



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 11:14 PM EDT

PDB ID : 4GZ9
Title : Mouse Neuropilin-1, extracellular domains 1-4 (a1a2b1b2)
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Deposited on : 2012-09-06
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

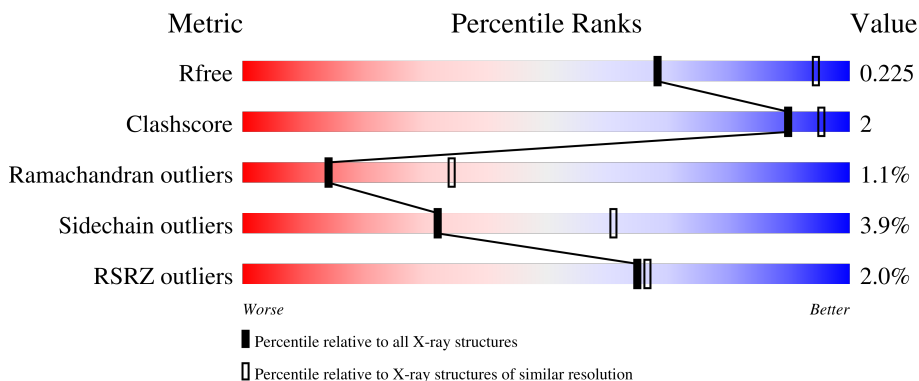
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	577	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>••</div> </div>
2	B	3	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4578 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.

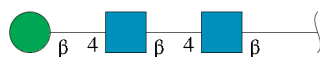
- Molecule 1 is a protein called Neuropilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4472	2842	753	852	25			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLU	-	expression tag	UNP P97333
A	20	THR	-	expression tag	UNP P97333
A	21	GLY	-	expression tag	UNP P97333
A	587	ARG	-	expression tag	UNP P97333
A	588	THR	-	expression tag	UNP P97333
A	589	LYS	-	expression tag	UNP P97333
A	590	HIS	-	expression tag	UNP P97333
A	591	HIS	-	expression tag	UNP P97333
A	592	HIS	-	expression tag	UNP P97333
A	593	HIS	-	expression tag	UNP P97333
A	594	HIS	-	expression tag	UNP P97333
A	595	HIS	-	expression tag	UNP P97333

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

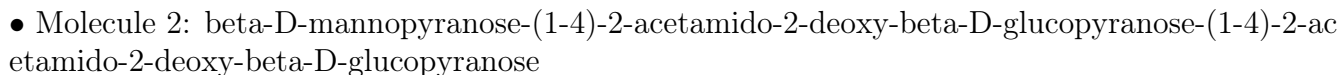


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	29	Total	O	0	0
			29	29		

- Molecule 1: Neuropilin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.36Å 245.36Å 47.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.00 – 2.70 80.31 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (81.00-2.70) 99.2 (80.31-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.199 , 0.223 0.203 , 0.225	Depositor DCC
R_{free} test set	2241 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4578	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: BMA, SO4, NAG, CA, EDO

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	0.55	1/4593 (0.0%)	0.68	0/6218

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	TRP	CD2-CE2	5.04	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	ARG	Peptide

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	4472	0	4310	16	0
2	B	39	0	34	0	0
3	A	14	0	13	1	0
4	A	2	0	0	0	0
5	A	10	0	0	0	0
6	A	12	0	18	0	0
7	A	29	0	0	0	0
All	All	4578	0	4375	16	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.

The worst 5 of 16 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:243:LEU:HD23	1:A:243:LEU:C	2.17	0.64
1:A:263:SER:OG	3:A:604:NAG:H81	2.08	0.52
1:A:437:MET:HG3	1:A:579:GLU:HA	1.95	0.48
1:A:243:LEU:HD23	1:A:244:SER:N	2.30	0.47
1:A:462:ILE:HG13	1:A:471:TRP:HB2	1.98	0.46

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	560/577 (97%)	532 (95%)	22 (4%)	6 (1%)	14 34

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ASP

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Mol	Chain	Res	Type
1	A	129	THR
1	A	253	ILE
1	A	413	THR
1	A	233	PRO

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	492/506 (97%)	473 (96%)	19 (4%)	32 61

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LYS
1	A	528	THR
1	A	572	SER
1	A	496	ARG
1	A	232	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

3 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	2,1	14,14,15	0.73	1 (7%)	17,19,21	1.85	5 (29%)
2	NAG	B	2	2	14,14,15	0.59	0	17,19,21	1.93	5 (29%)
2	BMA	B	3	2	11,11,12	0.71	0	15,15,17	1.72	5 (33%)

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	2,1	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	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	O5-C1	-2.03	1.40	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C4-C3-C2	-4.33	104.67	111.02
2	B	2	NAG	C2-N2-C7	4.19	128.52	122.90
2	B	1	NAG	C8-C7-N2	3.67	122.21	116.12
2	B	1	NAG	O4-C4-C3	-3.57	101.96	110.38
2	B	3	BMA	C1-O5-C5	3.39	116.72	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2

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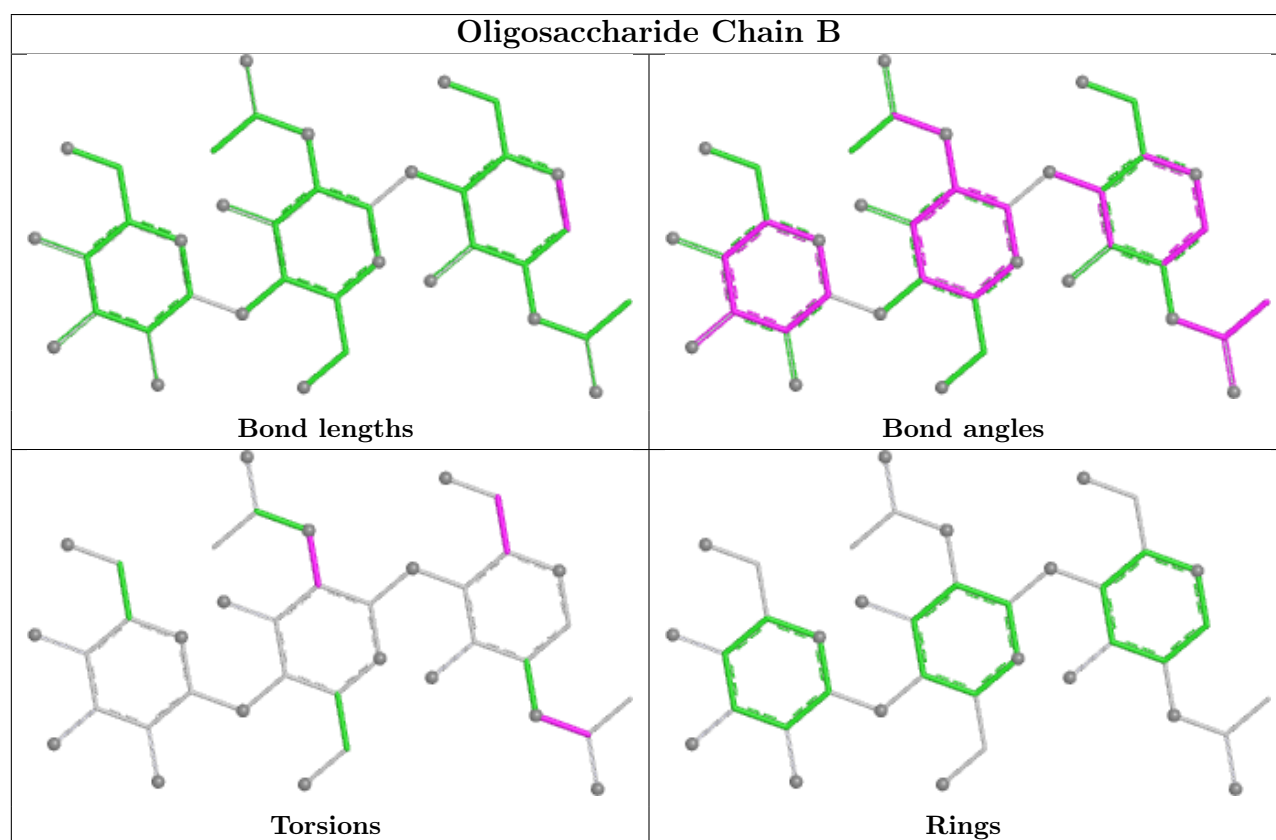
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Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C3-C2-N2-C7
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
5	SO4	A	608	-	4,4,4	0.43	0	6,6,6	0.40	0
6	EDO	A	610	-	3,3,3	0.36	0	2,2,2	0.42	0
5	SO4	A	607	-	4,4,4	0.53	0	6,6,6	0.29	0
6	EDO	A	611	-	3,3,3	0.39	0	2,2,2	0.39	0
3	NAG	A	604	1	14,14,15	0.60	0	17,19,21	1.27	1 (5%)
6	EDO	A	609	-	3,3,3	0.48	0	2,2,2	0.25	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
6	EDO	A	611	-	-	0/1/1/1	-
3	NAG	A	604	1	-	4/6/23/26	0/1/1/1
6	EDO	A	610	-	-	0/1/1/1	-
6	EDO	A	609	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	NAG	C1-O5-C5	4.32	117.97	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	NAG	O5-C5-C6-O6
3	A	604	NAG	C4-C5-C6-O6
3	A	604	NAG	C8-C7-N2-C2
3	A	604	NAG	O7-C7-N2-C2
6	A	609	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	NAG	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 [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	562/577 (97%)	0.22	11 (1%) 65 67	39, 61, 109, 133	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	ASN	3.2
1	A	98	ARG	2.9
1	A	203	GLY	2.8
1	A	96	GLY	2.6
1	A	205	PHE	2.5

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

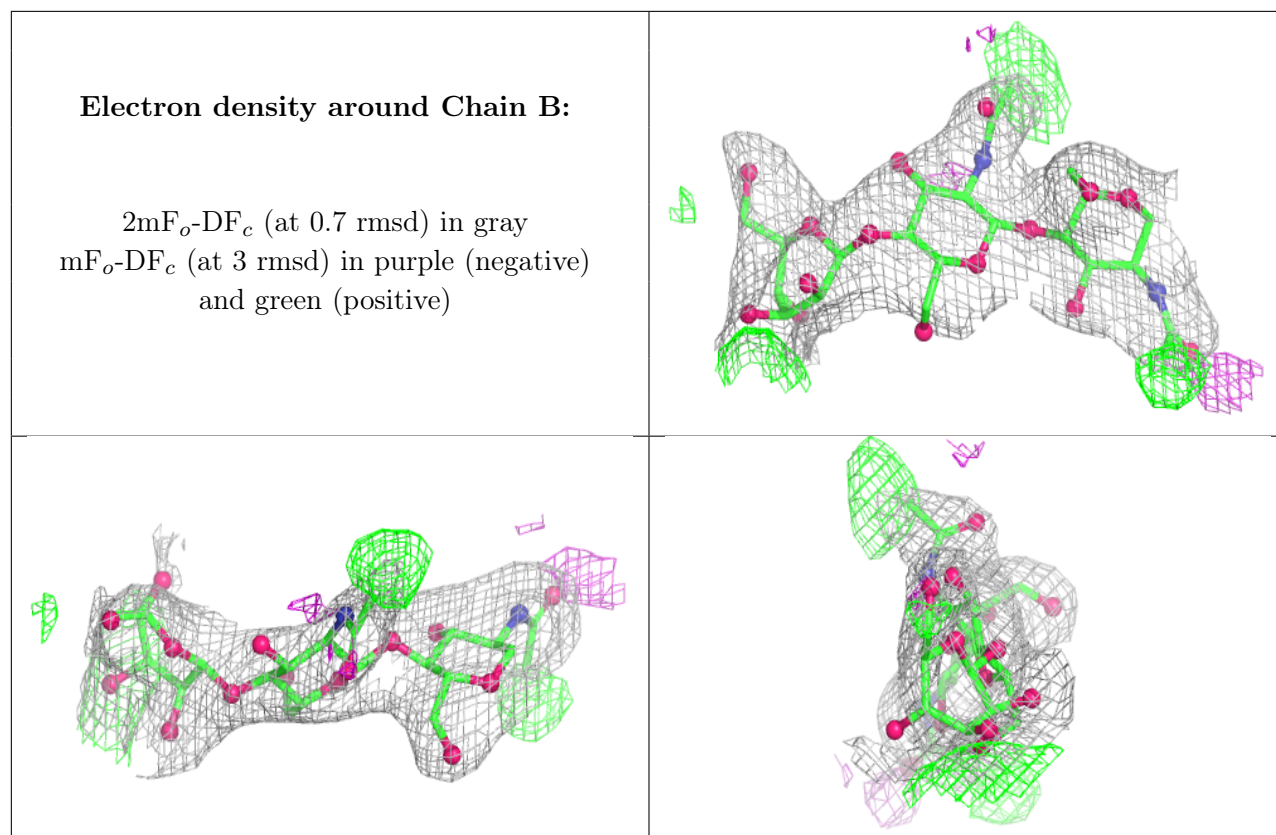
There are no non-standard protein/DNA/RNA residues in this entry.

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	BMA	B	3	11/12	0.75	0.23	117,124,130,133	0
2	NAG	B	2	14/15	0.87	0.24	85,100,113,116	0
2	NAG	B	1	14/15	0.96	0.14	69,77,84,86	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
6	EDO	A	609	4/4	0.87	0.14	71,73,75,75	0
3	NAG	A	604	14/15	0.88	0.22	75,98,110,113	0
4	CA	A	606	1/1	0.89	0.05	106,106,106,106	0
5	SO4	A	607	5/5	0.90	0.49	101,107,110,115	0
6	EDO	A	610	4/4	0.91	0.19	67,74,75,81	0
5	SO4	A	608	5/5	0.94	0.12	83,88,92,94	0
6	EDO	A	611	4/4	0.96	0.24	57,60,62,64	0
4	CA	A	605	1/1	0.99	0.08	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.