



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:28 PM UTC

PDB ID : 5HO9 / pdb_00005ho9
Title : Structure of truncated AbnA (domains 1-3), a GH43 arabinanase from *Geobacillus stearothermophilus*, in complex with arabinooctaose
Authors : Lansky, S.; Salama, R.; Azoulai, D.; Shwartstien, O.; Shoham, Y.; Shoham, G.
Deposited on : 2016-01-19
Resolution : 2.85 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

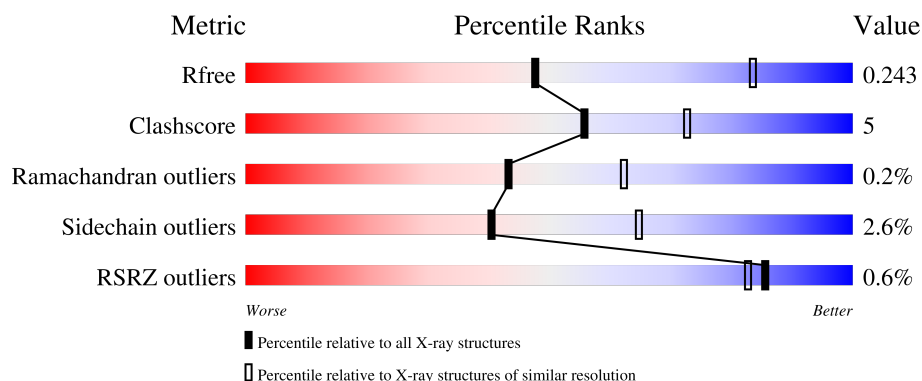
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	639	80% 13% 7%
1	B	639	84% 9% 7%
2	C	8	50% 50%
2	D	8	75% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9874 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 Extracellular arabinanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	1	0
			4695	2994	785	907	9			
1	B	596	Total	C	N	O	S	0	1	0
			4713	3004	788	912	9			

- Molecule 2 is an oligosaccharide called alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	8	Total	C	O	0	0	0
			73	40	33			
2	D	8	Total	C	O	0	0	0
			73	40	33			

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



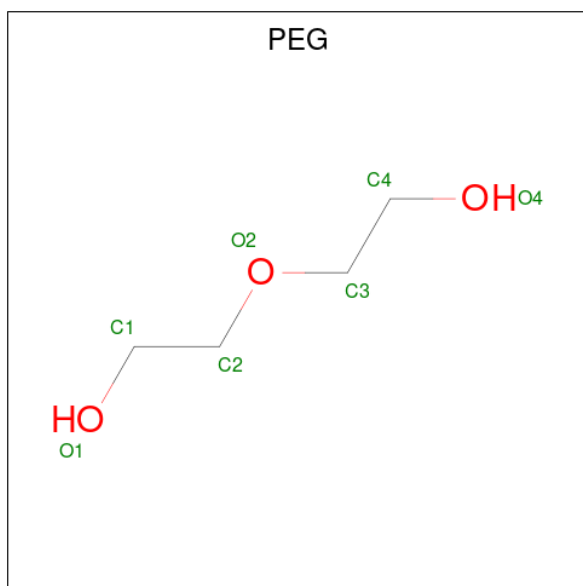
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

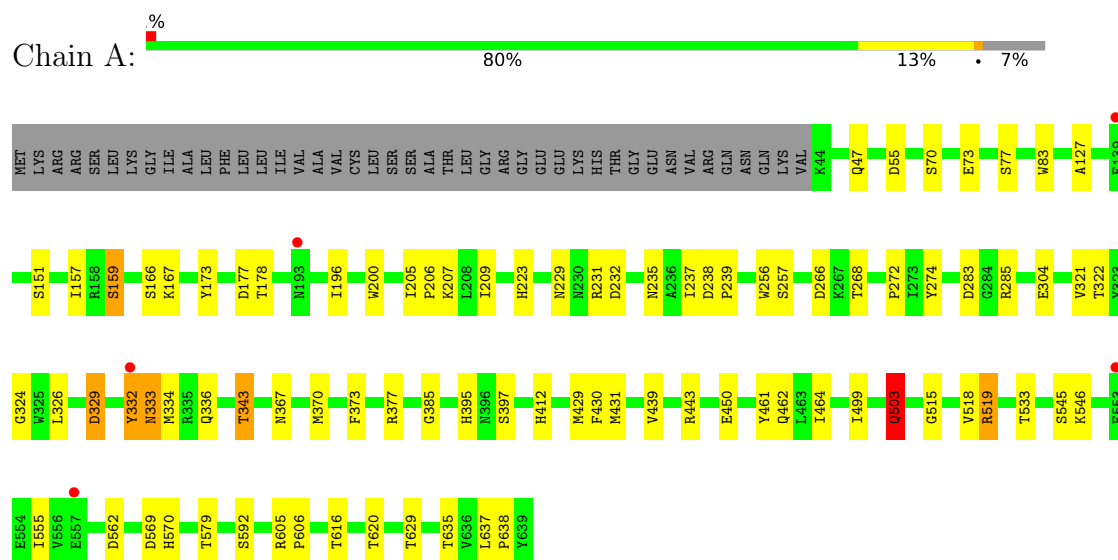
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total	O	0	0
			75	75		
5	B	82	Total	O	0	0
			82	82		

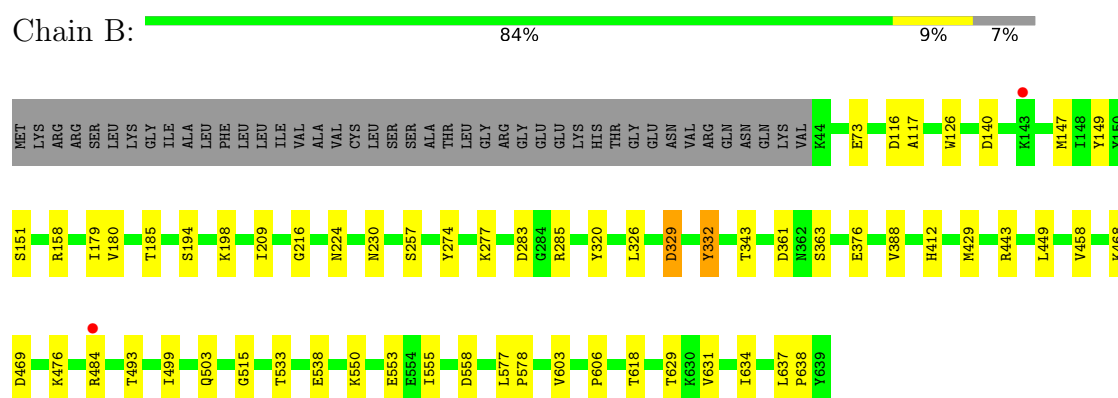
3 Residue-property plots

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: Extracellular arabinanase



- Molecule 1: Extracellular arabinanase

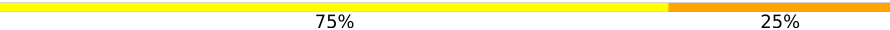


- Molecule 2: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose



AHR1
AHR2
AHR3
AHR4
AHR5
AHR6
AHR7
AHR8

- Molecule 2: α -L-arabinofuranose-(1-5)- α -L-arabinofuranose-(1-5)- α -L-arabinofuranose-(1-5)- α -L-arabinofuranose-(1-5)- α -L-arabinofuranose-(1-5)- α -L-arabinofuranose-(1-5)- α -L-arabinofuranose

Chain D: 

AHR1
AHR2
AHR3
AHR4
AHR5
AHR6
AHR7
AHR8

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.17Å 129.17Å 488.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.82 – 2.85 48.82 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.82-2.85) 99.8 (48.82-2.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.67 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.183 , 0.242 0.189 , 0.243	Depositor DCC
R_{free} test set	2101 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9874	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: PEG, AHR, 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	0.55	0/4830	0.86	3/6568 (0.0%)
1	B	0.55	0/4848	0.86	2/6589 (0.0%)
All	All	0.55	0/9678	0.86	5/13157 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	LEU	N-CA-C	6.89	119.63	111.71
1	A	503	GLN	N-CA-C	-6.06	99.40	109.46
1	A	257	SER	CB-CA-C	-5.44	110.28	116.54
1	B	274	TYR	CA-C-N	5.12	126.24	119.84
1	B	274	TYR	C-N-CA	5.12	126.24	119.84

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	4695	0	4460	53	0
1	B	4713	0	4492	33	0
2	C	73	0	0	6	0
2	D	73	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	60	0	0	5	0
3	B	40	0	0	1	0
4	A	28	0	40	0	0
4	B	35	0	50	2	0
5	A	75	0	0	1	0
5	B	82	0	0	1	0
All	All	9874	0	9042	89	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 5.

All (89) 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)
5:A:801:HOH:O	2:C:7:AHR:O2	1.96	0.81
1:A:285:ARG:NH2	1:A:343:THR:O	2.16	0.79
1:A:304:GLU:OE2	1:A:332:TYR:OH	2.03	0.75
1:A:637:LEU:HD21	2:D:3:AHR:O3	1.89	0.72
1:B:285:ARG:NH2	1:B:343:THR:O	2.24	0.70
1:A:70:SER:OG	2:C:5:AHR:O3	2.14	0.65
1:A:499:ILE:HB	1:A:503:GLN:HE21	1.67	0.59
1:B:458:VAL:HG21	1:B:484:ARG:HG3	1.83	0.59
1:A:151:SER:HB3	1:A:237:ILE:HG22	1.85	0.59
1:B:73:GLU:OE1	2:D:7:AHR:O3	2.22	0.58
1:A:443:ARG:NH1	3:A:711:SO4:O2	2.36	0.58
1:A:450:GLU:OE1	1:A:519:ARG:NH1	2.38	0.57
1:A:499:ILE:O	1:A:503:GLN:HB2	2.05	0.57
1:A:322:THR:HG23	1:A:333:ASN:O	2.05	0.56
1:B:618:THR:HG23	1:B:631:VAL:HG12	1.87	0.56
1:A:324:GLY:O	1:A:332:TYR:HE1	1.89	0.55
1:A:592:SER:HB3	1:A:616:THR:HG22	1.89	0.55
1:B:179:ILE:HG13	1:B:180:VAL:HG23	1.88	0.55
1:A:324:GLY:C	1:A:332:TYR:HE1	2.14	0.54
1:A:570:HIS:HD2	2:D:3:AHR:C3	2.20	0.54
1:B:126:TRP:O	1:B:151:SER:HB3	2.07	0.54
1:B:443:ARG:HG2	5:B:823:HOH:O	2.08	0.54
1:A:207:LYS:NZ	3:A:705:SO4:O3	2.36	0.54
1:B:637:LEU:CD2	2:C:3:AHR:O3	2.56	0.53
1:A:385:GLY:N	3:A:706:SO4:O1	2.27	0.53
1:A:177:ASP:OD1	1:A:178:THR:N	2.41	0.53
1:A:606:PRO:HD2	1:A:638:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:PHE:HB2	1:A:464:ILE:HD13	1.90	0.52
1:B:224:ASN:HB2	4:B:711:PEG:H11	1.92	0.51
1:B:637:LEU:HD21	2:C:3:AHR:O3	2.11	0.51
1:B:283:ASP:OD2	1:B:285:ARG:HD3	2.11	0.50
1:B:515:GLY:HA3	1:B:533:THR:O	2.11	0.50
1:A:515:GLY:HA3	1:A:533:THR:O	2.12	0.49
1:A:430:PHE:CZ	1:A:518:VAL:HG21	2.48	0.49
1:A:159:SER:OG	1:A:235:ASN:OD1	2.30	0.48
1:A:231:ARG:NH2	1:A:232:ASP:OD2	2.46	0.48
1:B:230:ASN:HB2	1:B:257:SER:HB3	1.95	0.48
1:A:73:GLU:OE2	2:C:7:AHR:O3	2.31	0.48
1:A:499:ILE:HB	1:A:503:GLN:NE2	2.28	0.48
1:B:209:ILE:HD13	1:B:216:GLY:HA2	1.96	0.48
1:A:336:GLN:HB3	1:A:367:ASN:HB2	1.96	0.47
1:A:462:GLN:HG3	1:A:545:SER:HB3	1.96	0.47
1:A:238:ASP:OD2	1:A:395:HIS:NE2	2.47	0.47
1:A:569:ASP:O	1:A:635:THR:HB	2.15	0.47
1:A:205:ILE:O	1:A:209:ILE:HG13	2.15	0.47
1:A:324:GLY:C	1:A:332:TYR:CE1	2.94	0.46
1:A:283:ASP:OD2	1:A:285:ARG:HD3	2.16	0.46
1:A:461:TYR:CE2	1:A:546:LYS:HB2	2.52	0.46
1:B:326:LEU:HA	1:B:332:TYR:CG	2.51	0.45
1:A:272:PRO:HB2	1:A:274:TYR:CZ	2.52	0.45
1:A:77:SER:HB2	1:A:83:TRP:CE3	2.53	0.44
1:B:469:ASP:N	3:B:707:SO4:O1	2.49	0.44
1:A:200:TRP:CZ3	1:A:206:PRO:HG3	2.53	0.44
1:A:127:ALA:O	1:A:239:PRO:HD2	2.18	0.44
1:A:412:HIS:CD2	1:A:412:HIS:C	2.96	0.44
1:B:606:PRO:HD2	1:B:638:PRO:HA	2.00	0.43
1:A:431:MET:HE2	1:A:431:MET:HB2	1.83	0.43
2:C:2:AHR:O5	2:C:3:AHR:O3	2.36	0.43
1:A:377:ARG:NH2	1:A:562:ASP:OD2	2.51	0.43
1:B:158:ARG:HD3	1:B:198:LYS:HG2	2.00	0.43
1:B:320:TYR:CE2	1:B:429:MET:HE1	2.54	0.43
1:A:429:MET:HE3	1:A:439:VAL:HG22	2.00	0.43
1:B:550:LYS:HE3	1:B:558:ASP:OD2	2.19	0.43
1:B:376:GLU:OE1	1:B:476:LYS:HD3	2.19	0.43
1:A:55:ASP:HB3	1:A:395:HIS:CE1	2.54	0.42
1:A:555:ILE:HD13	1:A:555:ILE:HA	1.89	0.42
1:B:326:LEU:HA	1:B:332:TYR:CD1	2.55	0.42
1:B:449:LEU:HD23	1:B:449:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:MET:HE3	1:A:370:MET:HB3	2.01	0.42
1:A:579:THR:N	3:A:710:SO4:O2	2.52	0.42
1:A:605:ARG:HA	1:A:606:PRO:HD3	1.92	0.42
1:A:223:HIS:NE2	1:A:229:ASN:HA	2.35	0.42
1:B:468:LYS:HE3	1:B:538:GLU:O	2.20	0.42
1:B:577:LEU:HA	1:B:578:PRO:HD2	1.85	0.42
1:B:499:ILE:O	1:B:503:GLN:HB3	2.20	0.41
1:B:555:ILE:HD13	1:B:555:ILE:HA	1.81	0.41
1:A:503:GLN:HE21	1:A:503:GLN:HB3	1.55	0.41
1:B:412:HIS:CD2	1:B:412:HIS:C	2.98	0.41
1:A:223:HIS:ND1	3:A:712:SO4:O2	2.54	0.41
1:B:116:ASP:OD1	1:B:194:SER:OG	2.36	0.41
1:B:147:MET:HE2	1:B:149:TYR:CE1	2.56	0.41
1:B:361:ASP:OD1	1:B:363:SER:HB2	2.21	0.41
1:A:166:SER:HB2	1:A:173:TYR:HA	2.03	0.41
1:A:266:ASP:OD1	1:A:268:THR:HB	2.21	0.41
1:B:224:ASN:H	4:B:711:PEG:H11	1.85	0.41
1:A:322:THR:HG21	1:A:332:TYR:CD2	2.56	0.41
2:D:7:AHR:O3	2:D:7:AHR:O5	2.39	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	595/639 (93%)	562 (94%)	32 (5%)	1 (0%)	43 62
1	B	595/639 (93%)	562 (94%)	32 (5%)	1 (0%)	43 62
All	All	1190/1278 (93%)	1124 (94%)	64 (5%)	2 (0%)	43 62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	TRP
1	B	117	ALA

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	495/536 (92%)	479 (97%)	16 (3%)	34	59
1	B	500/536 (93%)	488 (98%)	12 (2%)	43	67
All	All	995/1072 (93%)	967 (97%)	28 (3%)	40	62

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	157	ILE
1	A	159	SER
1	A	167	LYS
1	A	196	ILE
1	A	321	VAL
1	A	329[A]	ASP
1	A	329[B]	ASP
1	A	332	TYR
1	A	333	ASN
1	A	343	THR
1	A	397	SER
1	A	503	GLN
1	A	519	ARG
1	A	620	THR
1	A	629	THR
1	B	140	ASP
1	B	185	THR
1	B	277	LYS
1	B	329[A]	ASP
1	B	329[B]	ASP
1	B	332	TYR

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Mol	Chain	Res	Type
1	B	388	VAL
1	B	493	THR
1	B	553	GLU
1	B	603	VAL
1	B	629	THR
1	B	634	ILE

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	82	ASN
1	A	503	GLN
1	B	82	ASN
1	B	202	ASN
1	B	235	ASN
1	B	362	ASN
1	B	503	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 ⓘ

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AHR	C	1	2	10,10,10	1.47	1 (10%)	13,14,14	1.61	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AHR	C	2	2	9,9,10	1.87	2 (22%)	11,12,14	3.13	6 (54%)
2	AHR	C	3	2	9,9,10	2.55	5 (55%)	11,12,14	2.30	4 (36%)
2	AHR	C	4	2	9,9,10	2.46	3 (33%)	11,12,14	2.43	2 (18%)
2	AHR	C	5	2	9,9,10	1.81	5 (55%)	11,12,14	2.32	5 (45%)
2	AHR	C	6	2	9,9,10	1.50	2 (22%)	11,12,14	2.55	3 (27%)
2	AHR	C	7	2	9,9,10	1.41	2 (22%)	11,12,14	1.51	3 (27%)
2	AHR	C	8	2	9,9,10	1.41	3 (33%)	11,12,14	1.91	3 (27%)
2	AHR	D	1	2	10,10,10	2.26	2 (20%)	13,14,14	1.57	3 (23%)
2	AHR	D	2	2	9,9,10	2.42	4 (44%)	11,12,14	2.38	4 (36%)
2	AHR	D	3	2	9,9,10	1.73	3 (33%)	11,12,14	1.23	1 (9%)
2	AHR	D	4	2	9,9,10	2.66	4 (44%)	11,12,14	3.62	6 (54%)
2	AHR	D	5	2	9,9,10	2.32	3 (33%)	11,12,14	2.79	6 (54%)
2	AHR	D	6	2	9,9,10	1.69	3 (33%)	11,12,14	1.61	3 (27%)
2	AHR	D	7	2	9,9,10	1.74	2 (22%)	11,12,14	2.77	6 (54%)
2	AHR	D	8	2	9,9,10	1.45	1 (11%)	11,12,14	1.29	2 (18%)

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	AHR	C	1	2	-	2/2/18/18	0/1/1/1
2	AHR	C	2	2	-	1/2/15/18	0/1/1/1
2	AHR	C	3	2	-	0/2/15/18	0/1/1/1
2	AHR	C	4	2	-	2/2/15/18	0/1/1/1
2	AHR	C	5	2	-	1/2/15/18	0/1/1/1
2	AHR	C	6	2	-	0/2/15/18	0/1/1/1
2	AHR	C	7	2	-	0/2/15/18	0/1/1/1
2	AHR	C	8	2	-	2/2/15/18	0/1/1/1
2	AHR	D	1	2	-	0/2/18/18	0/1/1/1
2	AHR	D	2	2	-	2/2/15/18	0/1/1/1
2	AHR	D	3	2	-	2/2/15/18	0/1/1/1
2	AHR	D	4	2	-	2/2/15/18	0/1/1/1
2	AHR	D	5	2	-	0/2/15/18	0/1/1/1
2	AHR	D	6	2	-	0/2/15/18	0/1/1/1
2	AHR	D	7	2	-	0/2/15/18	0/1/1/1
2	AHR	D	8	2	-	2/2/15/18	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	AHR	C1-C2	-6.09	1.45	1.52
2	C	4	AHR	O4-C4	-5.44	1.35	1.44
2	D	5	AHR	C2-C3	-4.75	1.45	1.53
2	D	4	AHR	C3-C4	-4.72	1.41	1.53
2	D	4	AHR	C2-C3	-4.56	1.46	1.53
2	C	2	AHR	C2-C3	-4.53	1.46	1.53
2	C	3	AHR	C3-C4	-4.26	1.42	1.53
2	D	2	AHR	C2-C3	-4.24	1.46	1.53
2	D	2	AHR	O2-C2	-3.82	1.35	1.43
2	C	1	AHR	C1-C2	-3.73	1.48	1.52
2	C	4	AHR	C1-C2	-3.64	1.45	1.51
2	C	3	AHR	C1-C2	-3.64	1.45	1.51
2	D	5	AHR	C1-C2	-3.56	1.45	1.51
2	D	7	AHR	C2-C3	-3.53	1.47	1.53
2	D	2	AHR	C1-C2	-3.52	1.45	1.51
2	D	3	AHR	O4-C4	-3.44	1.38	1.44
2	D	4	AHR	C1-C2	-3.35	1.46	1.51
2	D	8	AHR	C2-C3	-3.35	1.48	1.53
2	C	6	AHR	O4-C1	-3.23	1.37	1.43
2	C	3	AHR	O4-C4	-3.21	1.39	1.44
2	D	6	AHR	O4-C1	-3.19	1.37	1.43
2	C	7	AHR	C2-C3	-3.01	1.48	1.53
2	C	8	AHR	C2-C3	-2.89	1.48	1.53
2	C	5	AHR	C1-C2	-2.72	1.47	1.51
2	D	1	AHR	C2-C3	-2.60	1.46	1.53
2	C	5	AHR	O4-C1	-2.60	1.38	1.43
2	D	4	AHR	O3-C3	-2.59	1.36	1.43
2	D	3	AHR	C2-C3	-2.50	1.49	1.53
2	D	5	AHR	C3-C4	-2.47	1.46	1.53
2	D	7	AHR	O4-C4	2.43	1.48	1.44
2	C	2	AHR	O2-C2	-2.43	1.38	1.43
2	D	6	AHR	C2-C3	-2.42	1.49	1.53
2	C	7	AHR	O4-C4	2.36	1.48	1.44
2	C	3	AHR	C2-C3	-2.34	1.49	1.53
2	C	3	AHR	O5-C5	-2.27	1.32	1.42
2	D	2	AHR	O4-C1	2.25	1.48	1.43
2	D	3	AHR	C3-C4	-2.25	1.47	1.53
2	C	5	AHR	C2-C3	-2.24	1.49	1.53
2	C	8	AHR	O4-C4	-2.15	1.40	1.44
2	C	5	AHR	O4-C4	-2.14	1.40	1.44
2	C	4	AHR	O2-C2	2.14	1.47	1.43
2	C	6	AHR	C2-C3	-2.09	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	8	AHR	C3-C4	-2.07	1.47	1.53
2	D	6	AHR	C1-C2	-2.02	1.48	1.51
2	C	5	AHR	C3-C4	-2.02	1.47	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	AHR	O4-C4-C3	-8.05	97.20	104.63
2	C	4	AHR	O4-C4-C5	-6.85	96.92	109.36
2	C	2	AHR	C1-C2-C3	-6.07	91.92	101.63
2	D	7	AHR	O4-C4-C5	5.99	120.26	109.36
2	C	2	AHR	O4-C4-C5	5.67	119.67	109.36
2	C	6	AHR	O4-C1-C2	-5.59	96.12	105.76
2	C	3	AHR	O4-C1-C2	-5.32	96.60	105.76
2	D	4	AHR	C1-C2-C3	-4.94	93.73	101.63
2	C	8	AHR	O4-C4-C3	-4.88	100.12	104.63
2	D	5	AHR	C5-C4-C3	-4.80	103.76	115.10
2	C	6	AHR	C1-C2-C3	-4.77	93.99	101.63
2	D	4	AHR	O4-C4-C5	4.62	117.76	109.36
2	D	2	AHR	O4-C4-C5	4.40	117.36	109.36
2	D	5	AHR	O4-C4-C5	4.20	117.00	109.36
2	D	2	AHR	C1-C2-C3	-4.19	94.93	101.63
2	D	7	AHR	C1-C2-C3	-4.16	94.98	101.63
2	C	1	AHR	O4-C4-C5	-4.13	100.49	109.22
2	C	5	AHR	O4-C1-C2	-4.13	98.65	105.76
2	C	5	AHR	C5-C4-C3	-4.12	105.37	115.10
2	D	5	AHR	O4-C1-C2	-3.96	98.93	105.76
2	D	4	AHR	C5-C4-C3	-3.88	105.94	115.10
2	C	2	AHR	O4-C4-C3	-3.82	101.10	104.63
2	D	7	AHR	O4-C4-C3	-3.62	101.29	104.63
2	D	4	AHR	O4-C1-C2	-3.45	99.81	105.76
2	D	6	AHR	O4-C1-C2	-3.42	99.87	105.76
2	C	3	AHR	C5-C4-C3	-3.40	107.08	115.10
2	D	5	AHR	C1-C2-C3	-3.33	96.29	101.63
2	D	2	AHR	O4-C4-C3	-3.25	101.63	104.63
2	C	2	AHR	O4-C1-C2	-3.24	100.18	105.76
2	C	7	AHR	O4-C4-C5	3.12	115.03	109.36
2	C	6	AHR	C5-C4-C3	-3.11	107.76	115.10
2	C	3	AHR	O3-C3-C4	-2.96	102.59	111.08
2	C	5	AHR	C1-C2-C3	-2.92	96.95	101.63
2	D	5	AHR	O4-C4-C3	-2.90	101.95	104.63
2	D	6	AHR	C5-C4-C3	-2.88	108.30	115.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	AHR	O1-C1-O4	2.69	114.55	111.12
2	C	2	AHR	C5-C4-C3	-2.69	108.75	115.10
2	D	8	AHR	O2-C2-C3	-2.69	106.13	111.43
2	D	2	AHR	O4-C1-C2	-2.68	101.14	105.76
2	D	5	AHR	O2-C2-C3	-2.66	106.19	111.43
2	D	1	AHR	C5-C4-C3	-2.61	108.94	115.10
2	C	5	AHR	O4-C4-C5	2.60	114.08	109.36
2	D	7	AHR	C5-C4-C3	-2.53	109.13	115.10
2	C	3	AHR	O3-C3-C2	-2.52	105.99	111.97
2	C	8	AHR	C5-C4-C3	-2.51	109.17	115.10
2	C	8	AHR	O4-C4-C5	-2.50	104.83	109.36
2	D	1	AHR	C1-C2-C3	-2.39	99.35	102.29
2	D	7	AHR	O4-C1-C2	-2.35	101.72	105.76
2	C	5	AHR	O4-C4-C3	-2.28	102.53	104.63
2	C	1	AHR	O1-C1-O4	-2.27	108.23	111.12
2	C	4	AHR	O3-C3-C2	-2.23	106.68	111.97
2	D	3	AHR	O3-C3-C4	-2.16	104.89	111.08
2	D	7	AHR	C1-O4-C4	-2.15	103.32	108.06
2	D	4	AHR	O3-C3-C4	-2.08	105.10	111.08
2	C	7	AHR	C1-C2-C3	-2.03	98.38	101.63
2	C	2	AHR	C1-O4-C4	-2.02	103.59	108.06
2	D	6	AHR	C1-C2-C3	-2.02	98.39	101.63
2	D	8	AHR	C5-C4-C3	-2.01	110.34	115.10
2	C	7	AHR	O2-C2-C3	-2.00	107.48	111.43
2	C	1	AHR	C1-C2-C3	-2.00	99.82	102.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	AHR	O4-C4-C5-O5
2	D	3	AHR	O4-C4-C5-O5
2	C	4	AHR	C3-C4-C5-O5
2	D	3	AHR	C3-C4-C5-O5
2	C	1	AHR	O4-C4-C5-O5
2	D	2	AHR	O4-C4-C5-O5
2	D	8	AHR	O4-C4-C5-O5
2	C	8	AHR	O4-C4-C5-O5
2	C	1	AHR	C3-C4-C5-O5
2	D	2	AHR	C3-C4-C5-O5
2	C	8	AHR	C3-C4-C5-O5
2	D	4	AHR	C3-C4-C5-O5

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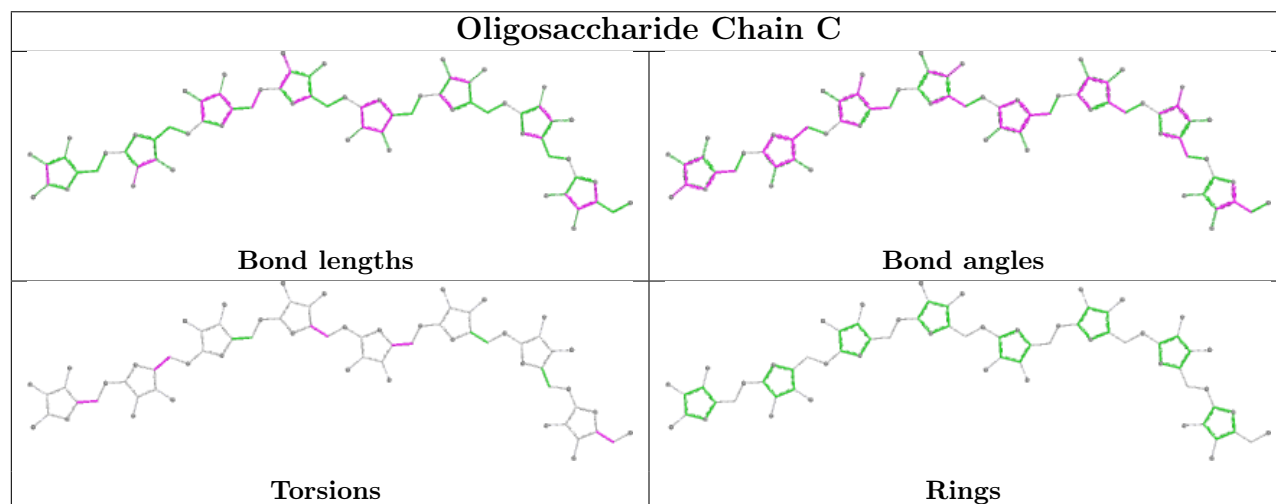
Mol	Chain	Res	Type	Atoms
2	D	8	AHR	C3-C4-C5-O5
2	D	4	AHR	O4-C4-C5-O5
2	C	2	AHR	O4-C4-C5-O5
2	C	5	AHR	C3-C4-C5-O5

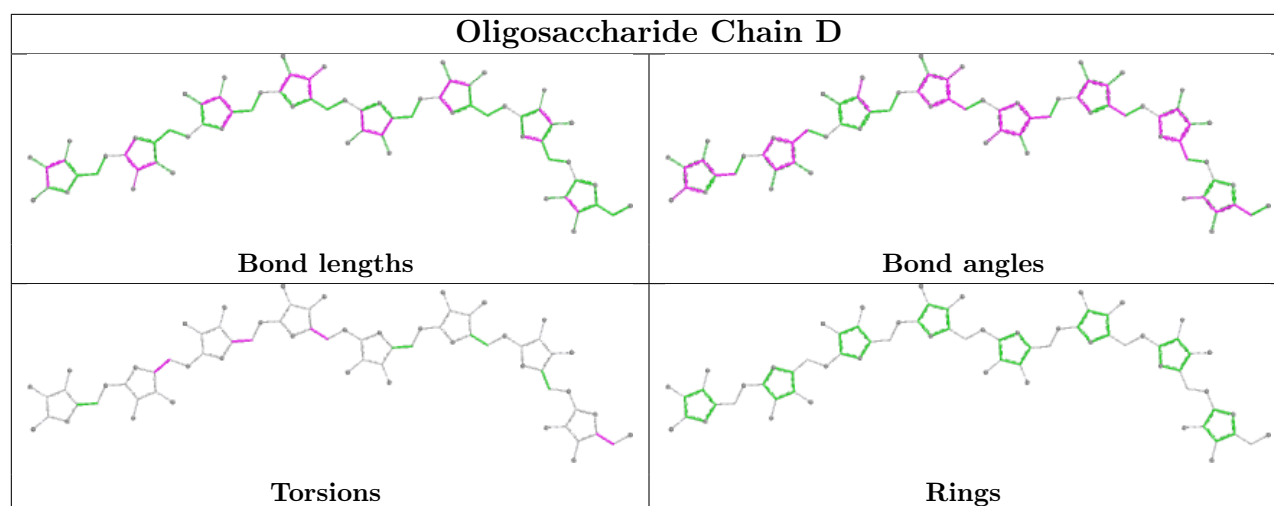
There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	AHR	2	0
2	C	5	AHR	1	0
2	D	7	AHR	2	0
2	C	3	AHR	3	0
2	C	2	AHR	1	0
2	C	7	AHR	2	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](#)

29 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	$\# Z > 2$
4	PEG	B	711	-	6,6,6	0.68	0	5,5,5	0.33	0
4	PEG	A	713	-	6,6,6	0.74	0	5,5,5	0.28	0
3	SO4	A	705	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	A	703	-	4,4,4	0.28	0	6,6,6	0.14	0
3	SO4	A	701	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	A	707	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	A	712	-	4,4,4	0.23	0	6,6,6	0.18	0
3	SO4	B	705	-	4,4,4	0.22	0	6,6,6	0.14	0
3	SO4	B	703	-	4,4,4	0.28	0	6,6,6	0.04	0
3	SO4	A	710	-	4,4,4	0.23	0	6,6,6	0.16	0
3	SO4	B	708	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	A	711	-	4,4,4	0.22	0	6,6,6	0.37	0
3	SO4	B	704	-	4,4,4	0.30	0	6,6,6	0.26	0
3	SO4	A	706	-	4,4,4	0.22	0	6,6,6	0.23	0
3	SO4	B	702	-	4,4,4	0.26	0	6,6,6	0.19	0
4	PEG	A	714	-	6,6,6	0.73	0	5,5,5	0.30	0
4	PEG	B	709	-	6,6,6	0.77	0	5,5,5	0.52	0
4	PEG	B	712	-	6,6,6	0.70	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	704	-	4,4,4	0.25	0	6,6,6	0.38	0
3	SO4	A	708	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	B	706	-	4,4,4	0.25	0	6,6,6	0.07	0
4	PEG	B	710	-	6,6,6	0.75	0	5,5,5	0.26	0
4	PEG	B	713	-	6,6,6	0.82	0	5,5,5	0.28	0
3	SO4	A	709	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	B	707	-	4,4,4	0.27	0	6,6,6	0.18	0
3	SO4	A	702	-	4,4,4	0.27	0	6,6,6	0.27	0
4	PEG	A	715	-	6,6,6	0.76	0	5,5,5	0.38	0
4	PEG	A	716	-	6,6,6	0.76	0	5,5,5	0.34	0
3	SO4	B	701	-	4,4,4	0.22	0	6,6,6	0.17	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	PEG	B	711	-	-	1/4/4/4	-
4	PEG	B	710	-	-	2/4/4/4	-
4	PEG	A	713	-	-	1/4/4/4	-
4	PEG	A	714	-	-	3/4/4/4	-
4	PEG	B	713	-	-	1/4/4/4	-
4	PEG	A	715	-	-	3/4/4/4	-
4	PEG	B	709	-	-	1/4/4/4	-
4	PEG	A	716	-	-	2/4/4/4	-
4	PEG	B	712	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	716	PEG	O1-C1-C2-O2
4	B	710	PEG	O2-C3-C4-O4
4	B	712	PEG	O1-C1-C2-O2
4	A	715	PEG	O1-C1-C2-O2
4	A	716	PEG	O2-C3-C4-O4
4	B	711	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	714	PEG	O1-C1-C2-O2
4	B	712	PEG	O2-C3-C4-O4
4	A	715	PEG	O2-C3-C4-O4
4	B	710	PEG	C4-C3-O2-C2
4	B	712	PEG	C4-C3-O2-C2
4	A	715	PEG	C1-C2-O2-C3
4	B	713	PEG	C4-C3-O2-C2
4	B	709	PEG	O2-C3-C4-O4
4	A	713	PEG	C4-C3-O2-C2
4	A	714	PEG	C4-C3-O2-C2
4	A	714	PEG	C1-C2-O2-C3

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	711	PEG	2	0
3	A	705	SO4	1	0
3	A	712	SO4	1	0
3	A	710	SO4	1	0
3	A	711	SO4	1	0
3	A	706	SO4	1	0
3	B	707	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	596/639 (93%)	-0.50	5 (0%) 82 78	20, 45, 71, 103	1 (0%)
1	B	596/639 (93%)	-0.56	2 (0%) 90 89	24, 42, 68, 95	1 (0%)
All	All	1192/1278 (93%)	-0.53	7 (0%) 85 83	20, 43, 69, 103	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	TYR	5.0
1	A	193	ASN	3.7
1	A	139	GLU	3.0
1	B	484	ARG	2.5
1	A	557	GLU	2.5
1	B	143	LYS	2.5
1	A	553	GLU	2.2

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.

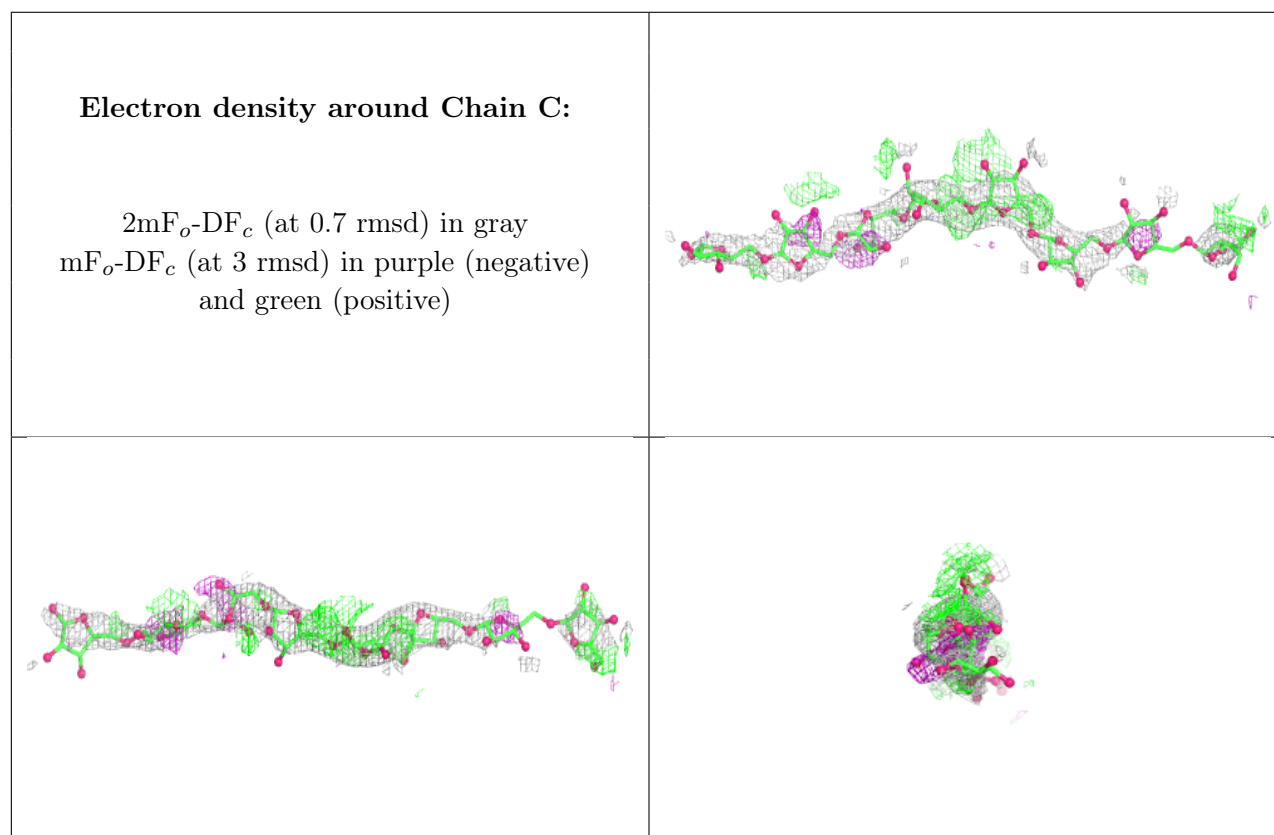
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AHR	C	8	9/10	0.55	0.27	77,83,89,91	9
2	AHR	D	8	9/10	0.72	0.24	91,97,102,105	9

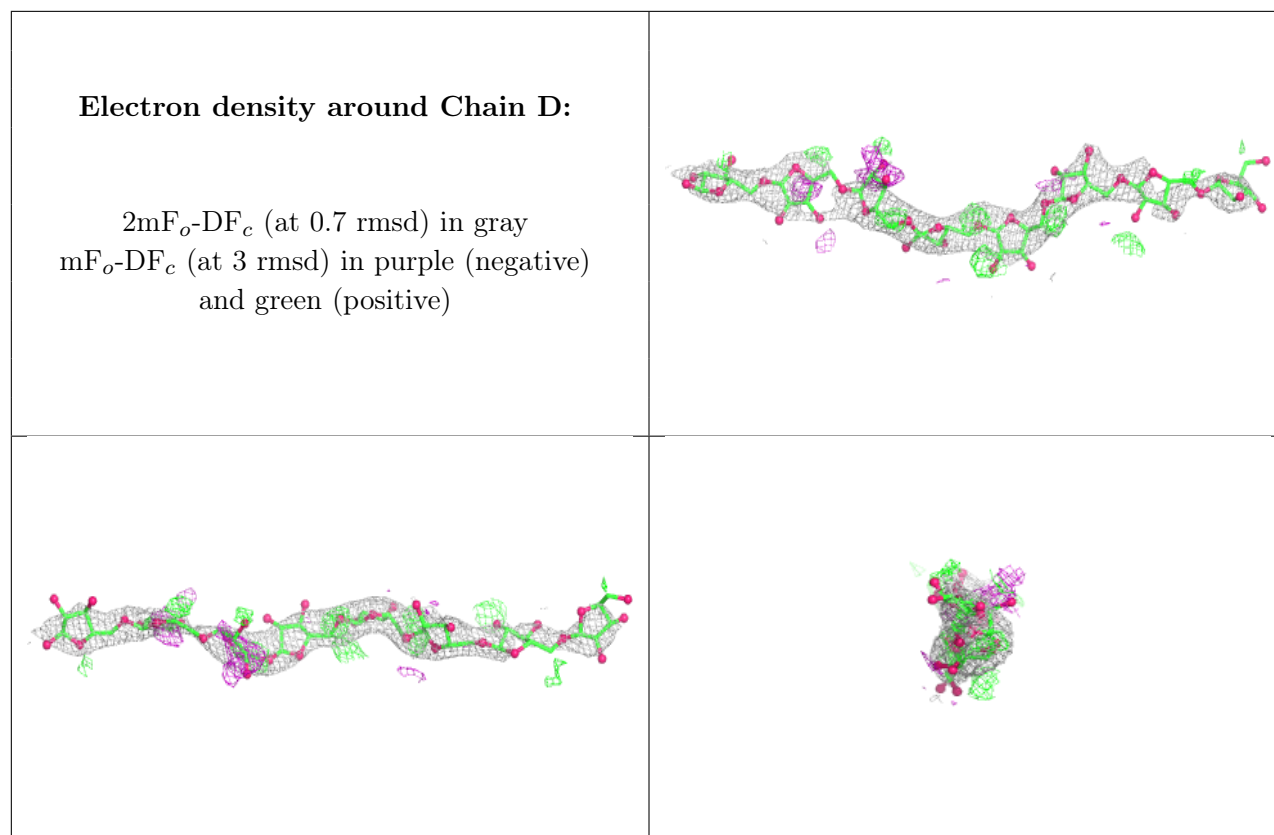
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AHR	C	7	9/10	0.74	0.33	75,82,93,94	9
2	AHR	C	5	9/10	0.80	0.28	49,55,65,67	9
2	AHR	D	7	9/10	0.81	0.30	88,96,107,108	9
2	AHR	C	1	10/10	0.81	0.23	59,66,74,74	10
2	AHR	C	2	9/10	0.83	0.28	53,61,65,67	9
2	AHR	D	3	9/10	0.85	0.31	63,70,76,77	9
2	AHR	D	5	9/10	0.85	0.26	63,69,79,81	9
2	AHR	C	4	9/10	0.86	0.24	49,53,61,65	9
2	AHR	D	1	10/10	0.86	0.17	73,80,88,88	10
2	AHR	D	6	9/10	0.88	0.22	70,78,86,86	9
2	AHR	C	3	9/10	0.88	0.26	49,56,62,63	9
2	AHR	D	2	9/10	0.88	0.26	67,74,78,81	9
2	AHR	C	6	9/10	0.89	0.19	57,64,72,73	9
2	AHR	D	4	9/10	0.91	0.24	63,67,75,79	9

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	SO4	A	703	5/5	0.54	0.18	93,99,115,134	5
3	SO4	A	705	5/5	0.56	0.13	125,130,132,141	5
3	SO4	A	712	5/5	0.66	0.16	135,135,135,135	0
3	SO4	B	705	5/5	0.71	0.10	119,119,124,135	0
3	SO4	A	709	5/5	0.75	0.10	114,118,120,140	0
3	SO4	B	703	5/5	0.79	0.15	80,82,90,100	5
3	SO4	B	706	5/5	0.79	0.15	118,118,127,143	0
3	SO4	B	704	5/5	0.80	0.12	81,84,91,105	0
4	PEG	A	716	7/7	0.80	0.25	83,83,83,83	0
3	SO4	A	708	5/5	0.81	0.17	85,101,115,117	5
3	SO4	A	707	5/5	0.81	0.09	112,118,137,140	0
4	PEG	B	711	7/7	0.81	0.18	74,78,83,94	0
3	SO4	B	707	5/5	0.83	0.16	33,43,67,75	5
3	SO4	B	708	5/5	0.83	0.23	111,111,111,111	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	701	5/5	0.84	0.12	64,69,87,87	5
3	SO4	A	710	5/5	0.86	0.16	74,80,83,92	5
3	SO4	A	711	5/5	0.86	0.17	54,54,54,54	5
3	SO4	A	706	5/5	0.86	0.14	73,82,85,89	5
3	SO4	A	701	5/5	0.86	0.11	75,82,93,95	0
4	PEG	B	712	7/7	0.87	0.14	60,64,78,80	0
4	PEG	A	714	7/7	0.88	0.14	64,67,71,72	0
3	SO4	B	702	5/5	0.88	0.14	66,69,87,93	5
4	PEG	A	715	7/7	0.89	0.16	59,68,72,83	0
4	PEG	A	713	7/7	0.89	0.18	74,82,91,94	0
4	PEG	B	713	7/7	0.89	0.15	54,59,67,73	0
4	PEG	B	710	7/7	0.90	0.17	64,76,81,84	0
4	PEG	B	709	7/7	0.93	0.12	47,55,59,62	0
3	SO4	A	704	5/5	0.96	0.07	61,64,68,70	0
3	SO4	A	702	5/5	0.98	0.06	53,56,63,68	0

6.5 Other polymers

There are no such residues in this entry.