



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:31 PM EDT

PDB ID : 4ZNQ / pdb_00004znq
Title : Crystal structure of Dln1 complexed with Man(alpha1-2)Man
Authors : Jia, N.; Jiang, Y.L.; Cheng, W.; Wang, H.W.; Zhou, C.Z.; Chen, Y.
Deposited on : 2015-05-05
Resolution : 1.90 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

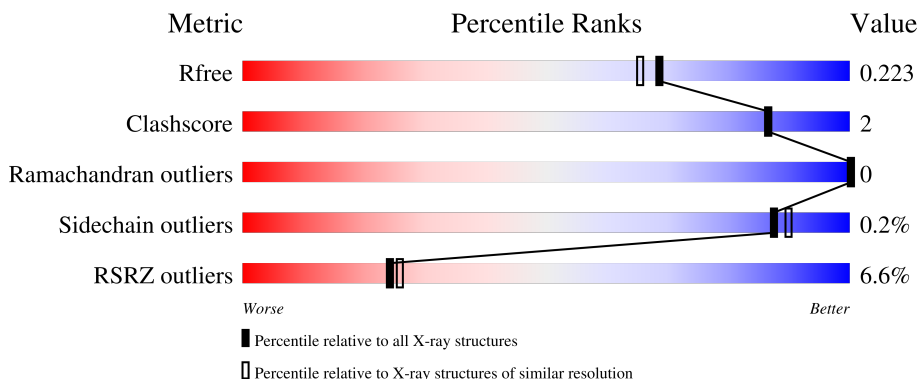
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	335	7% 90% • 5%
1	B	335	5% 89% 5% 5%
2	C	2	100%
2	D	2	100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5618 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	317	Total	C	N	O	S	0	4	0
			2444	1554	397	483	10			
1	B	317	Total	C	N	O	S	0	1	0
			2432	1544	397	481	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-(1-2)-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 (CCD ID: CL) (formula: Cl).

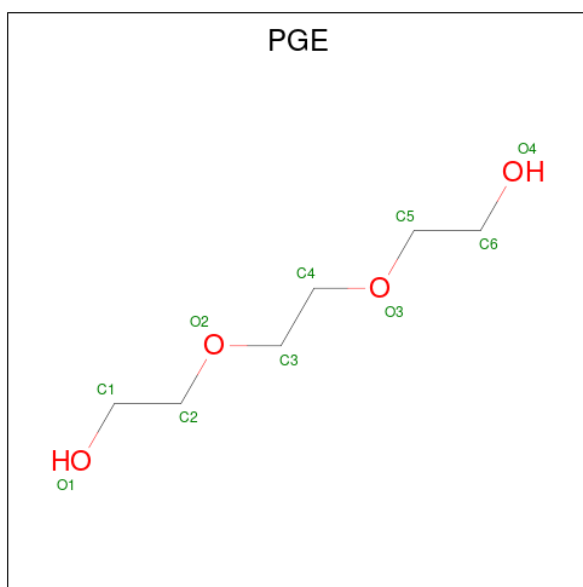
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



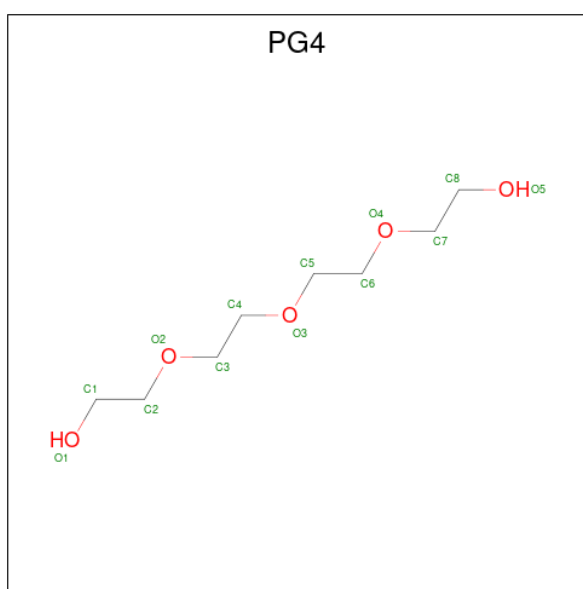
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

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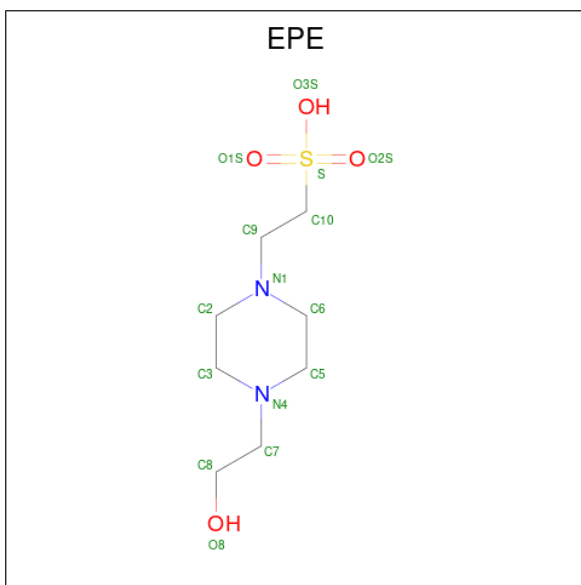
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



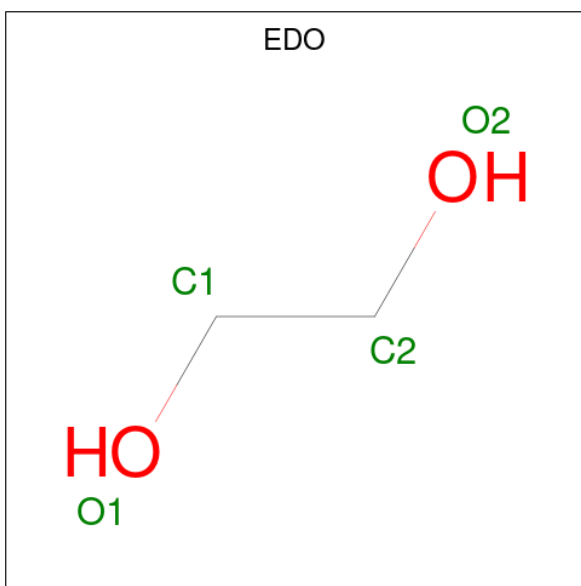
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

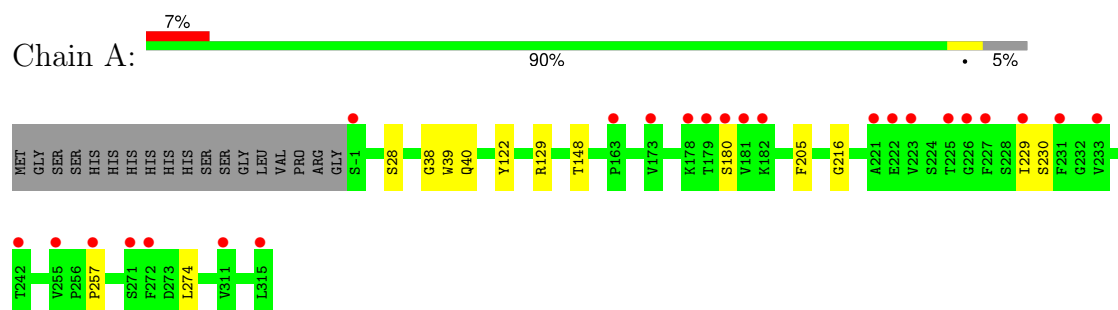
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	293	Total 293	O 293	0	0
9	B	298	Total 298	O 298	0	0

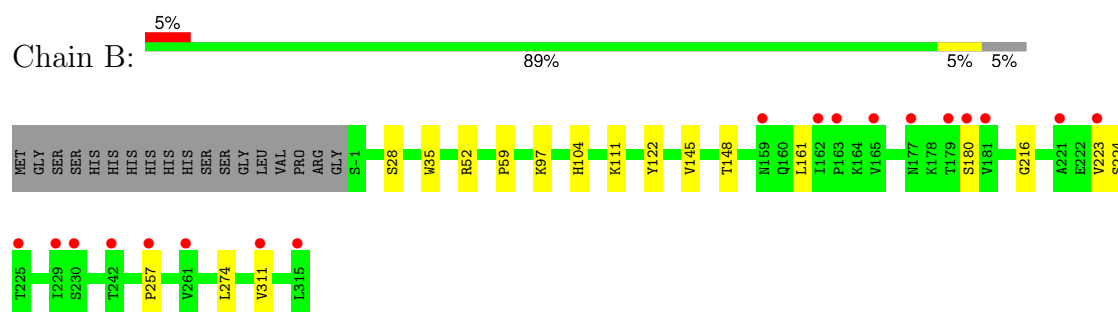
3 Residue-property plots [i](#)

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: Natterin-like protein



- Molecule 1: Natterin-like protein



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



- Molecule 2: alpha-D-mannopyranose-(1-2)-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 95.55Å 147.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.61 – 1.90 35.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (35.61-1.90) 99.2 (35.61-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.181 , 0.219 0.188 , 0.223	Depositor DCC
R_{free} test set	3237 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	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	0.96	EDS
Total number of atoms	5618	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.57% 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: EDO, EPE, CL, MAN, PEG, PGE, PG4

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	0.69	0/2509	0.82	2/3399 (0.1%)
1	B	0.67	0/2488	0.80	2/3369 (0.1%)
All	All	0.68	0/4997	0.81	4/6768 (0.1%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	216	GLY	N-CA-C	-6.01	104.53	112.82
1	A	274	LEU	N-CA-C	5.56	114.70	108.25
1	B	216	GLY	N-CA-C	-5.49	104.68	112.37
1	B	274	LEU	N-CA-C	5.16	114.23	108.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	GLN	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	2444	0	2418	8	0
1	B	2432	0	2395	13	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	7	0	10	0	0
4	B	14	0	20	1	0
5	A	30	0	42	3	0
5	B	20	0	28	0	0
6	A	13	0	18	0	0
7	B	15	0	18	0	0
8	B	4	0	6	0	0
9	A	293	0	0	1	0
9	B	298	0	0	4	0
All	All	5618	0	4997	21	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.

All (21) 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:223:VAL:HG12	1:B:224:SER:H	1.34	0.90
1:B:223:VAL:HG12	1:B:224:SER:N	1.92	0.82
1:B:223:VAL:CG1	1:B:224:SER:H	2.03	0.69
1:B:145[A]:VAL:HG11	1:B:148:THR:HG23	1.76	0.67
1:A:39:TRP:CD1	5:A:406:PGE:H4	2.38	0.58
1:B:97:LYS:NZ	9:B:504:HOH:O	2.38	0.49
1:A:38:GLY:HA3	5:A:406:PGE:C2	2.42	0.49
1:A:148[A]:THR:HG21	1:A:205:PHE:CZ	2.51	0.45
1:A:38:GLY:HA3	5:A:406:PGE:H22	1.98	0.45
1:B:180:SER:C	1:B:257:PRO:HB3	2.42	0.44
1:B:52:ARG:HD2	9:B:748:HOH:O	2.18	0.44
1:B:111:LYS:NZ	9:B:514:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:SER:HA	1:A:257:PRO:HB3	2.00	0.43
1:B:28:SER:HB3	1:B:122:TYR:CZ	2.53	0.43
1:B:161:LEU:HD12	9:B:596:HOH:O	2.20	0.42
1:A:129:ARG:NH2	9:A:503:HOH:O	2.45	0.41
1:B:35:TRP:CE2	1:B:59:PRO:HB3	2.55	0.41
1:A:229:ILE:HG22	1:A:230:SER:N	2.35	0.41
1:B:104:HIS:CE1	4:B:406:PEG:H41	2.56	0.41
1:A:28:SER:HB3	1:A:122:TYR:CZ	2.56	0.41
1:B:223:VAL:CG1	1:B:224:SER:N	2.61	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	319/335 (95%)	314 (98%)	5 (2%)	0	100	100
1	B	316/335 (94%)	311 (98%)	5 (2%)	0	100	100
All	All	635/670 (95%)	625 (98%)	10 (2%)	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	275/286 (96%)	275 (100%)	0	100	100
1	B	272/286 (95%)	271 (100%)	1 (0%)	84	87
All	All	547/572 (96%)	546 (100%)	1 (0%)	87	90

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

Mol	Chain	Res	Type
1	B	311	VAL

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	154	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 ⓘ

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	1.40	2 (16%)	17,17,17	1.23	2 (11%)
2	MAN	C	2	2	11,11,12	1.44	2 (18%)	15,15,17	1.40	1 (6%)
2	MAN	D	1	2	12,12,12	1.35	2 (16%)	17,17,17	1.56	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	D	2	2	11,11,12	1.25	1 (9%)	15,15,17	1.20	2 (13%)

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	-	0/2/22/22	0/1/1/1
2	MAN	C	2	2	-	0/2/19/22	0/1/1/1
2	MAN	D	1	2	-	1/2/22/22	0/1/1/1
2	MAN	D	2	2	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	MAN	O5-C5	-2.40	1.38	1.43
2	C	2	MAN	O2-C2	-2.27	1.38	1.43
2	C	1	MAN	O5-C5	-2.19	1.39	1.44
2	C	1	MAN	O4-C4	-2.13	1.37	1.43
2	D	1	MAN	O5-C5	-2.10	1.39	1.44
2	D	2	MAN	O2-C2	-2.06	1.39	1.43
2	D	1	MAN	O4-C4	-2.01	1.38	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	MAN	C1-O5-C5	4.11	117.70	112.19
2	D	1	MAN	O5-C5-C4	3.34	115.72	109.70
2	D	1	MAN	C1-O5-C5	2.94	119.33	113.65
2	D	2	MAN	C1-O5-C5	2.94	116.12	112.19
2	D	1	MAN	O5-C1-C2	2.89	115.38	110.30
2	C	1	MAN	O6-C6-C5	2.44	119.64	111.33
2	D	2	MAN	O2-C2-C3	2.27	114.86	110.15
2	D	1	MAN	O6-C6-C5	2.15	118.65	111.33
2	C	1	MAN	O5-C5-C4	2.07	113.43	109.70

There are no chirality outliers.

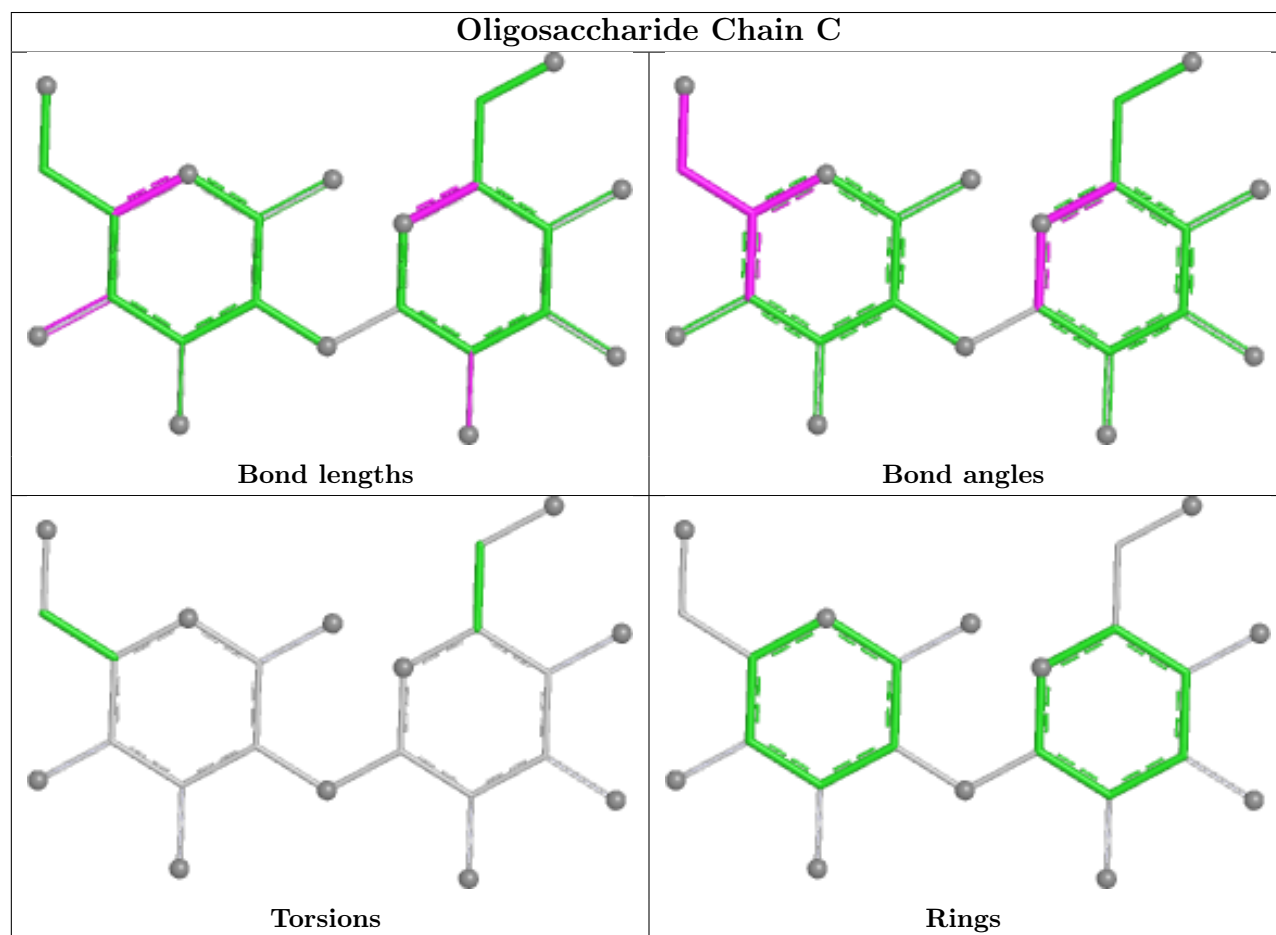
All (1) torsion outliers are listed below:

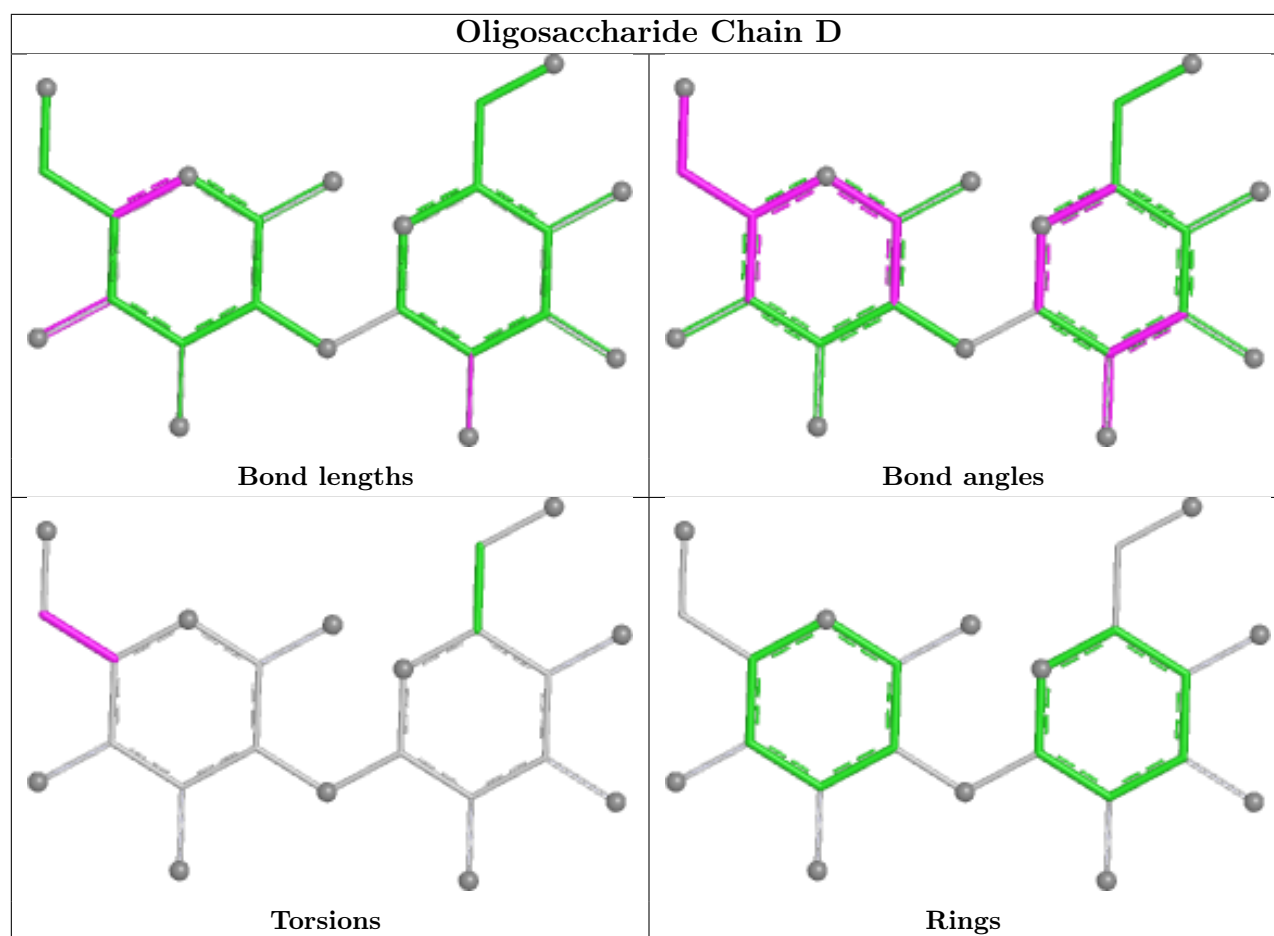
Mol	Chain	Res	Type	Atoms
2	D	1	MAN	C4-C5-C6-O6

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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	PGE	A	405	-	9,9,9	0.56	0	8,8,8	0.59	0
4	PEG	B	405	-	6,6,6	0.49	0	5,5,5	0.11	0
5	PGE	A	407	-	9,9,9	0.52	0	8,8,8	0.50	0
6	PG4	A	408	-	12,12,12	0.66	0	11,11,11	0.45	0
4	PEG	A	404	-	6,6,6	0.67	0	5,5,5	0.69	0
5	PGE	B	408	-	9,9,9	0.64	0	8,8,8	0.61	0
8	EDO	B	407	-	3,3,3	0.38	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PGE	B	409	-	9,9,9	0.69	0	8,8,8	0.51	0
5	PGE	A	406	-	9,9,9	0.44	0	8,8,8	0.41	0
4	PEG	B	406	-	6,6,6	0.45	0	5,5,5	0.59	0
7	EPE	B	404	-	15,15,15	1.88	1 (6%)	19,20,20	2.70	8 (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
5	PGE	A	405	-	-	4/7/7/7	-
4	PEG	B	405	-	-	1/4/4/4	-
5	PGE	A	407	-	-	3/7/7/7	-
6	PG4	A	408	-	-	5/10/10/10	-
4	PEG	A	404	-	-	1/4/4/4	-
5	PGE	B	408	-	-	2/7/7/7	-
8	EDO	B	407	-	-	1/1/1/1	-
5	PGE	B	409	-	-	2/7/7/7	-
5	PGE	A	406	-	-	4/7/7/7	-
4	PEG	B	406	-	-	3/4/4/4	-
7	EPE	B	404	-	-	5/9/19/19	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	404	EPE	C10-S	-7.00	1.67	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	404	EPE	C5-N4-C3	5.41	120.48	108.84
7	B	404	EPE	C6-N1-C2	5.40	120.47	108.84
7	B	404	EPE	O1S-S-C10	4.21	113.09	106.73
7	B	404	EPE	C7-N4-C5	3.66	121.00	111.24
7	B	404	EPE	C9-N1-C6	3.26	119.93	111.24
7	B	404	EPE	C9-N1-C2	3.14	119.60	111.24
7	B	404	EPE	C7-N4-C3	2.73	118.50	111.24
7	B	404	EPE	C3-C2-N1	-2.32	105.98	110.65

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	404	EPE	C10-C9-N1-C6
7	B	404	EPE	C9-C10-S-O2S
4	B	406	PEG	O2-C3-C4-O4
5	A	406	PGE	O2-C3-C4-O3
5	A	406	PGE	O1-C1-C2-O2
5	B	408	PGE	O3-C5-C6-O4
5	A	407	PGE	O2-C3-C4-O3
6	A	408	PG4	O1-C1-C2-O2
8	B	407	EDO	O1-C1-C2-O2
7	B	404	EPE	C9-C10-S-O3S
5	A	405	PGE	O3-C5-C6-O4
4	A	404	PEG	O1-C1-C2-O2
5	B	409	PGE	O2-C3-C4-O3
5	A	407	PGE	O3-C5-C6-O4
5	A	406	PGE	O3-C5-C6-O4
5	A	407	PGE	O1-C1-C2-O2
7	B	404	EPE	C9-C10-S-O1S
5	B	408	PGE	C1-C2-O2-C3
5	A	406	PGE	C1-C2-O2-C3
4	B	405	PEG	O1-C1-C2-O2
5	A	405	PGE	O1-C1-C2-O2
6	A	408	PG4	C4-C3-O2-C2
4	B	406	PEG	C1-C2-O2-C3
5	A	405	PGE	O2-C3-C4-O3
5	A	405	PGE	C1-C2-O2-C3
7	B	404	EPE	C8-C7-N4-C5
6	A	408	PG4	C1-C2-O2-C3
6	A	408	PG4	C3-C4-O3-C5
5	B	409	PGE	O3-C5-C6-O4
6	A	408	PG4	O3-C5-C6-O4
4	B	406	PEG	C4-C3-O2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	404	EPE	C2-C3-C5-C6-N1-N4

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	406	PGE	3	0
4	B	406	PEG	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	317/335 (94%)	0.39	24 (7%)	20 21	17, 30, 67, 100	4 (1%)
1	B	317/335 (94%)	0.33	18 (5%)	29 31	17, 30, 57, 91	1 (0%)
All	All	634/670 (94%)	0.36	42 (6%)	24 26	17, 30, 62, 100	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	LEU	6.6
1	B	315	LEU	5.6
1	A	223	VAL	5.2
1	B	223	VAL	4.9
1	A	181	VAL	4.8
1	B	163	PRO	4.0
1	A	229	ILE	3.9
1	A	180	SER	3.9
1	B	229	ILE	3.8
1	A	222	GLU	3.7
1	A	231	PHE	3.6
1	A	242	THR	3.5
1	B	181	VAL	3.5
1	A	227	PHE	3.5
1	A	179	THR	3.2
1	B	179	THR	3.2
1	A	271	SER	3.1
1	A	272	PHE	3.1
1	A	-1	SER	3.1
1	A	173	VAL	3.0
1	A	311	VAL	3.0
1	B	242	THR	3.0
1	A	182	LYS	2.8
1	A	163	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	226	GLY	2.7
1	A	233	VAL	2.6
1	A	225	THR	2.5
1	B	221	ALA	2.4
1	B	177	ASN	2.4
1	B	180	SER	2.4
1	B	162	ILE	2.3
1	B	225	THR	2.3
1	A	257	PRO	2.2
1	B	165	VAL	2.2
1	B	311	VAL	2.2
1	B	257	PRO	2.2
1	A	178	LYS	2.2
1	B	230	SER	2.2
1	B	261	VAL	2.1
1	A	255	VAL	2.1
1	A	221	ALA	2.0
1	B	159	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](#)

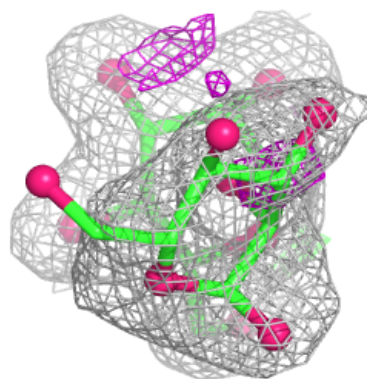
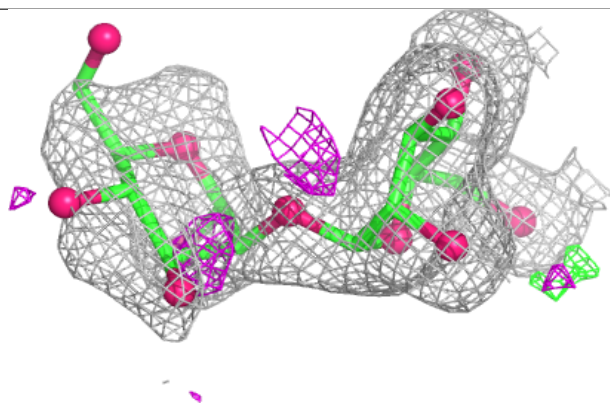
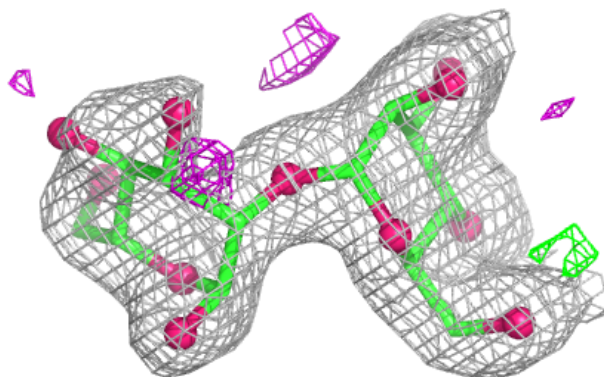
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	C	1	12/12	0.85	0.11	35,54,65,69	0
2	MAN	D	1	12/12	0.86	0.11	35,54,67,68	0
2	MAN	D	2	11/12	0.93	0.08	25,28,32,34	0
2	MAN	C	2	11/12	0.94	0.08	24,27,32,32	0

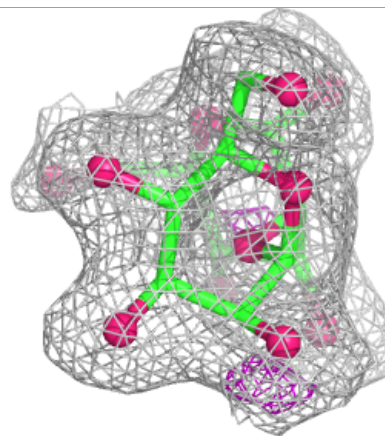
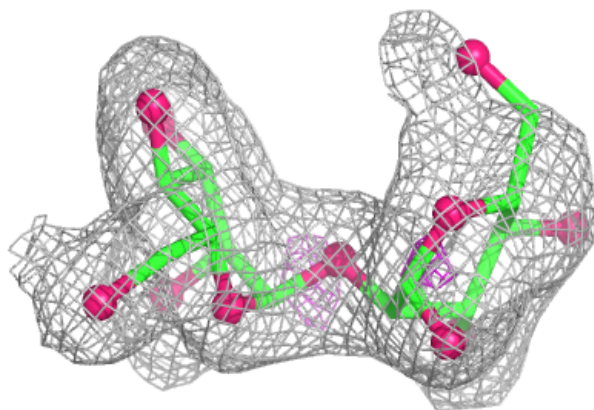
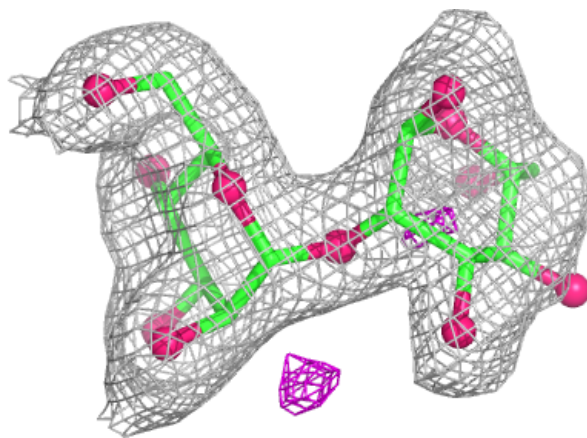
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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
5	PGE	B	409	10/10	0.75	0.17	51,54,58,60	0
5	PGE	B	408	10/10	0.77	0.15	46,51,56,57	0
5	PGE	A	407	10/10	0.77	0.16	47,53,56,56	0
6	PG4	A	408	13/13	0.82	0.16	53,55,60,61	0
5	PGE	A	405	10/10	0.83	0.15	48,50,60,66	0
5	PGE	A	406	10/10	0.85	0.15	47,51,54,54	0
4	PEG	B	405	7/7	0.86	0.14	49,50,52,53	0
7	EPE	B	404	15/15	0.86	0.15	46,61,73,76	0
8	EDO	B	407	4/4	0.87	0.15	41,48,49,49	0
4	PEG	A	404	7/7	0.88	0.11	42,43,46,47	0
4	PEG	B	406	7/7	0.90	0.11	47,48,50,54	0
3	CL	B	403	1/1	0.97	0.06	31,31,31,31	0
3	CL	A	403	1/1	0.98	0.04	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.