



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:25 PM EDT

PDB ID : 1KJR / pdb_00001kjr
Title : Crystal Structure of the human galectin-3 CRD in complex with a 3'-derivative of N-Acetyllactosamine
Authors : Sorme, P.; Arnoux, P.; Kahl-Knutsson, B.; Leffler, H.; Rini, J.M.; Nilsson, U.J.
Deposited on : 2001-12-05
Resolution : 1.55 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

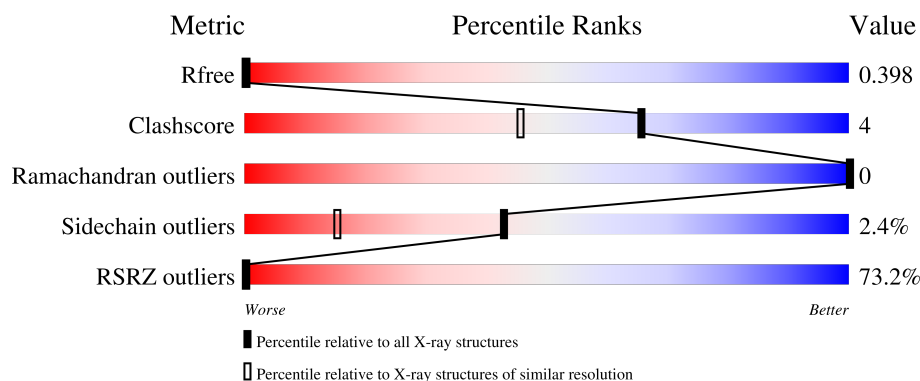
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	146	69% 84% 10% 5%
2	B	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BEK	A	500	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1384 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 Galectin-3.

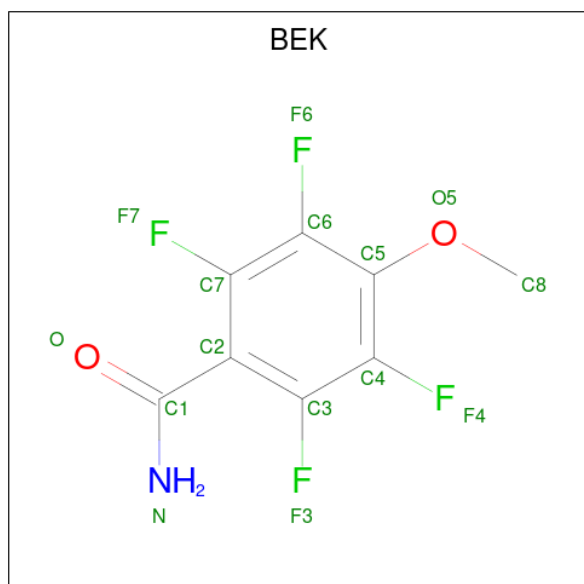
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	138	1144	728	207	206	3	0	5	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	25	14	1	10	0	0	0

- Molecule 3 is 2,3,5,6-TETRAFLUORO-4-METHOXY-BENZAMIDE (CCD ID: BEK) (formula: C₈H₅F₄NO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			15	8	4	1	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

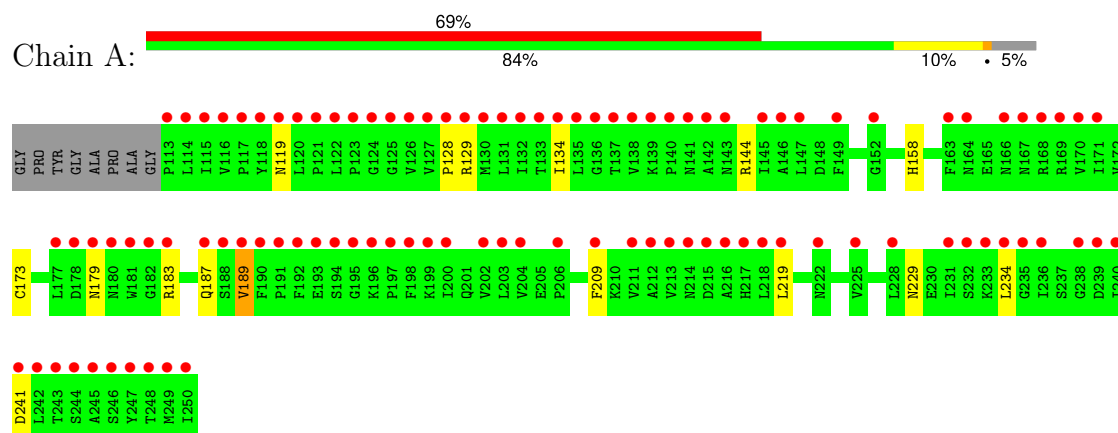
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	199	Total	O	0	0
			199	199		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Galectin-3



- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-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	37.60Å 58.40Å 64.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55 20.00 – 1.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.55) 96.2 (20.00-1.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.182 , 0.212 0.370 , 0.398	Depositor DCC
R_{free} test set	947 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 97.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	1384	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.59% 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: BEK, NAG, GAL, CL

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	1.01	0/1170	1.15	3/1586 (0.2%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ASP	N-CA-C	-6.23	98.57	108.73
1	A	209	PHE	N-CA-C	-6.12	99.29	109.46
1	A	189	VAL	N-CA-C	-5.32	102.65	109.30

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	1144	0	1148	9	0
2	B	25	0	22	0	0
3	A	15	0	4	1	0
4	A	1	0	0	0	0
5	A	199	0	0	2	0
All	All	1384	0	1174	9	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 4.

All (9) 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:119:ASN:HB3	5:A:700:HOH:O	1.70	0.91
1:A:134[A]:ILE:HD11	1:A:234:LEU:HD21	1.81	0.63
1:A:187:GLN:HE21	1:A:189:VAL:H	1.52	0.57
1:A:187:GLN:NE2	1:A:189:VAL:H	2.10	0.48
1:A:119:ASN:ND2	5:A:786:HOH:O	2.26	0.45
1:A:144:ARG:HG3	3:A:500:BEK:H83	1.99	0.45
1:A:158:HIS:O	1:A:173:CYS:HA	2.19	0.42
1:A:128:PRO:O	1:A:129:ARG:HB2	2.21	0.41
1:A:219:LEU:C	1:A:219:LEU:HD12	2.46	0.41

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	141/146 (97%)	139 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	129/127 (102%)	125 (97%)	4 (3%)	35 8

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

Mol	Chain	Res	Type
1	A	179[A]	ASN
1	A	179[B]	ASN
1	A	183	ARG
1	A	229	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	187	GLN
1	A	229	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	NAG	B	1	2	15,15,15	0.75	1 (6%)	21,21,21	1.15	1 (4%)
2	GAL	B	2	2,3	10,10,12	0.58	0	13,13,17	0.65	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	NAG	B	1	2	-	0/6/26/26	0/1/1/1
2	GAL	B	2	2,3	-	0/2/15/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.21	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-C2-C3	-3.63	105.60	110.54

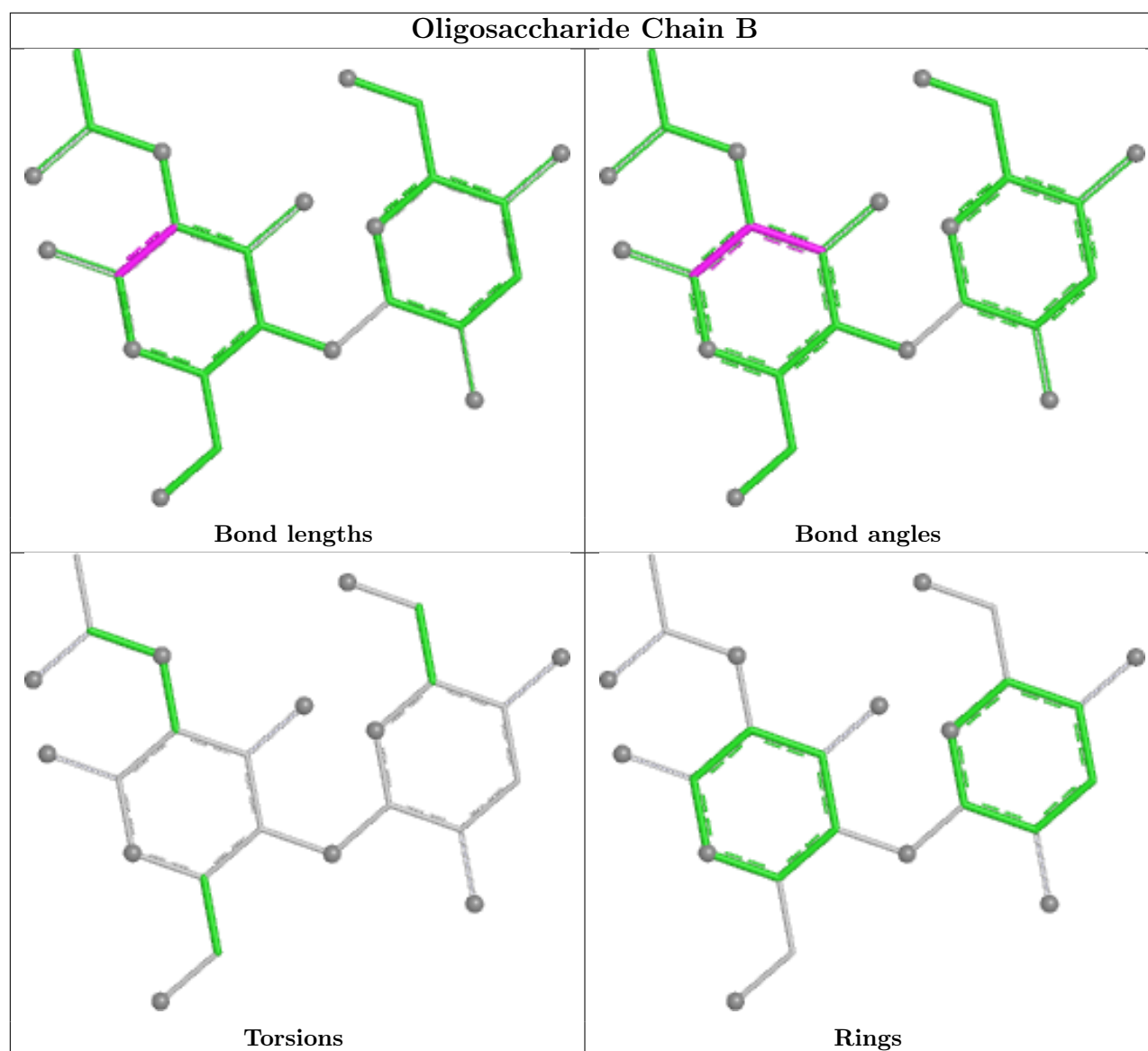
There are no chirality outliers.

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 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	$\# Z > 2$
3	BEK	A	500	2	15,15,15	8.78	14 (93%)	20,22,22	2.84	5 (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
3	BEK	A	500	2	-	1/6/6/6	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	BEK	F4-C4	-16.91	1.10	1.34
3	A	500	BEK	F6-C6	-16.36	1.11	1.34
3	A	500	BEK	O5-C5	-11.98	1.16	1.38
3	A	500	BEK	F3-C3	-11.14	1.19	1.34
3	A	500	BEK	F7-C7	-10.81	1.19	1.34
3	A	500	BEK	C2-C7	6.89	1.50	1.38
3	A	500	BEK	O-C1	6.22	1.35	1.24
3	A	500	BEK	C2-C1	-6.01	1.40	1.51
3	A	500	BEK	C5-C6	5.19	1.49	1.39
3	A	500	BEK	C5-C4	4.64	1.47	1.39
3	A	500	BEK	C6-C7	4.43	1.44	1.38
3	A	500	BEK	C2-C3	3.64	1.45	1.38
3	A	500	BEK	C4-C3	3.02	1.42	1.38
3	A	500	BEK	C1-N	2.33	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	BEK	O-C1-C2	8.15	131.38	120.07
3	A	500	BEK	O-C1-N	-5.83	114.19	122.62
3	A	500	BEK	C8-O5-C5	5.62	129.99	114.74
3	A	500	BEK	C7-C2-C3	2.96	120.79	116.29
3	A	500	BEK	C2-C7-C6	-2.28	118.93	122.07

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	BEK	C6-C5-O5-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	BEK	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	138/146 (94%)	3.04	101 (73%) 0 0	5, 14, 22, 30	5 (3%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	9.3
1	A	115	ILE	6.3
1	A	250	ILE	6.3
1	A	197	PRO	6.3
1	A	136	GLY	5.8
1	A	113	PRO	5.8
1	A	243	THR	5.7
1	A	119	ASN	5.5
1	A	242	LEU	5.5
1	A	244[A]	SER	5.4
1	A	198	PHE	5.4
1	A	137	THR	5.3
1	A	247	TYR	5.2
1	A	135	LEU	5.2
1	A	123	PRO	5.2
1	A	138	VAL	5.1
1	A	121	PRO	5.0
1	A	134[A]	ILE	5.0
1	A	118	TYR	4.8
1	A	241	ASP	4.8
1	A	142	ALA	4.8
1	A	132	ILE	4.8
1	A	117	PRO	4.8
1	A	116	VAL	4.6
1	A	214	ASN	4.6
1	A	140	PRO	4.4
1	A	183	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	120	LEU	4.3
1	A	213	VAL	4.3
1	A	215	ASP	4.3
1	A	238	GLY	4.2
1	A	216	ALA	4.2
1	A	133	THR	4.0
1	A	193	GLU	4.0
1	A	246	SER	4.0
1	A	170	VAL	4.0
1	A	188	SER	4.0
1	A	131	LEU	4.0
1	A	192	PHE	3.9
1	A	139	LYS	3.9
1	A	218	LEU	3.8
1	A	203	LEU	3.7
1	A	122	LEU	3.6
1	A	240	ILE	3.6
1	A	236	ILE	3.6
1	A	204	VAL	3.6
1	A	200	ILE	3.5
1	A	212	ALA	3.5
1	A	196	LYS	3.5
1	A	189	VAL	3.5
1	A	171	ILE	3.5
1	A	164	ASN	3.4
1	A	248	THR	3.4
1	A	199	LYS	3.3
1	A	194	SER	3.3
1	A	190	PHE	3.3
1	A	126	VAL	3.3
1	A	245	ALA	3.2
1	A	163	PHE	3.1
1	A	143	ASN	3.0
1	A	141	ASN	3.0
1	A	234	LEU	3.0
1	A	179[A]	ASN	2.9
1	A	195	GLY	2.9
1	A	249	MET	2.9
1	A	232[A]	SER	2.9
1	A	239	ASP	2.8
1	A	191	PRO	2.8
1	A	209	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLY	2.8
1	A	211	VAL	2.8
1	A	206	PRO	2.8
1	A	235	GLY	2.7
1	A	166	ASN	2.7
1	A	127	VAL	2.7
1	A	217	HIS	2.7
1	A	125	GLY	2.6
1	A	124	GLY	2.6
1	A	187	GLN	2.6
1	A	167	ASN	2.6
1	A	233	LYS	2.6
1	A	181	TRP	2.5
1	A	128	PRO	2.5
1	A	202	VAL	2.5
1	A	146	ALA	2.5
1	A	231	ILE	2.5
1	A	130	MET	2.5
1	A	129	ARG	2.5
1	A	222[A]	ASN	2.4
1	A	182	GLY	2.4
1	A	225	VAL	2.3
1	A	219	LEU	2.3
1	A	168	ARG	2.3
1	A	145	ILE	2.3
1	A	147	LEU	2.1
1	A	177	LEU	2.1
1	A	169	ARG	2.1
1	A	149	PHE	2.1
1	A	178	ASP	2.1
1	A	180	ASN	2.0
1	A	228	LEU	2.0

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

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

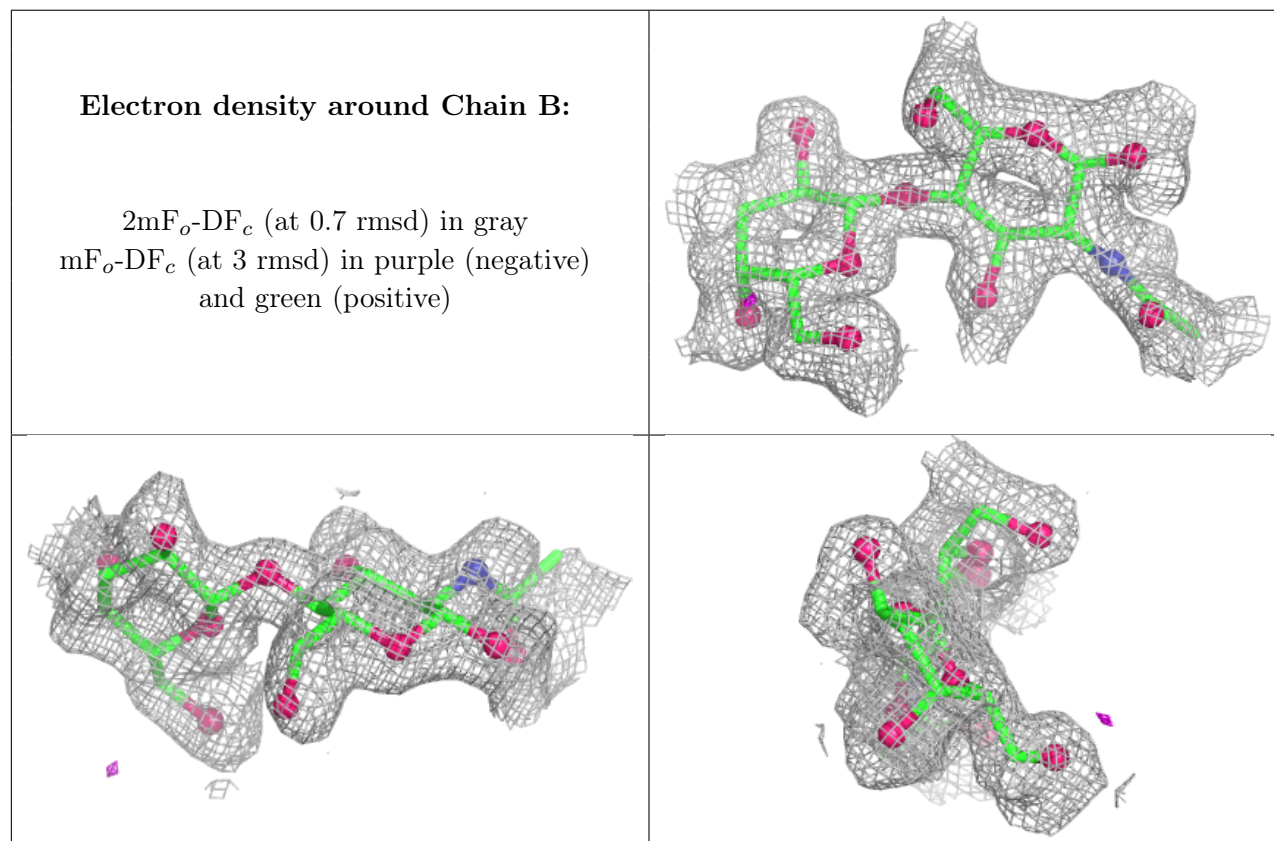
6.3 Carbohydrates [i](#)

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	NAG	B	1	15/15	0.76	0.17	18,25,31,32	0
2	GAL	B	2	10/12	0.89	0.10	13,15,18,20	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	CL	A	300	1/1	0.78	0.11	16,16,16,16	0
3	BEK	A	500	15/15	0.81	0.13	18,22,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.