



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:52 AM EDT

PDB ID : 2GMP / pdb_00002gmp
Title : Metal-free (apo) P. angolensis seed lectin in complex with GlcNAC-beta(1-2)Man
Authors : Garcia-Pino, A.; Buts, L.; Wyns, L.; Loris, R.
Deposited on : 2006-04-07
Resolution : 2.50 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

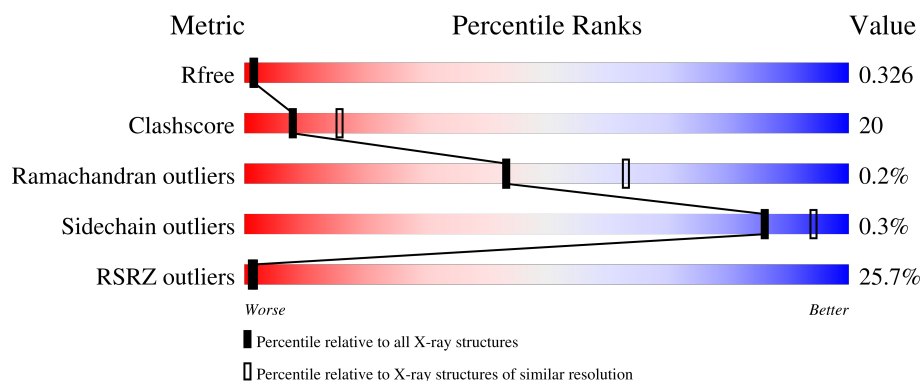
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	252	
1	B	252	
2	C	2	
2	D	2	

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	D	2	-	-	X	-

2 Entry composition [i](#)

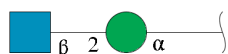
There are 4 unique types of molecules in this entry. The entry contains 3700 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 lectin.

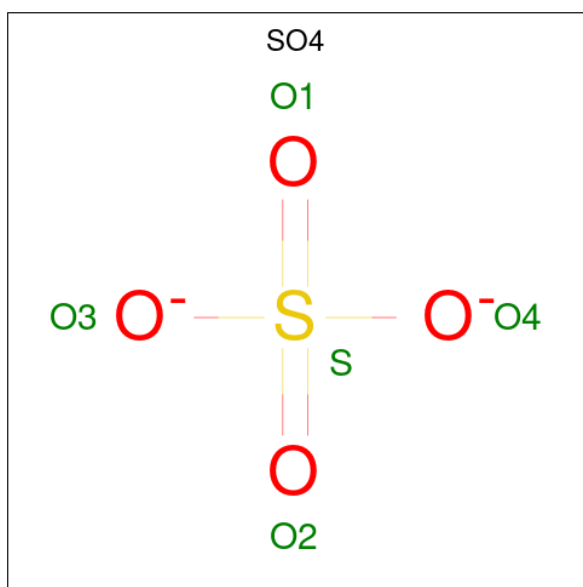
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	0	0	0
			1726	1099	289	338			
1	B	233	Total	C	N	O	0	0	1
			1744	1111	293	340			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	D	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

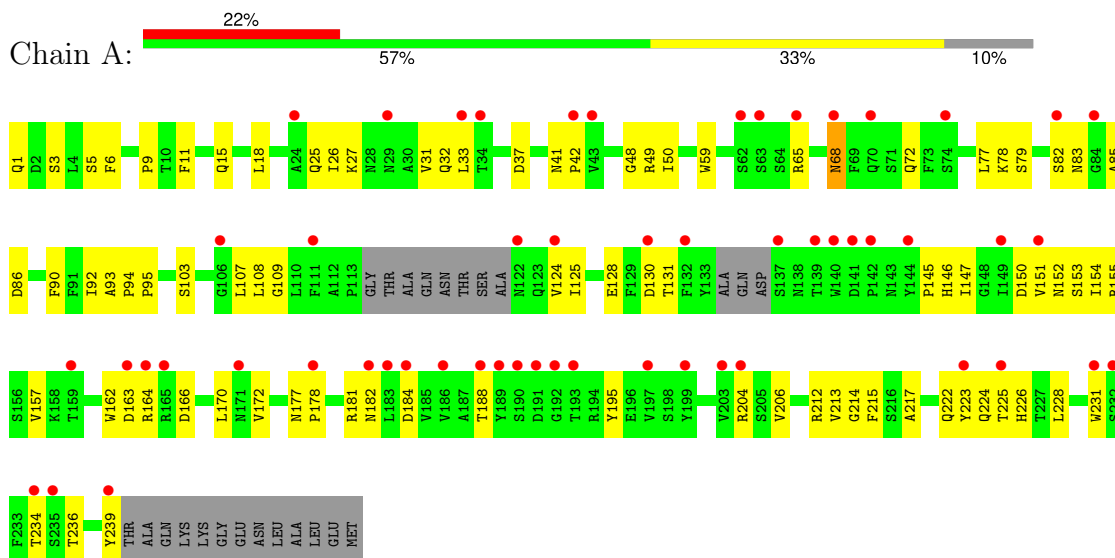
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total	O	0	0
			90	90		
4	B	83	Total	O	0	0
			83	83		

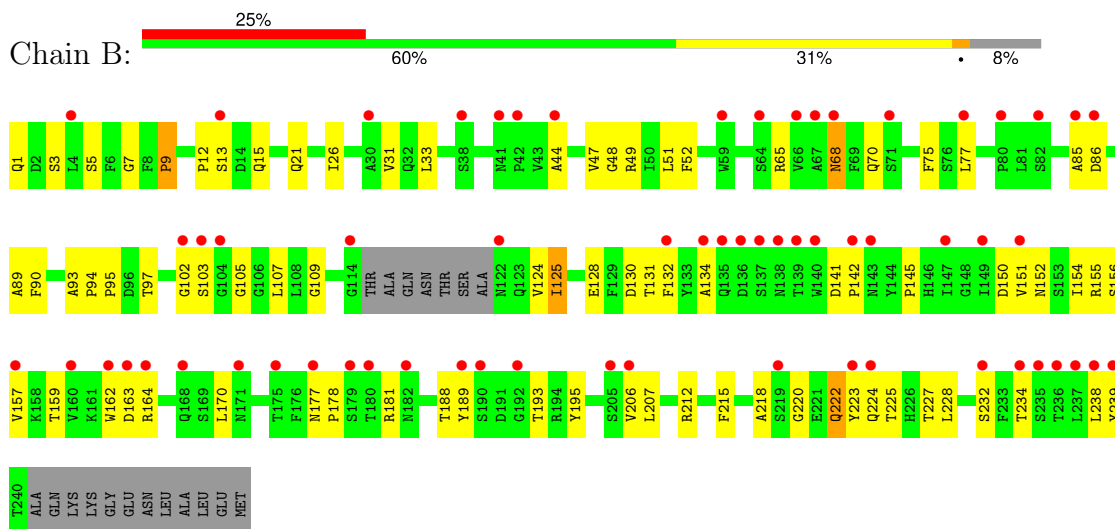
3 Residue-property plots

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: lectin



- Molecule 1: lectin



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



MAN1
MAG2

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

Chain D:

100%

MAN1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.11Å 61.00Å 128.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 99.3 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.49Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.255 0.296 , 0.326	Depositor DCC
R_{free} test set	1297 reflections (7.87%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for k,h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3700	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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: NAG, PCA, MAN, SO4

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	0.43	0/1760	0.98	6/2399 (0.3%)
1	B	0.43	0/1780	0.99	6/2428 (0.2%)
All	All	0.43	0/3540	0.98	12/4827 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ASN	N-CA-C	-6.82	97.41	108.52
1	B	68	ASN	N-CA-C	-6.00	98.94	108.73
1	B	9	PRO	N-CA-C	-5.82	105.95	113.57
1	B	125	ILE	N-CA-C	-5.81	100.12	108.48
1	B	152	ASN	CB-CA-C	-5.60	110.10	116.54
1	B	90	PHE	N-CA-C	-5.54	100.68	109.76
1	A	90	PHE	N-CA-C	-5.45	100.41	109.46
1	B	52	PHE	N-CA-C	-5.28	102.46	110.28
1	A	9	PRO	N-CA-C	-5.25	106.56	113.65
1	A	82	SER	N-CA-C	-5.13	106.79	113.16
1	A	146	HIS	N-CA-C	5.07	116.55	108.79
1	A	223	TYR	N-CA-C	5.04	116.65	109.14

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	1726	0	1625	60	0
1	B	1744	0	1628	67	0
2	C	26	0	23	7	0
2	D	26	0	25	9	0
3	A	5	0	0	0	0
4	A	90	0	0	4	0
4	B	83	0	0	0	0
All	All	3700	0	3301	132	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 20.

All (132) 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:102:GLY:O	2:D:2:NAG:H61	1.53	1.08
1:B:164:ARG:HE	1:B:224:GLN:HE22	1.08	0.95
1:A:164:ARG:HE	1:A:224:GLN:HE22	1.01	0.93
1:A:86:ASP:OD1	2:C:1:MAN:H61	1.70	0.91
1:A:164:ARG:HE	1:A:224:GLN:NE2	1.69	0.90
1:B:164:ARG:HE	1:B:224:GLN:NE2	1.72	0.88
2:C:1:MAN:C2	2:C:2:NAG:C1	2.55	0.84
1:B:21:GLN:HE22	1:B:49:ARG:HH21	1.28	0.81
1:B:164:ARG:HH11	1:B:224:GLN:HE21	1.29	0.80
1:B:145:PRO:HG2	1:B:162:TRP:O	1.84	0.78
1:B:102:GLY:O	2:D:2:NAG:C6	2.32	0.78
1:A:3:SER:HB2	1:A:236:THR:HG22	1.68	0.74
1:A:164:ARG:HH11	1:A:224:GLN:HE21	1.33	0.74
1:A:65:ARG:HG2	1:A:239:TYR:HA	1.69	0.73
2:D:1:MAN:O2	2:D:2:NAG:C2	2.36	0.72
1:A:5:SER:HB2	1:A:234:THR:HG22	1.73	0.70
1:A:145:PRO:HG2	1:A:162:TRP:O	1.91	0.70
1:A:3:SER:CB	1:A:236:THR:HG22	2.21	0.69
1:B:21:GLN:NE2	1:B:49:ARG:HE	1.92	0.67
1:B:95:PRO:HA	1:B:212:ARG:HG3	1.76	0.66
1:A:103:SER:OG	1:A:109:GLY:HA2	1.94	0.66
1:B:31:VAL:HB	1:B:228:LEU:HB3	1.79	0.65
1:B:85:ALA:HB1	1:B:86:ASP:HA	1.80	0.64
1:A:85:ALA:HB1	1:A:86:ASP:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MAN:O2	2:D:2:NAG:N2	2.31	0.63
1:A:93:ALA:HB1	1:A:94:PRO:HD2	1.80	0.62
2:C:1:MAN:O3	2:C:2:NAG:C1	2.49	0.61
1:A:147:ILE:HG13	1:A:162:TRP:HB2	1.84	0.60
1:B:124:VAL:HA	1:B:207:LEU:HD21	1.84	0.59
1:B:107:LEU:CD1	2:D:2:NAG:O6	2.51	0.58
1:B:156:SER:HB3	1:B:159:THR:CG2	2.33	0.58
1:B:77:LEU:HA	1:B:225:THR:O	2.04	0.57
1:B:33:LEU:O	1:B:48:GLY:HA3	2.03	0.57
1:A:78:LYS:HA	1:A:166:ASP:OD1	2.05	0.57
1:B:107:LEU:HD12	2:D:2:NAG:O6	2.04	0.57
1:B:154:ILE:CG2	1:B:157:VAL:HG12	2.34	0.57
1:A:131:THR:HA	1:A:145:PRO:HB3	1.87	0.57
1:B:47:VAL:HG22	1:B:218:ALA:CB	2.35	0.56
1:A:5:SER:CB	1:A:234:THR:HG22	2.34	0.56
1:B:105:GLY:HA3	2:D:1:MAN:O3	2.05	0.56
1:B:15:GLN:CG	1:B:26:ILE:HD11	2.36	0.55
4:A:256:HOH:O	1:B:9:PRO:HG2	2.07	0.55
1:B:154:ILE:HG21	1:B:157:VAL:HG12	1.87	0.55
2:C:1:MAN:O2	2:C:2:NAG:C2	2.53	0.54
1:A:151:VAL:CG1	1:A:206:VAL:HG11	2.38	0.54
1:A:92:ILE:HG12	1:A:213:VAL:HG12	1.90	0.53
1:A:164:ARG:NE	1:A:224:GLN:NE2	2.49	0.53
1:B:15:GLN:HG2	1:B:26:ILE:CD1	2.39	0.53
1:A:5:SER:OG	1:B:5:SER:HB2	2.09	0.52
1:B:15:GLN:HG3	1:B:26:ILE:HD11	1.91	0.52
1:A:124:VAL:HG22	1:A:125:ILE:N	2.25	0.52
1:B:13:SER:HA	1:B:26:ILE:HG21	1.92	0.52
1:B:177:ASN:O	1:B:181:ARG:N	2.42	0.51
1:B:21:GLN:HE22	1:B:49:ARG:NH2	2.02	0.51
1:B:47:VAL:HG22	1:B:218:ALA:HB1	1.92	0.51
1:B:7:GLY:HA2	1:B:232:SER:HA	1.93	0.51
1:B:164:ARG:NE	1:B:224:GLN:NE2	2.51	0.50
1:A:37:ASP:OD2	1:A:41:ASN:HB2	2.12	0.50
1:A:65:ARG:HD3	1:A:239:TYR:CE2	2.47	0.50
1:A:33:LEU:O	1:A:48:GLY:HA3	2.12	0.50
1:B:151:VAL:CG1	1:B:206:VAL:HG11	2.41	0.50
1:B:75:PHE:HA	1:B:227:THR:O	2.11	0.50
1:A:27:LYS:HB2	1:A:32:GLN:HG2	1.94	0.50
1:A:11:PHE:HB3	1:A:26:ILE:HD12	1.93	0.49
1:B:128:GLU:OE2	1:B:150:ASP:OD1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HB	1:A:228:LEU:HB3	1.93	0.49
1:B:75:PHE:CZ	1:B:170:LEU:HD23	2.47	0.49
1:B:103:SER:OG	1:B:109:GLY:HA2	2.13	0.49
1:B:130:ASP:HB3	1:B:132:PHE:CE1	2.47	0.49
1:B:21:GLN:HE21	1:B:49:ARG:HE	1.58	0.48
1:B:162:TRP:HA	1:B:195:TYR:CE2	2.49	0.48
1:B:131:THR:HA	1:B:145:PRO:HB3	1.95	0.48
1:A:6:PHE:HA	1:B:3:SER:O	2.15	0.47
1:B:85:ALA:O	1:B:224:GLN:HG2	2.14	0.47
1:A:59:TRP:CD2	1:A:204:ARG:HG2	2.49	0.47
1:A:79:SER:HB2	1:A:224:GLN:HB3	1.96	0.47
1:B:93:ALA:HB1	1:B:94:PRO:CD	2.44	0.46
1:A:107:LEU:CD1	2:C:2:NAG:H61	2.45	0.46
1:A:150:ASP:OD2	1:A:155:ARG:HA	2.15	0.46
1:A:50:ILE:O	1:A:214:GLY:HA3	2.15	0.46
1:B:164:ARG:HH11	1:B:224:GLN:NE2	2.04	0.46
1:A:152:ASN:OD1	1:A:206:VAL:HB	2.16	0.46
1:A:170:LEU:HD12	1:A:188:THR:O	2.16	0.46
1:B:222:GLN:OE1	1:B:222:GLN:N	2.49	0.46
1:A:182:ASN:ND2	1:A:184:ASP:OD1	2.49	0.46
1:A:164:ARG:HH11	1:A:224:GLN:NE2	2.07	0.45
2:D:1:MAN:C2	2:D:2:NAG:C1	2.87	0.45
1:A:164:ARG:NH1	1:A:224:GLN:HE21	2.09	0.45
1:B:65:ARG:HG2	1:B:239:TYR:HA	1.98	0.45
1:B:188:THR:HA	1:B:193:THR:O	2.17	0.45
1:B:128:GLU:CD	1:B:155:ARG:HH21	2.25	0.45
1:B:164:ARG:NH1	1:B:224:GLN:HE21	2.05	0.45
1:B:223:TYR:CD1	1:B:223:TYR:N	2.85	0.45
1:B:51:LEU:HD11	1:B:97:THR:HG23	1.99	0.45
1:B:85:ALA:CB	1:B:86:ASP:HA	2.42	0.45
2:C:1:MAN:O2	2:C:2:NAG:N2	2.50	0.45
1:A:152:ASN:HB3	1:A:153:SER:H	1.58	0.44
1:A:3:SER:HB3	1:A:236:THR:HG22	1.97	0.44
1:A:164:ARG:HH22	1:A:166:ASP:HB2	1.82	0.44
1:A:215:PHE:HE1	1:A:231:TRP:CD2	2.36	0.44
1:B:70:GLN:HB2	1:B:234:THR:HG22	2.00	0.44
1:A:68:ASN:HA	1:A:178:PRO:HD3	2.00	0.44
1:A:154:ILE:CG2	1:A:157:VAL:HG12	2.48	0.43
1:A:95:PRO:HB3	1:A:212:ARG:NH1	2.33	0.43
1:A:94:PRO:HA	1:A:95:PRO:HD3	1.88	0.43
1:A:15:GLN:HG3	1:A:18:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:O	1:A:166:ASP:HA	2.18	0.43
1:B:238:LEU:O	1:B:238:LEU:HD12	2.18	0.43
1:A:177:ASN:O	1:A:181:ARG:N	2.52	0.42
1:B:107:LEU:HD12	2:D:2:NAG:C6	2.49	0.42
1:A:217:ALA:HB1	1:A:226:HIS:CD2	2.55	0.42
1:A:49:ARG:HA	1:A:215:PHE:O	2.19	0.42
1:A:79:SER:HB2	1:A:224:GLN:CB	2.49	0.42
1:A:163:ASP:HB2	1:A:195:TYR:OH	2.20	0.42
1:A:25:GLN:HG2	4:A:293:HOH:O	2.19	0.42
4:A:262:HOH:O	1:B:12:PRO:HG2	2.20	0.42
1:A:225:THR:HA	4:A:296:HOH:O	2.20	0.41
1:B:156:SER:HB3	1:B:159:THR:HG21	2.01	0.41
1:A:83:ASN:ND2	1:A:222:GLN:HG2	2.35	0.41
1:A:107:LEU:HD12	2:C:2:NAG:H61	2.01	0.41
1:B:44:ALA:HB1	1:B:220:GLY:O	2.21	0.41
1:A:72:GLN:HA	1:A:172:VAL:O	2.20	0.41
1:B:124:VAL:CG2	1:B:125:ILE:N	2.84	0.41
1:A:128:GLU:OE1	1:A:130:ASP:OD2	2.38	0.41
1:B:163:ASP:O	1:B:189:TYR:OH	2.38	0.41
1:B:68:ASN:HA	1:B:178:PRO:HD3	2.03	0.41
1:B:89:ALA:O	1:B:215:PHE:HA	2.21	0.41
1:B:124:VAL:HG22	1:B:125:ILE:N	2.36	0.41
1:B:141:ASP:HA	1:B:142:PRO:HD2	1.91	0.41
1:B:134:ALA:O	1:B:142:PRO:HB3	2.21	0.41
1:B:47:VAL:HG22	1:B:218:ALA:HB2	2.03	0.40
1:A:42:PRO:HD3	1:A:225:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/252 (88%)	211 (95%)	10 (4%)	1 (0%)	24	43
1	B	229/252 (91%)	215 (94%)	14 (6%)	0	100	100
All	All	451/504 (90%)	426 (94%)	24 (5%)	1 (0%)	43	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	LEU

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	184/215 (86%)	184 (100%)	0	100	100
1	B	182/215 (85%)	181 (100%)	1 (0%)	81	92
All	All	366/430 (85%)	365 (100%)	1 (0%)	86	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	222	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	70	GLN
1	A	222	GLN
1	A	224	GLN
1	B	21	GLN
1	B	25	GLN
1	B	41	ASN
1	B	55	GLN
1	B	182	ASN

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Mol	Chain	Res	Type
1	B	224	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	B	1	1	7,8,9	2.79	2 (28%)	9,10,12	1.84	2 (22%)
1	PCA	A	1	1	7,8,9	2.82	3 (42%)	9,10,12	2.00	3 (33%)

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
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	PCA	CD-N	6.50	1.50	1.34
1	A	1	PCA	CD-N	6.41	1.50	1.34
1	A	1	PCA	CA-N	3.08	1.50	1.46
1	B	1	PCA	CA-N	2.96	1.49	1.46
1	A	1	PCA	CB-CG	-2.01	1.48	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	OE-CD-CG	-3.40	120.65	126.72
1	B	1	PCA	OE-CD-CG	-3.13	121.13	126.72
1	A	1	PCA	OE-CD-N	2.87	131.18	124.96
1	B	1	PCA	OE-CD-N	2.61	130.59	124.96
1	A	1	PCA	CB-CA-C	-2.23	109.59	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	MAN	C	1	2	12,12,12	1.93	2 (16%)	17,17,17	1.96	2 (11%)
2	NAG	C	2	2	14,14,15	0.77	1 (7%)	17,19,21	0.86	1 (5%)
2	MAN	D	1	2	12,12,12	0.44	0	17,17,17	1.99	2 (11%)
2	NAG	D	2	2	14,14,15	0.75	1 (7%)	17,19,21	0.85	1 (5%)

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	MAN	C	1	2	-	2/2/22/22	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	MAN	D	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	MAN	O6-C6	-6.19	1.16	1.42
2	C	2	NAG	C1-C2	2.39	1.55	1.52
2	D	2	NAG	C1-C2	2.31	1.55	1.52
2	C	1	MAN	C6-C5	-2.03	1.45	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	MAN	O2-C2-C1	7.51	126.59	109.25
2	C	1	MAN	C6-C5-C4	7.32	130.98	113.02
2	C	2	NAG	C1-O5-C5	2.42	115.44	112.19
2	D	2	NAG	C1-O5-C5	2.37	115.37	112.19
2	D	1	MAN	C3-C4-C5	2.08	114.00	110.23
2	C	1	MAN	C3-C4-C5	2.07	113.99	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

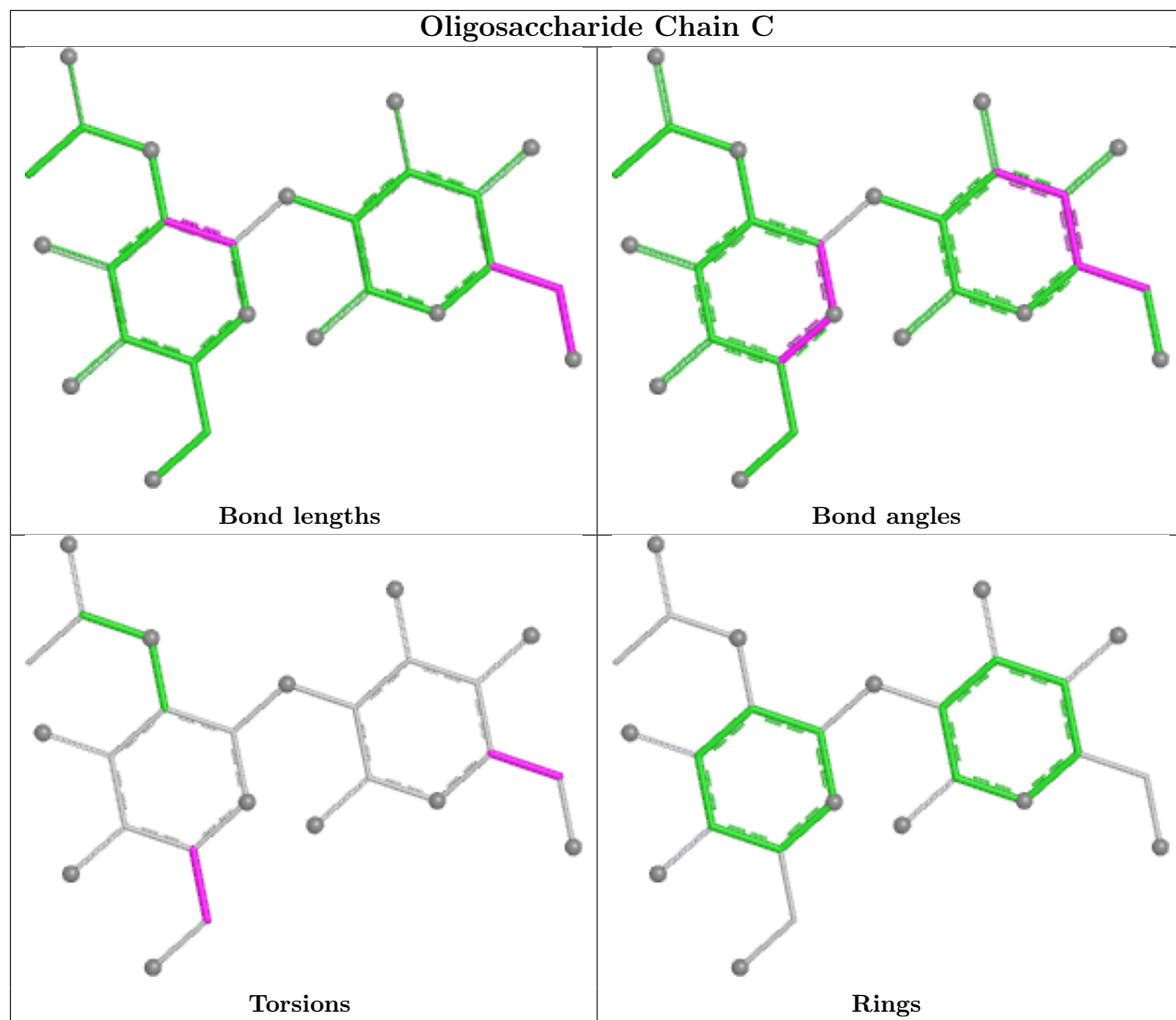
Mol	Chain	Res	Type	Atoms
2	C	1	MAN	O5-C5-C6-O6
2	C	1	MAN	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

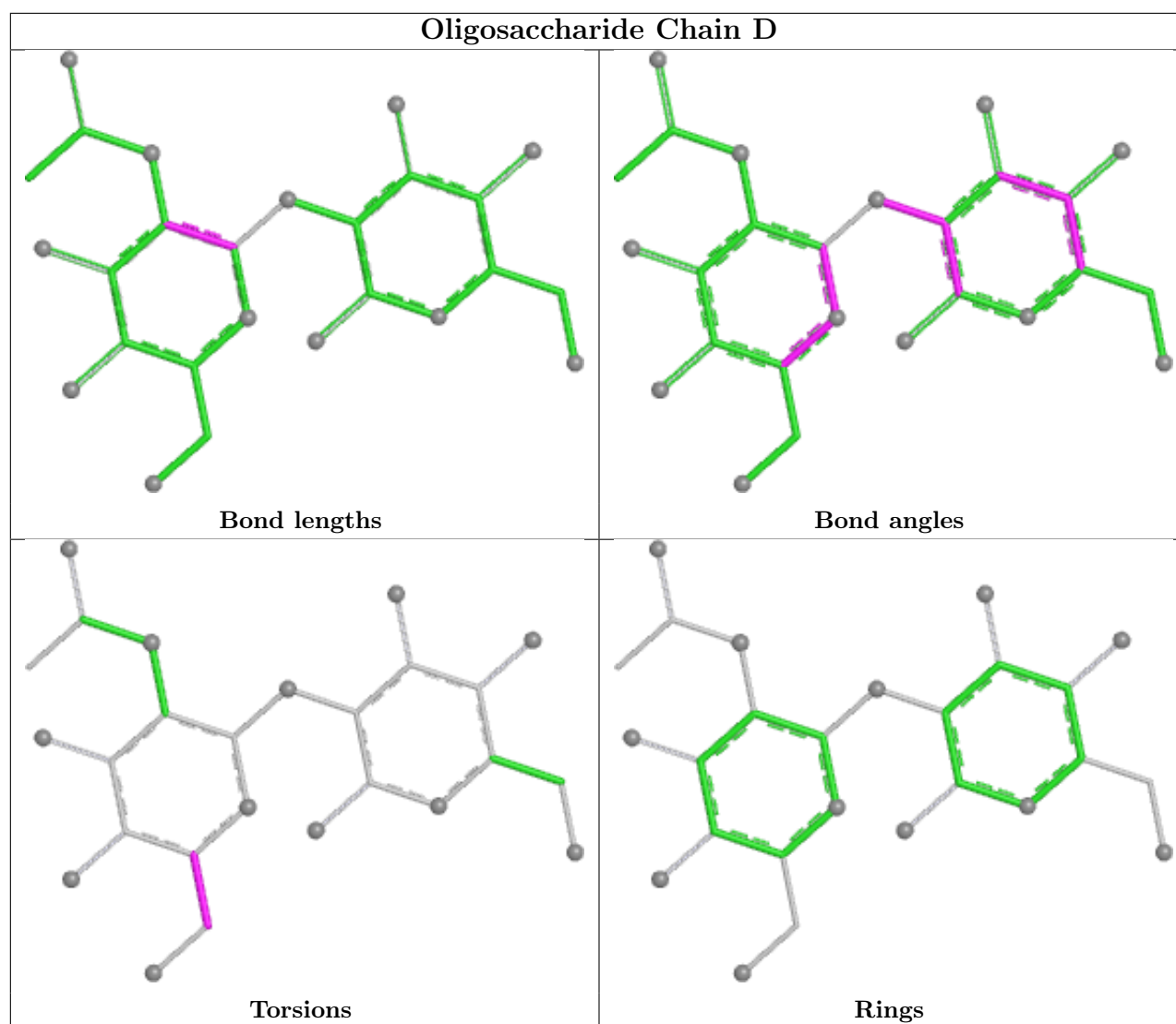
There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	MAN	5	0
2	C	2	NAG	6	0
2	D	2	NAG	8	0
2	D	1	MAN	4	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](#)

1 ligand is 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	SO4	A	255	-	4,4,4	0.41	0	6,6,6	0.08	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.

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	227/252 (90%)	1.49	55 (24%) 2 1	11, 26, 41, 69	8 (3%)
1	B	232/252 (92%)	1.50	63 (27%) 1 1	9, 26, 50, 72	5 (2%)
All	All	459/504 (91%)	1.50	118 (25%) 1 1	9, 26, 46, 72	13 (2%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	THR	5.3
1	B	135	GLN	5.0
1	A	140	TRP	4.5
1	B	140	TRP	4.3
1	A	235	SER	4.2
1	A	184	ASP	4.2
1	B	138	ASN	4.2
1	B	160	VAL	4.0
1	B	134	ALA	3.9
1	A	182	ASN	3.9
1	A	234	THR	3.8
1	B	85	ALA	3.6
1	A	192	GLY	3.5
1	A	144	TYR	3.4
1	A	122	ASN	3.4
1	A	142	PRO	3.3
1	A	239	TYR	3.2
1	B	114	GLY	3.2
1	B	219	SER	3.2
1	A	63	SER	3.1
1	B	139	THR	3.0
1	A	82	SER	3.0
1	B	224	GLN	3.0
1	B	177	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	141	ASP	2.9
1	B	189	TYR	2.9
1	A	190	SER	2.9
1	B	102	GLY	2.9
1	B	38	SER	2.8
1	B	71	SER	2.8
1	A	223	TYR	2.8
1	B	232	SER	2.8
1	A	130	ASP	2.8
1	A	165	ARG	2.8
1	B	179	SER	2.8
1	A	225	THR	2.8
1	B	142	PRO	2.7
1	B	190	SER	2.7
1	B	67	ALA	2.7
1	B	44	ALA	2.7
1	A	62	SER	2.7
1	B	163	ASP	2.6
1	A	186	VAL	2.6
1	A	159	THR	2.6
1	B	234	THR	2.6
1	A	231	TRP	2.6
1	B	157	VAL	2.6
1	A	189	TYR	2.6
1	B	192	GLY	2.6
1	B	132	PHE	2.6
1	B	147	ILE	2.5
1	A	183	LEU	2.5
1	A	171	ASN	2.5
1	B	64	SER	2.5
1	B	137	SER	2.5
1	B	162	TRP	2.5
1	B	77	LEU	2.5
1	B	42	PRO	2.5
1	A	163	ASP	2.5
1	B	175	THR	2.5
1	A	197	VAL	2.5
1	A	24	ALA	2.5
1	A	178	PRO	2.4
1	A	132	PHE	2.4
1	A	84	GLY	2.4
1	A	193	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	86	ASP	2.4
1	B	168	GLN	2.4
1	B	237	LEU	2.4
1	A	203	VAL	2.4
1	B	122	ASN	2.4
1	B	236	THR	2.4
1	A	106	GLY	2.4
1	B	239	TYR	2.4
1	B	59	TRP	2.4
1	A	151	VAL	2.3
1	B	151	VAL	2.3
1	A	68	ASN	2.3
1	B	66	VAL	2.3
1	B	182	ASN	2.3
1	A	74	SER	2.3
1	A	232	SER	2.3
1	B	238	LEU	2.2
1	A	29	ASN	2.2
1	B	143	ASN	2.2
1	B	223	TYR	2.2
1	A	34	THR	2.2
1	B	136	ASP	2.2
1	A	204	ARG	2.2
1	A	111	PHE	2.2
1	A	124	VAL	2.2
1	B	80	PRO	2.2
1	B	206	VAL	2.2
1	B	30	ALA	2.2
1	B	180	THR	2.2
1	A	191	ASP	2.2
1	A	33	LEU	2.2
1	B	4	LEU	2.2
1	B	13	SER	2.2
1	B	82	SER	2.2
1	B	103	SER	2.2
1	B	68	ASN	2.1
1	B	149	ILE	2.1
1	B	104	GLY	2.1
1	B	235	SER	2.1
1	A	42	PRO	2.1
1	A	164	ARG	2.1
1	B	164	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	41	ASN	2.1
1	A	65	ARG	2.1
1	A	188	THR	2.1
1	B	205	SER	2.1
1	A	70	GLN	2.0
1	A	43	VAL	2.0
1	B	171	ASN	2.0
1	A	149	ILE	2.0
1	A	137	SER	2.0
1	A	199	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	A	1	8/9	0.72	0.19	19,20,22,24	0
1	PCA	B	1	8/9	0.72	0.16	17,18,19,20	0

6.3 Carbohydrates [i](#)

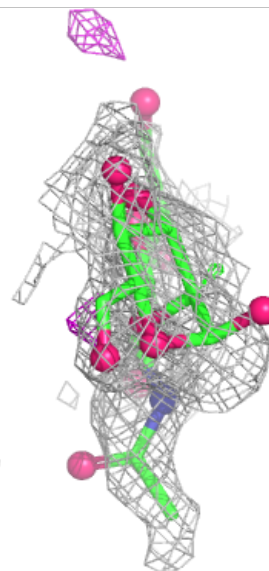
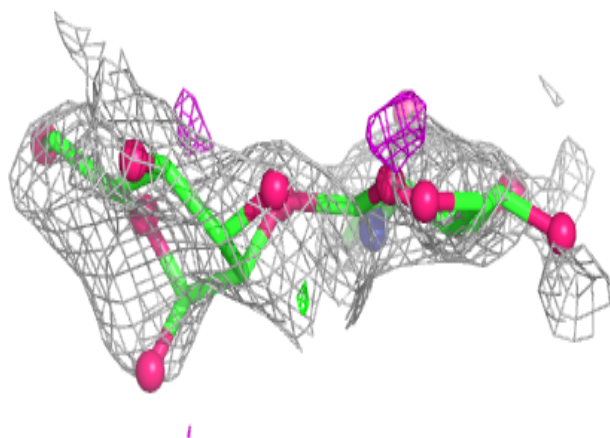
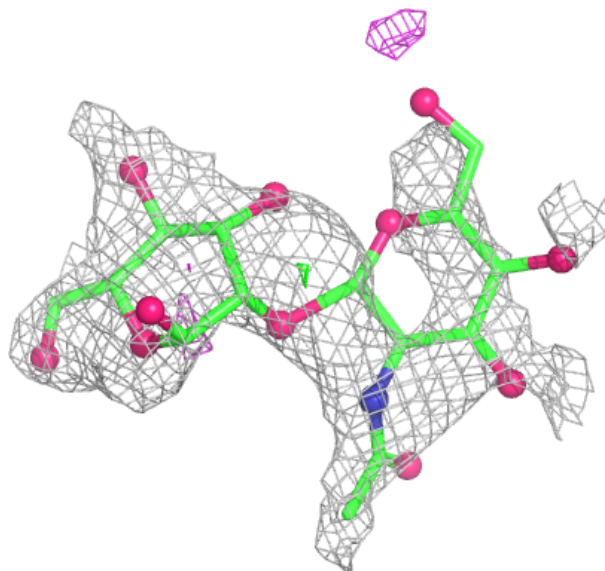
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

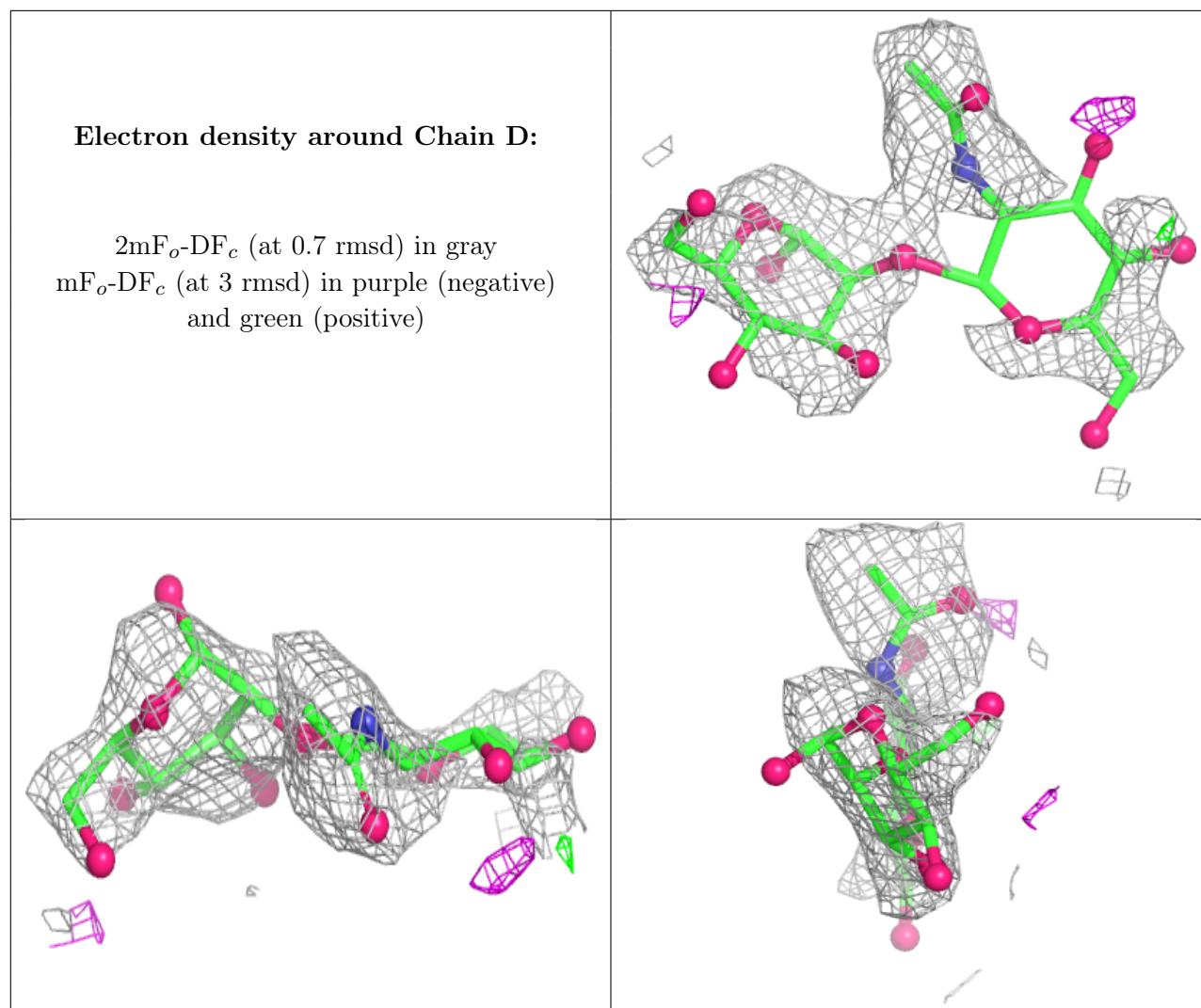
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.38	0.29	85,90,90,90	0
2	NAG	C	2	14/15	0.56	0.21	85,90,90,90	0
2	MAN	C	1	12/12	0.63	0.26	84,89,90,91	0
2	MAN	D	1	12/12	0.68	0.18	84,89,90,91	0

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($\text{\AA}^2$)	Q<0.9
3	SO4	A	255	5/5	0.74	0.18	97,98,98,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.