



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:55 PM UTC

PDB ID : 4ZLI / pdb_00004zli
Title : Cellobionic acid phosphorylase - 3-O-beta-D-glucopyranosyl-alpha-D-glucopyranuronic acid complex
Authors : Nam, Y.W.; Arakawa, T.; Fushinobu, S.
Deposited on : 2015-05-01
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	:	4-5-2 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

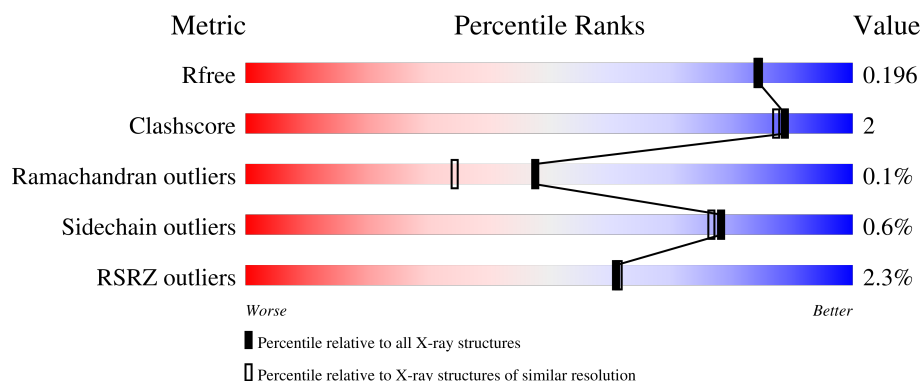
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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	796	2% 84% 14% ..
2	B	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6932 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.

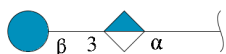
- Molecule 1 is a protein called Putative b-glycan phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	785	6228	3965	1060	1171	32	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	MET	engineered mutation	UNP Q21MB1
A	789	LEU	-	expression tag	UNP Q21MB1
A	790	GLU	-	expression tag	UNP Q21MB1
A	791	HIS	-	expression tag	UNP Q21MB1
A	792	HIS	-	expression tag	UNP Q21MB1
A	793	HIS	-	expression tag	UNP Q21MB1
A	794	HIS	-	expression tag	UNP Q21MB1
A	795	HIS	-	expression tag	UNP Q21MB1
A	796	HIS	-	expression tag	UNP Q21MB1

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-D-glucopyranuronic acid.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	2	24	12	12	0	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

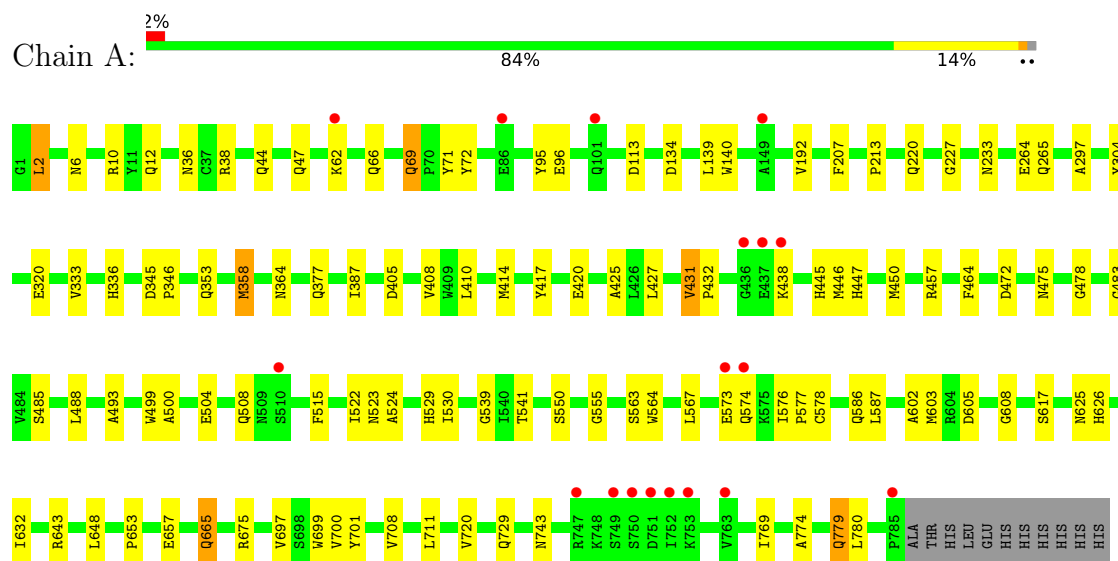
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	629	Total O 629 629	0	0

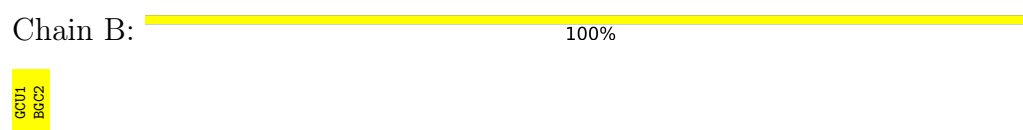
3 Residue-property plots

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: Putative b-glycan phosphorylase



- Molecule 2: beta-D-glucopyranose-(1-3)-alpha-D-glucopyranuronic acid



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.06Å 107.06Å 185.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.50 – 1.80 40.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.50-1.80) 99.4 (40.50-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.155 , 0.188 0.167 , 0.196	Depositor DCC
R_{free} test set	5709 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6932	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: CL, SO4, BGC, GOL, GCU

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	1.72	72/6393 (1.1%)	1.32	19/8683 (0.2%)

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	GLN	C-O	-9.40	1.12	1.24
1	A	608	GLY	C-O	-7.49	1.19	1.24
1	A	530	ILE	CA-C	-7.06	1.45	1.52
1	A	358	MET	SD-CE	-6.63	1.62	1.79
1	A	504	GLU	CA-C	6.60	1.61	1.52
1	A	653	PRO	CA-C	6.57	1.61	1.52
1	A	2	LEU	CA-C	-6.54	1.45	1.52
1	A	587	LEU	N-CA	6.49	1.54	1.46
1	A	524	ALA	N-CA	6.46	1.54	1.46
1	A	508	GLN	CD-NE2	6.38	1.46	1.33
1	A	364	ASN	CG-OD1	6.32	1.35	1.23
1	A	774	ALA	C-O	-6.31	1.16	1.23
1	A	113	ASP	CA-C	-6.26	1.45	1.52
1	A	675	ARG	CA-C	6.24	1.60	1.52
1	A	414	MET	CG-SD	-6.23	1.65	1.80
1	A	578	CYS	CA-C	6.21	1.60	1.52
1	A	264	GLU	CA-C	6.18	1.60	1.52
1	A	602	ALA	CA-C	-6.17	1.45	1.52
1	A	539	GLY	C-O	-6.00	1.16	1.24
1	A	405	ASP	CA-CB	-5.98	1.43	1.53
1	A	483	GLY	CA-C	5.95	1.57	1.52
1	A	550	SER	C-O	-5.84	1.16	1.24
1	A	493	ALA	N-CA	5.83	1.53	1.46
1	A	701	TYR	N-CA	5.75	1.53	1.46
1	A	427	LEU	CA-C	-5.72	1.44	1.52
1	A	539	GLY	N-CA	-5.69	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	500	ALA	CA-C	5.68	1.60	1.52
1	A	577	PRO	C-O	5.67	1.31	1.24
1	A	464	PHE	N-CA	5.63	1.52	1.46
1	A	139	LEU	N-CA	5.62	1.53	1.46
1	A	457	ARG	N-CA	-5.62	1.38	1.45
1	A	603	MET	N-CA	-5.60	1.38	1.46
1	A	446	MET	N-CA	-5.59	1.39	1.46
1	A	320	GLU	N-CA	5.57	1.53	1.46
1	A	626	HIS	N-CA	-5.51	1.39	1.46
1	A	586	GLN	CA-CB	-5.49	1.46	1.54
1	A	297	ALA	C-O	5.47	1.30	1.24
1	A	304	TYR	CA-C	-5.44	1.46	1.52
1	A	729	GLN	N-CA	5.44	1.53	1.46
1	A	708	VAL	C-O	5.42	1.30	1.24
1	A	475	ASN	CA-C	5.41	1.59	1.52
1	A	708	VAL	N-CA	-5.41	1.40	1.46
1	A	140	TRP	CA-C	5.39	1.58	1.52
1	A	478	GLY	CA-C	-5.38	1.44	1.51
1	A	515	PHE	CA-C	-5.38	1.45	1.52
1	A	574	GLN	C-O	-5.34	1.17	1.24
1	A	213	PRO	CA-C	5.33	1.58	1.53
1	A	44	GLN	CD-NE2	5.32	1.44	1.33
1	A	457	ARG	CA-C	5.31	1.58	1.52
1	A	192	VAL	CA-C	5.30	1.59	1.52
1	A	711	LEU	N-CA	-5.30	1.39	1.46
1	A	333	VAL	CA-CB	5.29	1.60	1.54
1	A	450	MET	N-CA	-5.27	1.39	1.46
1	A	563	SER	C-O	5.24	1.30	1.24
1	A	617	SER	CA-C	-5.22	1.46	1.52
1	A	207	PHE	N-CA	-5.21	1.40	1.46
1	A	472	ASP	C-O	-5.16	1.19	1.24
1	A	779	GLN	CA-C	-5.16	1.46	1.52
1	A	410	LEU	N-CA	-5.12	1.42	1.46
1	A	417	TYR	N-CA	-5.12	1.40	1.46
1	A	625	ASN	CG-OD1	5.10	1.33	1.23
1	A	564	TRP	N-CA	-5.10	1.39	1.46
1	A	563	SER	CA-C	-5.07	1.46	1.52
1	A	529	HIS	N-CA	5.06	1.52	1.45
1	A	523	ASN	N-CA	-5.06	1.40	1.46
1	A	632	ILE	C-O	5.06	1.29	1.24
1	A	720	VAL	CA-CB	5.06	1.59	1.53
1	A	265	GLN	CA-C	-5.05	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	425	ALA	C-O	-5.04	1.17	1.24
1	A	697	VAL	C-O	5.03	1.30	1.24
1	A	488	LEU	N-CA	-5.03	1.39	1.46
1	A	541	THR	CA-C	-5.02	1.46	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LEU	N-CA-C	6.74	118.63	111.28
1	A	71	TYR	N-CA-C	-6.33	101.09	110.46
1	A	336	HIS	O-C-N	-6.15	115.73	122.07
1	A	605	ASP	N-CA-C	6.05	120.28	113.02
1	A	431	VAL	N-CA-CB	6.01	118.07	111.64
1	A	485	SER	CA-C-N	5.96	126.55	119.94
1	A	485	SER	C-N-CA	5.96	126.55	119.94
1	A	47	GLN	N-CA-C	5.76	122.53	109.81
1	A	522	ILE	N-CA-C	5.63	116.36	110.62
1	A	576	ILE	N-CA-CB	5.59	114.26	110.52
1	A	665	GLN	N-CA-C	5.52	118.40	109.40
1	A	665	GLN	CA-CB-CG	5.47	125.04	114.10
1	A	541	THR	N-CA-C	5.41	117.30	110.33
1	A	220	GLN	N-CA-C	5.37	117.55	111.11
1	A	420	GLU	N-CA-C	5.34	117.19	111.36
1	A	643	ARG	N-CA-C	-5.31	105.40	111.14
1	A	555	GLY	O-C-N	5.14	127.25	122.57
1	A	72	TYR	N-CA-C	-5.10	101.16	108.60
1	A	134	ASP	CB-CA-C	-5.09	101.14	109.99

There are no chirality outliers.

There are no planarity outliers.

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	6228	0	6003	23	0
2	B	24	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	40	1	0
4	A	20	0	0	0	0
5	A	1	0	0	0	0
6	A	629	0	0	0	0
All	All	6932	0	6061	23	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 2.

All (23) 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:353:GLN:HE21	1:A:699:TRP:HE1	1.31	0.79
1:A:447:HIS:HD2	1:A:499:TRP:HE1	1.41	0.68
1:A:743:ASN:HD22	1:A:779:GLN:HE22	1.48	0.62
1:A:377:GLN:OE1	1:A:445:HIS:HD2	1.86	0.57
1:A:353:GLN:HE21	1:A:699:TRP:NE1	2.00	0.57
1:A:657:GLU:OE1	3:A:804:GOL:O1	2.18	0.57
1:A:447:HIS:CD2	1:A:499:TRP:HE1	2.23	0.57
1:A:431:VAL:O	1:A:445:HIS:HE1	1.92	0.52
1:A:6:ASN:HD22	1:A:10:ARG:HH11	1.58	0.51
1:A:377:GLN:OE1	1:A:445:HIS:CD2	2.63	0.50
1:A:573:GLU:H	1:A:573:GLU:CD	2.19	0.50
1:A:431:VAL:HB	1:A:432:PRO:HD2	1.93	0.50
1:A:6:ASN:ND2	1:A:10:ARG:HH11	2.16	0.44
1:A:66:GLN:H	1:A:69:GLN:NE2	2.16	0.44
1:A:36:ASN:ND2	1:A:38:ARG:H	2.17	0.43
1:A:227:GLY:H	1:A:233:ASN:HD22	1.66	0.43
1:A:358:MET:HE3	1:A:358:MET:HB3	1.71	0.42
1:A:769:ILE:HD11	1:A:780:LEU:HD21	2.01	0.42
1:A:38:ARG:HB3	1:A:96:GLU:HG2	2.02	0.41
1:A:346:PRO:HD2	1:A:387:ILE:O	2.20	0.41
1:A:2:LEU:HA	1:A:12:GLN:O	2.21	0.40
1:A:345:ASP:CG	1:A:345:ASP:O	2.65	0.40
1:A:648:LEU:HD11	1:A:700:VAL:HG13	2.03	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	783/796 (98%)	763 (97%)	19 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TYR

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	655/665 (98%)	651 (99%)	4 (1%)	78	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	408	VAL
1	A	438	LYS
1	A	665	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN

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Mol	Chain	Res	Type
1	A	36	ASN
1	A	69	GLN
1	A	103	ASN
1	A	233	ASN
1	A	313	GLN
1	A	340	ASN
1	A	353	GLN
1	A	355	ASN
1	A	368	GLN
1	A	445	HIS
1	A	447	HIS
1	A	529	HIS
1	A	560	ASN
1	A	586	GLN
1	A	693	ASN
1	A	721	GLN
1	A	723	GLN
1	A	743	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	GCU	B	1	2	13,13,13	1.43	3 (23%)	18,19,19	1.88	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	B	2	2	11,11,12	1.70	1 (9%)	15,15,17	1.13	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	GCU	B	1	2	-	0/4/24/24	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	C2-C3	4.55	1.59	1.52
2	B	1	GCU	C3-C2	2.47	1.58	1.52
2	B	1	GCU	O6B-C6	-2.39	1.23	1.30
2	B	1	GCU	C1-C2	2.32	1.57	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GCU	C1-C2-C3	3.78	118.06	110.36
2	B	1	GCU	O6B-C6-O6A	2.81	130.46	124.08
2	B	1	GCU	C4-C3-C2	-2.73	106.05	110.83
2	B	1	GCU	C1-O5-C5	2.63	116.09	112.22
2	B	1	GCU	O6A-C6-C5	-2.61	111.37	120.81
2	B	1	GCU	O1-C1-C2	-2.52	101.67	108.98
2	B	2	BGC	O2-C2-C1	-2.16	104.29	109.22
2	B	1	GCU	O4-C4-C3	-2.07	105.49	110.38

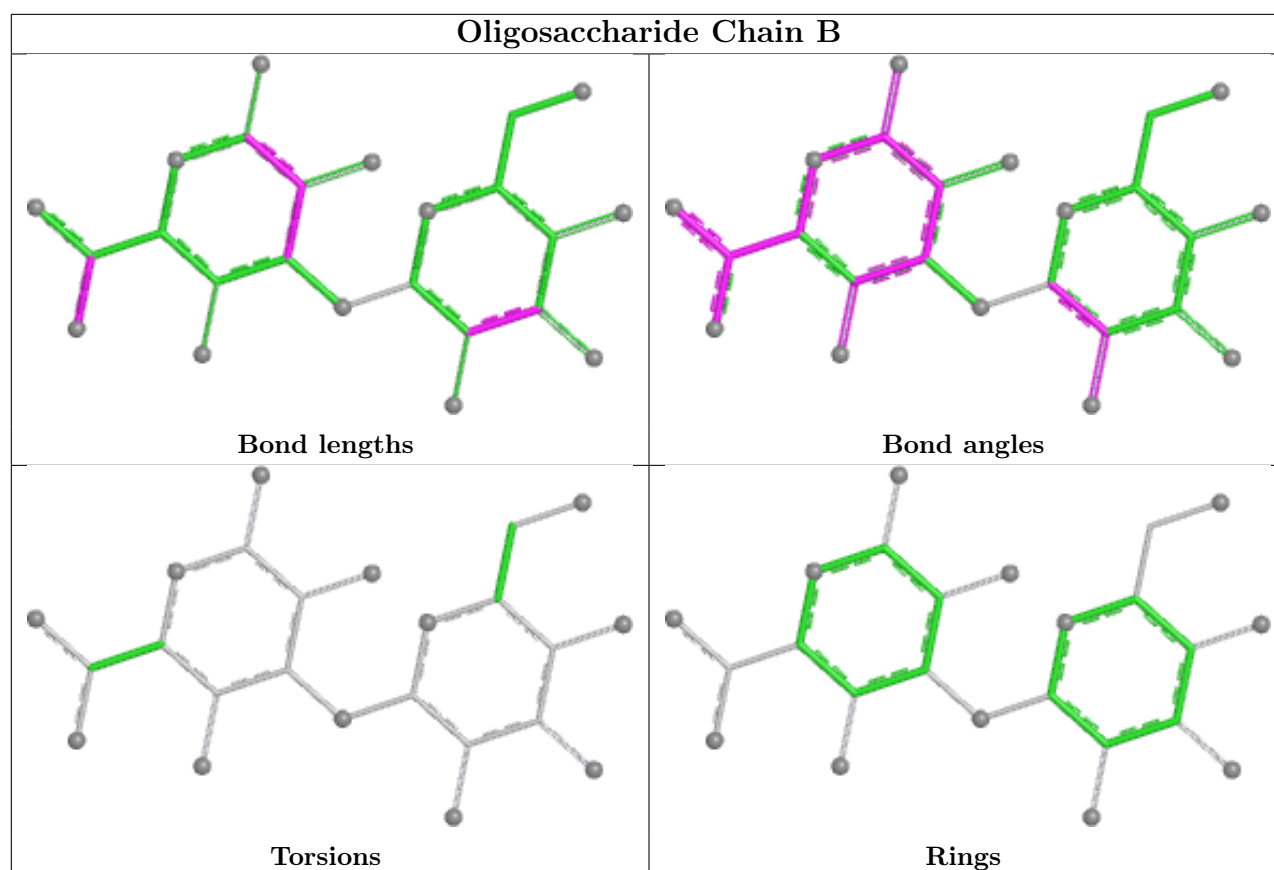
There are no chirality outliers.

There are no torsion outliers.

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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	$\# Z > 2$
3	GOL	A	803	-	5,5,5	1.56	1 (20%)	5,5,5	1.97	2 (40%)
4	SO4	A	808	-	4,4,4	0.62	0	6,6,6	0.82	0
3	GOL	A	801	-	5,5,5	1.05	0	5,5,5	0.84	0
3	GOL	A	802	-	5,5,5	0.47	0	5,5,5	0.47	0
3	GOL	A	805	-	5,5,5	0.80	0	5,5,5	0.69	0
4	SO4	A	809	-	4,4,4	0.79	0	6,6,6	0.65	0
4	SO4	A	810	-	4,4,4	0.84	0	6,6,6	0.96	1 (16%)
3	GOL	A	804	-	5,5,5	0.91	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	807	-	4,4,4	0.64	0	6,6,6	0.50	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
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	A	801	-	-	0/4/4/4	-
3	GOL	A	802	-	-	0/4/4/4	-
3	GOL	A	805	-	-	0/4/4/4	-
3	GOL	A	804	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	GOL	O2-C2	2.59	1.50	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	GOL	O3-C3-C2	3.01	123.95	110.38
3	A	803	GOL	O2-C2-C1	2.15	118.06	109.18
4	A	810	SO4	O3-S-O1	-2.01	99.05	109.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	GOL	C1-C2-C3-O3
3	A	803	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	GOL	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	785/796 (98%)	0.02	18 (2%) 61 61	18, 26, 42, 75	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	SER	4.4
1	A	785	PRO	4.2
1	A	752	ILE	4.0
1	A	438	LYS	3.5
1	A	751	ASP	3.2
1	A	749	SER	3.1
1	A	763	VAL	3.0
1	A	510	SER	2.9
1	A	574	GLN	2.9
1	A	149	ALA	2.7
1	A	436	GLY	2.7
1	A	747	ARG	2.7
1	A	573	GLU	2.3
1	A	437	GLU	2.3
1	A	753	LYS	2.3
1	A	62	LYS	2.2
1	A	86	GLU	2.1
1	A	101	GLN	2.1

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

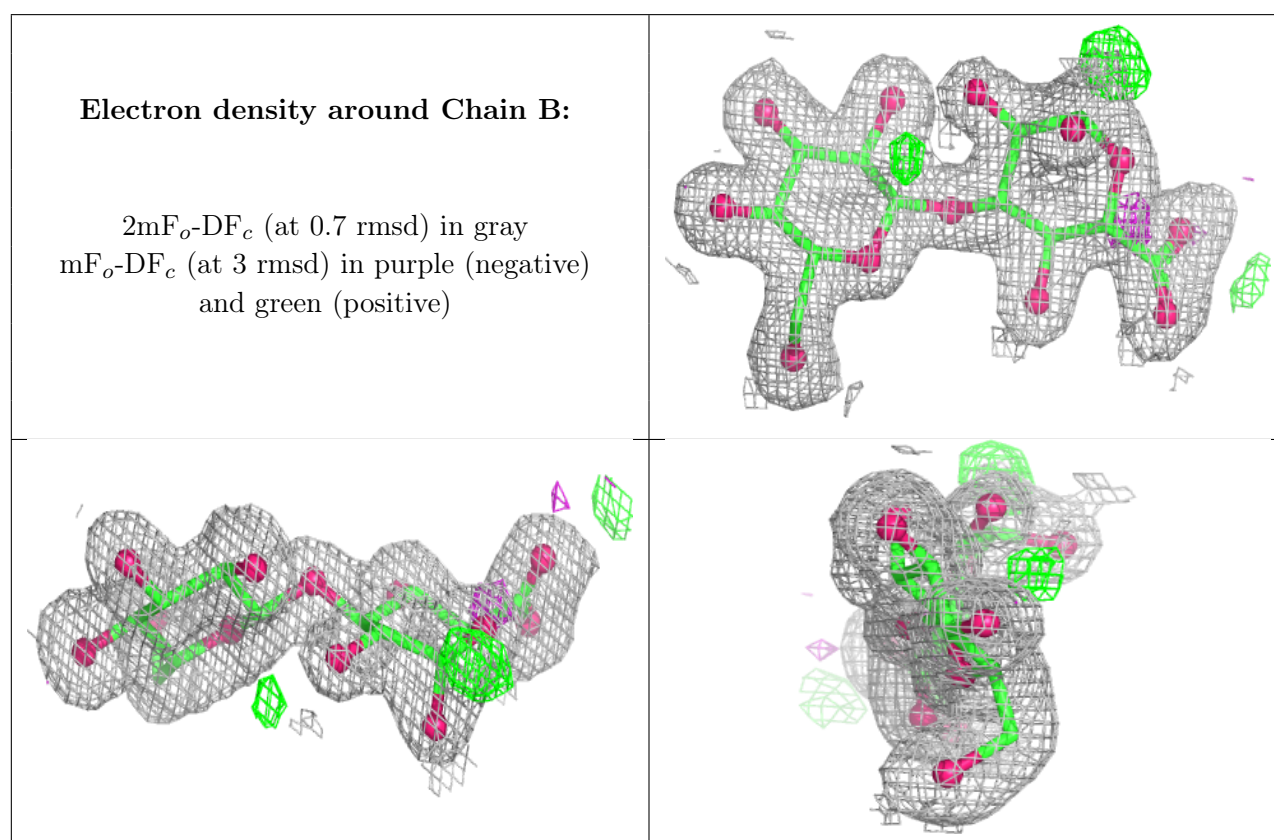
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	GCU	B	1	13/13	0.95	0.07	25,27,31,33	0
2	BGC	B	2	11/12	0.97	0.07	20,21,25,28	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	SO4	A	810	5/5	0.79	0.13	54,56,73,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	803	6/6	0.93	0.12	37,44,45,47	0
3	GOL	A	805	6/6	0.94	0.11	29,31,33,35	0
3	GOL	A	804	6/6	0.95	0.07	32,38,41,50	0
4	SO4	A	809	5/5	0.97	0.12	38,39,41,42	0
3	GOL	A	802	6/6	0.97	0.06	24,27,29,30	0
3	GOL	A	801	6/6	0.98	0.05	19,20,22,23	0
4	SO4	A	808	5/5	0.98	0.08	30,34,40,42	0
4	SO4	A	807	5/5	0.99	0.04	21,23,25,26	0
5	CL	A	811	1/1	0.99	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.