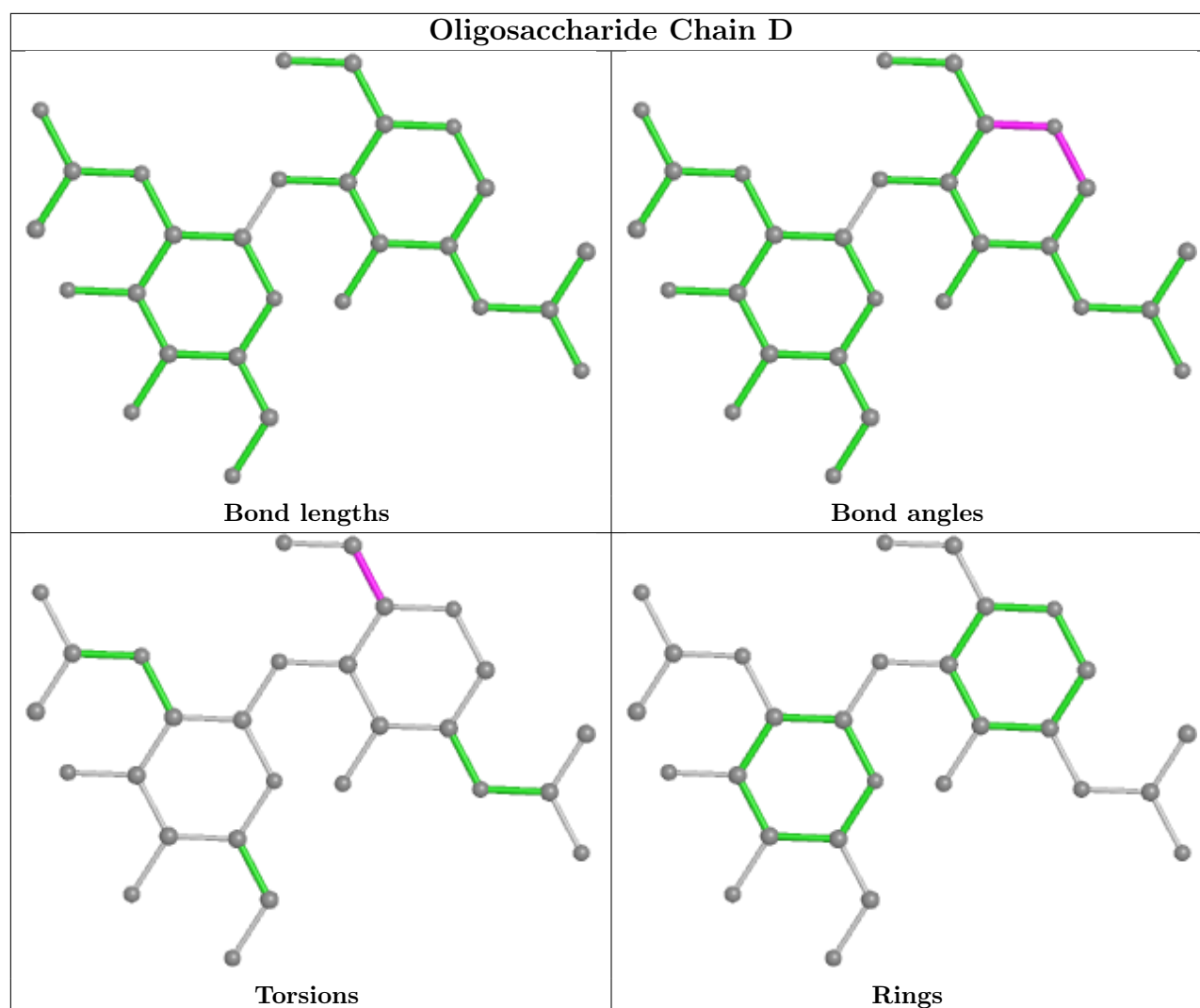
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
4	NAG	B	1021	1	14,14,15	0.39	0	17,19,21	0.68	1 (5%)
4	NAG	A	1021	1	14,14,15	0.47	0	17,19,21	0.71	0
4	NAG	A	1011	1	14,14,15	0.47	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1011	1	14,14,15	0.41	0	17,19,21	0.46	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
4	NAG	B	1021	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1021	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1011	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1011	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1021	NAG	C1-O5-C5	2.39	115.43	112.19
4	A	1011	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1021	NAG	O5-C5-C6-O6
4	B	1021	NAG	C4-C5-C6-O6
4	A	1011	NAG	C4-C5-C6-O6
4	A	1011	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	568/605 (93%)	0.09	27 (4%)	30 33	22, 40, 71, 99	0
1	B	568/605 (93%)	-0.10	15 (2%)	56 60	25, 40, 62, 96	0
All	All	1136/1210 (93%)	-0.01	42 (3%)	41 45	22, 40, 67, 99	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	VAL	4.1
1	A	500	ALA	4.0
1	A	272	PHE	4.0
1	A	121	LEU	4.0
1	A	186	ALA	4.0
1	B	48	ASN	3.6
1	B	39	VAL	3.5
1	A	117	GLN	3.5
1	A	190	GLN	3.1
1	B	549	LEU	3.1
1	A	187	THR	3.1
1	A	483	VAL	3.1
1	B	50	THR	3.0
1	B	277	LEU	3.0
1	A	122	ASN	2.9
1	A	175	THR	2.8
1	A	494	PRO	2.8
1	A	115	ILE	2.7
1	A	227	CYS	2.6
1	B	51	ALA	2.6
1	B	47	GLY	2.6
1	A	157	PHE	2.6
1	A	185	ARG	2.5
1	A	277	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	46	ASP	2.4
1	A	184	ASP	2.4
1	B	38	VAL	2.3
1	A	119	GLY	2.3
1	A	582	GLY	2.3
1	B	556	ARG	2.3
1	B	501	ASN	2.3
1	A	189	LYS	2.3
1	B	557	ARG	2.2
1	A	493	ALA	2.2
1	A	196	LEU	2.2
1	B	49	SER	2.2
1	A	487	HIS	2.1
1	A	497	THR	2.1
1	B	272	PHE	2.1
1	A	503	THR	2.1
1	A	486	MET	2.1
1	B	245	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

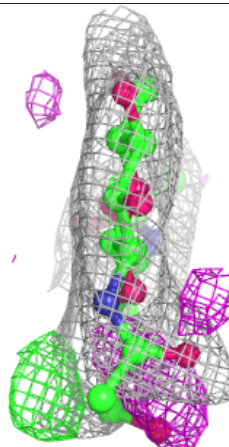
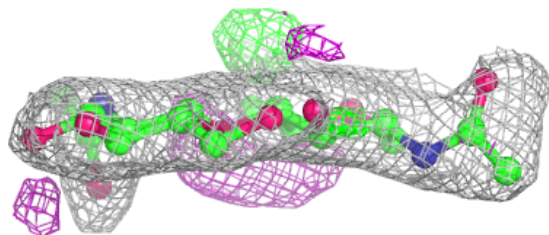
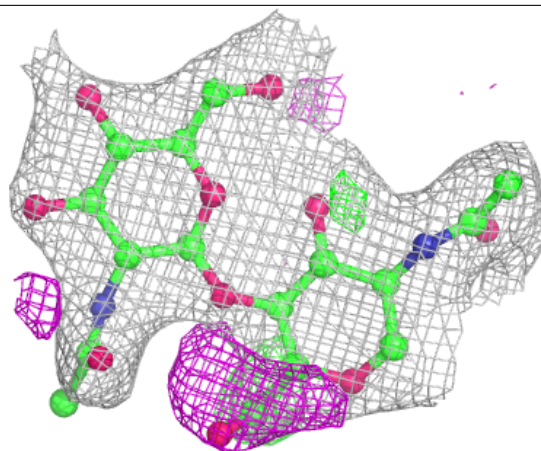
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

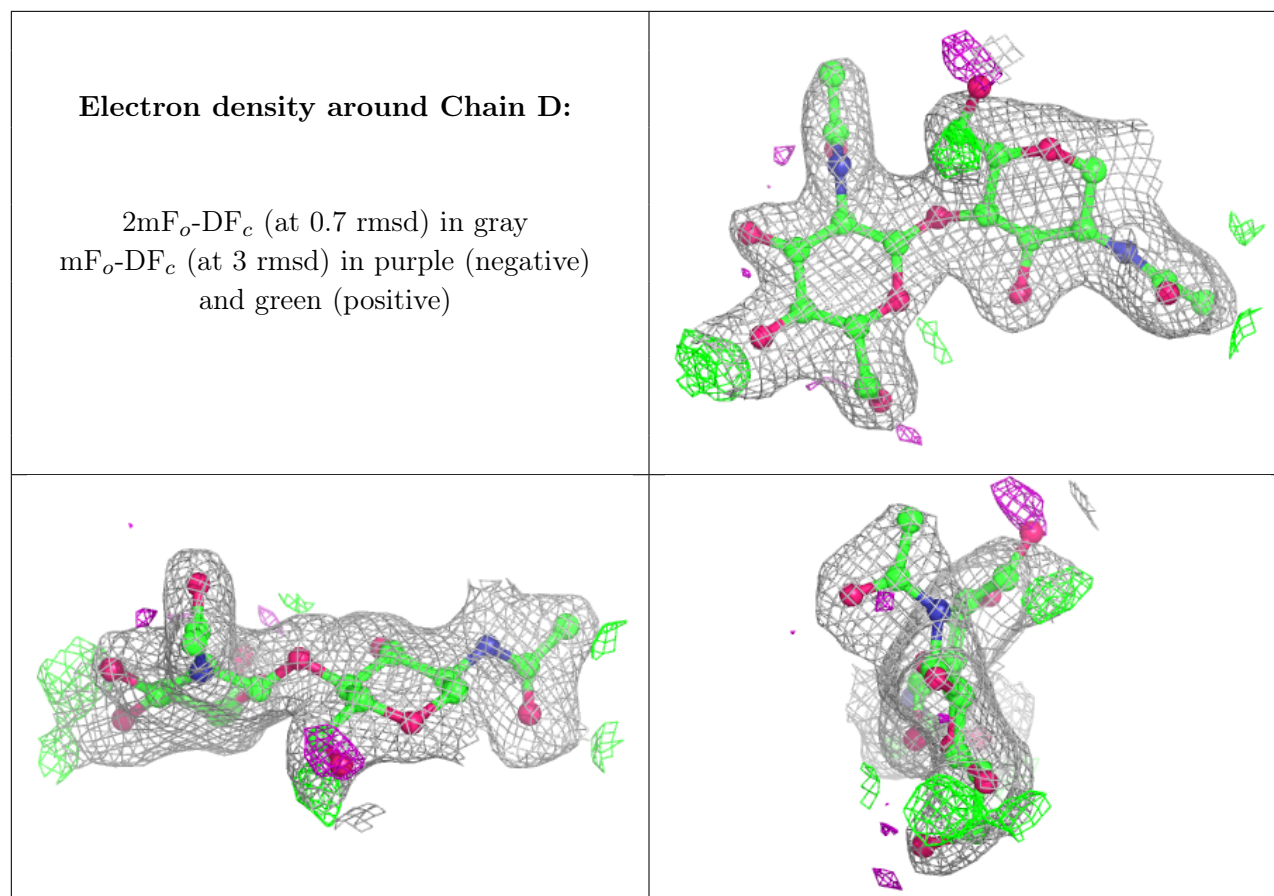
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	1	14/15	0.86	0.22	45,54,83,97	0
2	NAG	D	2	14/15	0.86	0.36	52,59,65,68	0
2	NAG	D	1	14/15	0.91	0.14	38,44,58,76	0
2	NAG	C	2	14/15	0.91	0.27	57,66,76,76	0

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 C:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
4	NAG	B	1011	14/15	0.78	0.28	72,78,81,83	0
4	NAG	A	1021	14/15	0.80	0.16	61,65,69,72	0
4	NAG	A	1011	14/15	0.86	0.24	63,67,72,72	0
4	NAG	B	1021	14/15	0.91	0.25	54,73,82,84	0
3	MN	A	606	1/1	0.99	0.10	33,33,33,33	0
3	MN	B	606	1/1	1.00	0.08	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.