



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2026 – 11:18 am BST

PDB ID : 9T91 / pdb_00009t91
Title : XN-IL lectin from *Xenorhabdus nematophila* in complex with hyaluronan tetrasaccharide
Authors : Korsak, M.; Wimmerova, M.
Deposited on : 2025-11-13
Resolution : 1.60 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 : 1.8.4, CSD as541be (2020)
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

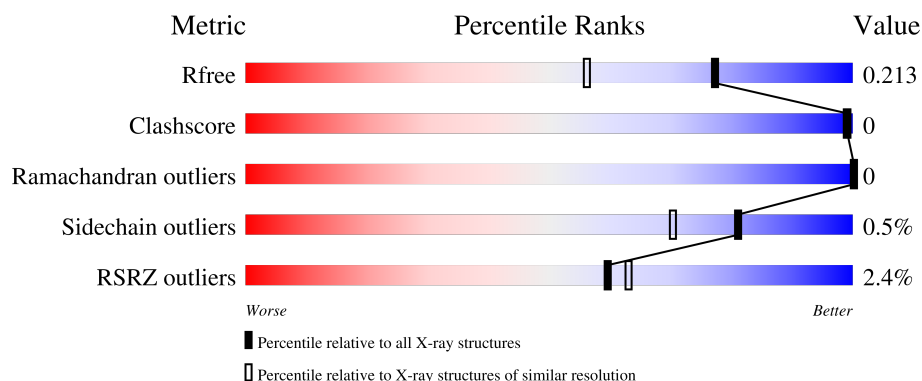
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	AAA	125	<div> <div>2%</div> <div>98%</div> <div>..</div> </div>
1	BBB	125	<div> <div>3%</div> <div>96%</div> <div>..</div> </div>
2	DDD	4	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2156 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 PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	AAA	124	Total	C	N	O	0	1	0
			953	618	154	181			
1	BBB	124	Total	C	N	O	0	0	0
			939	610	151	178			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	11	LYS	ARG	conflict	UNP D3VE08
BBB	11	LYS	ARG	conflict	UNP D3VE08

- Molecule 2 is an oligosaccharide called beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	DDD	4	Total	C	N	O	0	0	0
			53	28	2	23			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Ca 1 1	0	0
4	BBB	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	88	Total 88	O 88	0	0
5	BBB	89	Total 89	O 89	0	0

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.

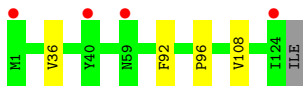
- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)

Chain AAA: 2% 98% ..



- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)

Chain BBB: 3% 96% ..



- Molecule 2: beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain DDD: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	65.80Å 65.80Å 129.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.88 – 1.60 42.88 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.88-1.60) 99.4 (42.88-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.202 0.194 , 0.213	Depositor DCC
R_{free} test set	2217 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2156	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: EDO, CA, BDP, NDG, NAG

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	AAA	1.01	0/980	1.15	1/1337 (0.1%)
1	BBB	1.10	1/965 (0.1%)	1.15	1/1319 (0.1%)
All	All	1.06	1/1945 (0.1%)	1.15	2/2656 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	108	VAL	C-O	5.29	1.29	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	85	ASP	CA-CB-CG	5.65	118.25	112.60
1	BBB	96	PRO	CA-C-O	-5.04	115.83	121.32

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	AAA	953	0	916	0	0
1	BBB	939	0	908	1	0
2	DDD	53	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	16	0	24	0	0
3	BBB	16	0	23	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	88	0	0	0	0
5	BBB	89	0	0	0	0
All	All	2156	0	1905	1	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 0.

All (1) 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:BBB:36:VAL:HG21	1:BBB:92:PHE:CE1	2.47	0.50

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	AAA	123/125 (98%)	123 (100%)	0	0	100	100
1	BBB	122/125 (98%)	122 (100%)	0	0	100	100
All	All	245/250 (98%)	245 (100%)	0	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	AAA	97/104 (93%)	96 (99%)	1 (1%)	68	50
1	BBB	96/104 (92%)	96 (100%)	0	100	100
All	All	193/208 (93%)	192 (100%)	1 (0%)	81	70

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	98	SER

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](#)

4 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	NDG	DDD	1	2	15,15,15	0.36	0	21,21,21	1.72	2 (9%)
2	BDP	DDD	2	4,2	12,12,13	0.96	1 (8%)	14,17,19	1.46	2 (14%)
2	NAG	DDD	3	2	14,14,15	1.00	1 (7%)	17,19,21	2.40	6 (35%)
2	BDP	DDD	4	4,2	12,12,13	1.10	0	14,17,19	2.23	6 (42%)

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	NDG	DDD	1	2	-	1/6/26/26	0/1/1/1
2	BDP	DDD	2	4,2	-	2/4/21/24	0/1/1/1
2	NAG	DDD	3	2	-	0/6/23/26	0/1/1/1
2	BDP	DDD	4	4,2	-	0/4/21/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	2	BDP	O6B-C6	-2.33	1.22	1.30
2	DDD	3	NAG	C6-C5	2.11	1.58	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	3	NAG	C1-O5-C5	7.73	122.67	112.19
2	DDD	1	NDG	C1-C2-N2	6.17	117.88	110.73
2	DDD	4	BDP	O3-C3-C2	-4.72	100.96	109.99
2	DDD	1	NDG	O3-C3-C2	-3.55	102.50	109.66
2	DDD	4	BDP	O3-C3-C4	3.32	118.03	110.35
2	DDD	4	BDP	O2-C2-C3	-2.94	104.26	110.14
2	DDD	3	NAG	C8-C7-N2	-2.75	111.45	116.10
2	DDD	4	BDP	O2-C2-C1	2.74	114.75	109.15
2	DDD	4	BDP	C2-C3-C4	-2.52	106.53	110.89
2	DDD	4	BDP	O4-C4-C3	-2.52	104.51	110.35
2	DDD	2	BDP	O3-C3-C2	-2.47	105.26	109.99
2	DDD	3	NAG	C3-C4-C5	2.47	114.64	110.24
2	DDD	3	NAG	O4-C4-C3	-2.46	104.67	110.35
2	DDD	3	NAG	O7-C7-N2	2.37	126.30	121.95
2	DDD	3	NAG	O6-C6-C5	2.32	119.26	111.29
2	DDD	2	BDP	O3-C3-C4	2.19	115.40	110.35

There are no chirality outliers.

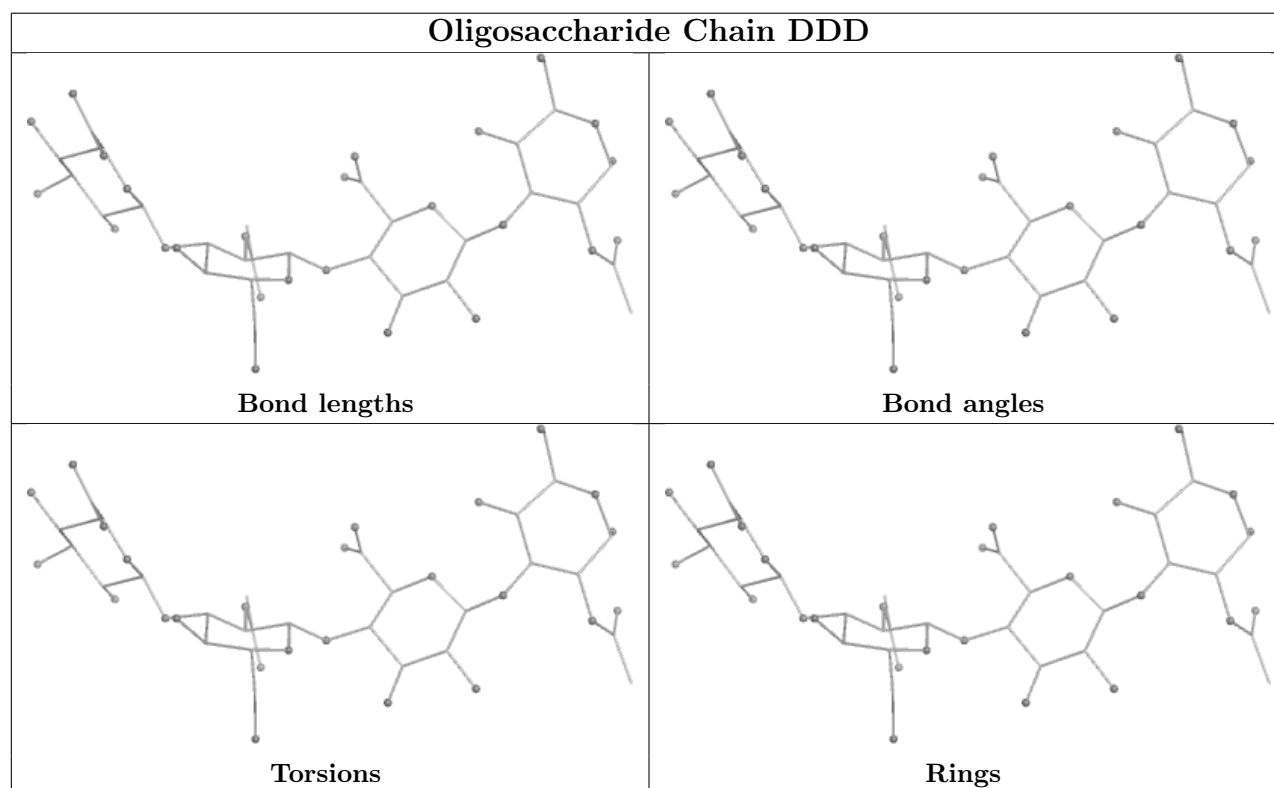
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DDD	1	NDG	C1-C2-N2-C7
2	DDD	2	BDP	O5-C5-C6-O6A
2	DDD	2	BDP	O5-C5-C6-O6B

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, 2 are monoatomic - leaving 8 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	EDO	AAA	201	-	3,3,3	0.29	0	2,2,2	0.43	0
3	EDO	BBB	204	-	3,3,3	0.06	0	2,2,2	0.27	0
3	EDO	BBB	201	-	3,3,3	0.37	0	2,2,2	0.27	0
3	EDO	AAA	203	-	3,3,3	0.36	0	2,2,2	0.54	0
3	EDO	AAA	202	-	3,3,3	0.16	0	2,2,2	0.34	0
3	EDO	BBB	203	-	3,3,3	0.32	0	2,2,2	0.43	0
3	EDO	BBB	202	-	3,3,3	0.77	0	2,2,2	0.37	0
3	EDO	AAA	204	-	3,3,3	0.30	0	2,2,2	0.16	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	EDO	AAA	201	-	-	1/1/1/1	-
3	EDO	BBB	204	-	-	0/1/1/1	-
3	EDO	BBB	201	-	-	1/1/1/1	-
3	EDO	AAA	203	-	-	0/1/1/1	-
3	EDO	AAA	202	-	-	0/1/1/1	-
3	EDO	BBB	203	-	-	1/1/1/1	-
3	EDO	BBB	202	-	-	0/1/1/1	-
3	EDO	AAA	204	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	201	EDO	O1-C1-C2-O2
3	BBB	201	EDO	O1-C1-C2-O2
3	BBB	203	EDO	O1-C1-C2-O2
3	AAA	204	EDO	O1-C1-C2-O2

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	AAA	124/125 (99%)	-0.00	2 (1%) 70 74	15, 30, 41, 56	1 (0%)
1	BBB	124/125 (99%)	0.15	4 (3%) 50 53	25, 32, 42, 54	0
All	All	248/250 (99%)	0.07	6 (2%) 59 63	15, 30, 42, 56	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	124	ILE	5.8
1	AAA	124	ILE	5.1
1	BBB	40	TYR	3.7
1	BBB	1	MET	2.8
1	AAA	1	MET	2.5
1	BBB	59	ASN	2.0

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

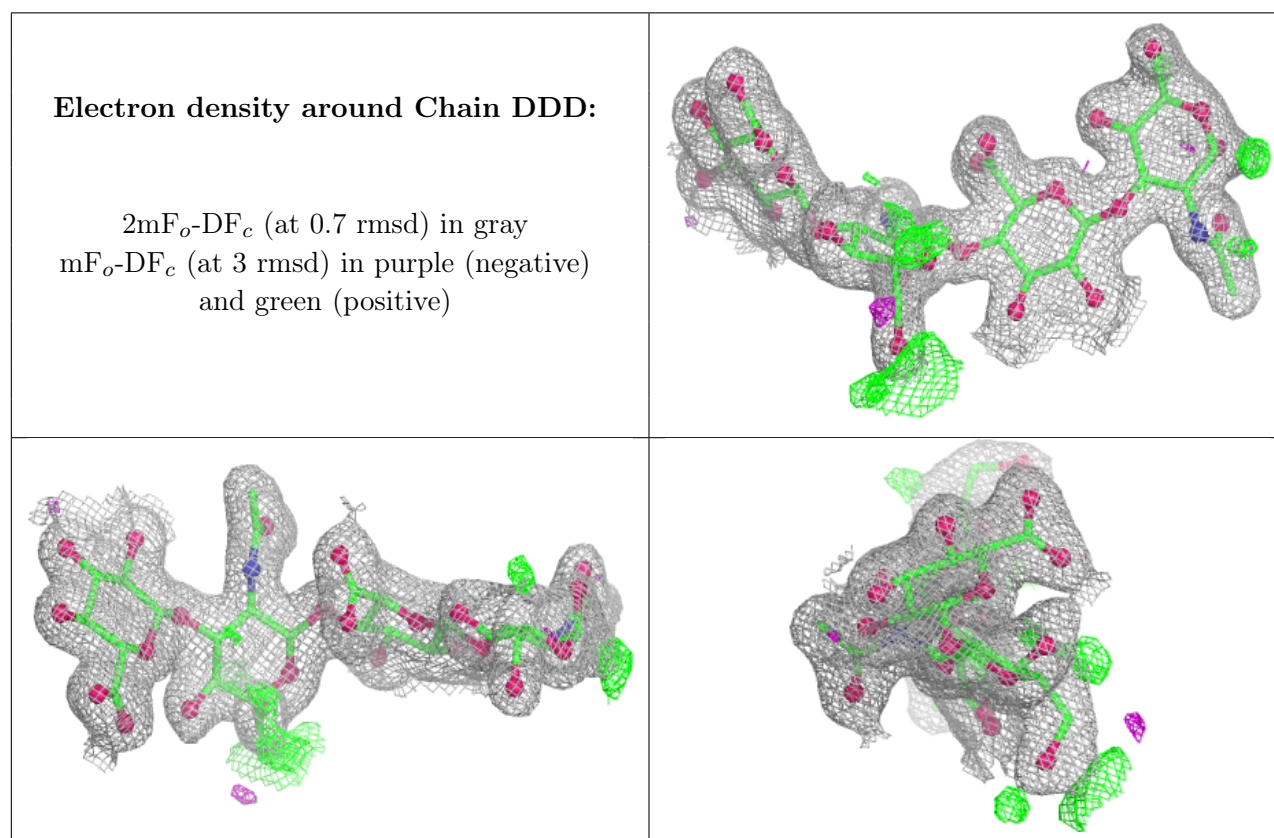
There are no non-standard protein/DNA/RNA residues in this entry.

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	NDG	DDD	1	15/15	-	-	31,44,50,56	0
2	BDP	DDD	2	12/13	-	-	26,31,36,38	0
2	NAG	DDD	3	14/15	-	-	28,31,36,39	0
2	BDP	DDD	4	12/13	-	-	29,30,37,38	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(\AA^2)	Q<0.9
3	EDO	BBB	203	4/4	0.82	0.25	55,57,62,67	0
3	EDO	AAA	204	4/4	0.85	0.14	44,49,52,57	0
3	EDO	AAA	203	4/4	0.89	0.14	45,45,47,50	0
3	EDO	AAA	202	4/4	0.92	0.13	43,50,51,55	0
3	EDO	BBB	202	4/4	0.92	0.14	42,43,46,47	0
3	EDO	AAA	201	4/4	0.92	0.12	35,40,44,44	0
3	EDO	BBB	204	4/4	0.94	0.09	46,46,49,54	0
3	EDO	BBB	201	4/4	0.96	0.07	35,35,38,47	0
4	CA	AAA	205	1/1	0.99	0.02	26,26,26,26	0
4	CA	BBB	205	1/1	0.99	0.05	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.