



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:31 AM UTC

PDB ID : 1BYH / pdb_00001byh
Title : MOLECULAR AND ACTIVE-SITE STRUCTURE OF A BACILLUS (1-3,1-4)-BETA-GLUCANASE
Authors : Keitel, T.; Heinemann, U.
Deposited on : 1992-12-31
Resolution : 2.80 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 : 4-5-2 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

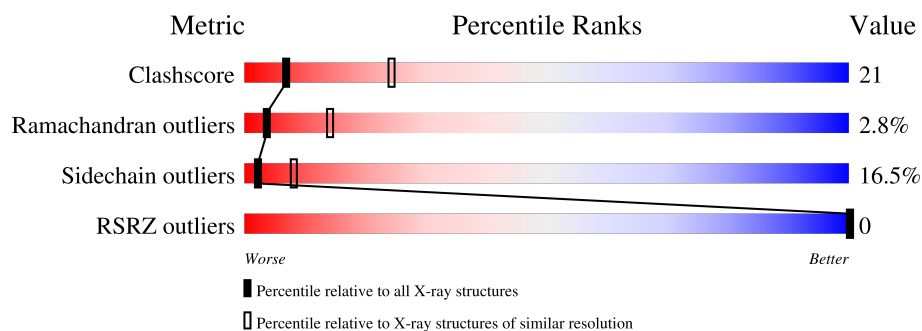
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	214	
2	B	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1797 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 HYBRID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1697	1090	273	329	5			

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

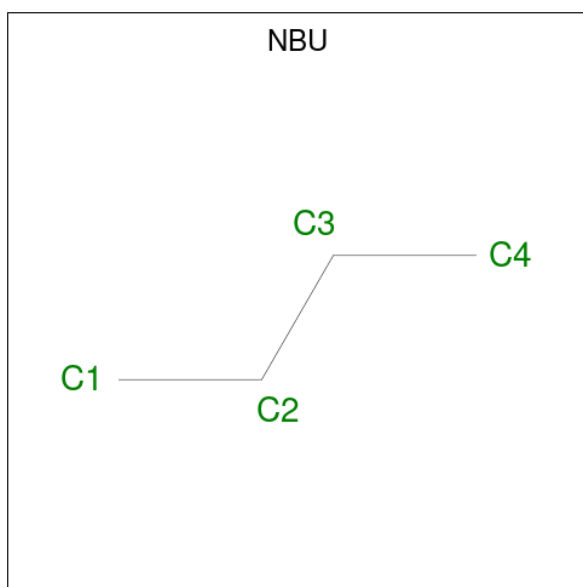


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is N-BUTANE (CCD ID: NBU) (formula: C₄H₁₀).



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

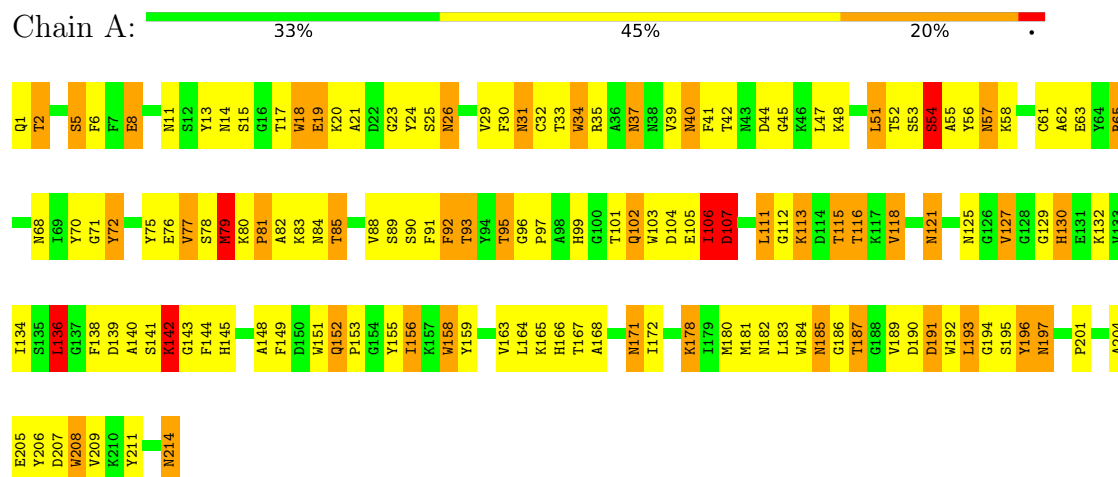
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	72	Total O 72 72	0	0

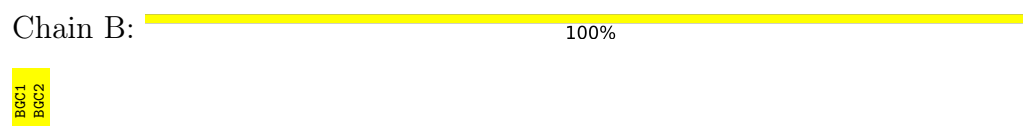
3 Residue-property plots

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: HYBRID



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.32Å 78.52Å 39.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 77.9 (8.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.87 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.168 , (Not available) 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1797	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.64% 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: CA, BGC, NBU

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	1.48	18/1753 (1.0%)	2.40	107/2384 (4.5%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	VAL	CA-CB	10.39	1.66	1.54
1	A	106	ILE	CA-CB	10.18	1.70	1.54
1	A	105	GLU	CD-OE2	10.14	1.44	1.25
1	A	172	ILE	CA-CB	8.08	1.64	1.54
1	A	145	HIS	CD2-NE2	-7.53	1.29	1.37
1	A	172	ILE	C-N	7.08	1.43	1.33
1	A	99	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	41	PHE	CA-CB	6.46	1.63	1.53
1	A	130	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	115	THR	CA-CB	6.11	1.61	1.53
1	A	21	ALA	CA-CB	-6.08	1.44	1.53
1	A	1	GLN	CA-CB	6.03	1.65	1.53
1	A	89	SER	CA-CB	-5.83	1.44	1.53
1	A	145	HIS	CG-ND1	-5.51	1.32	1.38
1	A	166	HIS	CD2-NE2	-5.39	1.31	1.37
1	A	57	ASN	CA-CB	5.20	1.62	1.53
1	A	191	ASP	CA-CB	5.19	1.61	1.53
1	A	70	TYR	CA-C	-5.05	1.46	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASN	CA-CB-CG	11.91	124.51	112.60
1	A	57	ASN	OD1-CG-ND2	-11.37	111.23	122.60
1	A	185	ASN	OD1-CG-ND2	-10.50	112.10	122.60
1	A	71	GLY	CA-C-O	10.30	131.68	121.28
1	A	107	ASP	CA-CB-CG	10.21	122.81	112.60
1	A	152	GLN	OE1-CD-NE2	-9.97	112.62	122.60
1	A	34	TRP	CG-CD2-CE3	9.61	143.51	133.90
1	A	40	ASN	CA-CB-CG	9.44	122.04	112.60
1	A	95	THR	CA-CB-OG1	-9.32	95.63	109.60
1	A	106	ILE	O-C-N	-9.28	113.23	122.97
1	A	121	ASN	OD1-CG-ND2	-8.89	113.71	122.60
1	A	207	ASP	CA-C-O	-8.74	111.62	120.80
1	A	44	ASP	CA-CB-CG	8.69	121.28	112.60
1	A	34	TRP	CB-CG-CD1	-8.58	114.03	126.90
1	A	214	ASN	OD1-CG-ND2	-8.56	114.04	122.60
1	A	182	ASN	CA-CB-CG	8.43	121.03	112.60
1	A	185	ASN	CB-CG-ND2	8.23	128.75	116.40
1	A	130	HIS	CA-CB-CG	8.19	121.99	113.80
1	A	68	ASN	CA-CB-CG	7.98	120.58	112.60
1	A	144	PHE	O-C-N	7.96	132.28	123.13
1	A	26	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	A	2	THR	N-CA-C	7.87	127.57	110.80
1	A	102	GLN	OE1-CD-NE2	-7.85	114.75	122.60
1	A	30	PHE	CA-CB-CG	7.72	121.53	113.80
1	A	37	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	A	14	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	A	26	ASN	CA-CB-CG	7.23	119.83	112.60
1	A	142	LYS	CB-CG-CD	7.17	127.79	111.30
1	A	214	ASN	CA-CB-CG	7.09	119.69	112.60
1	A	190	ASP	CA-C-N	6.99	129.53	120.44
1	A	190	ASP	C-N-CA	6.99	129.53	120.44
1	A	106	ILE	N-CA-C	-6.99	99.04	108.96
1	A	68	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	A	95	THR	CA-CB-CG2	6.91	122.25	110.50
1	A	11	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	A	41	PHE	N-CA-C	-6.79	98.15	109.07
1	A	172	ILE	N-CA-CB	-6.73	101.79	111.21
1	A	97	PRO	CA-C-N	6.70	130.16	120.38
1	A	97	PRO	C-N-CA	6.70	130.16	120.38
1	A	71	GLY	N-CA-C	6.43	120.75	112.13
1	A	14	ASN	CB-CG-ND2	6.42	126.04	116.40
1	A	14	ASN	CA-CB-CG	-6.38	106.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLN	CA-CB-CG	6.27	126.64	114.10
1	A	130	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	A	15	SER	N-CA-C	6.25	118.85	110.35
1	A	143	GLY	CA-C-N	6.24	130.72	122.30
1	A	143	GLY	C-N-CA	6.24	130.72	122.30
1	A	97	PRO	O-C-N	6.17	129.63	122.17
1	A	105	GLU	CA-CB-CG	6.16	126.42	114.10
1	A	166	HIS	CB-CG-ND1	6.13	131.90	122.70
1	A	19	GLU	CA-CB-CG	6.09	126.28	114.10
1	A	151	TRP	CD2-CE2-CZ2	-6.09	116.31	122.40
1	A	90	SER	CA-C-N	6.05	131.34	122.39
1	A	90	SER	C-N-CA	6.05	131.34	122.39
1	A	44	ASP	CA-C-O	6.02	126.39	119.35
1	A	208	TRP	CG-CD2-CE3	5.93	139.83	133.90
1	A	190	ASP	N-CA-C	5.89	118.48	111.71
1	A	190	ASP	CA-C-O	5.89	126.75	120.10
1	A	31	ASN	CB-CG-ND2	-5.86	107.61	116.40
1	A	190	ASP	O-C-N	5.84	129.06	122.22
1	A	166	HIS	CB-CG-CD2	-5.81	123.65	131.20
1	A	156	ILE	N-CA-C	-5.79	99.79	108.12
1	A	37	ASN	CB-CG-ND2	5.77	125.06	116.40
1	A	136	LEU	N-CA-C	-5.76	100.28	109.96
1	A	62	ALA	N-CA-C	5.74	118.86	108.69
1	A	149	PHE	CA-CB-CG	5.74	119.53	113.80
1	A	76	GLU	N-CA-C	5.70	118.39	108.76
1	A	40	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	34	TRP	CE2-CD2-CG	-5.67	100.40	107.20
1	A	130	HIS	CB-CG-ND1	5.67	131.20	122.70
1	A	26	ASN	CB-CG-ND2	5.65	124.88	116.40
1	A	158	TRP	CB-CA-C	-5.60	99.56	109.70
1	A	184	TRP	CA-C-O	5.58	127.36	121.33
1	A	57	ASN	CB-CG-ND2	5.56	124.74	116.40
1	A	78	SER	N-CA-C	-5.56	99.46	108.52
1	A	65	ARG	CA-CB-CG	5.49	125.08	114.10
1	A	152	GLN	CG-CD-NE2	5.48	124.62	116.40
1	A	77	VAL	CB-CA-C	-5.46	102.48	110.62
1	A	194	GLY	N-CA-C	-5.46	103.55	112.83
1	A	72	TYR	N-CA-CB	-5.45	100.89	109.51
1	A	79	MET	CA-CB-CG	5.41	124.93	114.10
1	A	54	SER	CA-C-O	5.40	126.33	120.55
1	A	81	PRO	N-CA-C	5.38	118.75	111.22
1	A	196	TYR	CA-C-O	5.36	126.79	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	TYR	CA-C-O	5.36	125.92	120.24
1	A	129	GLY	CA-C-O	5.33	125.90	119.82
1	A	65	ARG	N-CA-CB	-5.33	101.59	111.13
1	A	18	TRP	CE2-CD2-CG	-5.33	100.81	107.20
1	A	118	VAL	CG1-CB-CG2	-5.31	99.11	110.80
1	A	209	VAL	O-C-N	-5.29	117.18	123.05
1	A	82	ALA	CA-C-O	5.27	126.50	120.54
1	A	111	LEU	CA-C-O	-5.23	114.98	120.58
1	A	45	GLY	O-C-N	5.22	129.48	122.70
1	A	80	LYS	CA-CB-CG	-5.17	103.76	114.10
1	A	101	THR	CA-CB-CG2	5.17	119.29	110.50
1	A	104	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	24	TYR	CB-CG-CD2	-5.13	113.11	120.80
1	A	79	MET	N-CA-C	5.13	117.04	108.99
1	A	72	TYR	CB-CA-C	5.12	117.54	110.16
1	A	208	TRP	CB-CG-CD1	-5.12	119.22	126.90
1	A	158	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	A	116	THR	CA-C-O	5.04	125.90	119.95
1	A	91	PHE	CA-C-O	5.04	126.35	120.20
1	A	96	GLY	CA-C-N	5.02	125.30	119.47
1	A	96	GLY	C-N-CA	5.02	125.30	119.47
1	A	15	SER	O-C-N	5.01	128.97	122.81
1	A	92	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	TYR	Sidechain
1	A	196	TYR	Sidechain

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	1697	0	1557	67	1
2	B	23	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	4	0	6	0	0
5	A	72	0	0	10	1
All	All	1797	0	1583	67	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 21.

All (67) 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:32:CYS:HB3	1:A:185:ASN:HD21	1.37	0.87
1:A:31:ASN:HB2	5:A:282:HOH:O	1.80	0.82
1:A:52:THR:HG22	1:A:201:PRO:HB3	1.63	0.81
1:A:197:ASN:HD22	1:A:197:ASN:H	1.36	0.73
1:A:187:THR:OG1	5:A:282:HOH:O	2.07	0.71
1:A:121:ASN:HD21	1:A:130:HIS:H	1.37	0.71
1:A:106:ILE:HD12	1:A:107:ASP:N	2.06	0.70
1:A:55:ALA:HB3	1:A:58:LYS:HD3	1.75	0.67
1:A:88:VAL:HG23	1:A:193:LEU:HD11	1.77	0.67
1:A:48:LYS:HG3	5:A:268:HOH:O	1.97	0.65
1:A:106:ILE:HD12	1:A:107:ASP:H	1.63	0.63
1:A:31:ASN:HB3	1:A:185:ASN:OD1	2.00	0.62
1:A:32:CYS:HB3	1:A:185:ASN:ND2	2.14	0.61
1:A:75:TYR:O	1:A:148:ALA:HA	2.02	0.59
1:A:197:ASN:H	1:A:197:ASN:ND2	1.99	0.58
1:A:51:LEU:O	1:A:201:PRO:HA	2.04	0.58
1:A:197:ASN:HD22	1:A:197:ASN:N	2.00	0.57
1:A:102:GLN:OE1	1:A:125:ASN:HB2	2.03	0.57
1:A:65:ARG:HB2	1:A:65:ARG:HH11	1.69	0.56
1:A:204:ALA:HB3	5:A:287:HOH:O	2.05	0.56
1:A:61:CYS:HB2	1:A:183:LEU:O	2.06	0.55
1:A:134:ILE:HD13	1:A:165:LYS:HG2	1.88	0.55
1:A:83:LYS:HG3	1:A:115:THR:OG1	2.07	0.55
1:A:111:LEU:HD21	1:A:192:TRP:NE1	2.22	0.55
1:A:88:VAL:CG2	1:A:193:LEU:HD11	2.37	0.53
1:A:65:ARG:HD3	1:A:180:MET:HE3	1.91	0.53
1:A:136:LEU:HD13	1:A:138:PHE:CE1	2.44	0.53
1:A:85:THR:HB	1:A:195:SER:O	2.11	0.51
1:A:106:ILE:HD13	1:A:158:TRP:CZ2	2.45	0.50
1:A:152:GLN:HE22	1:A:214:ASN:HD21	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:HA	1:A:178:LYS:O	2.12	0.50
1:A:25:SER:HA	5:A:284:HOH:O	2.12	0.50
1:A:23:GLY:HA2	1:A:35:ARG:NH1	2.27	0.49
1:A:55:ALA:HB3	1:A:58:LYS:HB3	1.95	0.49
1:A:63:GLU:OE1	5:A:264:HOH:O	2.19	0.49
1:A:92:PHE:HB3	1:A:107:ASP:HB3	1.95	0.48
1:A:17:THR:HB	1:A:18:TRP:CD1	2.49	0.47
1:A:18:TRP:HA	1:A:65:ARG:O	2.14	0.47
1:A:155:TYR:HA	1:A:168:ALA:O	2.14	0.47
1:A:29:VAL:O	1:A:186:GLY:HA2	2.15	0.47
1:A:65:ARG:HH11	1:A:65:ARG:CB	2.28	0.47
1:A:187:THR:N	5:A:282:HOH:O	2.48	0.47
1:A:72:TYR:CE2	1:A:153:PRO:HG3	2.50	0.46
1:A:113:LYS:HG2	1:A:193:LEU:O	2.17	0.44
1:A:42:THR:HG21	1:A:48:LYS:NZ	2.33	0.44
1:A:139:ASP:HB3	1:A:142:LYS:HG3	1.99	0.44
1:A:34:TRP:CE3	1:A:61:CYS:SG	3.11	0.43
1:A:5:SER:HA	1:A:211:TYR:O	2.18	0.43
1:A:26:ASN:HA	5:A:237:HOH:O	2.18	0.43
1:A:6:PHE:HE2	1:A:8:GLU:HB2	1.84	0.43
1:A:8:GLU:O	1:A:208:TRP:HB2	2.19	0.42
1:A:79:MET:HE3	1:A:79:MET:HB2	1.49	0.42
1:A:65:ARG:CB	1:A:65:ARG:NH1	2.83	0.42
1:A:183:LEU:HB2	5:A:287:HOH:O	2.20	0.42
1:A:81:PRO:HD2	1:A:140:ALA:O	2.20	0.42
1:A:116:THR:HA	1:A:138:PHE:O	2.20	0.42
1:A:118:VAL:HG23	1:A:136:LEU:HD21	2.00	0.42
1:A:159:TYR:HA	1:A:163:VAL:O	2.20	0.41
1:A:18:TRP:CZ3	1:A:181:MET:HE1	2.55	0.41
1:A:54:SER:OG	1:A:58:LYS:HG2	2.19	0.41
1:A:57:ASN:N	5:A:226:HOH:O	2.49	0.41
1:A:156:ILE:O	1:A:167:THR:HA	2.20	0.41
1:A:20:LYS:HD3	1:A:39:VAL:HB	2.03	0.41
1:A:121:ASN:ND2	1:A:130:HIS:H	2.13	0.41
1:A:95:THR:O	1:A:103:TRP:HA	2.21	0.41
1:A:111:LEU:HD12	1:A:111:LEU:N	2.35	0.41
1:A:54:SER:HB2	1:A:58:LYS:NZ	2.36	0.41

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)
1:A:152:GLN:NE2	5:A:288:HOH:O[3_645]	2.12	0.08

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	212/214 (99%)	198 (93%)	8 (4%)	6 (3%)	4 14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	VAL
1	A	84	ASN
1	A	171	ASN
1	A	56	TYR
1	A	2	THR
1	A	112	GLY

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	176/176 (100%)	147 (84%)	29 (16%)	2 8

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	8	GLU
1	A	19	GLU
1	A	33	THR
1	A	37	ASN
1	A	40	ASN
1	A	47	LEU
1	A	51	LEU
1	A	53	SER
1	A	54	SER
1	A	77	VAL
1	A	79	MET
1	A	85	THR
1	A	93	THR
1	A	106	ILE
1	A	107	ASP
1	A	113	LYS
1	A	127	VAL
1	A	132	LYS
1	A	136	LEU
1	A	141	SER
1	A	142	LYS
1	A	164	LEU
1	A	178	LYS
1	A	187	THR
1	A	191	ASP
1	A	193	LEU
1	A	197	ASN
1	A	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	37	ASN
1	A	84	ASN
1	A	121	ASN
1	A	145	HIS
1	A	152	GLN
1	A	166	HIS
1	A	197	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 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	BGC	B	1	4,2	12,12,12	1.24	3 (25%)	17,17,17	1.86	4 (23%)
2	BGC	B	2	2	11,11,12	1.75	1 (9%)	15,15,17	0.88	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
2	BGC	B	1	4,2	-	2/2/22/22	0/1/1/1
2	BGC	B	2	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	BGC	C4-C5	4.68	1.63	1.53
2	B	1	BGC	O1-C1	2.38	1.47	1.39
2	B	1	BGC	C4-C3	2.17	1.58	1.52
2	B	1	BGC	C3-C2	2.08	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	BGC	C4-C3-C2	4.67	119.03	110.83
2	B	1	BGC	O3-C3-C4	-3.85	101.31	110.38
2	B	1	BGC	C3-C4-C5	2.39	114.57	110.23
2	B	1	BGC	O4-C4-C3	-2.31	104.93	110.38

There are no chirality outliers.

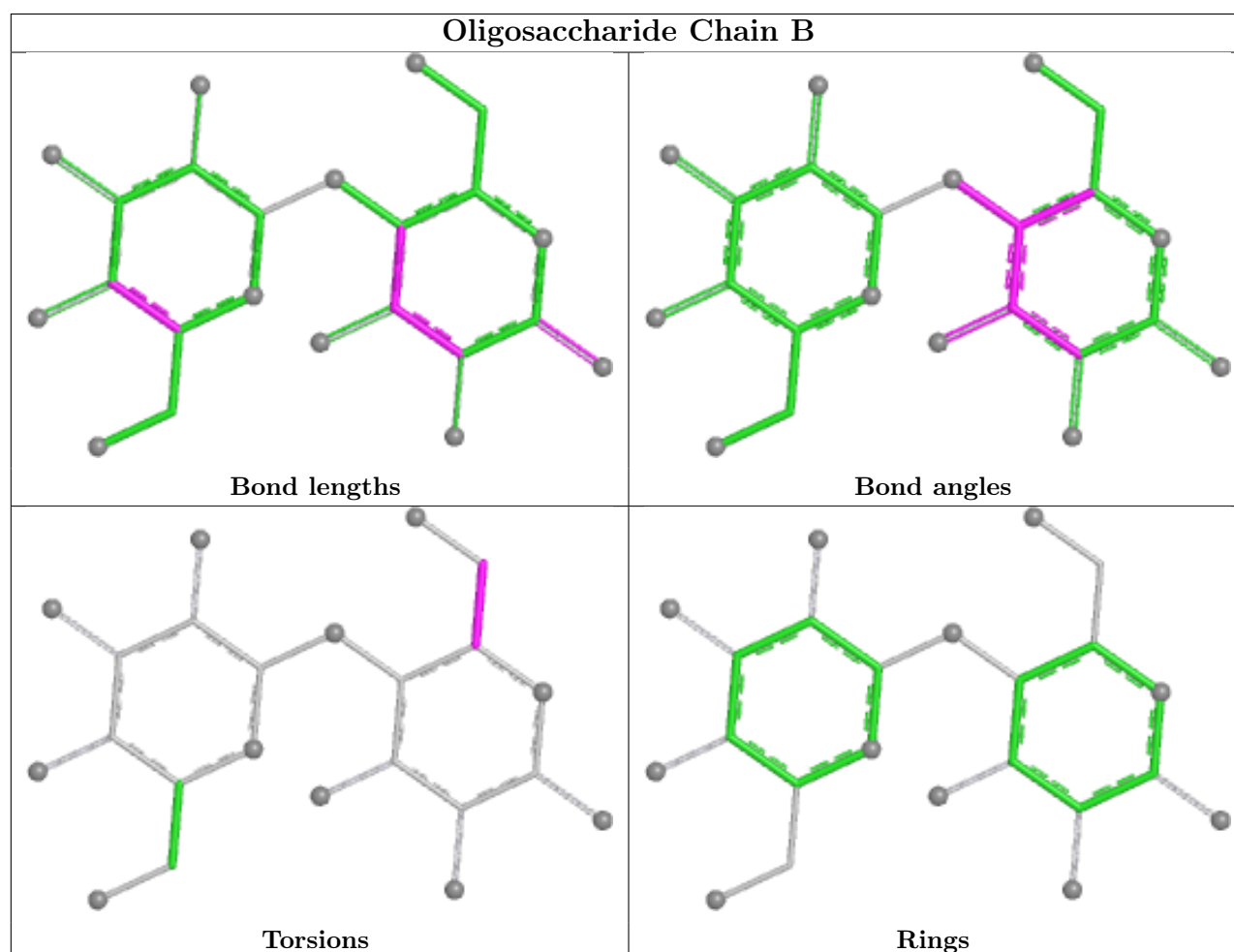
All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	NBU	A	215	2,1	3,3,3	0.43	0	2,2,2	0.32	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	NBU	A	215	2,1	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	215	NBU	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	214/214 (100%)	-0.58	0 100 100	7, 19, 26, 32	0

There are no RSRZ outliers to report.

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

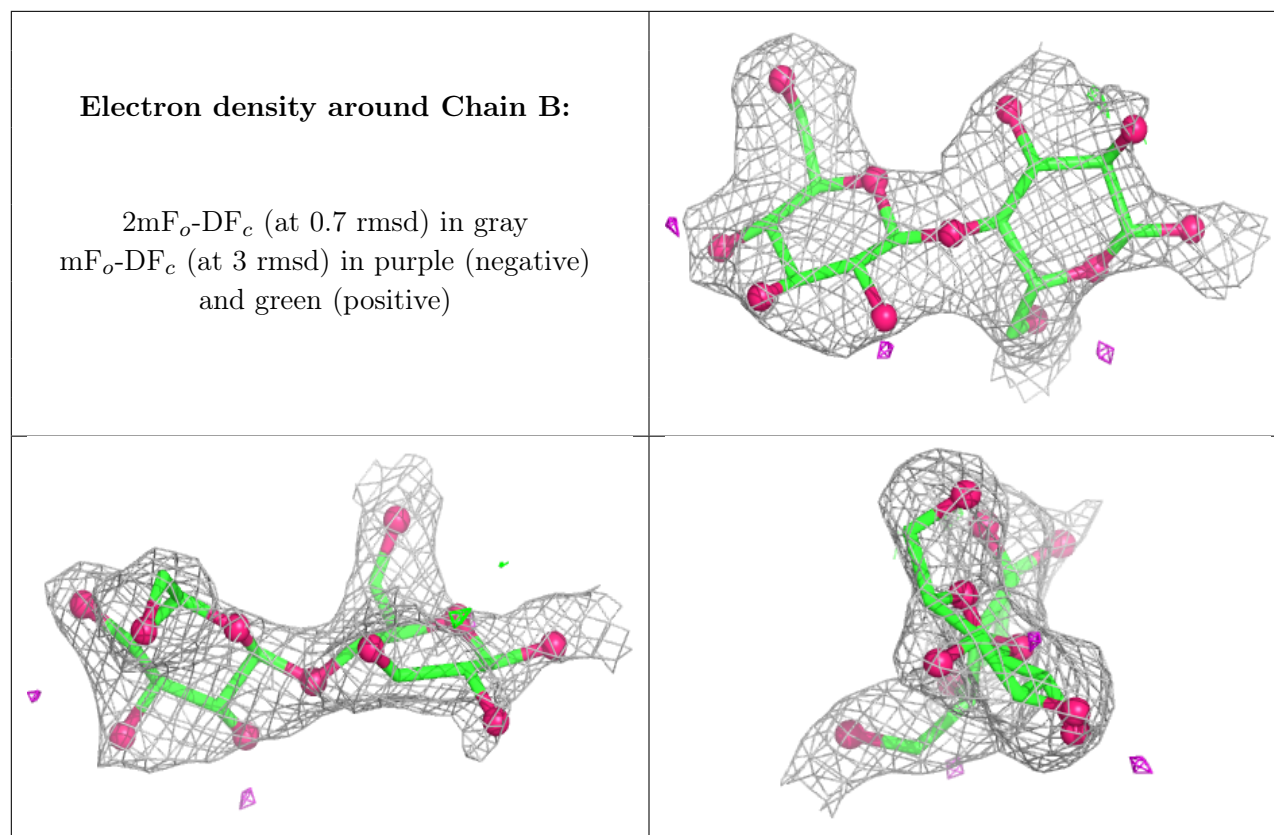
There are no non-standard protein/DNA/RNA residues in this entry.

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	BGC	B	2	11/12	0.89	0.08	13,22,26,27	0
2	BGC	B	1	12/12	0.91	0.07	18,28,32,32	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 [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	CA	A	218	1/1	0.66	0.25	32,32,32,32	0
4	NBU	A	215	4/4	0.83	0.10	23,25,29,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.