



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 12:10 PM JST

PDB ID : 6JG1
Title : Crystal structure of barley exohydrolaseI wildtype in complex with 4I,4III,4V-S-trithiocellohexaose
Authors : Luang, S.; Streltsov, V.A.; Hrmova, M.
Deposited on : 2019-02-13
Resolution : 1.78 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 : 2.31.2
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) : 2.31.2

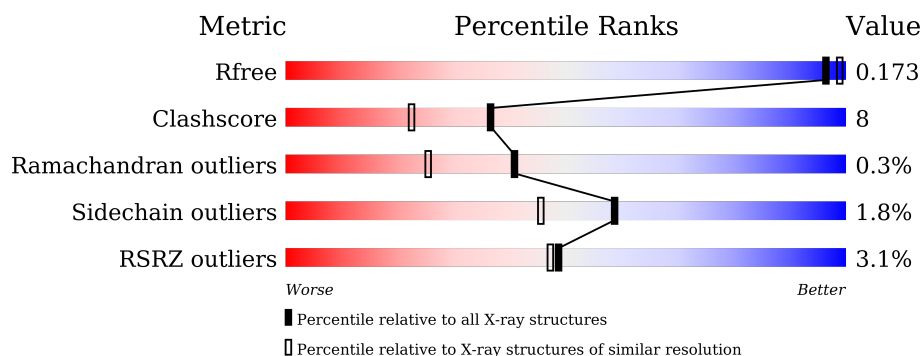
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	609	
2	B	3	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5347 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 Barley exohydrolase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	11	0
			4628	2929	801	870	28			

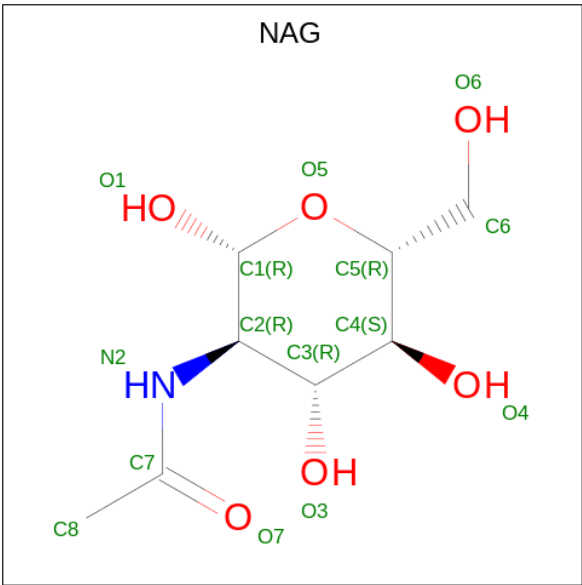
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP A0A287SCR5
A	-2	HIS	-	expression tag	UNP A0A287SCR5
A	-1	ALA	-	expression tag	UNP A0A287SCR5
A	0	ALA	-	expression tag	UNP A0A287SCR5
A	320	LYS	ASN	See sequence details	UNP A0A287SCR5

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1-thio-beta-D-glucopyranose.

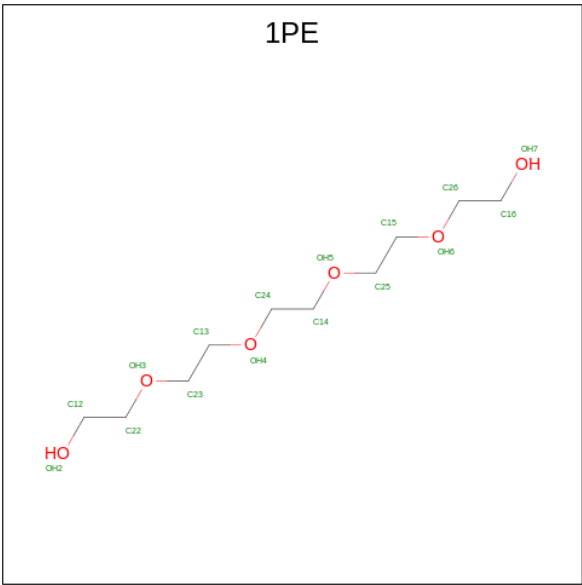
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	O	S	0	1	0
			35	18	15	2			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



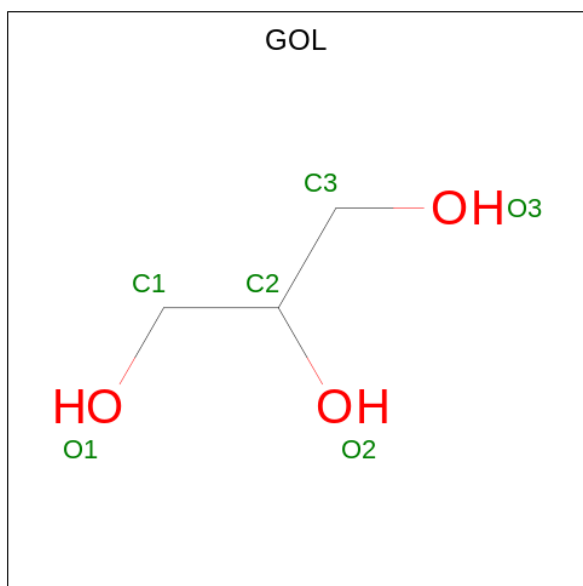
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

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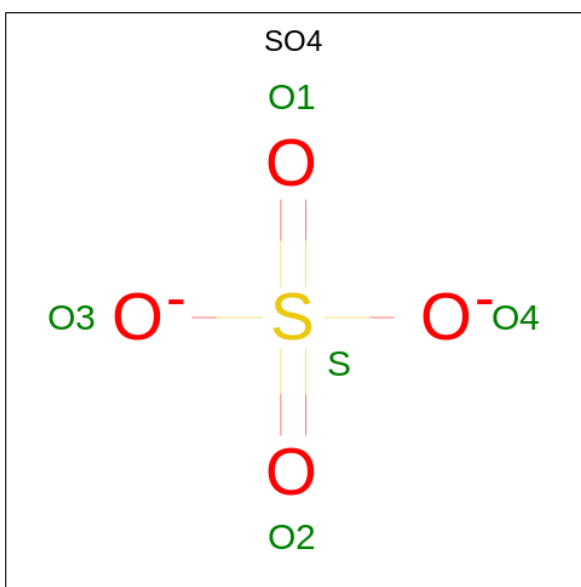
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 11 6 5	0	1
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 19 12 7	0	1

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

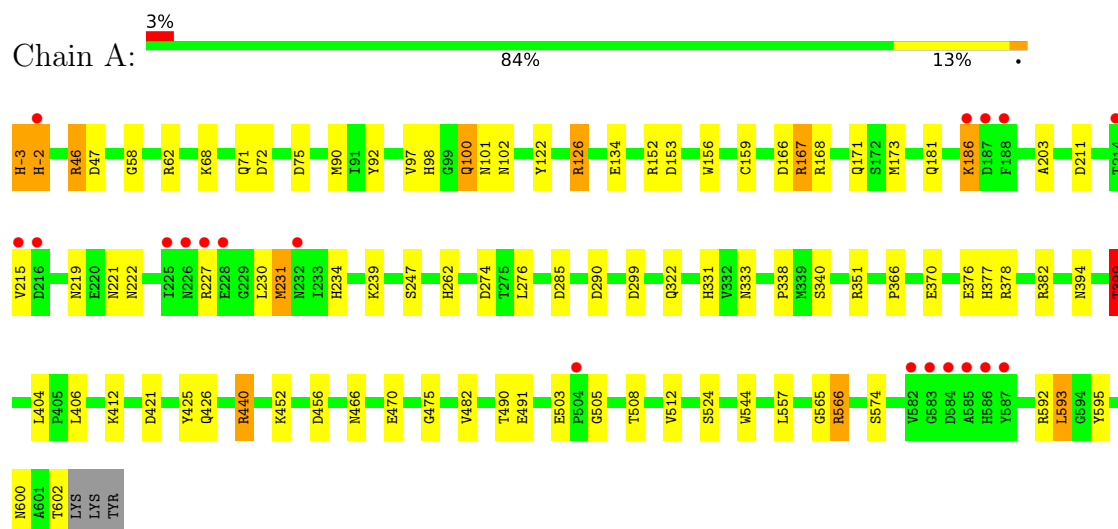
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	545	Total	O	0	0
			545	545		

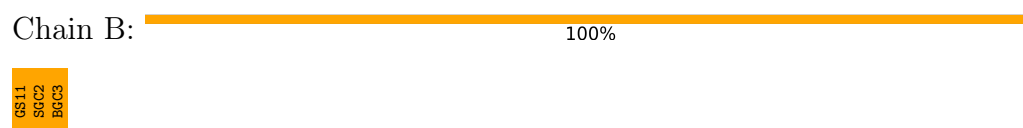
3 Residue-property plots [i](#)

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: Barley exohydrolase I



- Molecule 2: beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1-thio-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.76Å 99.76Å 183.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 1.78 48.13 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.17-1.78) 99.9 (48.13-1.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.136 , 0.164 0.148 , 0.173	Depositor DCC
R_{free} test set	4447 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5347	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 3.33% 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: SGC, GS1, GOL, SO4, BGC, NAG, 1PE

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	1.17	8/4784 (0.2%)	1.26	47/6496 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	503	GLU	CD-OE2	12.22	1.39	1.25
1	A	426	GLN	CB-CG	-7.02	1.33	1.52
1	A	126	ARG	CD-NE	-6.69	1.35	1.46
1	A	399	THR	CB-CG2	-6.32	1.31	1.52
1	A	333	ASN	CG-ND2	5.69	1.47	1.32
1	A	595	TYR	CE2-CZ	-5.45	1.31	1.38
1	A	574	SER	CA-CB	5.44	1.61	1.52
1	A	376	GLU	CD-OE2	5.24	1.31	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH1	20.76	130.68	120.30
1	A	126	ARG	NE-CZ-NH2	-20.00	110.30	120.30
1	A	68	LYS	CD-CE-NZ	11.57	138.32	111.70
1	A	46	ARG	NE-CZ-NH2	10.20	125.40	120.30
1	A	452	LYS	CD-CE-NZ	-9.96	88.80	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	A	152	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	A	351	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	62	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	153	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	376	GLU	OE1-CD-OE2	-7.54	114.25	123.30
1	A	211	ASP	CB-CG-OD1	7.09	124.69	118.30
1	A	47	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	72	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	A	592	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	A	126	ARG	CD-NE-CZ	6.74	133.03	123.60
1	A	274	ASP	CB-CG-OD1	6.66	124.30	118.30
1	A	440	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	421	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	399	THR	N-CA-CB	-6.30	98.34	110.30
1	A	593	LEU	CB-CG-CD2	6.28	121.68	111.00
1	A	46	ARG	CD-NE-CZ	6.28	132.39	123.60
1	A	46	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	A	456	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	A	173[A]	MET	CG-SD-CE	5.94	109.70	100.20
1	A	173[B]	MET	CG-SD-CE	5.94	109.70	100.20
1	A	159	CYS	CA-CB-SG	-5.83	103.50	114.00
1	A	231	MET	CG-SD-CE	-5.66	91.14	100.20
1	A	382	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	215[A]	VAL	CG1-CB-CG2	5.62	119.89	110.90
1	A	215[B]	VAL	CG1-CB-CG2	5.62	119.89	110.90
1	A	421	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	440	ARG	CG-CD-NE	-5.43	100.40	111.80
1	A	456	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	166	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	167	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	62	ARG	CG-CD-NE	-5.23	100.83	111.80
1	A	425	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	215[A]	VAL	CA-CB-CG2	5.18	118.68	110.90
1	A	215[B]	VAL	CA-CB-CG2	5.18	118.68	110.90
1	A	75	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	92	TYR	CB-CG-CD1	5.14	124.08	121.00
1	A	557	LEU	CB-CG-CD2	5.14	119.73	111.00
1	A	299	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	566[A]	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	566[B]	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	75	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	HIS	Peptide

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	4628	0	4621	64	0
2	B	35	0	27	7	0
3	A	42	0	39	8	0
4	A	64	0	54	7	0
5	A	18	0	24	4	0
6	A	15	0	0	0	0
7	A	545	0	0	22	0
All	All	5347	0	4765	75	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 8.

All (75) 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:600:ASN:HD21	3:A:703:NAG:C1	1.10	1.58
1:A:221:ASN:ND2	3:A:702:NAG:C1	1.72	1.48
1:A:600:ASN:ND2	3:A:703:NAG:C1	1.94	1.30
7:A:805:HOH:O	2:B:1:GS1:H5	0.98	1.14
1:A:394:ASN:HD21	1:A:404:LEU:H	1.17	0.91
1:A:600:ASN:HD21	3:A:703:NAG:C2	1.83	0.91
7:A:805:HOH:O	2:B:1:GS1:C5	1.70	0.85
1:A:156:TRP:HE1	1:A:219:ASN:HD22	1.28	0.81
1:A:466[A]:ASN:ND2	1:A:508:THR:OG1	2.15	0.79
2:B:2[B]:SGC:O6	2:B:3:BGC:C1	2.33	0.76
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.50	0.75
1:A:221:ASN:ND2	3:A:702:NAG:O5	2.20	0.75
1:A:167:ARG:HH21	1:A:171:GLN:HE22	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:709:1PE:OH2	7:A:804:HOH:O	2.07	0.71
1:A:181:GLN:HE21	1:A:203:ALA:H	1.39	0.70
7:A:805:HOH:O	2:B:1:GS1:O4	2.11	0.69
1:A:97:VAL:H	1:A:101:ASN:HD21	1.42	0.67
1:A:322:GLN:HG3	7:A:866:HOH:O	1.95	0.67
1:A:262:HIS:HE1	1:A:285:ASP:H	1.42	0.65
1:A:122:TYR:CE2	1:A:126:ARG:HD2	2.32	0.65
1:A:58:GLY:H	1:A:102:ASN:ND2	1.95	0.64
1:A:156:TRP:HE1	1:A:219:ASN:ND2	1.95	0.64
1:A:470[B]:GLU:HG3	7:A:1189:HOH:O	1.97	0.63
1:A:566[A]:ARG:NH2	5:A:712:GOL:O3	2.31	0.63
1:A:340:SER:H	4:A:710:1PE:H221	1.64	0.62
1:A:167:ARG:HH21	1:A:171:GLN:NE2	1.97	0.61
1:A:482[B]:VAL:CG2	1:A:512:VAL:HG11	2.30	0.61
7:A:805:HOH:O	2:B:1:GS1:C4	2.25	0.60
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.16	0.59
1:A:602:THR:O	7:A:806:HOH:O	2.17	0.57
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.87	0.57
1:A:168:ARG:HD3	5:A:713:GOL:O2	2.04	0.57
1:A:234:HIS:HD2	7:A:1096:HOH:O	1.87	0.57
1:A:566[B]:ARG:NH1	7:A:810:HOH:O	2.29	0.57
1:A:600:ASN:CG	3:A:703:NAG:C1	2.69	0.57
1:A:97:VAL:H	1:A:101:ASN:ND2	2.02	0.57
1:A:262:HIS:CE1	1:A:285:ASP:H	2.23	0.55
4:A:710:1PE:H222	7:A:1253:HOH:O	2.07	0.55
7:A:820:HOH:O	2:B:1:GS1:C6	2.55	0.54
1:A:331:HIS:HD2	7:A:1231:HOH:O	1.90	0.54
1:A:230:LEU:HD23	1:A:231:MET:CE	2.38	0.53
1:A:602:THR:C	7:A:806:HOH:O	2.47	0.53
1:A:600:ASN:ND2	3:A:703:NAG:C2	2.56	0.51
1:A:490:THR:HG22	1:A:491:GLU:HG3	1.93	0.51
1:A:234:HIS:HE1	7:A:1245:HOH:O	1.94	0.50
1:A:399:THR:HG23	7:A:963:HOH:O	2.11	0.50
4:A:705:1PE:C15	7:A:1081:HOH:O	2.59	0.50
1:A:186:LYS:N	1:A:186:LYS:HD2	2.28	0.49
1:A:566[B]:ARG:NE	7:A:818:HOH:O	2.45	0.48
1:A:370:GLU:OE2	7:A:807:HOH:O	2.20	0.48
1:A:602:THR:HG21	7:A:1326:HOH:O	2.13	0.47
1:A:167:ARG:HH22	5:A:713:GOL:H2	1.79	0.47
1:A:-3:HIS:HA	1:A:-2:HIS:HD2	1.80	0.47
1:A:338:PRO:HB2	4:A:710:1PE:H221	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239[A]:LYS:HD3	1:A:276:LEU:HD22	1.96	0.46
1:A:167:ARG:NH2	5:A:713:GOL:H2	2.30	0.46
1:A:222:ASN:HB2	3:A:702:NAG:H82	1.97	0.46
1:A:71:GLN:HE22	1:A:366:PRO:HA	1.80	0.45
1:A:181:GLN:HE22	1:A:247:SER:H	1.65	0.44
1:A:524:SER:O	1:A:544:TRP:HA	2.18	0.44
1:A:340:SER:H	4:A:710:1PE:C22	2.30	0.42
1:A:181:GLN:HE22	1:A:247:SER:N	2.18	0.42
1:A:-3:HIS:O	1:A:-2:HIS:HB2	2.20	0.42
1:A:58:GLY:H	1:A:102:ASN:HD21	1.68	0.41
1:A:399:THR:CG2	7:A:963:HOH:O	2.67	0.41
1:A:404:LEU:HD23	1:A:406:LEU:HG	2.02	0.41
1:A:482[B]:VAL:HG22	1:A:512:VAL:HG11	2.02	0.41
1:A:134:GLU:OE2	1:A:377:HIS:CD2	2.71	0.41
1:A:46:ARG:HD2	7:A:819:HOH:O	2.21	0.40
1:A:565:GLY:C	1:A:566[B]:ARG:HG2	2.40	0.40
1:A:167:ARG:NH2	1:A:171:GLN:HE22	2.12	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	615/609 (101%)	597 (97%)	16 (3%)	2 (0%)	41 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	505	GLY

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	498/490 (102%)	489 (98%)	9 (2%)	59 45

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

Mol	Chain	Res	Type
1	A	90	MET
1	A	98	HIS
1	A	100	GLN
1	A	186	LYS
1	A	227	ARG
1	A	290	ASP
1	A	399	THR
1	A	440	ARG
1	A	593	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	71	GLN
1	A	100	GLN
1	A	101	ASN
1	A	102	ASN
1	A	112	ASN
1	A	171	GLN
1	A	181	GLN
1	A	199	ASN
1	A	219	ASN
1	A	234	HIS
1	A	262	HIS
1	A	265	GLN
1	A	331	HIS
1	A	377	HIS
1	A	394	ASN

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Mol	Chain	Res	Type
1	A	600	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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$
3	NAG	A	702	-	14,14,15	0.56	0	17,19,21	2.81	5 (29%)
3	NAG	A	703	-	14,14,15	0.89	0	17,19,21	1.03	0
3	NAG	A	701	-	14,14,15	0.79	0	17,19,21	1.66	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	702	-	-	0/6/23/26	0/1/1/1
3	NAG	A	703	-	-	0/6/23/26	0/1/1/1
3	NAG	A	701	-	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAG	O5-C1-C2	7.39	122.96	111.29
3	A	702	NAG	C1-O5-C5	4.76	118.64	112.19
3	A	701	NAG	O5-C5-C6	4.31	113.96	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAG	C1-C2-N2	3.65	116.73	110.49
3	A	702	NAG	C3-C4-C5	3.44	116.38	110.24
3	A	702	NAG	C4-C3-C2	3.28	115.82	111.02
3	A	701	NAG	C1-C2-N2	-2.89	105.55	110.49
3	A	701	NAG	C1-O5-C5	-2.05	109.42	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NAG	3	0
3	A	703	NAG	5	0

5.5 Carbohydrates [i](#)

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	GS1	B	1	2	11,12,12	0.75	0	15,17,17	1.30	1 (6%)
2	SGC	B	2[A]	-	10,11,12	2.38	4 (40%)	12,15,17	2.24	4 (33%)
2	SGC	B	2[B]	-	10,11,12	2.34	4 (40%)	12,15,17	2.41	5 (41%)
2	BGC	B	3	2	11,11,12	0.89	0	15,15,17	3.44	7 (46%)

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	GS1	B	1	2	-	1/2/22/22	0/1/1/1
2	SGC	B	2[A]	-	-	0/2/19/22	0/1/1/1
2	SGC	B	2[B]	-	-	2/2/19/22	0/1/1/1
2	BGC	B	3	2	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2[A]	SGC	C5-C4	4.49	1.56	1.53
2	B	2[B]	SGC	C5-C4	4.49	1.56	1.53
2	B	2[A]	SGC	O5-C5	3.64	1.50	1.43
2	B	2[B]	SGC	O5-C5	3.64	1.50	1.43
2	B	2[A]	SGC	C6-C5	3.20	1.62	1.51
2	B	2[B]	SGC	C6-C5	3.20	1.62	1.51
2	B	2[A]	SGC	C2-C3	2.07	1.55	1.52
2	B	2[B]	SGC	C2-C3	2.07	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BGC	C1-O5-C5	9.06	124.47	112.19
2	B	3	BGC	O5-C1-C2	5.63	119.46	110.77
2	B	2[A]	SGC	O5-C5-C6	5.41	115.68	107.20
2	B	2[B]	SGC	O5-C5-C6	5.41	115.68	107.20
2	B	3	BGC	C1-C2-C3	4.47	115.16	109.67
2	B	3	BGC	O5-C5-C6	-4.15	100.70	107.20
2	B	2[B]	SGC	O6-C6-C5	-3.56	99.07	111.29
2	B	1	GS1	O2-C2-C1	-2.73	105.24	110.27
2	B	3	BGC	O2-C2-C1	2.64	114.55	109.15
2	B	3	BGC	C6-C5-C4	2.45	118.75	113.00
2	B	2[A]	SGC	C1-C2-C3	2.41	112.62	109.67
2	B	2[B]	SGC	C1-C2-C3	2.41	112.62	109.67
2	B	2[A]	SGC	O3-C3-C4	2.22	113.68	109.12
2	B	2[B]	SGC	O3-C3-C4	2.22	113.68	109.12
2	B	3	BGC	C2-C3-C4	-2.16	107.16	110.89
2	B	2[A]	SGC	O2-C2-C3	2.08	114.31	110.14
2	B	2[B]	SGC	O2-C2-C3	2.08	114.31	110.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

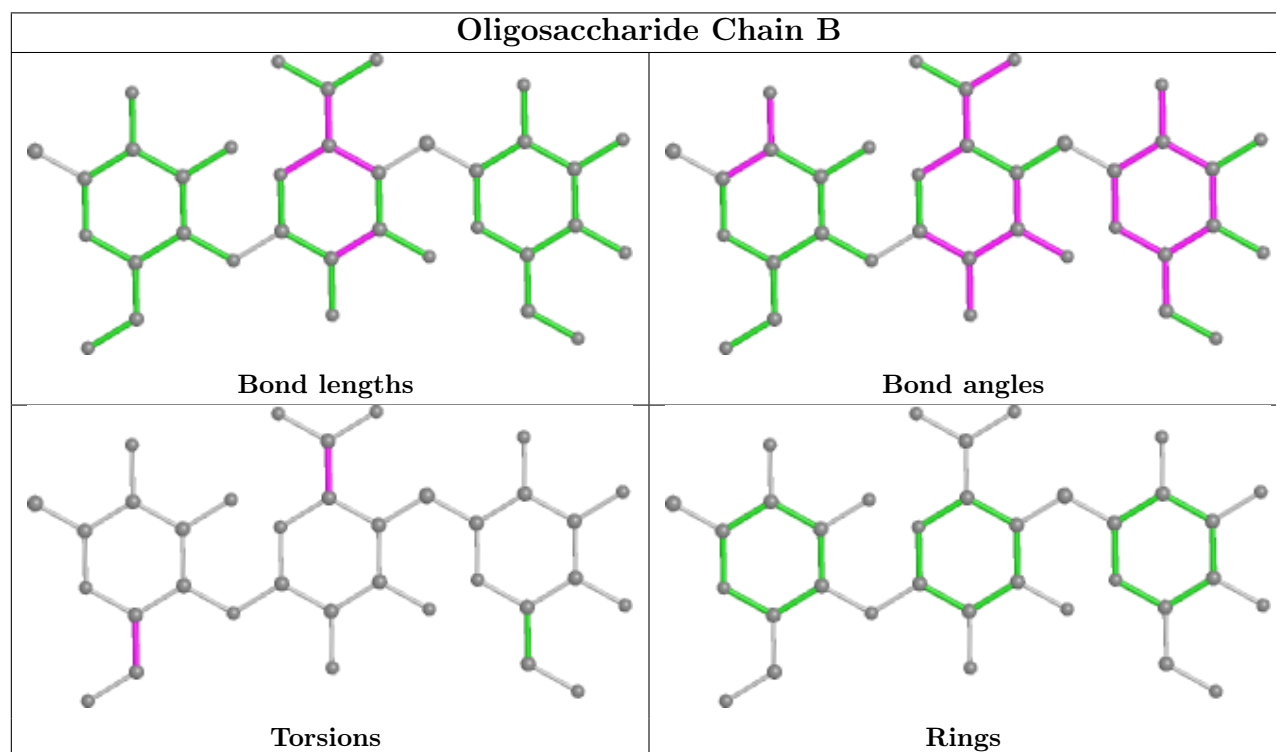
Mol	Chain	Res	Type	Atoms
2	B	2[B]	SGC	O5-C5-C6-O6
2	B	2[B]	SGC	C4-C5-C6-O6
2	B	1	GS1	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2[B]	SGC	2	0
2	B	1	GS1	5	0
2	B	3	BGC	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](#)

19 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	1PE	A	707	-	6,6,15	0.83	0	5,5,14	0.66	0
4	1PE	A	710	-	4,4,15	1.38	1 (25%)	3,3,14	0.76	0
4	1PE	A	711[A]	-	15,15,15	1.22	0	14,14,14	1.63	4 (28%)
5	GOL	A	712	-	5,5,5	0.64	0	5,5,5	0.90	0
6	SO4	A	716	-	4,4,4	0.55	0	6,6,6	0.75	0
3	NAG	A	701	-	14,14,15	0.79	0	17,19,21	1.66	3 (17%)
4	1PE	A	708[B]	-	9,9,15	0.47	0	8,8,14	1.55	1 (12%)
3	NAG	A	702	-	14,14,15	0.56	0	17,19,21	2.81	5 (29%)
4	1PE	A	711[B]	-	15,15,15	1.19	0	14,14,14	1.57	3 (21%)
5	GOL	A	713	-	5,5,5	0.35	0	5,5,5	0.70	0
5	GOL	A	714	-	5,5,5	0.18	0	5,5,5	0.96	0
4	1PE	A	709	-	4,4,15	0.63	0	3,3,14	0.33	0
4	1PE	A	704	-	6,6,15	0.46	0	5,5,14	0.68	0
6	SO4	A	715	-	4,4,4	0.44	0	6,6,6	0.84	0
4	1PE	A	706	-	4,4,15	0.68	0	3,3,14	0.35	0
3	NAG	A	703	-	14,14,15	0.89	0	17,19,21	1.03	0
6	SO4	A	717	-	4,4,4	0.39	0	6,6,6	0.94	0
4	1PE	A	708[A]	-	9,9,15	0.49	0	8,8,14	1.26	1 (12%)
4	1PE	A	705	-	4,4,15	1.04	0	3,3,14	0.89	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
5	GOL	A	713	-	-	2/4/4/4	-
4	1PE	A	704	-	-	1/4/4/13	-
4	1PE	A	707	-	-	1/4/4/13	-
4	1PE	A	710	-	-	1/2/2/13	-
4	1PE	A	711[A]	-	-	9/13/13/13	-
4	1PE	A	708[B]	-	-	4/7/7/13	-
4	1PE	A	706	-	-	1/2/2/13	-
3	NAG	A	703	-	-	0/6/23/26	0/1/1/1
5	GOL	A	714	-	-	2/4/4/4	-
4	1PE	A	709	-	-	0/2/2/13	-
3	NAG	A	702	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	712	-	-	2/4/4/4	-
4	1PE	A	711[B]	-	-	10/13/13/13	-
4	1PE	A	708[A]	-	-	4/7/7/13	-
4	1PE	A	705	-	-	0/2/2/13	-
3	NAG	A	701	-	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	710	1PE	OH3-C22	2.24	1.53	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAG	O5-C1-C2	7.39	122.96	111.29
3	A	702	NAG	C1-O5-C5	4.76	118.64	112.19
3	A	701	NAG	O5-C5-C6	4.31	113.96	107.20
4	A	708[B]	1PE	OH2-C12-C22	-3.79	89.84	111.81
3	A	702	NAG	C1-C2-N2	3.65	116.73	110.49
3	A	702	NAG	C3-C4-C5	3.44	116.38	110.24
3	A	702	NAG	C4-C3-C2	3.28	115.82	111.02
3	A	701	NAG	C1-C2-N2	-2.89	105.55	110.49
4	A	708[A]	1PE	OH2-C12-C22	-2.80	95.60	111.81
4	A	711[A]	1PE	OH4-C24-C14	2.62	122.20	110.39
4	A	711[B]	1PE	OH4-C24-C14	2.62	122.20	110.39
4	A	711[A]	1PE	C26-OH6-C15	-2.52	102.35	113.29
4	A	711[A]	1PE	C24-OH4-C13	2.47	123.97	113.29
4	A	711[B]	1PE	C24-OH4-C13	2.47	123.97	113.29
4	A	711[A]	1PE	OH3-C23-C13	2.46	121.49	110.39
4	A	711[B]	1PE	OH3-C23-C13	2.46	121.49	110.39
3	A	701	NAG	C1-O5-C5	-2.05	109.42	112.19

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	712	GOL	C1-C2-C3-O3
4	A	711[A]	1PE	C13-C23-OH3-C22
4	A	711[B]	1PE	C13-C23-OH3-C22
4	A	711[A]	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
4	A	711[B]	1PE	C14-C24-OH4-C13
4	A	711[A]	1PE	OH6-C15-C25-OH5
4	A	711[B]	1PE	OH6-C15-C25-OH5
4	A	711[A]	1PE	C16-C26-OH6-C15
4	A	711[A]	1PE	OH5-C14-C24-OH4
4	A	711[B]	1PE	OH5-C14-C24-OH4
5	A	712	GOL	O2-C2-C3-O3
4	A	711[B]	1PE	OH7-C16-C26-OH6
5	A	714	GOL	C1-C2-C3-O3
4	A	710	1PE	OH2-C12-C22-OH3
5	A	714	GOL	O2-C2-C3-O3
3	A	701	NAG	C4-C5-C6-O6
4	A	707	1PE	OH6-C15-C25-OH5
4	A	708[B]	1PE	OH2-C12-C22-OH3
4	A	708[A]	1PE	C23-C13-OH4-C24
4	A	708[B]	1PE	C23-C13-OH4-C24
4	A	708[A]	1PE	C12-C22-OH3-C23
4	A	708[B]	1PE	C12-C22-OH3-C23
4	A	711[B]	1PE	C16-C26-OH6-C15
4	A	708[A]	1PE	OH5-C14-C24-OH4
4	A	708[B]	1PE	OH5-C14-C24-OH4
4	A	711[A]	1PE	C12-C22-OH3-C23
4	A	711[B]	1PE	C12-C22-OH3-C23
4	A	711[A]	1PE	OH4-C13-C23-OH3
4	A	711[B]	1PE	OH4-C13-C23-OH3
4	A	706	1PE	OH7-C16-C26-OH6
4	A	704	1PE	C16-C26-OH6-C15
4	A	708[A]	1PE	OH2-C12-C22-OH3
5	A	713	GOL	O1-C1-C2-O2
5	A	713	GOL	O1-C1-C2-C3
4	A	711[A]	1PE	OH2-C12-C22-OH3
4	A	711[B]	1PE	OH2-C12-C22-OH3
4	A	711[A]	1PE	C23-C13-OH4-C24
4	A	711[B]	1PE	C23-C13-OH4-C24

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	710	1PE	5	0
5	A	712	GOL	1	0
3	A	702	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	713	GOL	3	0
4	A	709	1PE	1	0
3	A	703	NAG	5	0
4	A	705	1PE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	606/609 (99%)	-0.23	19 (3%)	49 47	12, 19, 36, 62	4 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	585	ALA	5.7
1	A	187	ASP	4.3
1	A	186	LYS	4.0
1	A	582	VAL	3.9
1	A	586	HIS	3.7
1	A	228	GLU	3.5
1	A	583	GLY	3.2
1	A	227	ARG	3.0
1	A	584	ASP	3.0
1	A	215[A]	VAL	2.8
1	A	226	ASN	2.8
1	A	-2	HIS	2.7
1	A	587	TYR	2.7
1	A	188	PHE	2.5
1	A	214	THR	2.5
1	A	504	PRO	2.4
1	A	216	ASP	2.2
1	A	232	ASN	2.1
1	A	225	ILE	2.0

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

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.

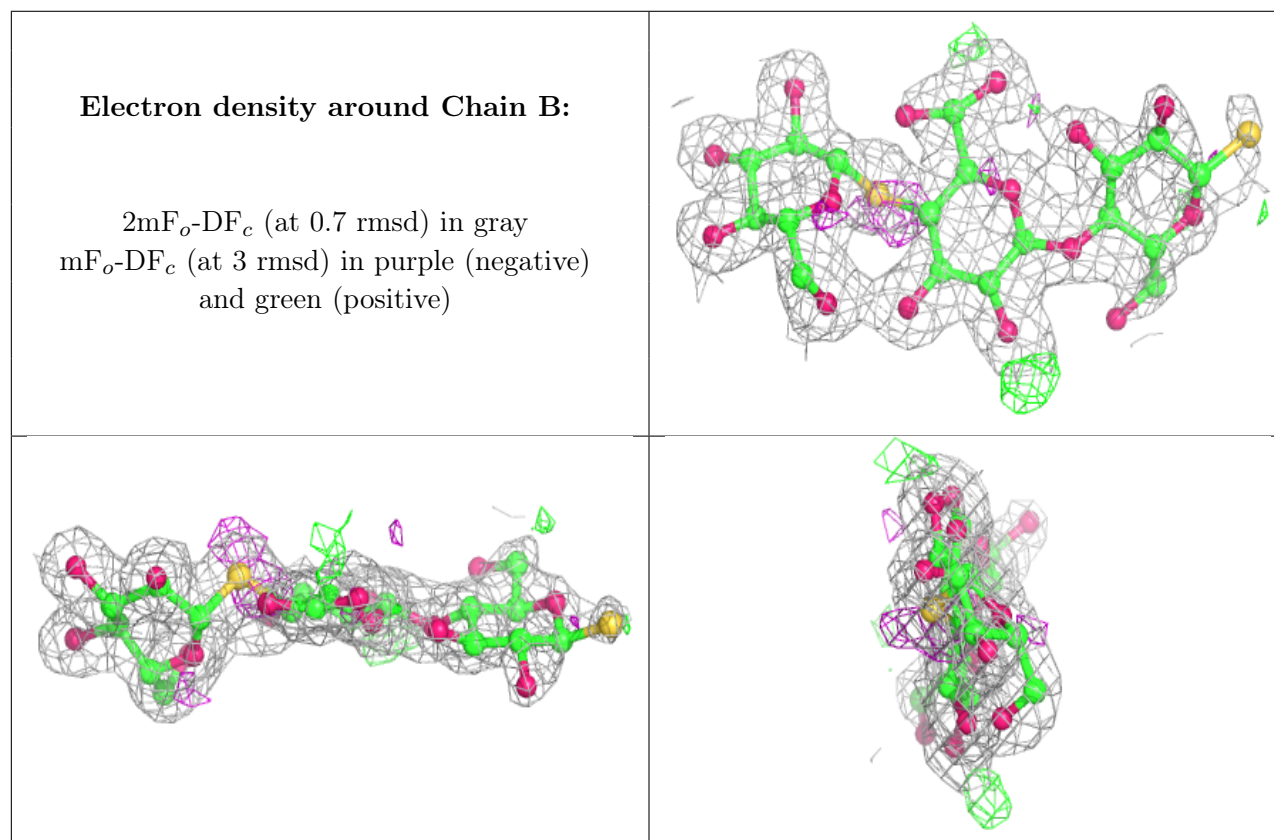
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	703	14/15	0.78	0.19	52,60,64,70	0
3	NAG	A	702	14/15	0.79	0.20	46,54,68,77	14
3	NAG	A	701	14/15	0.90	0.29	43,50,60,60	0

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(\AA^2)	Q<0.9
2	GS1	B	1	12/12	0.83	0.15	39,52,58,69	11
2	SGC	B	2[A]	11/12	0.92	0.12	21,29,31,34	1
2	SGC	B	2[B]	11/12	0.92	0.12	21,28,31,34	1
2	BGC	B	3	11/12	0.96	0.08	20,23,26,28	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands

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
4	1PE	A	706	5/16	0.73	0.15	56,57,66,71	0
4	1PE	A	707	7/16	0.76	0.16	44,50,64,68	0
4	1PE	A	711[A]	16/16	0.76	0.23	27,49,65,67	3
4	1PE	A	711[B]	16/16	0.76	0.23	36,49,65,67	3
3	NAG	A	703	14/15	0.78	0.19	52,60,64,70	0
3	NAG	A	702	14/15	0.79	0.20	46,54,68,77	14
5	GOL	A	712	6/6	0.79	0.30	50,53,65,66	0
5	GOL	A	713	6/6	0.85	0.28	62,69,75,81	0
4	1PE	A	709	5/16	0.86	0.15	54,59,63,70	0
4	1PE	A	710	5/16	0.86	0.17	24,26,43,49	0
4	1PE	A	704	7/16	0.87	0.15	49,53,57,59	0
6	SO4	A	717	5/5	0.87	0.16	36,42,45,45	5
4	1PE	A	705	5/16	0.88	0.17	35,36,55,64	0
4	1PE	A	708[B]	10/16	0.89	0.12	35,40,48,49	1
5	GOL	A	714	6/6	0.89	0.28	54,61,67,68	0
4	1PE	A	708[A]	10/16	0.89	0.12	34,40,48,49	1
3	NAG	A	701	14/15	0.90	0.29	43,50,60,60	0
6	SO4	A	716	5/5	0.92	0.13	31,35,44,45	5
6	SO4	A	715	5/5	0.94	0.13	32,33,40,41	5

6.5 Other polymers

There are no such residues in this entry.