



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:58 PM UTC

PDB ID : 1KTW / pdb_00001ktw
Title : IOTA-CARRAGEENASE COMPLEXED TO IOTA-CARRAGEENAN FRAGMENTS
Authors : Michel, G.; Kahn, R.; Dideberg, O.
Deposited on : 2002-01-18
Resolution : 2.00 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

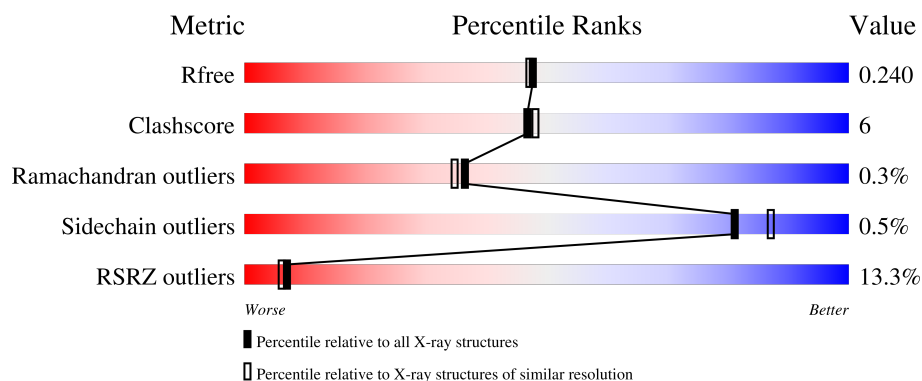
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	A	464	10% 83% 14% ..
1	B	464	17% 83% 14% ..
2	C	2	50% 50%
3	D	4	50% 25% 25%

2 Entry composition [i](#)

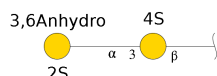
There are 7 unique types of molecules in this entry. The entry contains 7837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 IOTA-CARRAGEENASE.

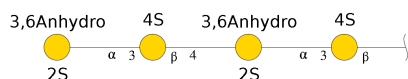
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	16	0	0
			3605	2259	639	692	15			
1	B	457	Total	C	N	O	S	37	0	0
			3605	2259	639	692	15			

- Molecule 2 is an oligosaccharide called 3,6-anhydro-2-O-sulfo- α -D-galactopyranose-(1-3)-4-O-sulfo- β -D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	S	0	0	0
			30	12	16	2			

- Molecule 3 is an oligosaccharide called 3,6-anhydro-2-O-sulfo- α -D-galactopyranose-(1-3)-4-O-sulfo- β -D-galactopyranose-(1-4)-3,6-anhydro-2-O-sulfo- α -D-galactopyranose-(1-3)-4-O-sulfo- β -D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	O	S	0	0	0
			59	24	31	4			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Ca 5 5	0	0
4	B	5	Total Ca 5 5	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0
5	B	2	Total Na 2 2	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0

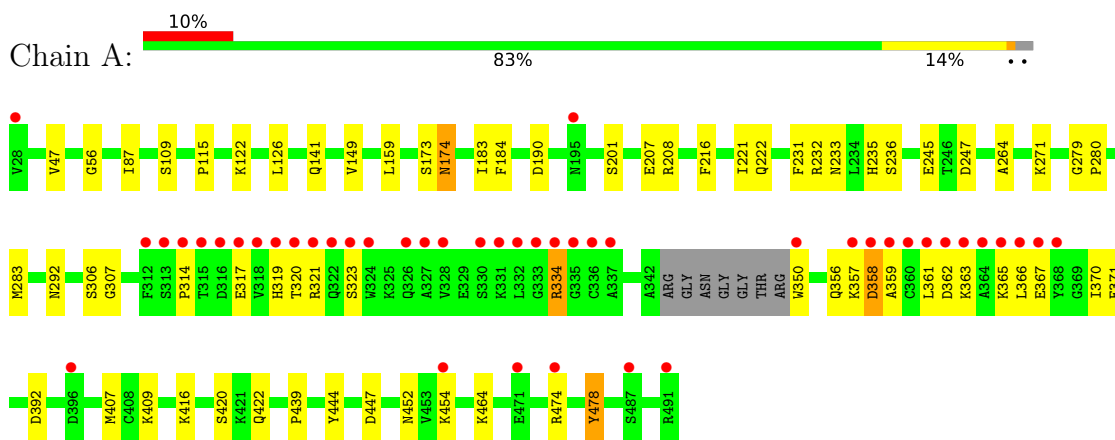
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	289	Total O 289 289	0	0
7	B	233	Total O 233 233	0	0

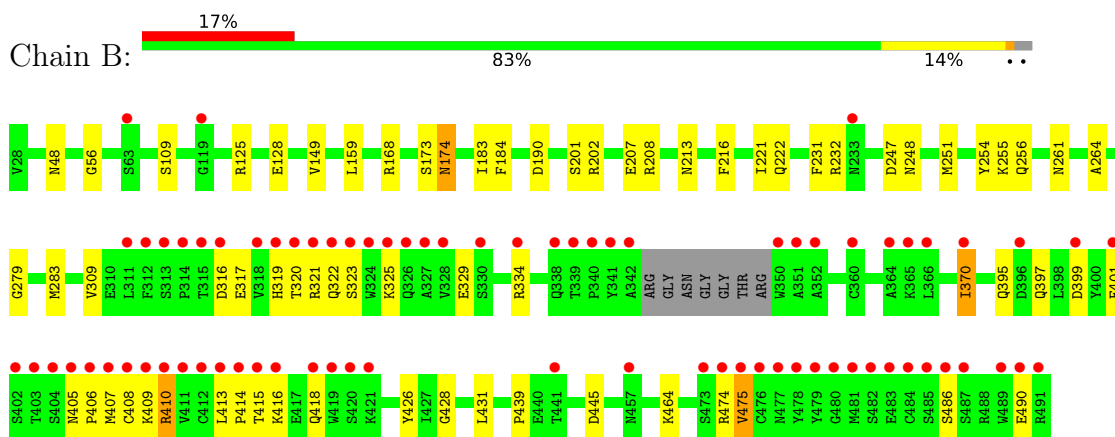
3 Residue-property plots [i](#)

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

- Molecule 1: IOTA-CARRAGEENASE



- Molecule 1: IOTA-CARRAGEENASE



- Molecule 2: 3,6-anhydro-2-O-sulfo-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose



- Molecule 3: 3,6-anhydro-2-O-sulfo-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose-(1-4)-3,6-anhydro-2-O-sulfo-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.73Å 122.31Å 91.94Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	23.17 – 2.00 23.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (23.17-2.00) 97.1 (23.17-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 1.99Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.238 0.206 , 0.240	Depositor DCC
R_{free} test set	3986 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7837	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: NA, CL, G4S, DGS, CA

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	0.69	0/3678	0.99	24/4970 (0.5%)
1	B	0.62	0/3678	0.99	20/4970 (0.4%)
All	All	0.66	0/7356	0.99	44/9940 (0.4%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	SER	N-CA-C	8.88	122.79	108.76
1	B	173	SER	N-CA-C	8.37	121.99	108.76
1	A	109	SER	N-CA-C	8.14	122.31	112.38
1	B	109	SER	N-CA-C	7.94	122.06	112.38
1	A	190	ASP	N-CA-C	7.33	120.51	109.95
1	A	307	GLY	N-CA-C	-7.19	102.89	112.82
1	B	190	ASP	N-CA-C	6.96	120.69	110.17
1	A	174	ASN	N-CA-C	6.43	124.49	110.80
1	B	207	GLU	N-CA-C	6.33	118.40	108.96
1	A	247	ASP	N-CA-C	6.33	120.64	112.41
1	A	216	PHE	N-CA-C	6.25	118.90	111.33
1	A	207	GLU	N-CA-C	6.14	118.11	108.96
1	A	149	VAL	N-CA-C	-6.13	98.91	107.80
1	B	464	LYS	N-CA-C	-6.09	104.57	112.68
1	B	174	ASN	N-CA-C	6.03	123.63	110.80
1	B	216	PHE	N-CA-C	5.85	118.41	111.33
1	B	221	ILE	CB-CA-C	-5.85	101.90	110.62
1	B	283	MET	N-CA-C	5.78	119.68	109.96
1	B	56	GLY	N-CA-C	5.71	123.70	114.90
1	B	428	GLY	CA-C-N	5.69	125.64	119.78
1	B	428	GLY	C-N-CA	5.69	125.64	119.78
1	B	401	PHE	N-CA-C	-5.66	106.42	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	PRO	N-CA-C	5.60	120.86	113.86
1	B	201	SER	N-CA-C	5.53	118.66	110.48
1	A	283	MET	N-CA-C	5.46	119.13	109.96
1	A	201	SER	N-CA-C	5.40	118.47	110.48
1	B	279	GLY	CA-C-N	5.39	125.00	119.56
1	B	279	GLY	C-N-CA	5.39	125.00	119.56
1	A	56	GLY	N-CA-C	5.33	123.12	114.90
1	A	392	ASP	N-CA-C	-5.27	100.71	109.46
1	A	464	LYS	N-CA-C	-5.27	104.54	111.96
1	B	213	ASN	N-CA-C	5.18	118.54	111.39
1	A	87	ILE	N-CA-C	-5.18	102.06	107.60
1	A	141	GLN	N-CA-C	5.16	117.83	109.06
1	B	159	LEU	N-CA-C	5.16	117.85	109.24
1	A	420	SER	N-CA-C	5.15	118.66	112.38
1	A	221	ILE	CB-CA-C	-5.14	102.99	110.81
1	A	447	ASP	N-CA-C	5.09	117.87	109.72
1	A	292	ASN	N-CA-C	5.08	116.85	110.91
1	A	159	LEU	N-CA-C	5.06	117.68	109.24
1	B	247	ASP	N-CA-C	5.05	120.06	112.94
1	A	478	TYR	N-CA-C	5.02	119.65	111.37
1	B	149	VAL	N-CA-C	-5.02	100.53	107.80
1	A	47	VAL	N-CA-C	5.01	115.92	108.65

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	3605	0	3500	40	0
1	B	3605	0	3500	40	0
2	C	30	0	18	1	0
3	D	59	0	32	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	1	0
7	A	289	0	0	1	0
7	B	233	0	0	2	0
All	All	7837	0	7050	81	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 6.

All (81) 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:405:ASN:HD21	1:B:409:LYS:H	1.01	0.95
1:B:320:THR:HG22	1:B:321:ARG:N	1.97	0.80
1:B:405:ASN:ND2	1:B:409:LYS:H	1.83	0.73
1:B:320:THR:CG2	1:B:321:ARG:H	2.03	0.71
1:A:334:ARG:H	1:A:334:ARG:CD	2.03	0.71
1:A:320:THR:H	1:A:323:SER:HB3	1.56	0.70
1:B:405:ASN:HD21	1:B:409:LYS:N	1.82	0.69
1:B:320:THR:CG2	1:B:321:ARG:N	2.56	0.68
1:A:407:MET:HE3	1:A:409:LYS:HE3	1.74	0.68
1:B:415:THR:OG1	1:B:418:GLN:HG3	1.94	0.68
1:A:334:ARG:H	1:A:334:ARG:HD3	1.58	0.67
1:B:261:ASN:HB3	7:B:738:HOH:O	1.94	0.67
1:B:320:THR:HG22	1:B:321:ARG:H	1.59	0.67
1:A:334:ARG:HD3	1:A:334:ARG:N	2.12	0.65
1:A:416:LYS:CE	1:A:416:LYS:H	2.09	0.65
1:B:416:LYS:HD3	1:B:416:LYS:H	1.63	0.64
1:B:254:TYR:O	1:B:256:GLN:HG3	1.99	0.63
1:B:248:ASN:HB3	1:B:251:MET:HE2	1.80	0.62
1:B:125:ARG:HD3	1:B:128:GLU:OE2	1.99	0.61
1:B:320:THR:H	1:B:323:SER:HB3	1.65	0.60
1:A:115:PRO:HB3	1:A:126:LEU:HD21	1.84	0.60
1:A:407:MET:HE3	1:A:409:LYS:CE	2.32	0.59
1:B:399:ASP:OD1	1:B:474:ARG:HA	2.02	0.59
1:B:416:LYS:H	1:B:416:LYS:CD	2.16	0.58
1:B:416:LYS:HD3	1:B:416:LYS:N	2.20	0.57
1:A:365:LYS:CD	1:A:371:GLU:HG2	2.36	0.56
1:B:409:LYS:O	1:B:410:ARG:HB2	2.06	0.55
3:D:2:DGS:O8	3:D:2:DGS:H3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PRO:HG2	1:A:317:GLU:HB3	1.87	0.55
1:A:321:ARG:NH1	1:A:350:TRP:HZ3	2.05	0.55
1:A:365:LYS:HE2	1:A:371:GLU:HG2	1.89	0.54
1:B:183:ILE:O	1:B:184:PHE:HB2	2.07	0.53
1:A:365:LYS:CE	1:A:371:GLU:HG2	2.38	0.53
1:B:413:LEU:HD12	1:B:414:PRO:HD2	1.90	0.52
1:A:416:LYS:HD3	1:A:422:GLN:NE2	2.25	0.51
1:A:317:GLU:CD	1:A:319:HIS:HE2	2.19	0.51
1:A:416:LYS:H	1:A:416:LYS:CD	2.22	0.51
1:A:334:ARG:CD	1:A:334:ARG:N	2.72	0.50
1:B:168:ARG:NE	1:B:202:ARG:HD3	2.26	0.50
1:A:416:LYS:H	1:A:416:LYS:HE2	1.75	0.50
1:B:329:GLU:OE1	1:B:334:ARG:HA	2.12	0.49
1:A:231:PHE:O	1:A:264:ALA:HA	2.13	0.49
1:B:395:GLN:NE2	1:B:426:TYR:OH	2.37	0.49
1:A:271:LYS:HE2	7:A:818:HOH:O	2.12	0.48
1:A:365:LYS:HD3	1:A:371:GLU:HG2	1.96	0.48
1:A:361:LEU:O	1:A:365:LYS:HG3	2.13	0.48
1:B:486:SER:HB3	1:B:490:GLU:OE2	2.13	0.48
1:A:416:LYS:HD3	1:A:416:LYS:N	2.29	0.48
1:A:365:LYS:NZ	1:A:444:TYR:HE2	2.13	0.47
1:A:362:ASP:O	1:A:366:LEU:HG	2.14	0.47
1:A:416:LYS:CD	1:A:416:LYS:N	2.78	0.46
1:B:317:GLU:HB3	1:B:319:HIS:CD2	2.50	0.46
1:B:168:ARG:CZ	1:B:202:ARG:HD3	2.45	0.46
1:B:309:VAL:HG13	1:B:370:ILE:HG21	1.98	0.46
1:A:356:GLN:O	1:A:356:GLN:HG3	2.15	0.45
1:B:174:ASN:HA	1:B:208:ARG:O	2.15	0.45
1:A:174:ASN:HA	1:A:208:ARG:O	2.16	0.45
1:A:306:SER:HB2	1:A:439:PRO:HD3	1.98	0.45
1:B:407:MET:O	1:B:408:CYS:C	2.59	0.45
1:B:320:THR:HG22	1:B:322:GLN:H	1.82	0.45
1:A:122:LYS:HA	2:C:2:DGS:O7	2.17	0.45
1:B:325:LYS:HE2	1:B:329:GLU:OE2	2.17	0.44
1:A:365:LYS:HG2	1:A:370:ILE:O	2.17	0.44
1:A:232:ARG:HG2	1:A:233:ASN:ND2	2.33	0.44
1:B:222:GLN:NE2	6:B:531:CL:CL	2.88	0.43
1:B:231:PHE:O	1:B:264:ALA:HA	2.19	0.43
1:A:183:ILE:O	1:A:184:PHE:HB2	2.17	0.43
1:B:397:GLN:HB3	1:B:431:LEU:CD1	2.49	0.43
1:A:222:GLN:NE2	6:A:530:CL:CL	2.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LYS:O	1:A:358:ASP:C	2.62	0.42
1:B:406:PRO:O	1:B:475:VAL:HB	2.18	0.42
1:A:474:ARG:HH21	1:A:478:TYR:H	1.66	0.42
1:A:359:ALA:O	1:A:363:LYS:HG3	2.20	0.42
1:A:245:GLU:HA	1:A:279:GLY:O	2.20	0.42
1:B:232:ARG:HD2	7:B:615:HOH:O	2.19	0.42
1:A:235:HIS:HD2	1:A:236:SER:N	2.18	0.42
1:B:255:LYS:C	1:B:256:GLN:HG3	2.45	0.42
1:A:452:ASN:OD1	1:A:454:LYS:HE2	2.20	0.41
1:B:316:ASP:OD1	1:B:316:ASP:C	2.63	0.41
1:B:439:PRO:O	1:B:445:ASP:HB2	2.20	0.40
1:B:409:LYS:O	1:B:410:ARG:CB	2.69	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	453/464 (98%)	429 (95%)	23 (5%)	1 (0%)	43	42
1	B	453/464 (98%)	418 (92%)	33 (7%)	2 (0%)	30	27
All	All	906/928 (98%)	847 (94%)	56 (6%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	ASP
1	B	410	ARG
1	B	475	VAL

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	395/399 (99%)	393 (100%)	2 (0%)	81	87
1	B	395/399 (99%)	393 (100%)	2 (0%)	81	87
All	All	790/798 (99%)	786 (100%)	4 (0%)	81	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	ARG
1	A	367	GLU
1	B	48	ASN
1	B	370	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	93	HIS
1	A	123	ASN
1	A	195	ASN
1	A	203	ASN
1	A	222	GLN
1	A	228	ASN
1	A	233	ASN
1	A	235	HIS
1	A	266	ASN
1	A	422	GLN
1	B	45	GLN
1	B	60	ASN
1	B	123	ASN
1	B	203	ASN
1	B	222	GLN
1	B	228	ASN
1	B	235	HIS

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Mol	Chain	Res	Type
1	B	292	ASN
1	B	395	GLN
1	B	405	ASN

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	G4S	C	1	2	16,16,16	0.54	0	21,24,24	0.58	0
2	DGS	C	2	2	15,15,16	1.03	1 (6%)	16,23,25	1.90	4 (25%)
3	G4S	D	1	3	16,16,16	0.46	0	21,24,24	0.64	0
3	DGS	D	2	3	15,15,16	0.89	0	16,23,25	2.07	2 (12%)
3	G4S	D	3	3	15,15,16	0.73	0	19,22,24	0.70	0
3	DGS	D	4	3	15,15,16	0.88	0	16,23,25	2.80	4 (25%)

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	G4S	C	1	2	-	1/7/27/27	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGS	C	2	2	-	2/5/27/30	0/3/2/2
3	G4S	D	1	3	-	1/7/27/27	0/1/1/1
3	DGS	D	2	3	-	2/5/27/30	0/3/2/2
3	G4S	D	3	3	-	1/7/24/27	0/1/1/1
3	DGS	D	4	3	-	2/5/27/30	0/3/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	DGS	C1-C2	2.53	1.55	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	DGS	O2-C2-C3	9.63	117.31	106.65
3	D	2	DGS	O2-C2-C3	6.48	113.82	106.65
2	C	2	DGS	O2-C2-C3	4.74	111.89	106.65
2	C	2	DGS	C1-O5-C5	3.18	116.44	112.19
3	D	2	DGS	O5-C5-C6	-2.82	109.20	113.33
2	C	2	DGS	C2-C3-C4	-2.67	107.35	113.84
3	D	4	DGS	O5-C5-C6	-2.50	109.68	113.33
3	D	4	DGS	O9-S-O8	-2.45	102.79	112.24
3	D	4	DGS	C1-O5-C5	2.39	115.39	112.19
2	C	2	DGS	O5-C5-C6	-2.28	109.99	113.33

There are no chirality outliers.

All (9) torsion outliers are listed below:

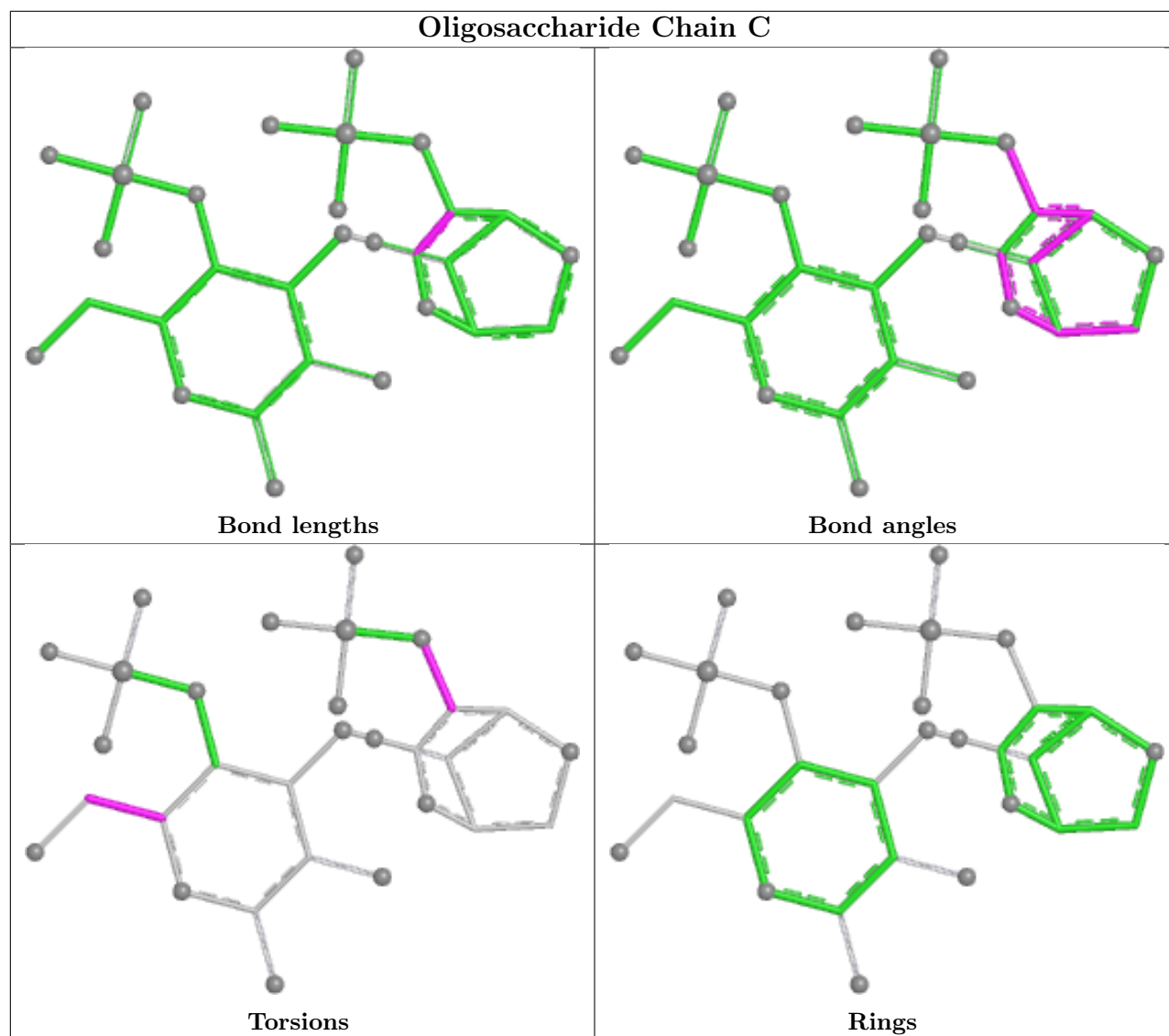
Mol	Chain	Res	Type	Atoms
2	C	2	DGS	C1-C2-O2-S
2	C	2	DGS	C3-C2-O2-S
3	D	2	DGS	C1-C2-O2-S
3	D	2	DGS	C3-C2-O2-S
3	D	4	DGS	C1-C2-O2-S
3	D	4	DGS	C3-C2-O2-S
2	C	1	G4S	O5-C5-C6-O6
3	D	3	G4S	O5-C5-C6-O6
3	D	1	G4S	O5-C5-C6-O6

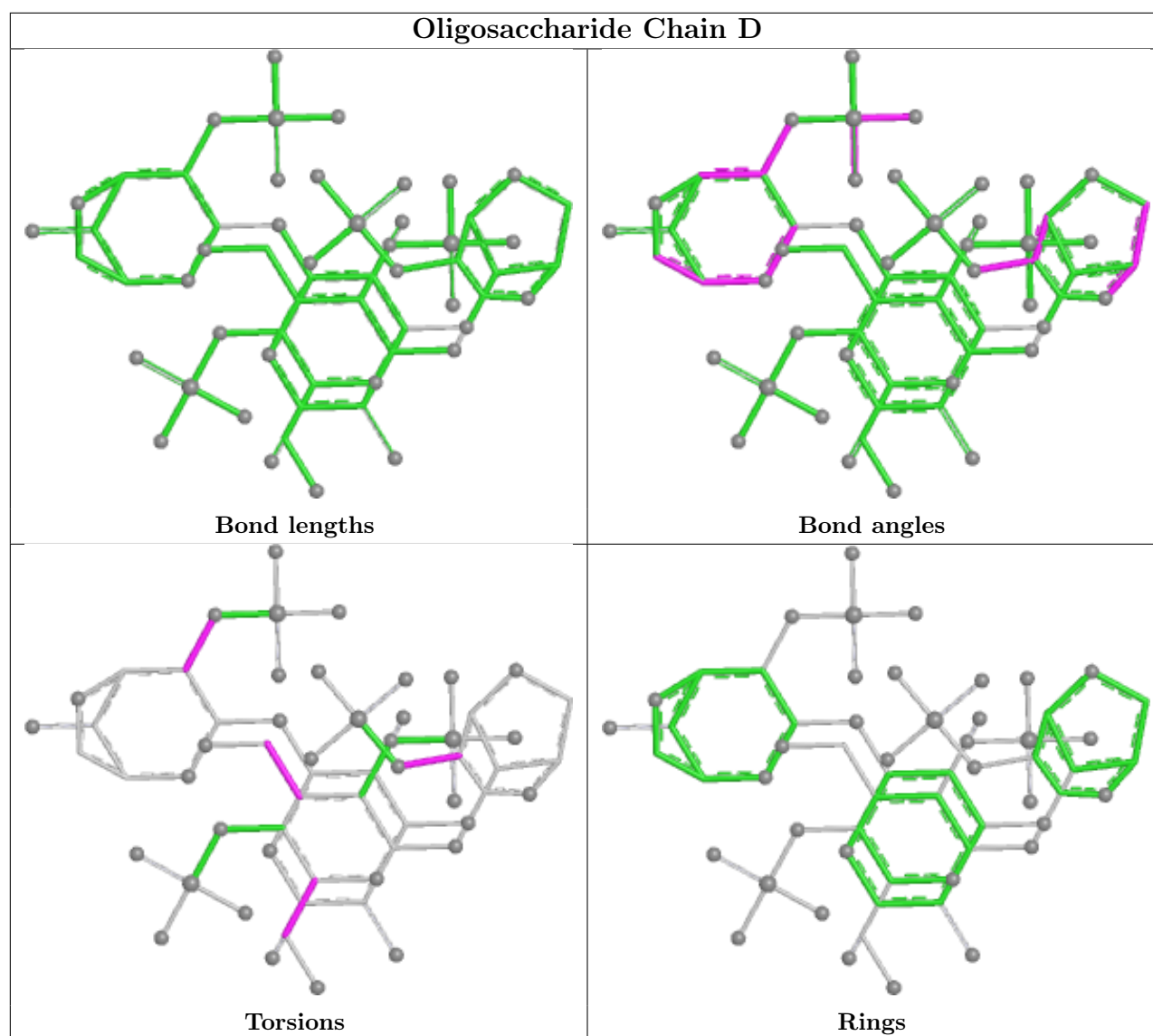
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	DGS	1	0
3	D	2	DGS	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 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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	457/464 (98%)	0.18	45 (9%) 13 12	7, 16, 51, 61	7 (1%)
1	B	457/464 (98%)	0.66	77 (16%) 4 4	8, 19, 57, 71	12 (2%)
All	All	914/928 (98%)	0.42	122 (13%) 7 6	7, 17, 55, 71	19 (2%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	477	ASN	8.6
1	B	475	VAL	7.9
1	B	476	CYS	7.8
1	B	408	CYS	7.7
1	B	406	PRO	7.0
1	B	409	LYS	6.3
1	B	402	SER	6.3
1	B	478	TYR	6.2
1	B	482	SER	6.0
1	A	327	ALA	5.9
1	B	480	GLY	5.9
1	B	411	VAL	5.9
1	B	407	MET	5.7
1	B	405	ASN	5.6
1	B	316	ASP	5.5
1	B	479	TYR	5.4
1	B	490	GLU	5.4
1	A	366	LEU	5.3
1	B	481	MET	5.0
1	B	404	SER	5.0
1	A	360	CYS	4.9
1	B	313	SER	4.8
1	A	330	SER	4.8
1	B	401	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	342	ALA	4.6
1	B	320	THR	4.6
1	B	486	SER	4.6
1	B	403	THR	4.5
1	B	314	PRO	4.4
1	B	414	PRO	4.3
1	A	358	ASP	4.2
1	B	366	LEU	4.2
1	B	483	GLU	4.2
1	B	413	LEU	4.2
1	A	315	THR	4.1
1	B	323	SER	4.1
1	B	485	SER	4.1
1	A	316	ASP	4.0
1	A	350	TRP	3.9
1	A	331	LYS	3.9
1	B	318	VAL	3.8
1	A	359	ALA	3.8
1	B	416	LYS	3.7
1	A	319	HIS	3.6
1	A	332	LEU	3.6
1	B	327	ALA	3.6
1	B	473	SER	3.5
1	A	363	LYS	3.5
1	A	365	LYS	3.5
1	A	361	LEU	3.4
1	B	474	ARG	3.4
1	A	328	VAL	3.4
1	A	362	ASP	3.4
1	B	396	ASP	3.4
1	A	321	ARG	3.4
1	A	491	ARG	3.4
1	B	410	ARG	3.3
1	A	323	SER	3.3
1	B	491	ARG	3.3
1	B	412	CYS	3.3
1	A	335	GLY	3.2
1	B	484	CYS	3.2
1	A	320	THR	3.2
1	A	357	LYS	3.2
1	A	333	GLY	3.2
1	B	350	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	334	ARG	3.1
1	B	415	THR	3.1
1	A	28	VAL	3.1
1	A	317	GLU	3.1
1	B	351	ALA	3.1
1	A	324	TRP	3.0
1	A	322	GLN	3.0
1	A	334	ARG	3.0
1	B	487	SER	3.0
1	A	367	GLU	3.0
1	A	471	GLU	3.0
1	B	340	PRO	3.0
1	B	421	LYS	2.9
1	A	314	PRO	2.9
1	A	318	VAL	2.9
1	B	312	PHE	2.9
1	A	326	GLN	2.8
1	A	364	ALA	2.8
1	A	337	ALA	2.8
1	B	324	TRP	2.8
1	B	341	TYR	2.7
1	B	489	TRP	2.7
1	A	312	PHE	2.7
1	A	454	LYS	2.7
1	A	396	ASP	2.7
1	B	319	HIS	2.6
1	B	330	SER	2.6
1	A	487	SER	2.6
1	B	328	VAL	2.6
1	B	321	ARG	2.6
1	B	326	GLN	2.5
1	B	233	ASN	2.5
1	B	315	THR	2.5
1	B	457	ASN	2.5
1	B	370	ILE	2.5
1	A	368	TYR	2.4
1	B	352	ALA	2.4
1	B	119	GLY	2.4
1	B	63	SER	2.4
1	B	360	CYS	2.3
1	B	325	LYS	2.2
1	A	336	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	365	LYS	2.2
1	B	311	LEU	2.2
1	B	399	ASP	2.2
1	B	364	ALA	2.1
1	B	419	TRP	2.1
1	B	338	GLN	2.1
1	A	313	SER	2.1
1	B	441	THR	2.1
1	A	195	ASN	2.1
1	B	418	GLN	2.1
1	B	420	SER	2.1
1	A	474	ARG	2.0
1	B	322	GLN	2.0
1	B	339	THR	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](#)

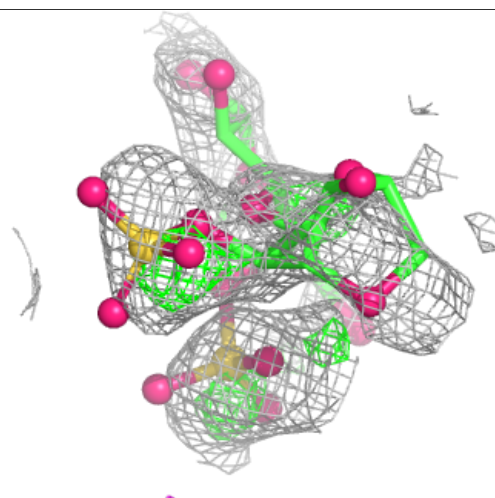
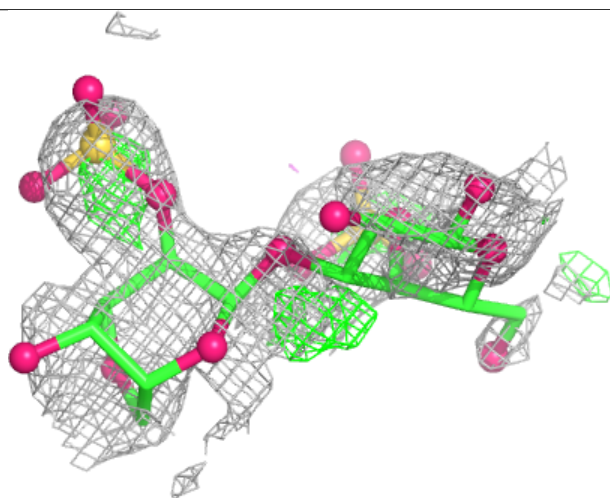
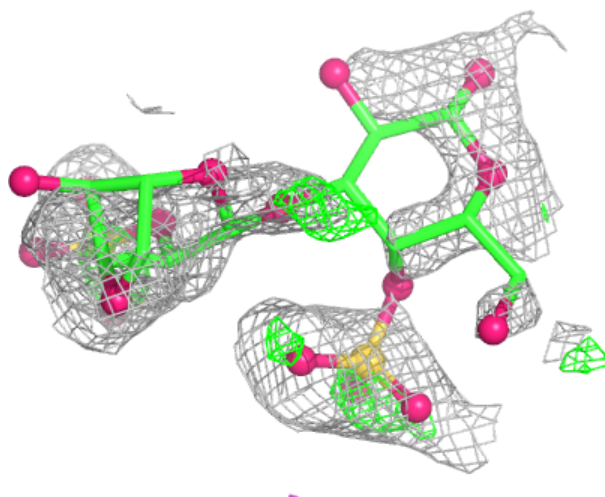
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

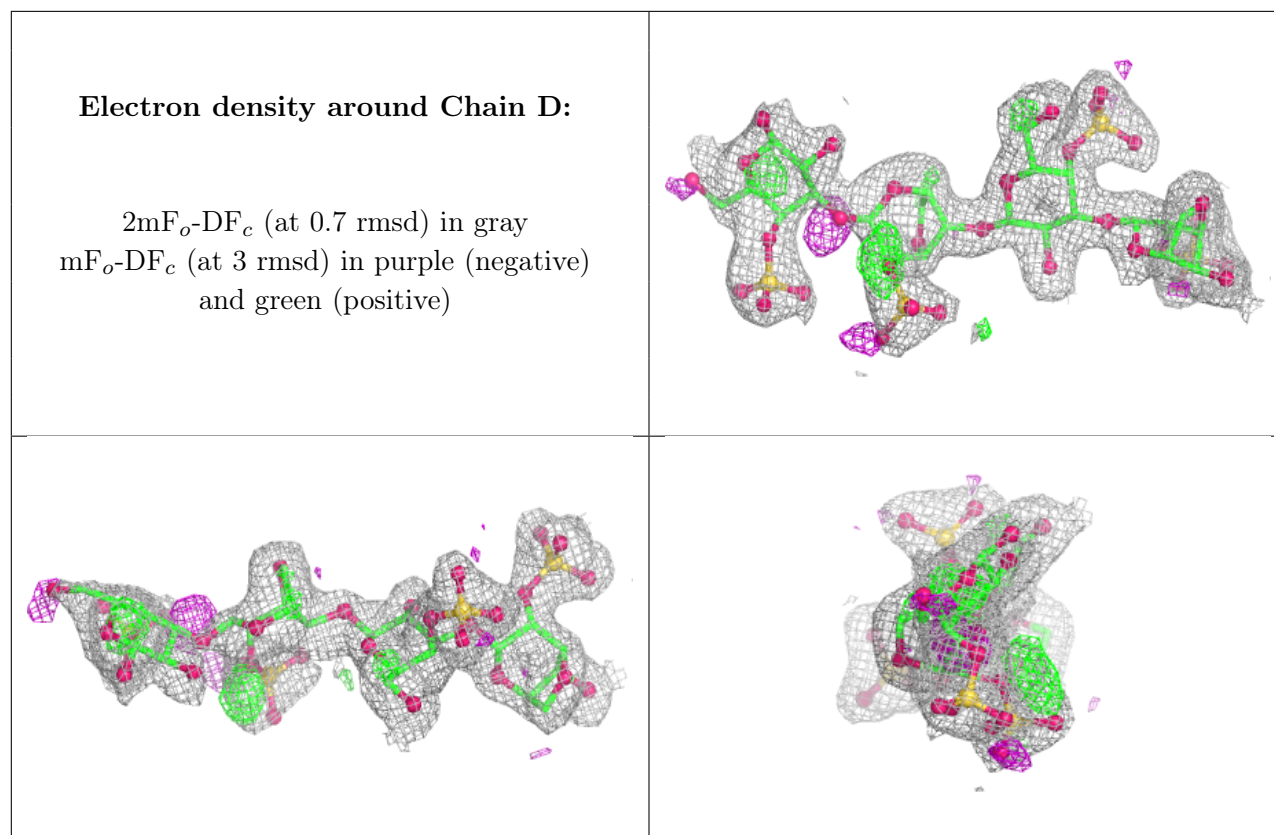
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DGS	C	2	14/15	0.65	0.35	69,70,70,70	14
2	G4S	C	1	16/16	0.79	0.38	66,67,68,69	16
3	G4S	D	1	16/16	0.80	0.19	47,52,54,56	0
3	DGS	D	2	14/15	0.80	0.18	27,37,50,50	0
3	G4S	D	3	15/16	0.95	0.07	17,20,24,26	0
3	DGS	D	4	14/15	0.97	0.07	17,21,21,22	0

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
4	CA	B	8	1/1	0.96	0.05	24,24,24,24	0
4	CA	B	10	1/1	0.97	0.05	27,27,27,27	0
4	CA	A	5	1/1	0.98	0.04	15,15,15,15	0
4	CA	A	9	1/1	0.98	0.05	22,22,22,22	0
5	NA	A	11	1/1	0.98	0.03	13,13,13,13	0
5	NA	A	13	1/1	0.98	0.11	14,14,14,14	0
5	NA	B	12	1/1	0.98	0.04	19,19,19,19	0
5	NA	B	14	1/1	0.98	0.07	19,19,19,19	0
6	CL	B	531	1/1	0.98	0.18	37,37,37,37	0
4	CA	A	7	1/1	0.99	0.02	15,15,15,15	0
4	CA	A	3	1/1	0.99	0.02	15,15,15,15	0
4	CA	B	2	1/1	0.99	0.02	16,16,16,16	0
4	CA	B	4	1/1	0.99	0.03	17,17,17,17	0
4	CA	B	6	1/1	0.99	0.04	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	A	530	1/1	0.99	0.12	30,30,30,30	0
4	CA	A	496	1/1	0.99	0.03	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.