



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 05:23 pm BST

PDB ID : 1UR0
Title : The structure of endo-beta-1,4-galactanase from *Bacillus licheniformis* in complex with two oligosaccharide products.
Authors : Ryttersgaard, C.; Le Nours, J.; Lo Leggio, L.; Jorgensen, C.T.; Christensen, L.L.H.; Bjornvad, M.; Larsen, S.
Deposited on : 2003-10-24
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

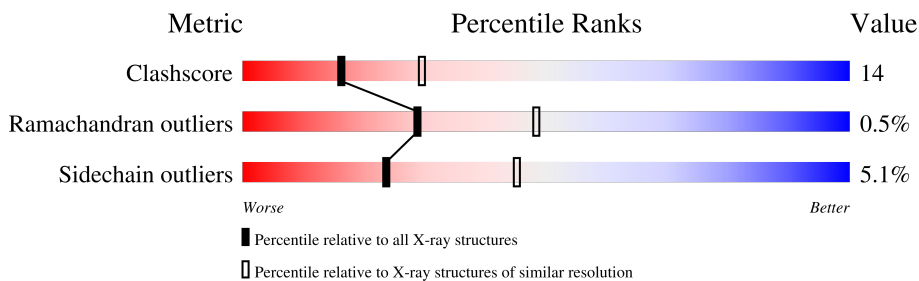
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	399	
1	B	399	
2	C	3	
2	D	3	

2 Entry composition [i](#)

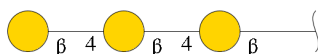
There are 5 unique types of molecules in this entry. The entry contains 6233 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GALACTANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	1
			2998	1905	510	578	5			
1	B	388	Total	C	N	O	S	0	0	1
			3009	1914	511	579	5			

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

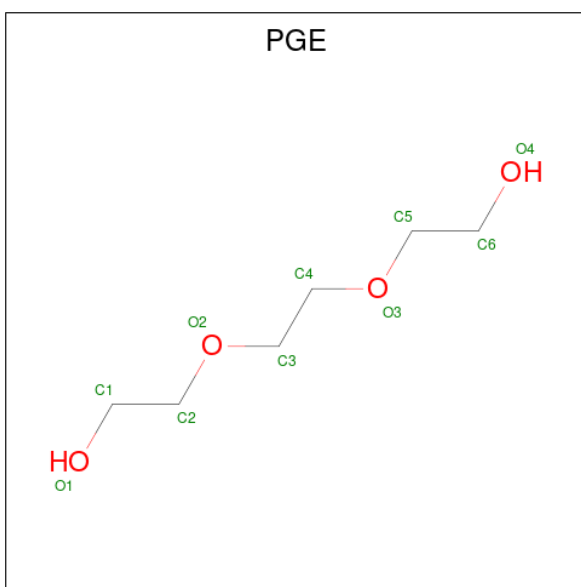


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			
2	D	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	78	Total O 78 78	0	0
5	B	58	Total O 58 58	0	0



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain D: 33% 33% 33%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.57Å 80.14Å 103.22Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	19.66 – 2.50	Depositor
% Data completeness (in resolution range)	95.3 (19.66-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6233	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, CA, GAL

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	0.78	10/3077 (0.3%)	0.98	6/4183 (0.1%)
1	B	0.75	9/3089 (0.3%)	0.95	7/4199 (0.2%)
All	All	0.76	19/6166 (0.3%)	0.96	13/8382 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ARG	CZ-NH1	-20.50	1.06	1.33
1	B	191	ARG	CZ-NH1	-18.50	1.08	1.33
1	A	221	ARG	CZ-NH1	-17.38	1.10	1.33
1	B	221	ARG	CZ-NH1	-16.44	1.11	1.33
1	A	221	ARG	CZ-NH2	-12.77	1.16	1.33
1	B	221	ARG	CZ-NH2	-12.62	1.16	1.33
1	A	191	ARG	CZ-NH2	-11.76	1.17	1.33
1	B	191	ARG	CZ-NH2	-10.34	1.19	1.33
1	B	71	ASN	CG-ND2	-7.64	1.13	1.32
1	B	71	ASN	CG-OD1	-7.33	1.07	1.24
1	A	71	ASN	CG-ND2	-7.27	1.14	1.32
1	A	71	ASN	CG-OD1	-7.23	1.08	1.24
1	B	93	GLN	CD-OE1	-6.79	1.09	1.24
1	A	93	GLN	CD-OE1	-6.54	1.09	1.24
1	B	93	GLN	CD-NE2	-6.54	1.16	1.32
1	A	289	ASN	CG-ND2	-6.34	1.17	1.32
1	A	93	GLN	CD-NE2	-6.14	1.17	1.32
1	B	289	ASN	CG-ND2	-5.07	1.20	1.32
1	A	289	ASN	CG-OD1	-5.02	1.12	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH2	35.43	138.01	120.30
1	B	191	ARG	NE-CZ-NH2	32.12	136.36	120.30
1	B	221	ARG	NE-CZ-NH2	26.32	133.46	120.30
1	A	221	ARG	NE-CZ-NH2	25.39	133.00	120.30
1	A	221	ARG	NH1-CZ-NH2	-12.03	106.17	119.40
1	A	191	ARG	NE-CZ-NH1	-11.84	114.38	120.30
1	B	221	ARG	NH1-CZ-NH2	-11.59	106.65	119.40
1	B	191	ARG	NH1-CZ-NH2	-11.42	106.84	119.40
1	A	191	ARG	NH1-CZ-NH2	-11.35	106.92	119.40
1	B	191	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	A	221	ARG	CD-NE-CZ	5.72	131.60	123.60
1	B	394	GLY	N-CA-C	-5.33	99.78	113.10
1	B	221	ARG	NE-CZ-NH1	-5.18	117.71	120.30

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	2998	0	2860	79	0
1	B	3009	0	2869	92	0
2	C	34	0	30	0	0
2	D	34	0	30	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	20	0	28	8	0
5	A	78	0	0	2	0
5	B	58	0	0	3	0
All	All	6233	0	5817	171	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 14.

All (171) 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:274:ASP:HB3	1:A:326:PRO:HB3	1.55	0.85
1:A:333:LEU:HD22	1:A:337:LYS:HE3	1.58	0.85
1:B:66:ARG:HG3	1:B:106:LEU:HD13	1.56	0.85
1:B:333:LEU:HD22	1:B:337:LYS:HE3	1.59	0.83
1:A:66:ARG:HG3	1:A:106:LEU:HD13	1.62	0.80
1:B:117:ASP:HB2	1:B:118:PRO:CD	2.12	0.80
1:B:376:ASP:OD2	1:B:380:ARG:HB2	1.81	0.80
1:A:117:ASP:HB2	1:A:118:PRO:CD	2.12	0.79
1:B:133:GLU:O	1:B:137:THR:HG22	1.82	0.78
1:A:133:GLU:O	1:A:137:THR:HG22	1.84	0.77
1:A:325:ILE:HB	1:A:326:PRO:HD2	1.66	0.77
1:B:325:ILE:HB	1:B:326:PRO:HD2	1.67	0.75
1:B:294:GLN:HG2	5:B:2001:HOH:O	1.88	0.74
1:A:289:ASN:HD22	1:A:298:ASN:HB2	1.53	0.73
1:B:354:GLU:HG3	1:B:355:TYR:H	1.54	0.73
1:B:25:ILE:HB	1:B:316:GLY:HA3	1.70	0.72
1:B:274:ASP:HB3	1:B:326:PRO:HB3	1.71	0.71
1:B:79:ASN:HB3	1:B:351:TYR:CD2	2.25	0.71
1:A:378:LYS:HA	1:A:378:LYS:HE2	1.72	0.71
1:A:293:VAL:HG11	1:A:383:PRO:HG2	1.73	0.71
1:B:293:VAL:HG11	1:B:383:PRO:HG2	1.73	0.70
1:A:272:ASP:HA	1:A:278:ASN:HD21	1.56	0.69
1:B:354:GLU:HG3	1:B:355:TYR:N	2.07	0.69
1:B:55:LYS:O	1:B:59:GLU:HG3	1.93	0.69
1:B:66:ARG:CG	1:B:106:LEU:HD13	2.22	0.69
1:B:136:LYS:HD3	4:B:1399:PGE:H22	1.75	0.67
1:B:258:LYS:HE2	4:B:1398:PGE:H52	1.76	0.67
1:A:274:ASP:HB3	1:A:326:PRO:CB	2.25	0.66
1:B:358:GLU:O	1:B:362:LYS:HE3	1.95	0.66
1:A:55:LYS:O	1:A:59:GLU:HG3	1.95	0.66
1:B:389:GLN:HB3	5:B:2053:HOH:O	1.94	0.66
1:B:272:ASP:HA	1:B:278:ASN:HD21	1.59	0.66
1:A:354:GLU:HG3	1:A:355:TYR:N	2.11	0.66
1:A:289:ASN:ND2	1:A:298:ASN:CB	2.60	0.65
1:A:272:ASP:HA	1:A:278:ASN:ND2	2.14	0.63
1:A:354:GLU:HG3	1:A:355:TYR:H	1.63	0.63
1:B:136:LYS:HD3	4:B:1399:PGE:H32	1.83	0.61
1:B:272:ASP:HA	1:B:278:ASN:ND2	2.15	0.60
1:B:21:ARG:NH1	1:B:312:GLU:O	2.33	0.60
1:A:289:ASN:ND2	1:A:298:ASN:HB2	2.17	0.60
1:B:176:TRP:CG	1:B:179:MET:HE3	2.36	0.60
1:A:289:ASN:ND2	1:A:298:ASN:HB3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASP:HB3	1:A:197:ILE:HG13	1.84	0.59
1:B:131:ASN:ND2	1:B:133:GLU:HB2	2.18	0.58
1:A:131:ASN:ND2	1:A:133:GLU:HB2	2.19	0.58
1:B:117:ASP:HB2	1:B:118:PRO:HD3	1.85	0.58
1:B:212:TYR:HB2	1:B:247:VAL:CG2	2.34	0.57
1:B:329:PRO:HD2	1:B:332:ARG:HD3	1.87	0.57
1:A:117:ASP:HB2	1:A:118:PRO:HD2	1.87	0.57
1:B:194:ASP:HB3	1:B:197:ILE:HG13	1.86	0.57
1:B:258:LYS:NZ	4:B:1398:PGE:H22	2.19	0.57
1:A:217:GLU:OE2	1:A:221:ARG:NH1	2.38	0.57
1:B:66:ARG:CD	1:B:106:LEU:HD13	2.34	0.57
1:A:299:ALA:O	1:A:303:VAL:HG23	2.05	0.56
1:B:31:SER:HB2	1:B:68:ARG:NH1	2.19	0.56
1:B:117:ASP:HB2	1:B:118:PRO:HD2	1.88	0.56
1:B:258:LYS:HG3	4:B:1398:PGE:H4	1.87	0.56
1:B:34:ILE:O	1:B:38:GLU:HG3	2.06	0.55
1:A:34:ILE:O	1:A:38:GLU:HG3	2.05	0.55
1:B:87:ASP:OD1	1:B:89:GLU:HG3	2.06	0.55
1:A:289:ASN:HD21	1:A:298:ASN:HB3	1.71	0.54
1:B:299:ALA:O	1:B:303:VAL:HG23	2.08	0.54
1:B:181:GLN:HG2	4:B:1399:PGE:H12	1.90	0.54
1:A:31:SER:HB2	1:A:68:ARG:NH1	2.22	0.54
1:A:188:GLN:NE2	1:A:192:GLU:OE2	2.42	0.53
1:B:113:ASP:HB2	1:B:355:TYR:CZ	2.43	0.53
1:A:25:ILE:HB	1:A:316:GLY:HA3	1.90	0.53
1:B:205:ASN:HA	1:B:207:GLU:OE2	2.08	0.53
1:A:16:LYS:HE2	1:A:392:ASP:O	2.09	0.52
1:A:117:ASP:HB2	1:A:118:PRO:HD3	1.87	0.52
1:B:124:PRO:HD2	1:B:127:TRP:CE3	2.45	0.52
1:B:276:HIS:CD2	1:B:365:GLY:HA3	2.45	0.52
1:A:373:ALA:HB2	5:A:2066:HOH:O	2.09	0.52
1:B:373:ALA:HB2	5:B:2043:HOH:O	2.10	0.52
1:A:66:ARG:CG	1:A:106:LEU:HD13	2.34	0.52
1:B:185:ALA:HA	4:B:1399:PGE:H3	1.92	0.52
1:B:117:ASP:CB	1:B:118:PRO:CD	2.85	0.51
1:A:333:LEU:CD2	1:A:337:LYS:HE3	2.37	0.51
1:A:124:PRO:HD2	1:A:127:TRP:CE3	2.45	0.51
1:A:205:ASN:HA	1:A:207:GLU:OE2	2.10	0.51
1:B:332:ARG:NH2	1:B:335:LYS:HG2	2.26	0.51
1:A:12:LEU:HD22	1:A:383:PRO:O	2.11	0.51
1:A:226:TYR:CE1	1:A:257:LYS:HE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LYS:HZ2	4:B:1398:PGE:H22	1.75	0.50
1:A:208:THR:OG1	1:A:211:ARG:NH1	2.45	0.50
1:B:12:LEU:HD22	1:B:383:PRO:O	2.12	0.50
1:B:104:LYS:HD3	1:B:156:ASP:OD2	2.12	0.50
1:B:208:THR:OG1	1:B:211:ARG:NH1	2.45	0.49
1:A:68:ARG:HA	1:A:108:ASP:HB3	1.93	0.49
1:B:390:TYR:CE1	1:B:396:PRO:HD3	2.47	0.49
1:B:333:LEU:CD2	1:B:337:LYS:HE3	2.37	0.49
1:B:176:TRP:CD2	1:B:179:MET:HE3	2.47	0.49
1:A:117:ASP:CB	1:A:118:PRO:CD	2.85	0.48
1:B:347:TRP:CZ2	2:D:2:GAL:H5	2.49	0.48
1:B:236:PHE:HB3	1:B:285:GLN:HB3	1.96	0.47
1:B:226:TYR:CE1	1:B:257:LYS:HE3	2.50	0.47
1:A:376:ASP:OD2	1:A:380:ARG:HB2	2.15	0.47
1:B:53:ILE:HG12	1:B:57:LEU:HD22	1.96	0.47
1:B:68:ARG:HA	1:B:108:ASP:HB3	1.95	0.47
1:A:53:ILE:HG12	1:A:57:LEU:HD22	1.97	0.47
1:A:206:PRO:HB3	1:A:212:TYR:CE2	2.50	0.46
1:A:73:PRO:HG2	1:A:74:TYR:CE1	2.51	0.46
1:B:241:LEU:HD13	1:B:302:ASP:HB3	1.97	0.46
1:B:340:TRP:CE2	1:B:366:GLY:HA3	2.51	0.46
1:B:73:PRO:HG2	1:B:74:TYR:CE1	2.51	0.45
1:B:363:TRP:HA	1:B:363:TRP:CE3	2.51	0.45
1:A:44:TYR:CD1	1:A:44:TYR:N	2.85	0.45
1:A:301:ARG:C	1:A:301:ARG:HD3	2.37	0.45
1:B:139:LEU:C	1:B:139:LEU:HD23	2.36	0.45
1:B:143:THR:HG22	1:B:147:LEU:HD22	1.98	0.45
1:A:104:LYS:HD3	1:A:156:ASP:OD2	2.16	0.45
1:B:106:LEU:HD12	1:B:318:PHE:CZ	2.51	0.45
1:A:66:ARG:CD	1:A:106:LEU:HD13	2.46	0.45
1:B:347:TRP:CE2	2:D:2:GAL:H5	2.51	0.45
1:B:207:GLU:CG	1:B:238:HIS:HA	2.47	0.45
1:A:337:LYS:HA	1:A:340:TRP:CE3	2.52	0.45
1:B:337:LYS:HA	1:B:340:TRP:CE3	2.52	0.44
1:A:66:ARG:HG3	1:A:106:LEU:CD1	2.42	0.44
1:A:75:ASP:HB2	5:A:2069:HOH:O	2.16	0.44
1:A:96:LYS:HE3	1:A:153:ALA:HB1	1.99	0.44
1:B:96:LYS:HE3	1:B:153:ALA:HB1	1.99	0.44
1:B:301:ARG:HD3	1:B:301:ARG:C	2.38	0.44
1:B:67:VAL:O	1:B:67:VAL:HG13	2.17	0.44
1:B:206:PRO:HB3	1:B:212:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:OD1	1:A:49:LYS:HG2	2.18	0.44
1:A:66:ARG:HD2	1:A:106:LEU:HD13	2.00	0.44
1:A:13:TYR:OH	1:A:15:GLU:HB2	2.18	0.43
1:A:241:LEU:HD13	1:A:302:ASP:HB3	1.99	0.43
1:A:67:VAL:O	1:A:67:VAL:HG13	2.19	0.43
1:A:143:THR:HG22	1:A:147:LEU:HD22	1.99	0.43
1:A:280:ALA:HB1	1:A:281:PRO:HA	2.01	0.43
1:B:387:VAL:O	1:B:391:VAL:HG13	2.18	0.43
1:A:340:TRP:CE2	1:A:366:GLY:HA3	2.53	0.43
1:B:44:TYR:CD1	1:B:44:TYR:N	2.86	0.43
1:B:66:ARG:NH2	1:B:263:GLU:OE2	2.51	0.43
1:A:66:ARG:NH2	1:A:263:GLU:OE2	2.51	0.43
1:A:387:VAL:O	1:A:391:VAL:HG13	2.18	0.43
1:B:116:ALA:HA	1:B:120:LYS:O	2.19	0.42
1:A:17:VAL:HG13	1:A:305:GLN:HA	2.02	0.42
1:B:280:ALA:HB1	1:B:281:PRO:HA	2.00	0.42
1:B:347:TRP:CH2	1:B:360:ALA:HA	2.54	0.42
1:A:139:LEU:C	1:A:139:LEU:HD23	2.39	0.42
1:B:244:LEU:O	1:B:247:VAL:HG12	2.20	0.42
1:A:57:LEU:HD12	1:A:57:LEU:HA	1.90	0.42
1:A:132:PHE:CE1	1:A:178:LYS:HB3	2.55	0.42
1:A:386:HIS:HB3	1:A:390:TYR:CE2	2.55	0.42
1:B:211:ARG:HG2	1:B:212:TYR:HD1	1.85	0.42
1:B:276:HIS:O	1:B:277:GLY:C	2.58	0.42
1:B:356:ASP:OD2	1:B:359:ASP:HB3	2.20	0.42
1:B:261:VAL:HG23	1:B:307:VAL:CG2	2.50	0.42
1:B:290:PRO:O	1:B:295:GLY:HA3	2.20	0.42
1:B:114:PHE:O	1:B:115:TRP:C	2.57	0.41
1:A:347:TRP:CH2	1:A:360:ALA:HA	2.55	0.41
1:B:176:TRP:CD1	1:B:179:MET:HE3	2.56	0.41
1:A:207:GLU:CG	1:A:238:HIS:HA	2.51	0.41
1:B:333:LEU:O	1:B:337:LYS:HG3	2.20	0.41
1:B:276:HIS:CD2	1:B:366:GLY:H	2.38	0.41
1:B:24:PHE:CE2	1:B:304:ILE:HG23	2.56	0.41
1:B:113:ASP:HB2	1:B:355:TYR:CE1	2.56	0.41
1:B:241:LEU:CD1	1:B:302:ASP:HB3	2.51	0.41
1:A:60:ALA:O	1:A:389:GLN:HG3	2.21	0.41
1:A:66:ARG:HG3	1:A:106:LEU:HB3	2.03	0.41
1:A:114:PHE:O	1:A:115:TRP:C	2.59	0.41
1:A:276:HIS:O	1:A:277:GLY:C	2.59	0.41
1:B:132:PHE:CE1	1:B:178:LYS:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASN:HD22	1:A:298:ASN:CB	2.19	0.40
1:A:358:GLU:OE1	1:A:358:GLU:N	2.38	0.40
1:A:261:VAL:HG23	1:A:307:VAL:CG2	2.51	0.40
1:A:333:LEU:O	1:A:337:LYS:HG3	2.22	0.40
1:A:188:GLN:HE21	1:A:192:GLU:HG3	1.87	0.40
1:A:191:ARG:NH2	1:A:227:ASP:OD1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/399 (96%)	359 (93%)	24 (6%)	2 (0%)	29	48
1	B	386/399 (97%)	361 (94%)	23 (6%)	2 (0%)	29	48
All	All	771/798 (97%)	720 (93%)	47 (6%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	363	TRP
1	A	117	ASP
1	A	333	LEU
1	B	117	ASP

5.3.2 Protein sidechains [i](#)

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	305/315 (97%)	290 (95%)	15 (5%)	25	47
1	B	306/315 (97%)	290 (95%)	16 (5%)	23	44
All	All	611/630 (97%)	580 (95%)	31 (5%)	24	45

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	64	TYR
1	A	106	LEU
1	A	114	PHE
1	A	129	ASN
1	A	134	ASP
1	A	137	THR
1	A	147	LEU
1	A	173	GLU
1	A	191	ARG
1	A	207	GLU
1	A	236	PHE
1	A	294	GLN
1	A	333	LEU
1	A	341	GLU
1	B	57	LEU
1	B	64	TYR
1	B	106	LEU
1	B	114	PHE
1	B	129	ASN
1	B	134	ASP
1	B	137	THR
1	B	147	LEU
1	B	173	GLU
1	B	207	GLU
1	B	294	GLN
1	B	333	LEU
1	B	335	LYS
1	B	341	GLU
1	B	362	LYS
1	B	363	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	188	GLN
1	A	289	ASN
1	B	51	GLN
1	B	276	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GAL	C	1	2	12,12,12	0.84	0	17,17,17	0.58	0
2	GAL	C	2	2	11,11,12	1.17	1 (9%)	15,15,17	0.80	0
2	GAL	C	3	2	11,11,12	0.98	0	15,15,17	0.89	1 (6%)
2	GAL	D	1	2	12,12,12	0.84	0	17,17,17	0.56	0
2	GAL	D	2	2	11,11,12	1.09	1 (9%)	15,15,17	0.68	0
2	GAL	D	3	2	11,11,12	1.00	0	15,15,17	0.91	1 (6%)

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	GAL	C	1	2	-	1/2/22/22	0/1/1/1
2	GAL	C	2	2	-	1/2/19/22	0/1/1/1
2	GAL	C	3	2	-	2/2/19/22	0/1/1/1
2	GAL	D	1	2	-	1/2/22/22	0/1/1/1
2	GAL	D	2	2	-	1/2/19/22	0/1/1/1
2	GAL	D	3	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GAL	O5-C5	2.22	1.47	1.43
2	D	2	GAL	O5-C5	2.15	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	GAL	C1-C2-C3	-2.22	106.94	109.67
2	C	3	GAL	C1-C2-C3	-2.12	107.06	109.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	GAL	O5-C5-C6-O6
2	C	3	GAL	O5-C5-C6-O6
2	D	3	GAL	C4-C5-C6-O6
2	C	3	GAL	C4-C5-C6-O6
2	C	1	GAL	O5-C5-C6-O6
2	D	1	GAL	O5-C5-C6-O6
2	D	2	GAL	C4-C5-C6-O6
2	C	2	GAL	C4-C5-C6-O6

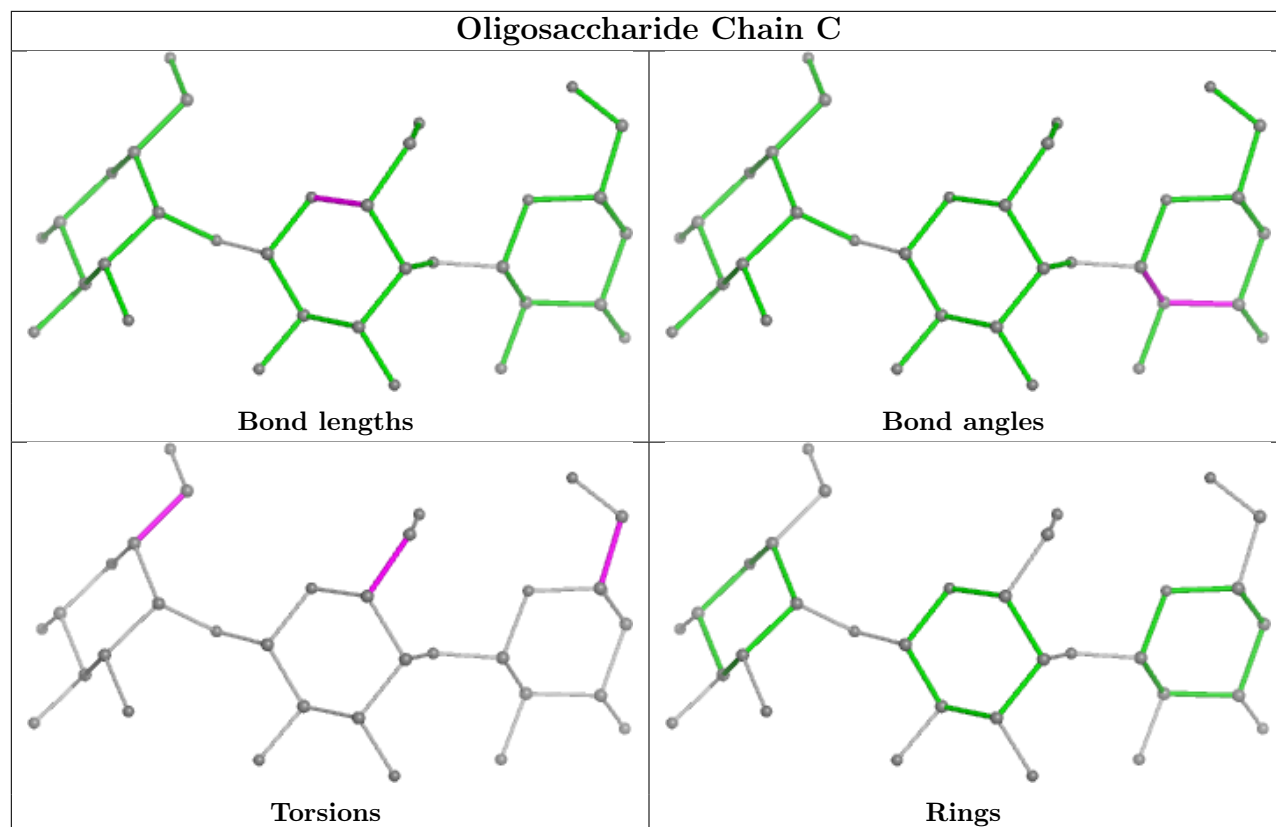
There are no ring outliers.

1 monomer is involved in 2 short contacts:

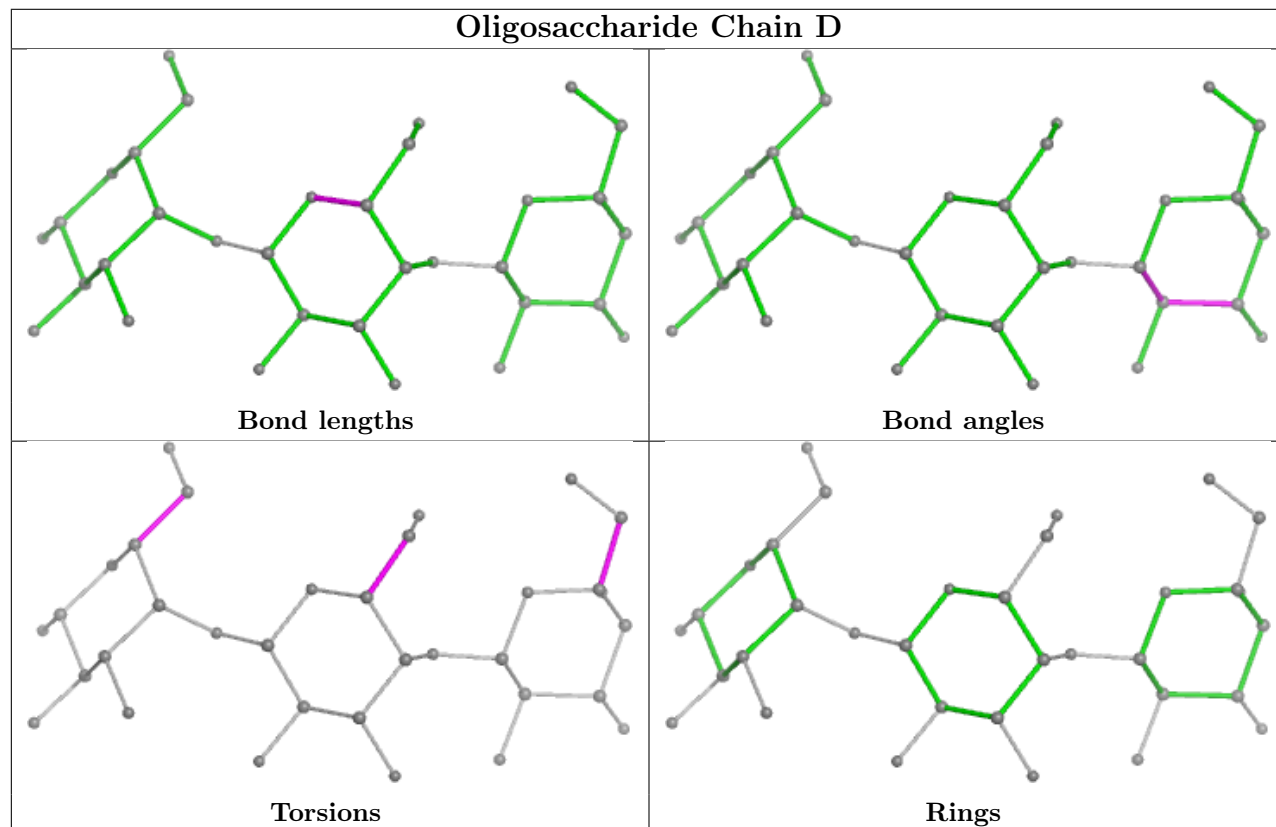
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GAL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	PGE	B	1399	-	9,9,9	0.88	0	8,8,8	1.61	2 (25%)
4	PGE	B	1398	-	9,9,9	0.85	0	8,8,8	1.61	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	B	1399	-	-	2/7/7/7	-
4	PGE	B	1398	-	-	6/7/7/7	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1398	PGE	C5-O3-C4	2.81	125.46	113.29
4	B	1399	PGE	C5-O3-C4	2.58	124.46	113.29
4	B	1399	PGE	O2-C2-C1	2.57	121.34	110.07
4	B	1398	PGE	O2-C2-C1	2.46	120.86	110.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1398	PGE	O2-C3-C4-O3
4	B	1398	PGE	O1-C1-C2-O2
4	B	1399	PGE	O2-C3-C4-O3
4	B	1399	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
4	B	1398	PGE	O3-C5-C6-O4
4	B	1398	PGE	C3-C4-O3-C5
4	B	1398	PGE	C4-C3-O2-C2
4	B	1398	PGE	C6-C5-O3-C4

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1399	PGE	4	0
4	B	1398	PGE	4	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.