



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:25 PM BST

PDB ID : 4ZNR
Title : Crystal structure of Dln1 complexed with Man(alpha1-3)Man
Authors : Jia, N.; Jiang, Y.L.; Cheng, W.; Wang, H.W.; Zhou, C.Z.; Chen, Y.
Deposited on : 2015-05-05
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

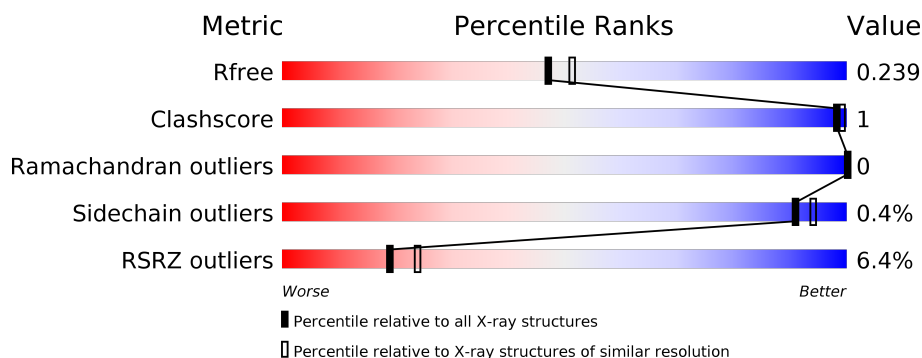
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	335	<div> <div>8%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	B	335	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div>100%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	D	1	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5459 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 Natterin-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	2	0
			2444	1550	401	483	10			
1	B	318	Total	C	N	O	S	0	1	0
			2441	1548	400	483	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q5CZR5
A	-18	GLY	-	expression tag	UNP Q5CZR5
A	-17	SER	-	expression tag	UNP Q5CZR5
A	-16	SER	-	expression tag	UNP Q5CZR5
A	-15	HIS	-	expression tag	UNP Q5CZR5
A	-14	HIS	-	expression tag	UNP Q5CZR5
A	-13	HIS	-	expression tag	UNP Q5CZR5
A	-12	HIS	-	expression tag	UNP Q5CZR5
A	-11	HIS	-	expression tag	UNP Q5CZR5
A	-10	HIS	-	expression tag	UNP Q5CZR5
A	-9	SER	-	expression tag	UNP Q5CZR5
A	-8	SER	-	expression tag	UNP Q5CZR5
A	-7	GLY	-	expression tag	UNP Q5CZR5
A	-6	LEU	-	expression tag	UNP Q5CZR5
A	-5	VAL	-	expression tag	UNP Q5CZR5
A	-4	PRO	-	expression tag	UNP Q5CZR5
A	-3	ARG	-	expression tag	UNP Q5CZR5
A	-2	GLY	-	expression tag	UNP Q5CZR5
A	-1	SER	-	expression tag	UNP Q5CZR5
A	0	HIS	-	expression tag	UNP Q5CZR5
B	-19	MET	-	expression tag	UNP Q5CZR5
B	-18	GLY	-	expression tag	UNP Q5CZR5
B	-17	SER	-	expression tag	UNP Q5CZR5
B	-16	SER	-	expression tag	UNP Q5CZR5
B	-15	HIS	-	expression tag	UNP Q5CZR5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q5CZR5
B	-13	HIS	-	expression tag	UNP Q5CZR5
B	-12	HIS	-	expression tag	UNP Q5CZR5
B	-11	HIS	-	expression tag	UNP Q5CZR5
B	-10	HIS	-	expression tag	UNP Q5CZR5
B	-9	SER	-	expression tag	UNP Q5CZR5
B	-8	SER	-	expression tag	UNP Q5CZR5
B	-7	GLY	-	expression tag	UNP Q5CZR5
B	-6	LEU	-	expression tag	UNP Q5CZR5
B	-5	VAL	-	expression tag	UNP Q5CZR5
B	-4	PRO	-	expression tag	UNP Q5CZR5
B	-3	ARG	-	expression tag	UNP Q5CZR5
B	-2	GLY	-	expression tag	UNP Q5CZR5
B	-1	SER	-	expression tag	UNP Q5CZR5
B	0	HIS	-	expression tag	UNP Q5CZR5

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

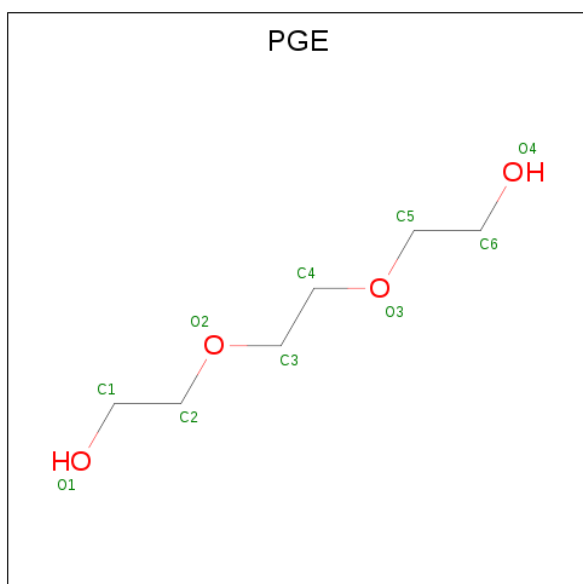
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



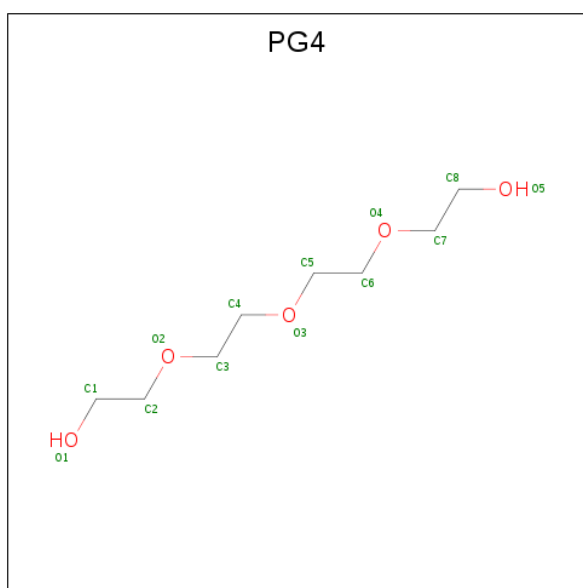
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



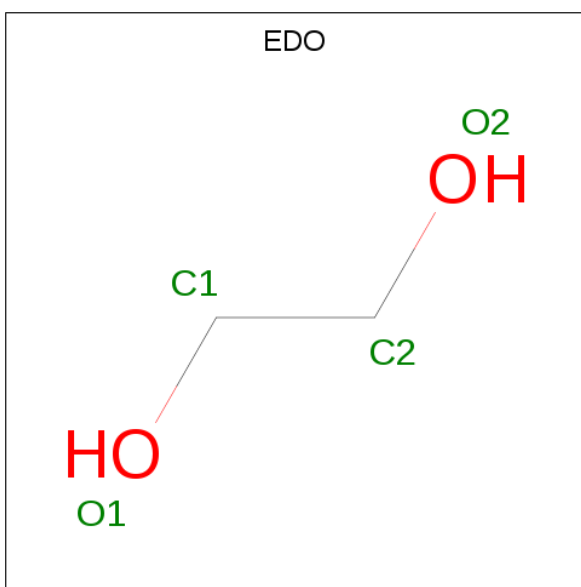
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



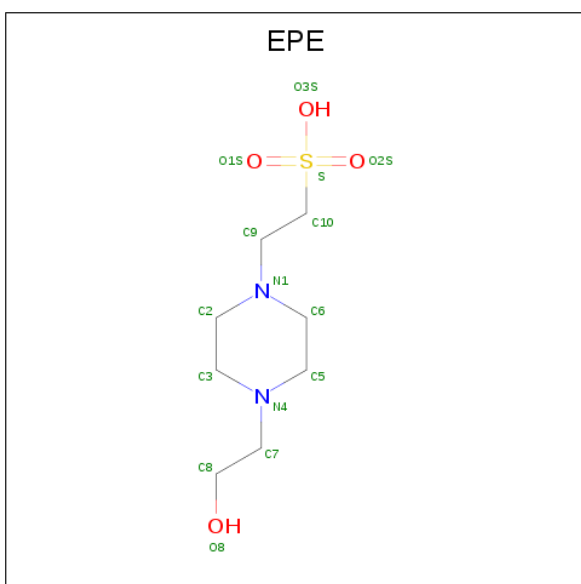
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



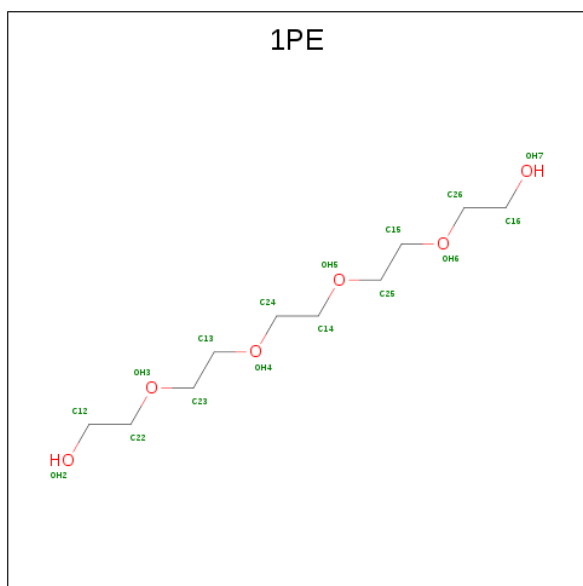
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			16	10	6		

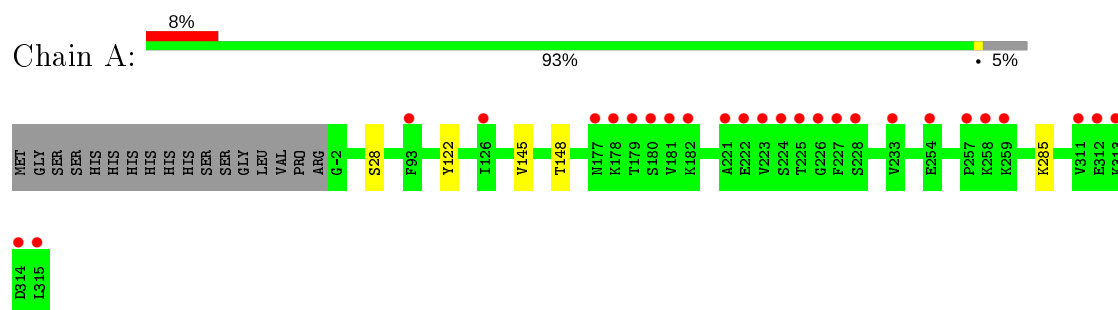
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	157	Total	O	0	0
			157	157		
10	B	212	Total	O	0	0
			212	212		

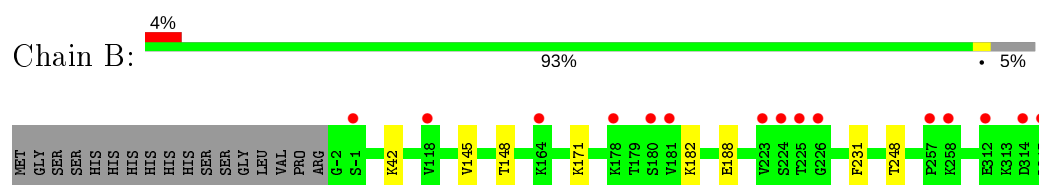
3 Residue-property plots [i](#)

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.

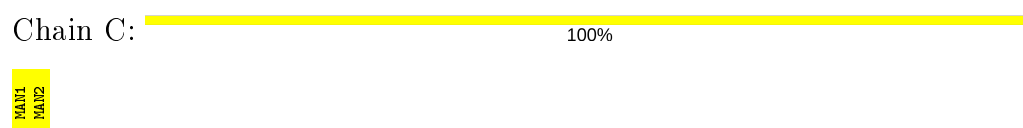
- Molecule 1: Natterin-like protein



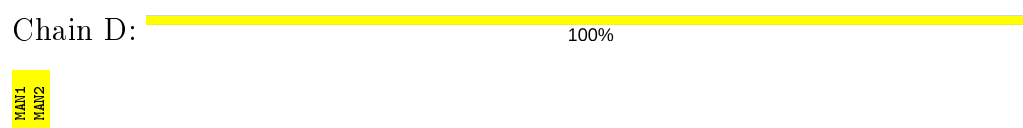
- Molecule 1: Natterin-like protein



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.17Å 95.21Å 146.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.57 – 2.10 34.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (34.57-2.10) 95.1 (34.55-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.207 , 0.241 0.208 , 0.239	Depositor DCC
R_{free} test set	2265 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.924	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.8	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	0.94	EDS
Total number of atoms	5459	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.90% 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: EPE, PGE, CL, EDO, 1PE, PG4, PEG, MAN

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	0.33	0/2503	0.53	0/3388
1	B	0.34	0/2494	0.54	0/3375
All	All	0.33	0/4997	0.54	0/6763

There are no bond length outliers.

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	2444	0	2409	3	0
1	B	2441	0	2401	4	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	20	0	0
4	B	21	0	30	0	0
5	A	20	0	28	0	0
5	B	20	0	28	0	0
6	A	26	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	13	0	18	0	0
7	A	4	0	6	0	0
7	B	8	0	12	0	0
8	B	15	0	18	0	0
9	B	16	0	22	0	0
10	A	157	0	0	0	0
10	B	212	0	0	1	0
All	All	5459	0	5070	6	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 1.

All (6) 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:B:171:LYS:NZ	1:B:188:GLU:O	2.44	0.48
1:A:285:LYS:HD2	1:B:248:THR:HB	1.99	0.45
1:B:145:VAL:HG11	1:B:148:THR:HG23	1.98	0.44
1:A:145:VAL:HG11	1:A:148:THR:HG23	2.00	0.43
1:A:28:SER:HB3	1:A:122:TYR:CZ	2.55	0.40
1:B:182:LYS:NZ	10:B:502:HOH:O	2.50	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	318/335 (95%)	314 (99%)	4 (1%)	0	100	100
1	B	317/335 (95%)	310 (98%)	7 (2%)	0	100	100
All	All	635/670 (95%)	624 (98%)	11 (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	273/286 (96%)	273 (100%)	0	100	100
1	B	272/286 (95%)	270 (99%)	2 (1%)	84	88
All	All	545/572 (95%)	543 (100%)	2 (0%)	91	94

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

Mol	Chain	Res	Type
1	B	42	LYS
1	B	231	PHE

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

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 ⓘ

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	MAN	C	1	2	12,12,12	2.14	3 (25%)	17,17,17	1.12	1 (5%)
2	MAN	C	2	2	11,11,12	2.14	4 (36%)	15,15,17	0.77	1 (6%)
2	MAN	D	1	2	12,12,12	2.16	3 (25%)	17,17,17	1.19	3 (17%)
2	MAN	D	2	2	11,11,12	2.09	3 (27%)	15,15,17	0.94	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	MAN	C	1	2	-	2/2/22/22	0/1/1/1
2	MAN	C	2	2	-	0/2/19/22	0/1/1/1
2	MAN	D	1	2	-	0/2/22/22	0/1/1/1
2	MAN	D	2	2	-	0/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	MAN	C2-C3	-4.59	1.45	1.52
2	D	2	MAN	C2-C3	-4.45	1.46	1.52
2	C	1	MAN	C3-C2	-4.21	1.41	1.52
2	C	1	MAN	C4-C3	-4.14	1.41	1.52
2	D	1	MAN	C4-C3	-4.09	1.41	1.52
2	D	1	MAN	C3-C2	-3.98	1.42	1.52
2	D	1	MAN	O3-C3	3.85	1.52	1.43
2	C	2	MAN	C4-C3	-3.69	1.42	1.52
2	D	2	MAN	C4-C3	-3.63	1.43	1.52
2	C	1	MAN	O3-C3	3.54	1.51	1.43
2	D	2	MAN	O3-C3	2.35	1.48	1.43
2	C	2	MAN	O3-C3	2.34	1.48	1.43
2	C	2	MAN	O5-C1	-2.09	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	MAN	C1-C2-C3	2.23	114.94	110.31
2	D	2	MAN	C1-C2-C3	2.18	112.35	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	MAN	O6-C6-C5	2.14	118.63	111.29
2	C	1	MAN	O6-C6-C5	2.11	118.55	111.29
2	C	2	MAN	O6-C6-C5	2.04	118.30	111.29
2	D	1	MAN	O5-C1-C2	2.02	113.89	110.28

There are no chirality outliers.

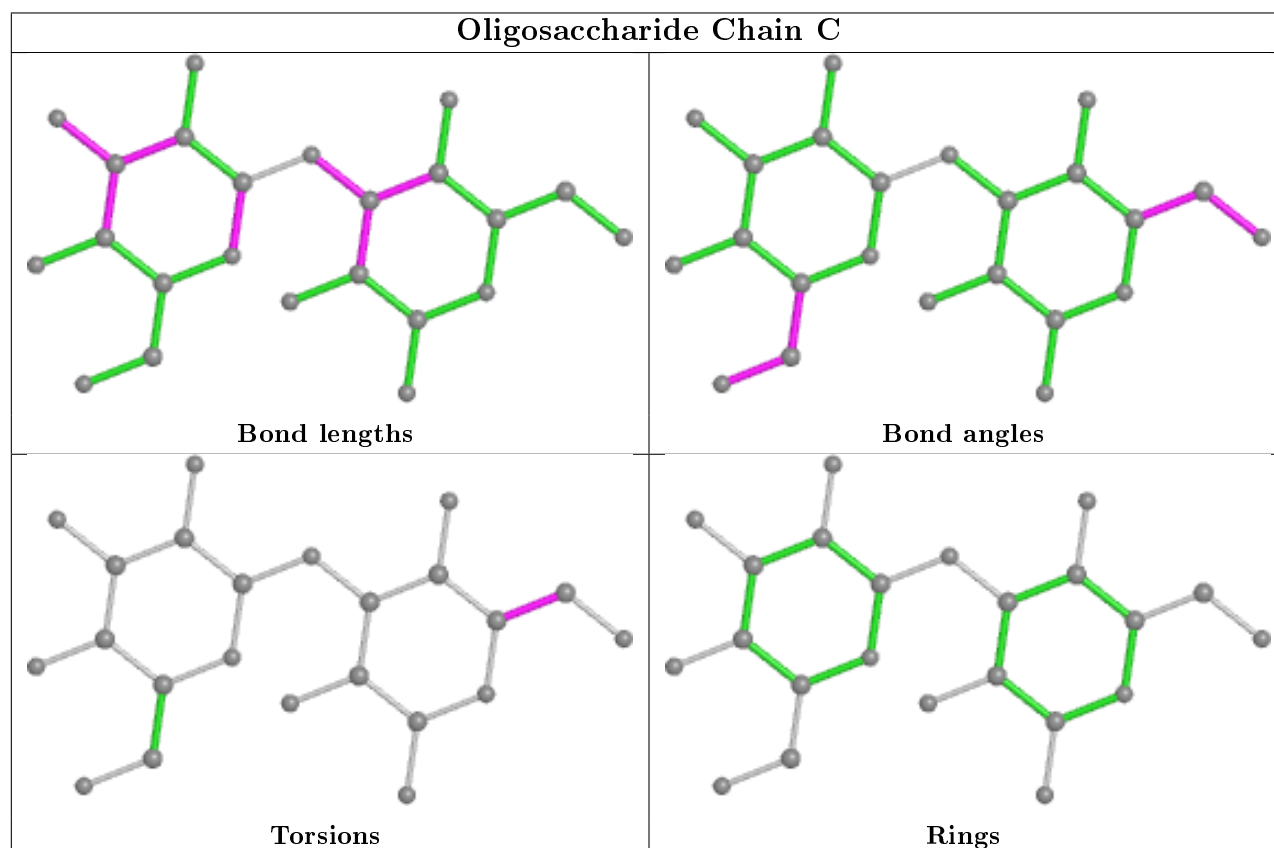
All (2) torsion outliers are listed below:

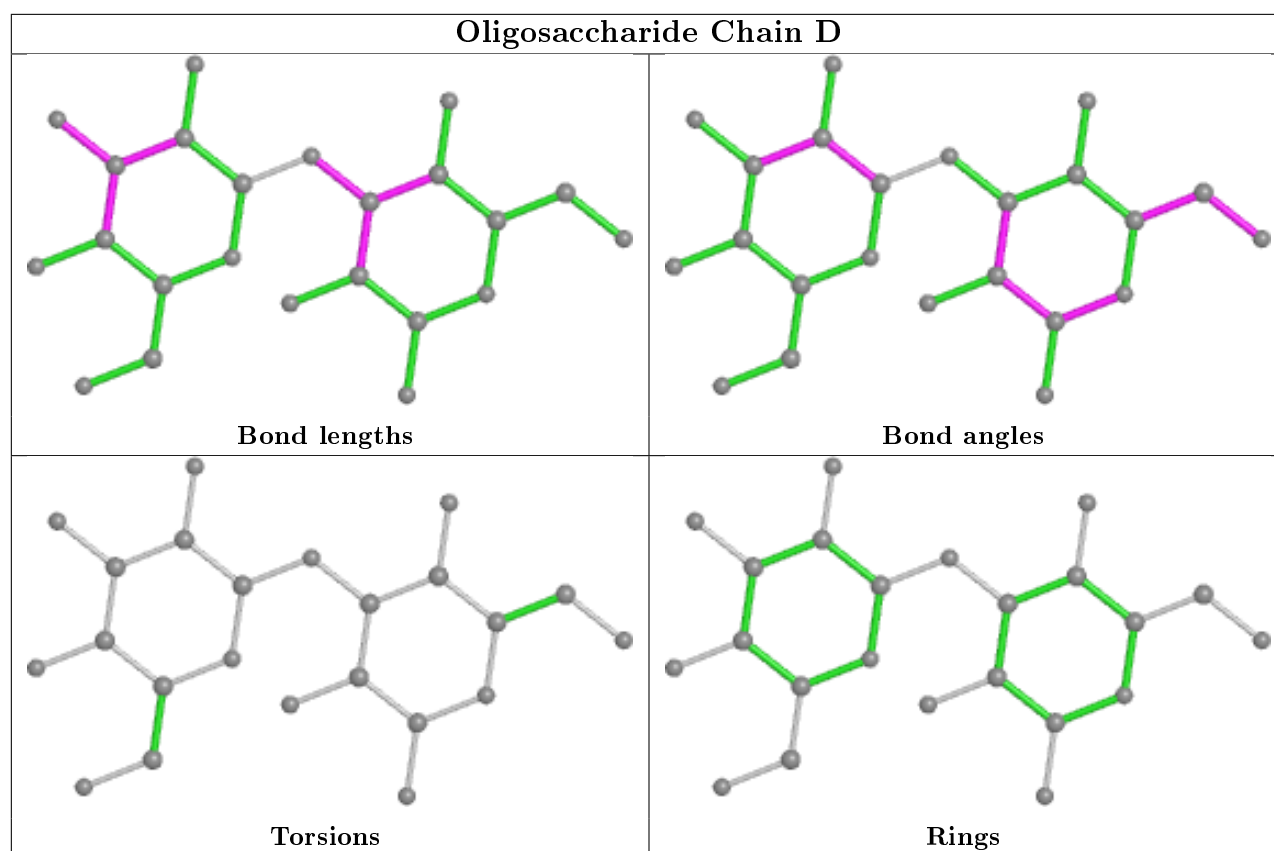
Mol	Chain	Res	Type	Atoms
2	C	1	MAN	O5-C5-C6-O6
2	C	1	MAN	C4-C5-C6-O6

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 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\# Z > 2$
7	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.27	0
4	PEG	A	404	-	6,6,6	0.50	0	5,5,5	0.23	0
4	PEG	B	408	-	6,6,6	0.48	0	5,5,5	0.58	0
4	PEG	B	409	-	6,6,6	0.50	0	5,5,5	0.20	0
5	PGE	A	406	-	9,9,9	0.48	0	8,8,8	0.19	0
5	PGE	B	410	-	9,9,9	0.49	0	8,8,8	0.21	0
5	PGE	A	407	-	9,9,9	0.48	0	8,8,8	0.15	0
4	PEG	A	405	-	6,6,6	0.51	0	5,5,5	0.32	0
4	PEG	B	407	-	6,6,6	0.46	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PGE	B	411	-	9,9,9	0.45	0	8,8,8	0.34	0
8	EPE	B	404	-	15,15,15	2.03	1 (6%)	18,20,20	2.91	11 (61%)
9	1PE	B	413	-	15,15,15	0.52	0	14,14,14	0.21	0
6	PG4	B	412	-	12,12,12	0.49	0	11,11,11	0.15	0
7	EDO	A	410	-	3,3,3	0.48	0	2,2,2	0.27	0
6	PG4	A	409	-	12,12,12	0.49	0	11,11,11	0.23	0
7	EDO	B	406	-	3,3,3	0.44	0	2,2,2	0.24	0
6	PG4	A	408	-	12,12,12	0.50	0	11,11,11	0.15	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
7	EDO	B	405	-	-	0/1/1/1	-
4	PEG	A	404	-	-	2/4/4/4	-
4	PEG	B	408	-	-	2/4/4/4	-
4	PEG	B	409	-	-	3/4/4/4	-
5	PGE	A	406	-	-	3/7/7/7	-
5	PGE	B	410	-	-	3/7/7/7	-
5	PGE	A	407	-	-	3/7/7/7	-
4	PEG	A	405	-	-	2/4/4/4	-
4	PEG	B	407	-	-	2/4/4/4	-
5	PGE	B	411	-	-	3/7/7/7	-
8	EPE	B	404	-	-	7/9/19/19	0/1/1/1
9	1PE	B	413	-	-	3/13/13/13	-
6	PG4	B	412	-	-	4/10/10/10	-
7	EDO	A	410	-	-	1/1/1/1	-
6	PG4	A	409	-	-	4/10/10/10	-
7	EDO	B	406	-	-	1/1/1/1	-
6	PG4	A	408	-	-	2/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	404	EPE	C10-S	-7.58	1.66	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	404	EPE	C5-N4-C3	5.60	121.44	108.83
8	B	404	EPE	C3-C2-N1	-4.59	101.22	110.64
8	B	404	EPE	C9-N1-C2	4.58	122.95	111.23
8	B	404	EPE	C9-N1-C6	3.96	121.37	111.23
8	B	404	EPE	C7-N4-C5	3.64	120.55	111.23
8	B	404	EPE	O1S-S-C10	3.19	110.75	106.92
8	B	404	EPE	C6-N1-C2	3.02	115.63	108.83
8	B	404	EPE	C2-C3-N4	-2.65	105.20	110.64
8	B	404	EPE	C7-N4-C3	2.64	117.98	111.23
8	B	404	EPE	C8-C7-N4	-2.41	104.76	113.40
8	B	404	EPE	O2S-S-C10	2.21	109.58	106.92

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	408	PEG	C4-C3-O2-C2
5	A	407	PGE	O2-C3-C4-O3
6	A	409	PG4	O3-C5-C6-O4
5	B	410	PGE	O1-C1-C2-O2
8	B	404	EPE	N4-C7-C8-O8
4	B	409	PEG	O2-C3-C4-O4
5	B	411	PGE	O3-C5-C6-O4
6	A	408	PG4	O4-C7-C8-O5
8	B	404	EPE	C9-C10-S-O3S
5	A	407	PGE	O1-C1-C2-O2
4	A	405	PEG	O2-C3-C4-O4
4	B	407	PEG	O2-C3-C4-O4
6	B	412	PG4	O4-C7-C8-O5
6	A	409	PG4	O2-C3-C4-O3
6	B	412	PG4	O2-C3-C4-O3
4	B	409	PEG	O1-C1-C2-O2
5	B	411	PGE	O1-C1-C2-O2
6	A	409	PG4	O4-C7-C8-O5
8	B	404	EPE	C10-C9-N1-C2
8	B	404	EPE	C10-C9-N1-C6
5	B	410	PGE	O3-C5-C6-O4
5	A	407	PGE	O3-C5-C6-O4
4	A	405	PEG	O1-C1-C2-O2
4	A	404	PEG	O1-C1-C2-O2
5	A	406	PGE	O3-C5-C6-O4
9	B	413	1PE	C23-C13-OH4-C24
6	A	409	PG4	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
4	B	407	PEG	O1-C1-C2-O2
5	A	406	PGE	O1-C1-C2-O2
6	A	408	PG4	O1-C1-C2-O2
8	B	404	EPE	C9-C10-S-O1S
8	B	404	EPE	C9-C10-S-O2S
5	B	410	PGE	O2-C3-C4-O3
4	B	408	PEG	O2-C3-C4-O4
4	B	409	PEG	C4-C3-O2-C2
6	B	412	PG4	C5-C6-O4-C7
9	B	413	1PE	OH6-C15-C25-OH5
9	B	413	1PE	OH4-C13-C23-OH3
5	A	406	PGE	C1-C2-O2-C3
5	B	411	PGE	C6-C5-O3-C4
6	B	412	PG4	O1-C1-C2-O2
7	B	406	EDO	O1-C1-C2-O2
7	A	410	EDO	O1-C1-C2-O2
4	A	404	PEG	O2-C3-C4-O4
8	B	404	EPE	C8-C7-N4-C5

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	318/335 (94%)	0.29	26 (8%) 11 15	20, 34, 71, 90	0
1	B	318/335 (94%)	0.15	15 (4%) 31 37	20, 32, 58, 84	0
All	All	636/670 (94%)	0.22	41 (6%) 19 24	20, 33, 65, 90	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	LEU	7.1
1	B	225	THR	6.0
1	A	223	VAL	6.0
1	A	181	VAL	5.9
1	A	224	SER	5.9
1	A	225	THR	5.1
1	B	224	SER	4.8
1	A	180	SER	4.8
1	A	226	GLY	4.5
1	B	181	VAL	4.3
1	A	233	VAL	4.2
1	B	223	VAL	4.2
1	A	182	LYS	4.2
1	B	315	LEU	4.1
1	A	178	LYS	3.6
1	A	179	THR	3.6
1	B	314	ASP	3.0
1	B	258	LYS	2.9
1	B	178	LYS	2.9
1	A	258	LYS	2.8
1	A	314	ASP	2.8
1	A	312	GLU	2.8
1	B	226	GLY	2.7
1	A	259	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	2.6
1	A	257	PRO	2.6
1	A	177	ASN	2.6
1	A	311	VAL	2.5
1	B	180	SER	2.5
1	B	-1	SER	2.5
1	A	93	PHE	2.3
1	A	313	LYS	2.3
1	A	254	GLU	2.2
1	A	126	ILE	2.2
1	A	221	ALA	2.2
1	B	312	GLU	2.1
1	A	228	SER	2.1
1	B	118	VAL	2.1
1	B	164	LYS	2.1
1	A	227	PHE	2.1
1	B	257	PRO	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 ⓘ

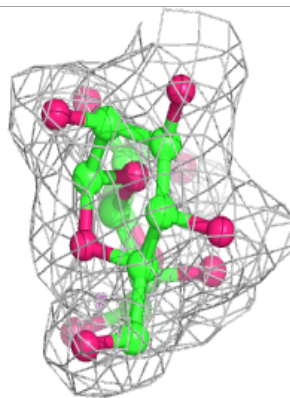
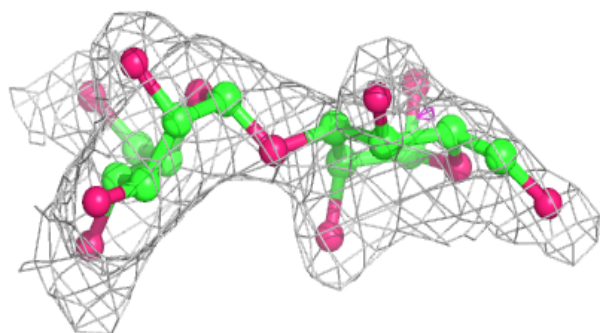
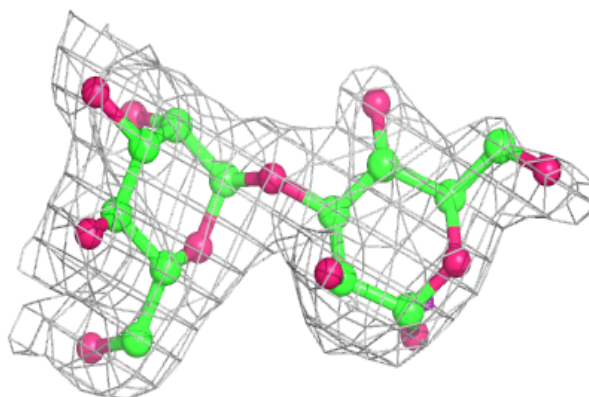
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	D	1	12/12	0.78	0.41	47,60,65,69	0
2	MAN	C	1	12/12	0.79	0.37	47,58,62,63	0
2	MAN	D	2	11/12	0.92	0.13	33,36,39,42	0
2	MAN	C	2	11/12	0.94	0.09	34,35,38,41	0

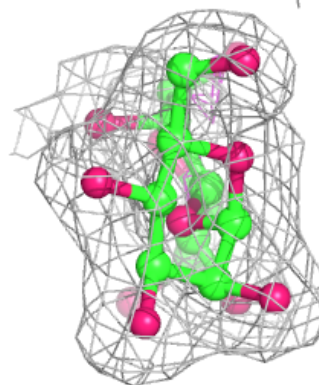
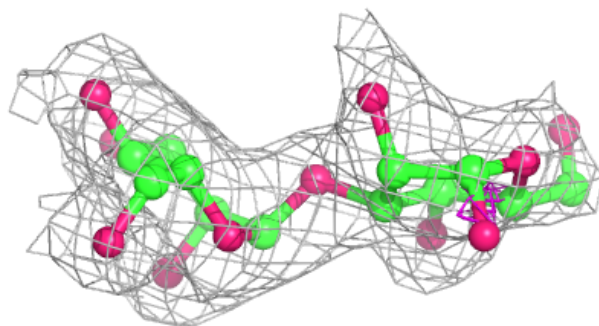
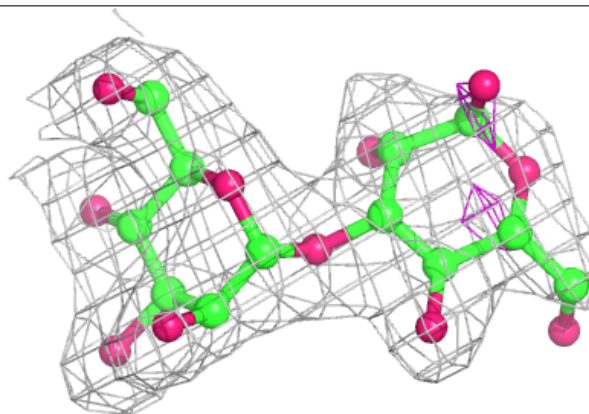
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain D:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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	PEG	A	404	7/7	0.68	0.17	54,55,56,56	0
4	PEG	B	407	7/7	0.70	0.21	59,59,61,62	0
4	PEG	A	405	7/7	0.73	0.19	65,66,66,67	0
7	EDO	A	410	4/4	0.75	0.12	57,57,57,57	0
6	PG4	A	409	13/13	0.75	0.16	49,50,53,53	0
9	1PE	B	413	16/16	0.76	0.19	49,55,64,64	0
4	PEG	B	409	7/7	0.79	0.21	67,70,72,72	0
6	PG4	A	408	13/13	0.79	0.20	44,48,49,51	0
7	EDO	B	406	4/4	0.80	0.13	56,57,57,58	0
8	EPE	B	404	15/15	0.81	0.33	56,61,67,69	5
5	PGE	B	410	10/10	0.83	0.17	44,48,49,49	0
7	EDO	B	405	4/4	0.84	0.28	58,59,59,59	0
4	PEG	B	408	7/7	0.85	0.16	54,57,58,60	0
6	PG4	B	412	13/13	0.87	0.14	50,53,54,55	0
5	PGE	A	406	10/10	0.88	0.12	45,46,49,50	0
5	PGE	B	411	10/10	0.88	0.13	49,50,52,55	0
5	PGE	A	407	10/10	0.89	0.15	51,52,54,55	0
3	CL	A	403	1/1	0.98	0.07	32,32,32,32	0
3	CL	B	403	1/1	1.00	0.05	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.