



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 01:01 AM UTC

PDB ID : 2WNF / pdb_00002wnf
Title : Crystal Structure of a Mammalian Sialyltransferase in complex with Gal-beta-1-3GalNAc-ortho-nitrophenol
Authors : Rao, F.V.; Rich, J.R.; Raikic, B.; Wakarchuk, W.W.; Withers, S.G.; Strynadka, N.C.J.
Deposited on : 2009-07-09
Resolution : 1.25 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

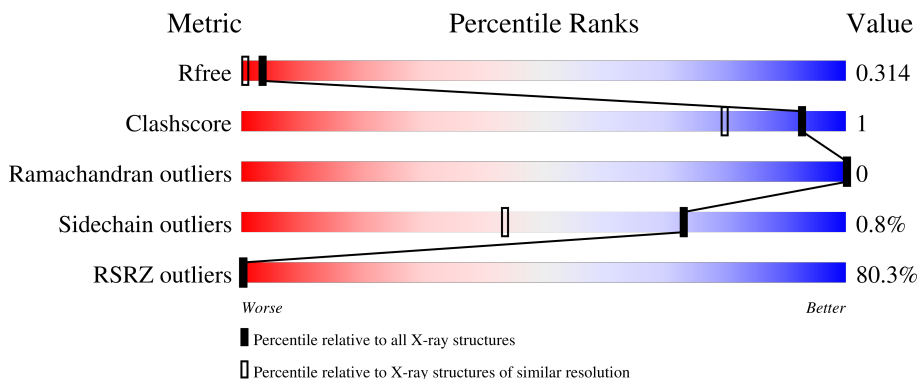
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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	298	72% 86% 5% • 9%
2	B	2	100%

2 Entry composition [i](#)

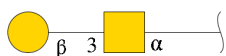
There are 4 unique types of molecules in this entry. The entry contains 2699 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CMP-N-ACETYLNEURAMINATE-BETA-GALACTOSAMIDE-ALPHA-2,3-SIALYLTRANSFERASE.

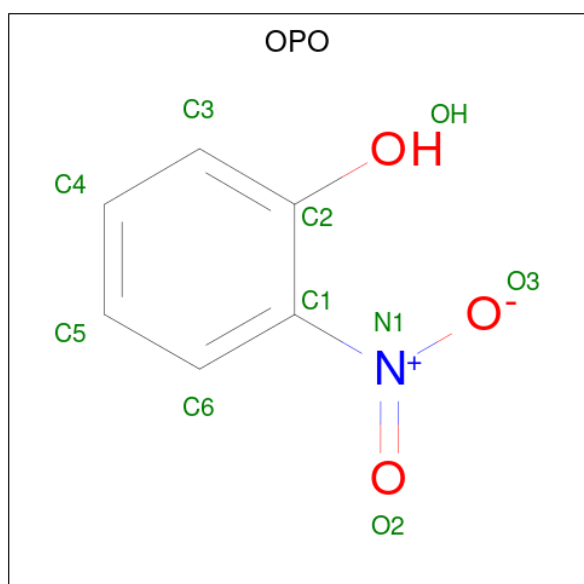
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	Se	0	17	0
			2343	1493	415	424	8	3			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



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

- Molecule 3 is O-NITROPHENOL (CCD ID: OPO) (formula: $C_6H_5NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	321	Total	O	0	0
			321	321		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.99Å 78.35Å 99.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.11 – 1.25 33.11 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.11-1.25) 99.9 (33.11-1.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.24Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.180 , 0.195 0.307 , 0.314	Depositor DCC
R_{free} test set	4261 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	9.1	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2699	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% 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: OPO, A2G, 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	1.36	6/2423 (0.2%)	1.06	0/3271

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	VAL	CA-C	9.17	1.61	1.52
1	A	220	VAL	CA-CB	9.00	1.65	1.54
1	A	143	ARG	CA-CB	-5.46	1.46	1.53
1	A	112	GLN	C-O	5.39	1.26	1.23
1	A	297	LYS	CG-CD	-5.03	1.37	1.52
1	A	245	GLU	CD-OE1	5.03	1.34	1.25

There are no bond angle outliers.

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	2343	0	2294	7	0
2	B	25	0	21	0	0
3	A	10	0	4	0	0
4	A	321	0	0	3	1
All	All	2699	0	2319	7	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 1.

All (7) 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:122[A]:GLU:HG2	4:A:690:HOH:O	1.60	1.02
1:A:106:ARG:O	1:A:109:ARG:HD2	2.01	0.61
1:A:122[A]:GLU:CG	4:A:690:HOH:O	2.35	0.57
1:A:181:GLU:HB2	4:A:511:HOH:O	2.08	0.54
1:A:143:ARG:HG2	1:A:284[B]:CYS:SG	2.59	0.42
1:A:107:LEU:HD22	1:A:269:TYR:HB3	2.02	0.41
1:A:64:CYS:HB2	1:A:66:ARG:O	2.21	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)
4:A:788:HOH:O	4:A:802:HOH:O[4_566]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/298 (96%)	278 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/263 (99%)	259 (99%)	2 (1%)	73	43

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	343	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN

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	A2G	B	1	3,2	14,14,15	1.32	2 (14%)	17,19,21	1.60	4 (23%)
2	GAL	B	2	2	11,11,12	1.49	2 (18%)	15,15,17	1.03	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	A2G	B	1	3,2	-	1/6/23/26	0/1/1/1
2	GAL	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	1	A2G	C1-C2	3.41	1.57	1.52
2	B	2	GAL	O5-C5	3.11	1.49	1.43
2	B	2	GAL	O2-C2	2.30	1.48	1.43
2	B	1	A2G	O5-C5	2.15	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	A2G	C1-O5-C5	2.97	116.17	112.19
2	B	1	A2G	O5-C1-C2	-2.86	106.87	111.29
2	B	1	A2G	O3-C3-C2	-2.06	105.11	109.40
2	B	2	GAL	C2-C3-C4	-2.04	107.27	110.86
2	B	1	A2G	C8-C7-N2	-2.03	112.75	116.12

There are no chirality outliers.

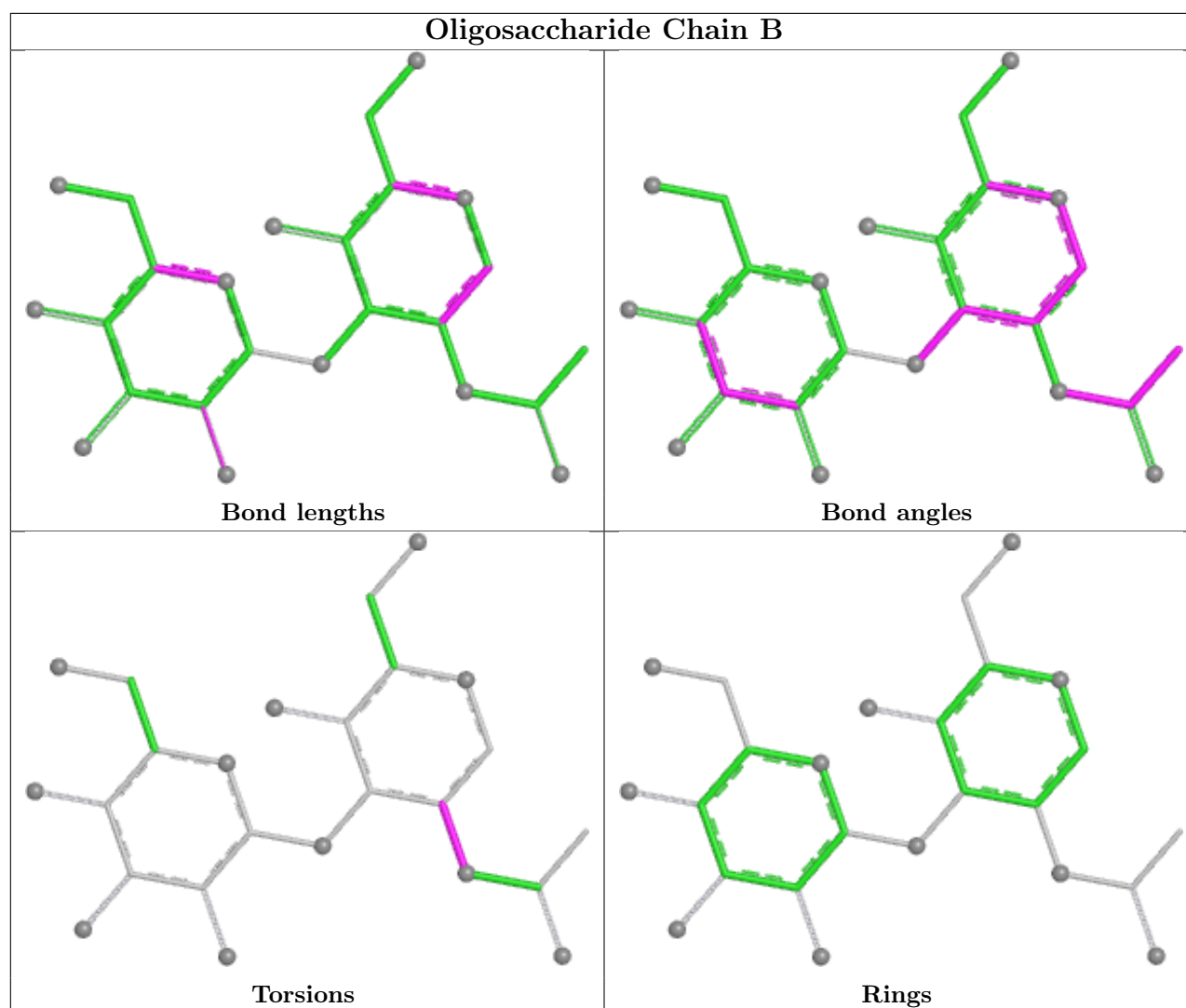
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	A2G	C1-C2-N2-C7

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](#)

1 ligand is 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	$\# Z > 2$
3	OPO	A	401	2	10,10,10	4.41	4 (40%)	10,13,13	3.54	6 (60%)

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	OPO	A	401	2	-	0/2/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	OPO	O2-N1	11.28	1.42	1.22
3	A	401	OPO	C1-N1	-6.11	1.34	1.45
3	A	401	OPO	C4-C3	3.72	1.45	1.38
3	A	401	OPO	OH-C2	2.80	1.42	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	OPO	C4-C5-C6	7.22	129.15	120.24
3	A	401	OPO	C3-C2-C1	5.07	125.28	118.94
3	A	401	OPO	O2-N1-C1	3.73	125.42	119.03
3	A	401	OPO	C4-C3-C2	-3.51	115.72	120.05
3	A	401	OPO	C5-C6-C1	-2.95	113.75	118.60
3	A	401	OPO	C5-C4-C3	-2.94	116.61	120.24

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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	269/298 (90%)	3.00	216 (80%) 0 0	5, 12, 18, 26	17 (6%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	GLY	7.6
1	A	232	THR	7.6
1	A	300	TRP	6.2
1	A	341[A]	LYS	5.5
1	A	304	TRP	5.5
1	A	180	PHE	5.4
1	A	318	VAL	5.3
1	A	154	LEU	5.3
1	A	290	TYR	5.2
1	A	182	ALA	5.1
1	A	234	VAL	5.1
1	A	158	TYR	5.0
1	A	159	TYR	5.0
1	A	303	TYR	5.0
1	A	184	VAL	5.0
1	A	301	HIS	4.9
1	A	147	VAL	4.9
1	A	236	VAL	4.9
1	A	240	ILE	4.9
1	A	292	PHE	4.8
1	A	201	LEU	4.8
1	A	185	GLY	4.7
1	A	340	PHE	4.5
1	A	212	PHE	4.5
1	A	294	ALA	4.4
1	A	176	PRO	4.4
1	A	106	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	193	VAL	4.3
1	A	242	VAL	4.3
1	A	177	THR	4.3
1	A	208	ILE	4.2
1	A	233	TYR	4.2
1	A	339	ILE	4.2
1	A	148	VAL	4.2
1	A	299	ASN	4.2
1	A	223	ALA	4.2
1	A	247	ILE	4.2
1	A	169	VAL	4.1
1	A	168	PHE	4.1
1	A	289	LEU	4.1
1	A	219	TRP	4.1
1	A	146	ALA	4.1
1	A	238	ALA	4.0
1	A	205	VAL	4.0
1	A	170	LEU	4.0
1	A	198	PHE	4.0
1	A	221	ILE	3.9
1	A	229	ILE	3.9
1	A	160	GLY	3.8
1	A	179	GLY	3.8
1	A	175	ALA	3.8
1	A	250	TYR	3.8
1	A	104	TRP	3.8
1	A	298	GLY	3.8
1	A	202	ALA	3.8
1	A	105	LEU	3.8
1	A	103	TRP	3.8
1	A	151	SER	3.7
1	A	163	ILE	3.7
1	A	228[A]	ARG	3.7
1	A	186[A]	SER	3.7
1	A	192	PHE	3.7
1	A	342	GLY	3.7
1	A	274	ILE	3.7
1	A	275	LEU	3.7
1	A	194	TYR	3.7
1	A	157	SER	3.7
1	A	83	ARG	3.6
1	A	231[A]	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	262	TRP	3.6
1	A	296	SER	3.6
1	A	203	GLN	3.6
1	A	204[A]	GLU	3.6
1	A	283	ILE	3.6
1	A	188	THR	3.6
1	A	225	THR	3.6
1	A	230	SER	3.6
1	A	94	ALA	3.5
1	A	237	PRO	3.5
1	A	272	THR	3.5
1	A	305	GLU	3.5
1	A	153	ASN	3.5
1	A	277	VAL	3.5
1	A	279	PHE	3.5
1	A	325[A]	SER	3.5
1	A	295	ASP	3.5
1	A	224	THR	3.4
1	A	155	LYS	3.4
1	A	210	VAL	3.4
1	A	150	ASN	3.4
1	A	209	LEU	3.4
1	A	287	VAL	3.4
1	A	268	ARG	3.4
1	A	123	LEU	3.3
1	A	183	ASP	3.3
1	A	259	PHE	3.3
1	A	302	HIS	3.3
1	A	127	VAL	3.3
1	A	142	CYS	3.3
1	A	69	GLU	3.3
1	A	189	THR	3.3
1	A	329	THR	3.3
1	A	124	PHE	3.3
1	A	68	ILE	3.3
1	A	173	ASN	3.3
1	A	239	LYS	3.3
1	A	327	VAL	3.3
1	A	330	ILE	3.3
1	A	65	THR	3.2
1	A	109	ARG	3.2
1	A	284[A]	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	255	ILE	3.2
1	A	337	ILE	3.2
1	A	161	PRO	3.2
1	A	149	GLY	3.2
1	A	111	LYS	3.2
1	A	215	THR	3.1
1	A	133	PRO	3.1
1	A	235	PRO	3.1
1	A	140	VAL	3.1
1	A	220	VAL	3.1
1	A	107	LEU	3.1
1	A	291	GLY	3.1
1	A	126	VAL	3.1
1	A	332	ALA	3.0
1	A	293	GLY	3.0
1	A	61	PRO	3.0
1	A	321	GLY	3.0
1	A	152	GLY	3.0
1	A	116	LEU	3.0
1	A	297	LYS	2.9
1	A	81	PHE	2.9
1	A	199	ARG	2.9
1	A	191	HIS	2.9
1	A	226	THR	2.9
1	A	328	THR	2.9
1	A	128	PRO	2.9
1	A	217	LEU	2.9
1	A	331	LEU	2.9
1	A	243	LYS	2.9
1	A	323	PHE	2.8
1	A	190	HIS	2.8
1	A	276[A]	SER	2.8
1	A	338	ARG	2.8
1	A	178	GLU	2.8
1	A	99	ASP	2.8
1	A	73	VAL	2.8
1	A	214	THR	2.8
1	A	343	ARG	2.8
1	A	248	LEU	2.8
1	A	263	LEU	2.8
1	A	76	TRP	2.8
1	A	278	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	273	GLY	2.8
1	A	67	CYS	2.8
1	A	326	ASN	2.7
1	A	135	LEU	2.7
1	A	227	GLY	2.7
1	A	119	THR	2.7
1	A	269	TYR	2.7
1	A	195	PRO	2.7
1	A	271	SER	2.7
1	A	145[A]	CYS	2.6
1	A	95[A]	HIS	2.6
1	A	334	ILE	2.6
1	A	121[A]	ARG	2.6
1	A	96	LEU	2.6
1	A	254	PHE	2.6
1	A	249	ILE	2.6
1	A	156[A]	GLU	2.6
1	A	63	THR	2.6
1	A	241	LYS	2.6
1	A	98	GLU	2.6
1	A	218	GLU	2.6
1	A	72	ARG	2.5
1	A	88	LEU	2.5
1	A	89	LEU	2.5
1	A	181	GLU	2.5
1	A	197	SER	2.5
1	A	281	LEU	2.5
1	A	139	LEU	2.5
1	A	319	HIS	2.4
1	A	112	GLN	2.4
1	A	97	GLU	2.4
1	A	113	PRO	2.4
1	A	270	PRO	2.4
1	A	120	ILE	2.4
1	A	134	LEU	2.4
1	A	257	TYR	2.4
1	A	100	THR	2.4
1	A	71[A]	GLN	2.4
1	A	62	CYS	2.4
1	A	130	ASN	2.4
1	A	75	ALA	2.4
1	A	162	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	79	GLU	2.3
1	A	131	VAL	2.3
1	A	91	ALA	2.3
1	A	222	SER	2.3
1	A	110	GLU	2.3
1	A	164	ASP	2.3
1	A	165	SER	2.3
1	A	206	SER	2.3
1	A	122[A]	GLU	2.3
1	A	200	GLU	2.3
1	A	252	PRO	2.3
1	A	211	PRO	2.2
1	A	101	TYR	2.2
1	A	258	VAL	2.2
1	A	167	ASP	2.1
1	A	74	SER	2.1
1	A	322	ASP	2.1
1	A	246	LYS	2.1
1	A	171	ARG	2.1
1	A	125	GLN	2.1
1	A	102	LYS	2.0

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

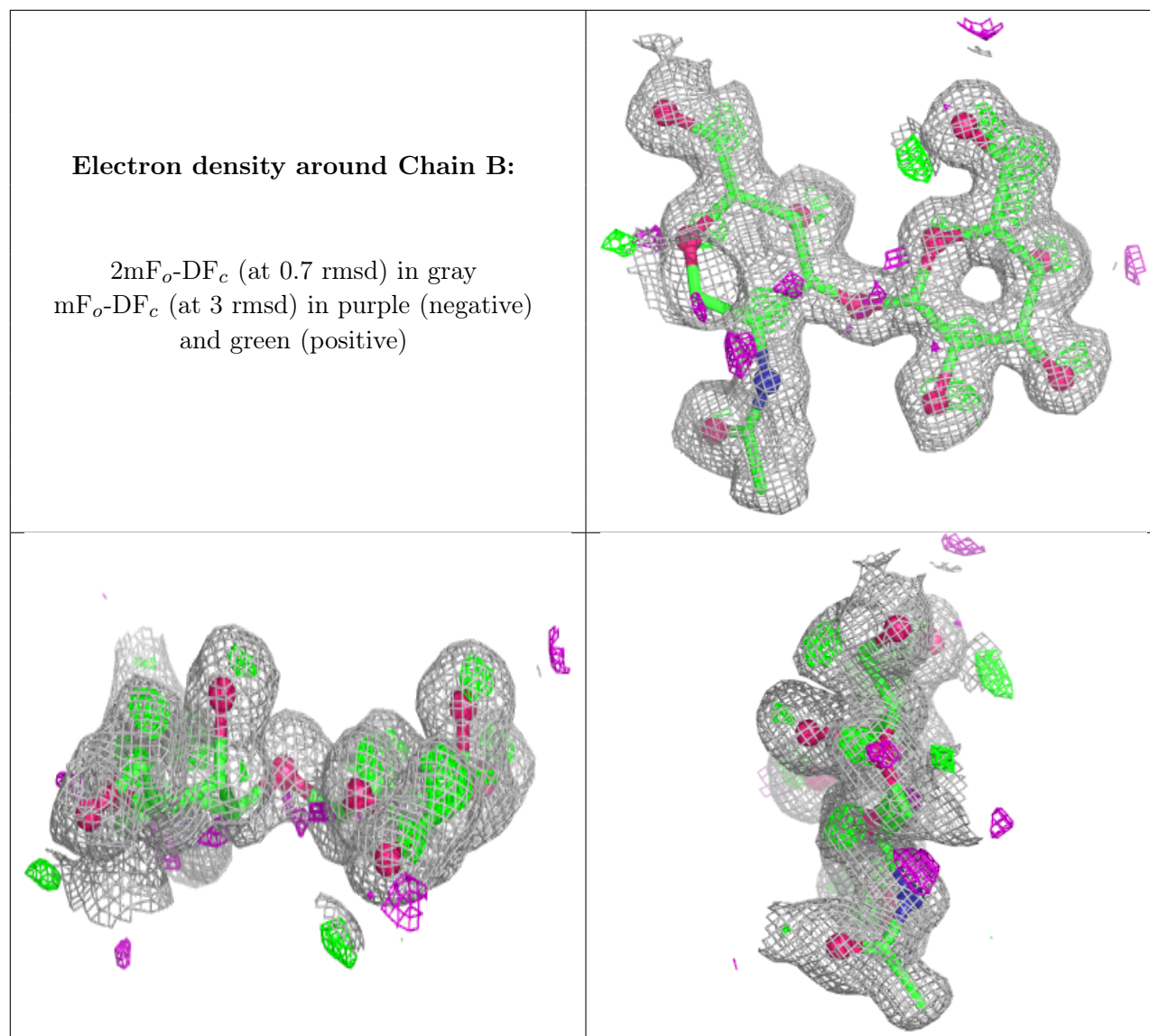
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	A2G	B	1	14/15	0.83	0.18	16,17,22,23	0
2	GAL	B	2	11/12	0.86	0.16	13,14,16,18	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(Å ²)	Q<0.9
3	OPO	A	401	10/10	0.75	0.19	20,23,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.