



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 12:27 PM JST

PDB ID : 6LBB
Title : Crystal structure of barley exohydrolaseI W434A mutant in complex with 4I, 4III,4V-S-trithiocellohexaose
Authors : Luang, S.; Streltsov, V.A.; Hrmova, M.
Deposited on : 2019-11-14
Resolution : 1.80 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

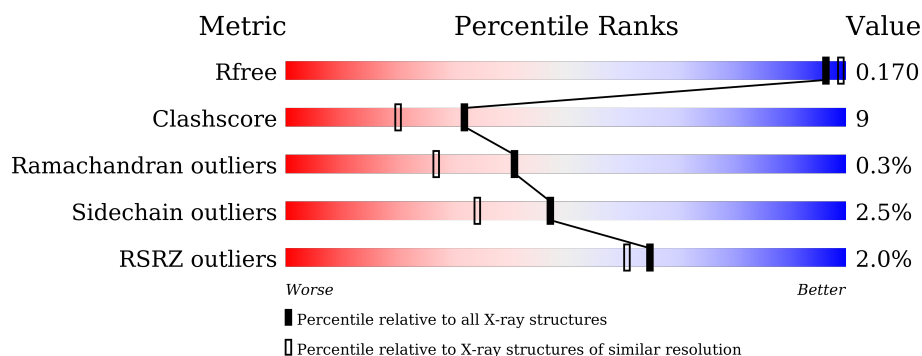
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
2	B	3	<div> <div>33%</div> <div>67%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5548 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 Beta-D-glucan exohydrolase isoenzyme ExoI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	10	16	0
			4627	2917	807	872	31			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP Q9XEI3
A	-2	HIS	-	expression tag	UNP Q9XEI3
A	-1	ALA	-	expression tag	UNP Q9XEI3
A	320	LYS	ASN	See sequence details	UNP Q9XEI3
A	434	ALA	TRP	engineered mutation	UNP Q9XEI3

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

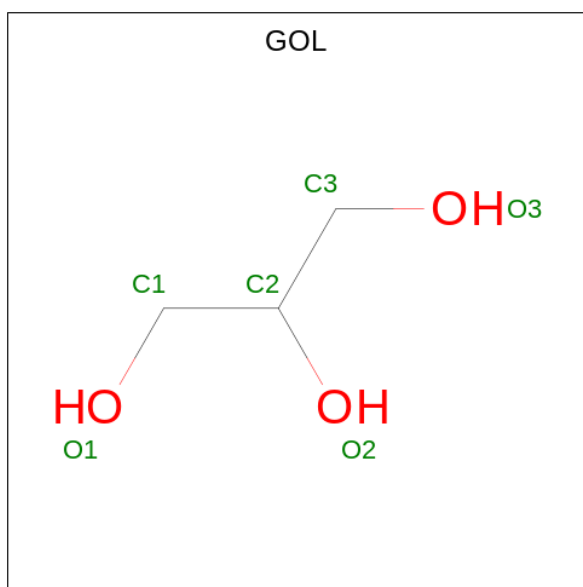
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	O	S	0	0	0
			34	18	14	2			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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



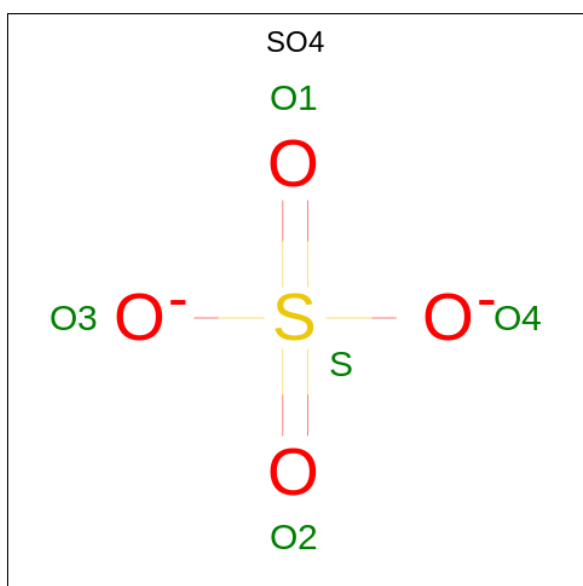
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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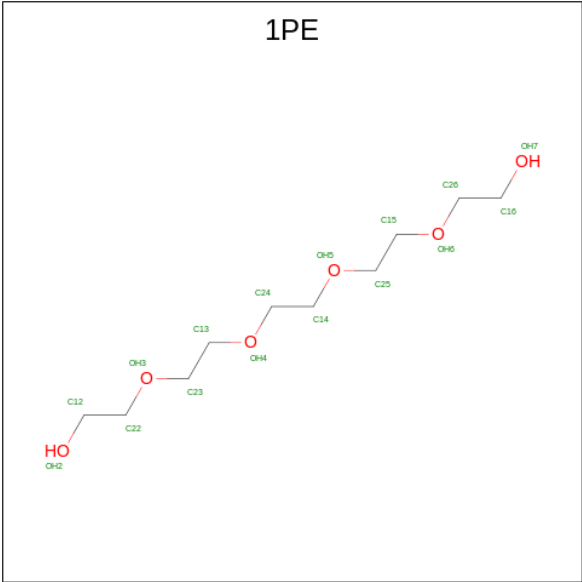
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



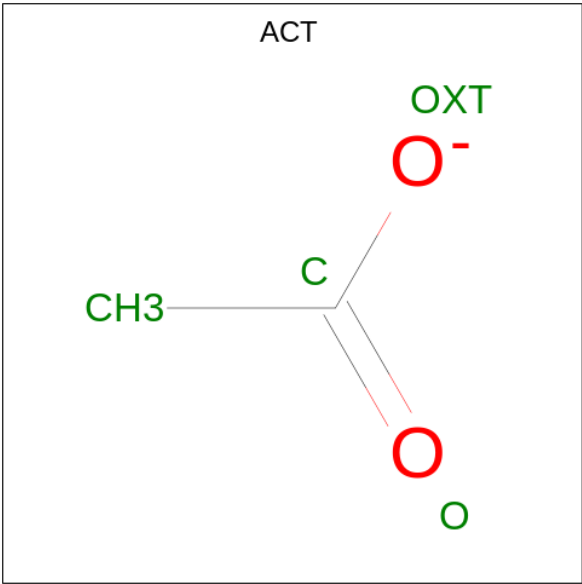
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0

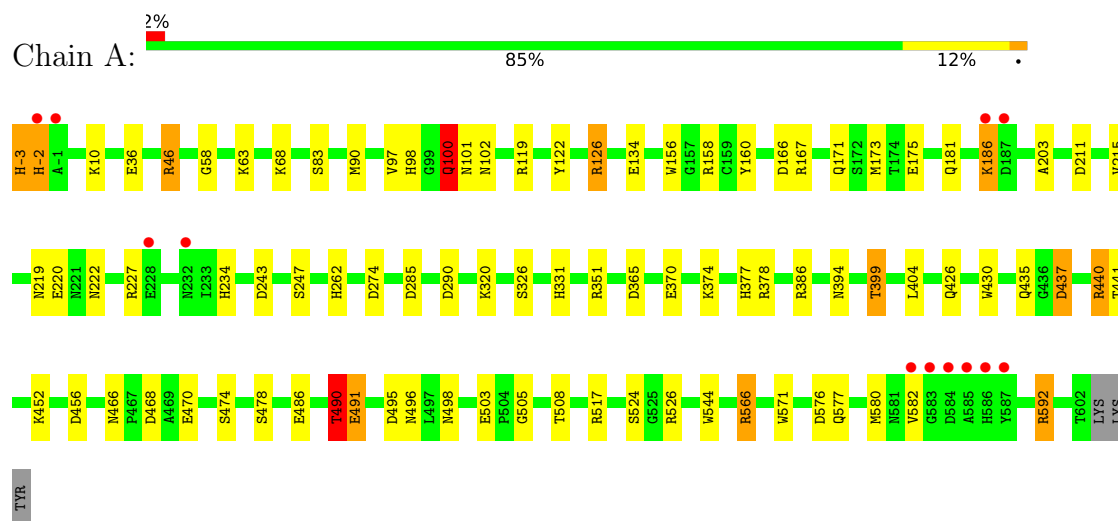
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	755	Total O 755 755	0	0

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: Beta-D-glucan exohydrolase isoenzyme ExoI



- 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	100.56Å 100.56Å 182.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.24 – 1.80 45.58 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.24-1.80) 99.8 (45.58-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.137 , 0.161 0.149 , 0.170	Depositor DCC
R_{free} test set	4367 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5548	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SGC, SO4, ACT, BGC, 1PE, NAG, GOL, GS1

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	1.16	14/4806 (0.3%)	1.24	45/6521 (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	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	503	GLU	CD-OE2	13.44	1.40	1.25
1	A	517	ARG	CZ-NH1	9.78	1.45	1.33
1	A	370	GLU	CD-OE2	8.66	1.35	1.25
1	A	399	THR	CB-CG2	-7.83	1.26	1.52
1	A	126	ARG	CD-NE	-7.62	1.33	1.46
1	A	491[B]	GLU	CG-CD	7.21	1.62	1.51
1	A	571	TRP	CE3-CZ3	7.03	1.50	1.38
1	A	220	GLU	CD-OE1	6.63	1.32	1.25
1	A	426	GLN	CB-CG	-6.50	1.35	1.52
1	A	440	ARG	CZ-NH1	6.47	1.41	1.33
1	A	326	SER	CB-OG	5.58	1.49	1.42
1	A	175	GLU	CD-OE1	-5.30	1.19	1.25
1	A	100	GLN	CD-OE1	5.16	1.35	1.24
1	A	370	GLU	CG-CD	5.15	1.59	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH1	25.19	132.89	120.30
1	A	126	ARG	NE-CZ-NH2	-22.98	108.81	120.30
1	A	440	ARG	NE-CZ-NH2	-11.27	114.67	120.30
1	A	-3	HIS	O-C-N	-10.86	105.33	122.70
1	A	46[A]	ARG	NE-CZ-NH1	-9.97	115.31	120.30
1	A	46[B]	ARG	NE-CZ-NH1	-9.97	115.31	120.30
1	A	517	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	A	46[A]	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	A	46[B]	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	A	126	ARG	CD-NE-CZ	8.29	135.21	123.60
1	A	158	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	A	68	LYS	CD-CE-NZ	7.61	129.20	111.70
1	A	592	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	274	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	211	ASP	CB-CG-OD1	6.86	124.48	118.30
1	A	243	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	A	468	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	-3	HIS	CA-C-N	6.69	131.92	117.20
1	A	495	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	440	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	490	THR	CB-CA-C	-6.49	94.07	111.60
1	A	351	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	456	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	A	437	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	173[A]	MET	CG-SD-CE	6.13	110.01	100.20
1	A	173[B]	MET	CG-SD-CE	6.13	110.01	100.20
1	A	490	THR	N-CA-CB	6.09	121.87	110.30
1	A	119	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	378	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	365	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	211	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	440	ARG	CG-CD-NE	-5.72	99.78	111.80
1	A	166	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	526	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	566[A]	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	566[B]	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	166	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	576	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	365	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	592	ARG	CG-CD-NE	-5.17	100.95	111.80
1	A	10	LYS	CD-CE-NZ	-5.15	99.86	111.70
1	A	491[B]	GLU	CG-CD-OE1	5.14	128.59	118.30
1	A	490	THR	OG1-CB-CG2	5.12	121.77	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	A	452	LYS	CD-CE-NZ	-5.02	100.16	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	HIS	Mainchain,Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4627	0	4585	75	0
2	B	34	0	29	10	0
3	A	42	0	39	0	0
4	A	36	0	48	10	0
5	A	10	0	0	0	0
6	A	28	0	34	10	0
7	A	16	0	12	0	0
8	A	755	0	0	22	1
All	All	5548	0	4747	85	1

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 9.

All (85) 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)
6:A:712[A]:1PE:H221	8:A:886:HOH:O	1.47	1.15
1:A:498:ASN:HB3	8:A:1361:HOH:O	1.45	1.15
6:A:712[B]:1PE:H221	8:A:886:HOH:O	1.52	1.09
1:A:490:THR:HG22	8:A:851:HOH:O	1.64	0.96
1:A:466[A]:ASN:ND2	1:A:508:THR:OG1	1.98	0.96
1:A:577:GLN:HB3	1:A:580[B]:MET:CE	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:THR:CG2	8:A:851:HOH:O	2.14	0.91
1:A:435:GLN:HE21	2:B:1:GS1:H62	1.35	0.89
1:A:394:ASN:HD21	1:A:404:LEU:H	1.22	0.84
1:A:167:ARG:HH21	1:A:171:GLN:HE22	1.25	0.84
6:A:712[B]:1PE:OH2	8:A:804:HOH:O	1.96	0.83
1:A:491[B]:GLU:HG3	2:B:2:SGC:O3	1.78	0.83
1:A:435:GLN:HE21	2:B:1:GS1:C6	1.92	0.82
1:A:122:TYR:CE2	1:A:126:ARG:HD2	2.18	0.79
1:A:430:TRP:HE1	1:A:490:THR:HG21	1.48	0.77
1:A:435:GLN:HG2	2:B:1:GS1:H62	1.66	0.75
1:A:156:TRP:HE1	1:A:219:ASN:HD22	1.35	0.75
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.52	0.75
4:A:706:GOL:O2	8:A:803:HOH:O	1.95	0.74
1:A:491[B]:GLU:OE2	2:B:2:SGC:O3	2.05	0.73
1:A:374:LYS:NZ	8:A:806:HOH:O	2.01	0.72
4:A:709:GOL:O1	8:A:805:HOH:O	2.01	0.71
1:A:430:TRP:NE1	1:A:490:THR:HG21	2.07	0.70
1:A:496:ASN:HD22	6:A:713:1PE:H221	1.58	0.67
1:A:399:THR:HG23	8:A:872:HOH:O	1.95	0.67
1:A:577:GLN:HB3	1:A:580[B]:MET:HE2	1.75	0.67
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.08	0.66
1:A:435:GLN:NE2	2:B:1:GS1:H62	2.08	0.66
1:A:262:HIS:HE1	1:A:285:ASP:H	1.43	0.65
1:A:167:ARG:NH2	1:A:171:GLN:HE22	1.95	0.64
1:A:496:ASN:ND2	6:A:713:1PE:H221	2.14	0.63
1:A:97:VAL:H	1:A:101:ASN:HD21	1.46	0.62
1:A:435:GLN:CG	2:B:1:GS1:H62	2.30	0.61
1:A:181:GLN:HE21	1:A:203:ALA:H	1.46	0.61
1:A:167:ARG:HH21	1:A:171:GLN:NE2	1.98	0.61
1:A:490:THR:HG23	8:A:851:HOH:O	1.93	0.60
1:A:491[B]:GLU:OE2	2:B:2:SGC:C3	2.48	0.60
1:A:386:ARG:NH1	8:A:808:HOH:O	2.14	0.60
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.85	0.60
6:A:712[B]:1PE:C12	8:A:804:HOH:O	2.48	0.60
1:A:181:GLN:HE22	1:A:247:SER:H	1.52	0.57
1:A:577:GLN:CB	1:A:580[B]:MET:CE	2.79	0.56
1:A:63:LYS:HG2	8:A:1109:HOH:O	2.06	0.56
1:A:386:ARG:HH22	4:A:706:GOL:H32	1.70	0.56
1:A:491[B]:GLU:OE2	2:B:2:SGC:H3	2.06	0.56
1:A:46[B]:ARG:HD2	1:A:83:SER:OG	2.04	0.55
1:A:156:TRP:HE1	1:A:219:ASN:ND2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566[A]:ARG:NH1	4:A:705:GOL:H2	2.22	0.55
4:A:709:GOL:H12	8:A:1324:HOH:O	2.08	0.54
1:A:234:HIS:HD2	8:A:1147:HOH:O	1.91	0.54
1:A:262:HIS:CE1	1:A:285:ASP:H	2.25	0.54
1:A:331:HIS:HD2	8:A:1389:HOH:O	1.91	0.54
1:A:234:HIS:HE1	8:A:1398:HOH:O	1.90	0.53
1:A:478:SER:O	4:A:709:GOL:H32	2.09	0.53
1:A:58:GLY:H	1:A:102:ASN:ND2	2.07	0.53
1:A:577:GLN:HB3	1:A:580[B]:MET:HE1	1.89	0.53
1:A:577:GLN:CD	1:A:580[B]:MET:HE3	2.32	0.51
4:A:707:GOL:O3	4:A:707:GOL:O1	2.26	0.50
1:A:496:ASN:HD22	6:A:713:1PE:C22	2.22	0.49
1:A:122:TYR:O	1:A:126:ARG:HD3	2.13	0.49
1:A:486:GLU:OE2	6:A:713:1PE:H122	2.14	0.48
1:A:566[A]:ARG:HH12	4:A:705:GOL:C2	2.27	0.48
1:A:97:VAL:H	1:A:101:ASN:ND2	2.11	0.48
1:A:437:ASP:HB3	1:A:441:THR:HG21	1.95	0.47
1:A:491[B]:GLU:CG	2:B:2:SGC:O3	2.54	0.47
1:A:566[A]:ARG:NH1	4:A:705:GOL:C2	2.77	0.47
6:A:714:1PE:C23	8:A:1389:HOH:O	2.61	0.47
1:A:524:SER:O	1:A:544:TRP:HA	2.16	0.46
1:A:160:TYR:OH	1:A:490:THR:HG23	2.17	0.45
1:A:46[A]:ARG:NH1	8:A:822:HOH:O	2.50	0.45
1:A:215:VAL:HG23	1:A:222:ASN:O	2.18	0.43
6:A:713:1PE:H131	6:A:713:1PE:H222	1.52	0.43
1:A:122:TYR:CD2	1:A:126:ARG:HD2	2.53	0.43
1:A:186:LYS:N	1:A:186:LYS:HD3	2.33	0.43
1:A:100:GLN:HA	1:A:100:GLN:NE2	2.29	0.43
1:A:399:THR:CG2	8:A:1393:HOH:O	2.67	0.42
1:A:134:GLU:OE2	1:A:377:HIS:CD2	2.68	0.42
1:A:227[A]:ARG:NH1	8:A:807:HOH:O	2.02	0.41
1:A:577:GLN:CD	1:A:580[B]:MET:CE	2.89	0.41
1:A:386:ARG:HH22	4:A:706:GOL:C3	2.32	0.41
1:A:470:GLU:O	1:A:474[B]:SER:OG	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1306:HOH:O	8:A:1370:HOH:O[8_565]	1.92	0.28

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	618/609 (102%)	599 (97%)	17 (3%)	2 (0%)	41 27

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	500/489 (102%)	488 (98%)	12 (2%)	49 36

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	36	GLU
1	A	90	MET
1	A	98	HIS
1	A	100	GLN
1	A	186	LYS
1	A	290	ASP
1	A	320	LYS
1	A	440	ARG

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Mol	Chain	Res	Type
1	A	490	THR
1	A	582	VAL
1	A	592	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
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	331	HIS
1	A	377	HIS
1	A	394	ASN
1	A	435	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

3 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	0.78	0	15,17,17	2.25	7 (46%)
2	SGC	B	2	2	10,11,12	2.55	2 (20%)	12,15,17	2.48	5 (41%)
2	BGC	B	3	2	11,11,12	2.59	6 (54%)	15,15,17	2.96	8 (53%)

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	-	2/2/22/22	0/1/1/1
2	SGC	B	2	2	-	0/2/19/22	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	SGC	C3-C4	6.30	1.59	1.53
2	B	3	BGC	O3-C3	4.62	1.53	1.43
2	B	2	SGC	C5-C4	4.27	1.56	1.53
2	B	3	BGC	C1-C2	4.08	1.61	1.52
2	B	3	BGC	O4-C4	-3.22	1.35	1.43
2	B	3	BGC	C4-C3	2.68	1.59	1.52
2	B	3	BGC	C4-C5	2.46	1.58	1.53
2	B	3	BGC	O5-C5	-2.24	1.38	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BGC	C1-O5-C5	5.30	119.37	112.19
2	B	3	BGC	O5-C5-C6	-5.25	98.97	107.20
2	B	2	SGC	O5-C5-C6	-4.66	99.89	107.20
2	B	3	BGC	O4-C4-C3	-4.24	100.55	110.35
2	B	2	SGC	O3-C3-C4	4.22	117.78	109.12
2	B	1	GS1	C4-C3-C2	-4.07	103.71	110.82
2	B	1	GS1	C6-C5-C4	-4.01	103.61	113.00
2	B	3	BGC	O5-C5-C4	-3.70	101.82	110.83
2	B	2	SGC	C6-C5-C4	3.49	120.36	112.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GS1	O2-C2-C3	-3.38	102.54	110.35
2	B	3	BGC	O2-C2-C1	3.38	116.06	109.15
2	B	1	GS1	O4-C4-C5	-3.21	101.33	109.30
2	B	3	BGC	C1-C2-C3	2.87	113.20	109.67
2	B	1	GS1	O5-C5-C6	2.85	113.51	106.44
2	B	2	SGC	C1-C2-C3	-2.74	106.29	109.67
2	B	3	BGC	C2-C3-C4	-2.64	106.33	110.89
2	B	3	BGC	O3-C3-C2	2.52	114.82	109.99
2	B	2	SGC	O3-C3-C2	-2.46	105.28	109.99
2	B	1	GS1	O2-C2-C1	-2.42	105.82	110.27
2	B	1	GS1	O4-C4-C3	2.05	115.08	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

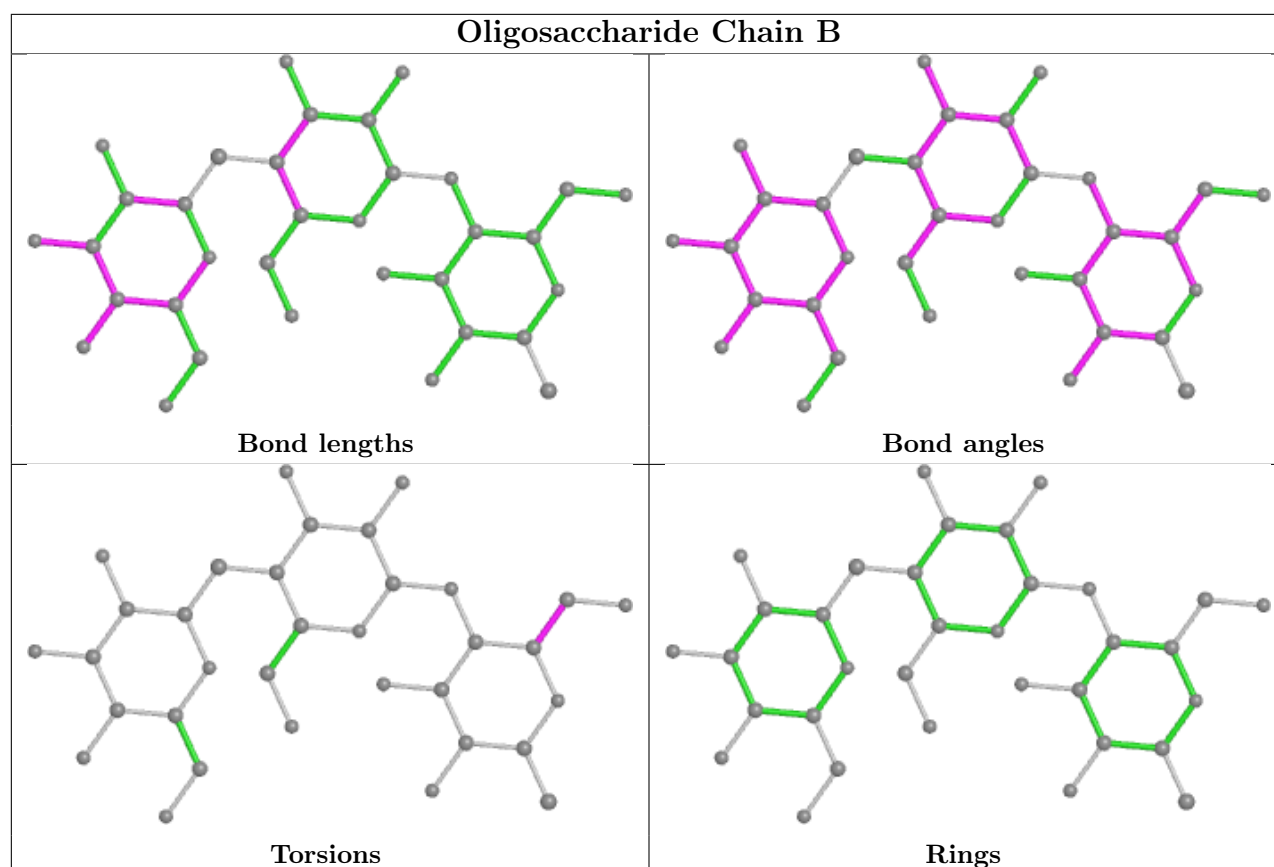
Mol	Chain	Res	Type	Atoms
2	B	1	GS1	O5-C5-C6-O6
2	B	1	GS1	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 10 short contacts:

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

21 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	GOL	A	708	-	5,5,5	0.23	0	5,5,5	0.60	0
7	ACT	A	718	-	3,3,3	0.69	0	3,3,3	0.84	0
6	1PE	A	713	-	6,6,15	1.28	0	5,5,14	1.54	1 (20%)
7	ACT	A	720	-	3,3,3	1.09	0	3,3,3	1.39	0
3	NAG	A	703	1	14,14,15	0.84	1 (7%)	17,19,21	1.31	3 (17%)
7	ACT	A	717	-	3,3,3	0.61	0	3,3,3	1.62	1 (33%)
6	1PE	A	716	-	4,4,15	0.65	0	3,3,14	0.40	0
4	GOL	A	704	-	5,5,5	0.67	0	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	A	712[B]	-	4,4,15	0.60	0	3,3,14	1.77	1 (33%)
4	GOL	A	706	-	5,5,5	0.56	0	5,5,5	1.01	0
3	NAG	A	701	1	14,14,15	0.73	0	17,19,21	2.00	8 (47%)
4	GOL	A	709	-	5,5,5	0.49	0	5,5,5	1.21	1 (20%)
6	1PE	A	714	-	4,4,15	0.80	0	3,3,14	0.48	0
3	NAG	A	702	1	14,14,15	1.22	1 (7%)	17,19,21	2.05	4 (23%)
6	1PE	A	712[A]	-	4,4,15	0.84	0	3,3,14	1.80	1 (33%)
7	ACT	A	719	-	3,3,3	0.77	0	3,3,3	1.83	1 (33%)
5	SO4	A	710	-	4,4,4	0.48	0	6,6,6	0.44	0
5	SO4	A	711	-	4,4,4	0.67	0	6,6,6	1.36	1 (16%)
6	1PE	A	715	-	3,3,15	0.43	0	2,2,14	0.36	0
4	GOL	A	707	-	5,5,5	0.59	0	5,5,5	0.82	0
4	GOL	A	705	-	5,5,5	0.80	0	5,5,5	1.32	1 (20%)

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
6	1PE	A	712[B]	-	-	2/2/2/13	-
4	GOL	A	706	-	-	4/4/4/4	-
3	NAG	A	703	1	-	1/6/23/26	0/1/1/1
4	GOL	A	708	-	-	2/4/4/4	-
6	1PE	A	713	-	-	2/4/4/13	-
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
6	1PE	A	715	-	-	1/1/1/13	-
4	GOL	A	709	-	-	2/4/4/4	-
6	1PE	A	714	-	-	0/2/2/13	-
6	1PE	A	716	-	-	0/2/2/13	-
4	GOL	A	707	-	-	0/4/4/4	-
3	NAG	A	702	1	-	0/6/23/26	0/1/1/1
6	1PE	A	712[A]	-	-	1/2/2/13	-
4	GOL	A	704	-	-	4/4/4/4	-
4	GOL	A	705	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAG	C2-N2	3.15	1.51	1.46
3	A	703	NAG	C1-C2	2.05	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAG	O7-C7-C8	-4.94	112.88	122.06
3	A	702	NAG	C8-C7-N2	4.14	123.11	116.10
3	A	701	NAG	O5-C1-C2	-3.38	105.96	111.29
6	A	712[A]	1PE	C23-OH3-C22	2.98	131.53	112.96
6	A	712[B]	1PE	C23-OH3-C22	2.98	131.53	112.96
3	A	701	NAG	C1-O5-C5	-2.90	108.26	112.19
3	A	702	NAG	C1-C2-N2	2.67	115.06	110.49
3	A	701	NAG	O3-C3-C2	-2.66	103.97	109.47
3	A	702	NAG	O3-C3-C2	-2.59	104.11	109.47
7	A	719	ACT	OXT-C-CH3	2.51	125.56	115.18
3	A	701	NAG	O7-C7-N2	2.45	126.46	121.95
5	A	711	SO4	O4-S-O2	2.44	122.06	109.31
3	A	703	NAG	C6-C5-C4	2.39	118.61	113.00
3	A	703	NAG	O3-C3-C4	2.39	115.88	110.35
3	A	701	NAG	O3-C3-C4	2.27	115.59	110.35
7	A	717	ACT	OXT-C-CH3	2.25	124.50	115.18
3	A	701	NAG	C6-C5-C4	2.21	118.17	113.00
3	A	701	NAG	C2-N2-C7	2.18	126.00	122.90
3	A	703	NAG	O5-C5-C6	2.09	110.49	107.20
6	A	713	1PE	C23-OH3-C22	-2.08	104.27	113.29
4	A	705	GOL	O1-C1-C2	-2.07	100.29	110.20
3	A	701	NAG	O4-C4-C5	2.04	114.36	109.30
4	A	709	GOL	C3-C2-C1	2.02	119.56	111.70

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	704	GOL	O1-C1-C2-C3
4	A	704	GOL	C1-C2-C3-O3
4	A	706	GOL	O1-C1-C2-O2
4	A	706	GOL	O1-C1-C2-C3
4	A	708	GOL	C1-C2-C3-O3
4	A	708	GOL	O2-C2-C3-O3
6	A	713	1PE	C13-C23-OH3-C22
4	A	705	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	705	GOL	C1-C2-C3-O3
4	A	706	GOL	C1-C2-C3-O3
4	A	709	GOL	O1-C1-C2-C3
4	A	704	GOL	O2-C2-C3-O3
4	A	704	GOL	O1-C1-C2-O2
6	A	712[B]	1PE	C12-C22-OH3-C23
4	A	705	GOL	O1-C1-C2-O2
4	A	705	GOL	O2-C2-C3-O3
4	A	709	GOL	O1-C1-C2-O2
6	A	715	1PE	OH7-C16-C26-OH6
6	A	712[B]	1PE	OH2-C12-C22-OH3
6	A	713	1PE	C12-C22-OH3-C23
3	A	703	NAG	C4-C5-C6-O6
4	A	706	GOL	O2-C2-C3-O3
6	A	712[A]	1PE	C12-C22-OH3-C23

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	713	1PE	5	0
6	A	712[B]	1PE	3	0
4	A	706	GOL	3	0
4	A	709	GOL	3	0
6	A	714	1PE	1	0
6	A	712[A]	1PE	1	0
4	A	707	GOL	1	0
4	A	705	GOL	3	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	605/609 (99%)	-0.41	12 (1%) 65 61	14, 21, 37, 81	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	586	HIS	6.6
1	A	585	ALA	5.2
1	A	-2	HIS	5.2
1	A	582	VAL	4.6
1	A	187	ASP	3.6
1	A	-1	ALA	3.0
1	A	186	LYS	3.0
1	A	587	TYR	2.9
1	A	228	GLU	2.6
1	A	583	GLY	2.2
1	A	584	ASP	2.2
1	A	232[A]	ASN	2.1

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

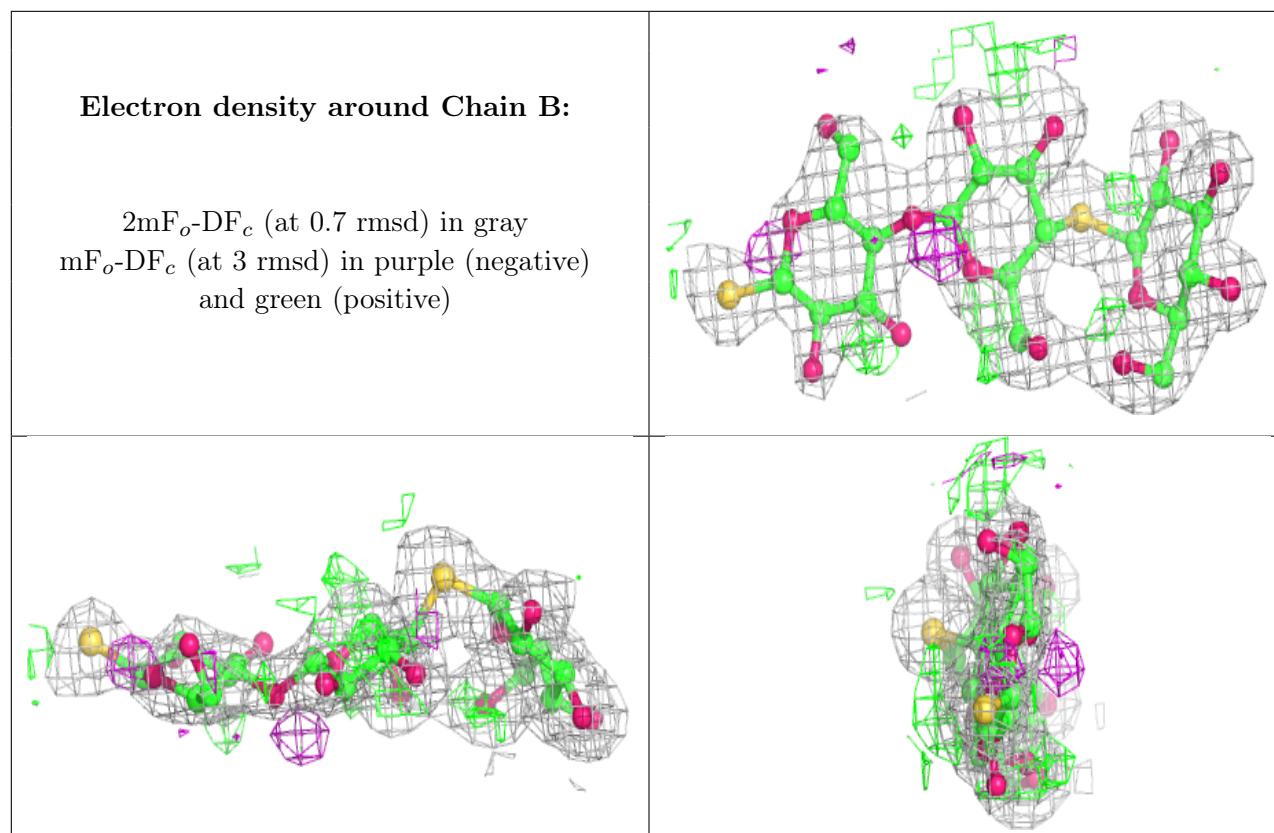
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GS1	B	1	12/12	0.88	0.18	41,49,58,60	0
2	SGC	B	2	11/12	0.92	0.13	22,33,42,43	0
2	BGC	B	3	11/12	0.96	0.14	17,22,24,24	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(\AA^2)	Q<0.9
6	1PE	A	712[A]	5/16	0.75	0.22	23,29,41,45	2
6	1PE	A	712[B]	5/16	0.75	0.22	23,32,41,45	2
4	GOL	A	705	6/6	0.77	0.23	43,56,58,64	0
4	GOL	A	708	6/6	0.78	0.19	50,67,75,81	0
6	1PE	A	714	5/16	0.78	0.20	47,48,56,69	0
6	1PE	A	713	7/16	0.82	0.20	45,54,58,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	706	6/6	0.82	0.15	51,54,61,62	0
6	1PE	A	715	4/16	0.82	0.15	62,64,64,68	0
3	NAG	A	703	14/15	0.84	0.28	47,68,76,85	0
6	1PE	A	716	5/16	0.84	0.15	48,55,61,63	0
3	NAG	A	701	14/15	0.86	0.24	46,51,71,72	0
3	NAG	A	702	14/15	0.86	0.18	51,66,73,75	0
7	ACT	A	719	4/4	0.89	0.13	49,63,64,69	0
7	ACT	A	720	4/4	0.89	0.16	39,53,57,70	0
7	ACT	A	717	4/4	0.92	0.14	53,66,68,70	0
4	GOL	A	704	6/6	0.92	0.16	16,36,37,43	6
4	GOL	A	709	6/6	0.92	0.16	33,39,45,53	0
5	SO4	A	710	5/5	0.94	0.18	49,49,56,59	5
4	GOL	A	707	6/6	0.94	0.12	44,53,57,63	0
5	SO4	A	711	5/5	0.95	0.16	27,29,39,42	5
7	ACT	A	718	4/4	0.96	0.19	38,51,59,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.