



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:48 PM UTC

PDB ID : 6ZBW / pdb_00006zbw
Title : Structure of the D125N mutant of the catalytic domain of the Bacillus circulans alpha-1,6 Mannanase in complex with an alpha-1,6-alpha-manno-cyclophellitol trisaccharide inhibitor
Authors : Davies, G.J.; Offen, W.A.
Deposited on : 2020-06-09
Resolution : 1.40 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

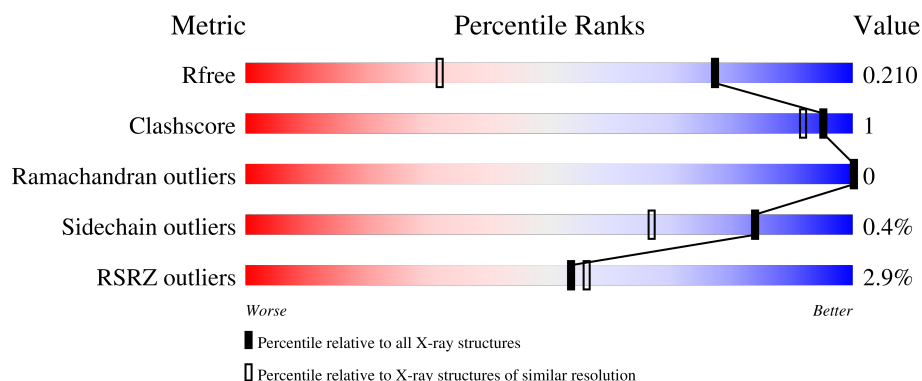
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

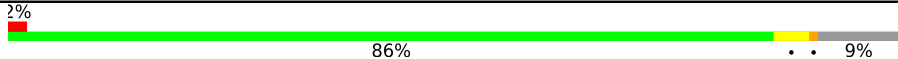
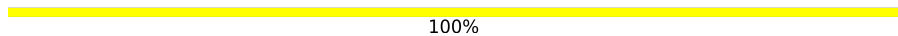
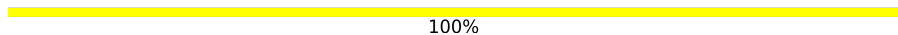
The reported resolution of this entry is 1.40 Å.

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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	362	 2% 86% 9%
1	B	362	 3% 89% 7%
2	C	2	 100%
2	D	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5878 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 Alpha-1,6-mannanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	3	0
			2653	1688	443	512	10			
1	B	335	Total	C	N	O	S	0	6	0
			2686	1712	450	514	10			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	initiating methionine	UNP Q9Z4P9
A	15	GLY	-	expression tag	UNP Q9Z4P9
A	16	SER	-	expression tag	UNP Q9Z4P9
A	17	SER	-	expression tag	UNP Q9Z4P9
A	18	HIS	-	expression tag	UNP Q9Z4P9
A	19	HIS	-	expression tag	UNP Q9Z4P9
A	20	HIS	-	expression tag	UNP Q9Z4P9
A	21	HIS	-	expression tag	UNP Q9Z4P9
A	22	HIS	-	expression tag	UNP Q9Z4P9
A	23	HIS	-	expression tag	UNP Q9Z4P9
A	24	SER	-	expression tag	UNP Q9Z4P9
A	25	SER	-	expression tag	UNP Q9Z4P9
A	26	GLY	-	expression tag	UNP Q9Z4P9
A	27	LEU	-	expression tag	UNP Q9Z4P9
A	28	GLU	-	expression tag	UNP Q9Z4P9
A	29	VAL	-	expression tag	UNP Q9Z4P9
A	30	LEU	-	expression tag	UNP Q9Z4P9
A	31	PHE	-	expression tag	UNP Q9Z4P9
A	32	GLN	-	expression tag	UNP Q9Z4P9
A	33	GLY	-	expression tag	UNP Q9Z4P9
A	34	PRO	-	expression tag	UNP Q9Z4P9
A	125	ASN	ASP	engineered mutation	UNP Q9Z4P9
A	341	GLN	ARG	engineered mutation	UNP Q9Z4P9
B	14	MET	-	initiating methionine	UNP Q9Z4P9
B	15	GLY	-	expression tag	UNP Q9Z4P9

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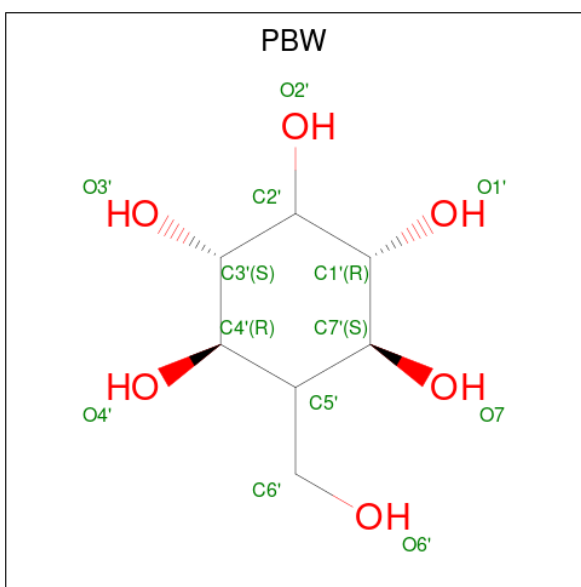
Chain	Residue	Modelled	Actual	Comment	Reference
B	16	SER	-	expression tag	UNP Q9Z4P9
B	17	SER	-	expression tag	UNP Q9Z4P9
B	18	HIS	-	expression tag	UNP Q9Z4P9
B	19	HIS	-	expression tag	UNP Q9Z4P9
B	20	HIS	-	expression tag	UNP Q9Z4P9
B	21	HIS	-	expression tag	UNP Q9Z4P9
B	22	HIS	-	expression tag	UNP Q9Z4P9
B	23	HIS	-	expression tag	UNP Q9Z4P9
B	24	SER	-	expression tag	UNP Q9Z4P9
B	25	SER	-	expression tag	UNP Q9Z4P9
B	26	GLY	-	expression tag	UNP Q9Z4P9
B	27	LEU	-	expression tag	UNP Q9Z4P9
B	28	GLU	-	expression tag	UNP Q9Z4P9
B	29	VAL	-	expression tag	UNP Q9Z4P9
B	30	LEU	-	expression tag	UNP Q9Z4P9
B	31	PHE	-	expression tag	UNP Q9Z4P9
B	32	GLN	-	expression tag	UNP Q9Z4P9
B	33	GLY	-	expression tag	UNP Q9Z4P9
B	34	PRO	-	expression tag	UNP Q9Z4P9
B	125	ASN	ASP	engineered mutation	UNP Q9Z4P9
B	341	GLN	ARG	engineered mutation	UNP Q9Z4P9

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			22	12	10			
2	D	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 3 is (1 {S},4 {S},5 {R})-6-(hydroxymethyl)cyclohexane-1,2,3,4,5-pentol (CCD ID: PBW) (formula: C₇H₁₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	7	5		
3	B	1	Total	C	O	0	0
			12	7	5		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	221	Total O 222 222	0	1
5	B	216	Total O 217 217	0	1

- Molecule 1: Alpha-1,6-mannanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.86Å 66.42Å 98.89Å 90.00° 100.13° 90.00°	Depositor
Resolution (Å)	48.72 – 1.40 48.72 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.72-1.40) 96.3 (48.72-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.154 , 0.206 0.162 , 0.210	Depositor DCC
R_{free} test set	5531 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5878	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0544e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, PBW, 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	1.16	5/2732 (0.2%)	1.23	5/3721 (0.1%)
1	B	1.15	4/2770 (0.1%)	1.25	3/3774 (0.1%)
All	All	1.16	9/5502 (0.2%)	1.24	8/7495 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	125	ASN	C-O	5.96	1.30	1.24
1	B	124	ASP	CG-OD2	5.68	1.36	1.25
1	A	124	ASP	CG-OD2	5.50	1.35	1.25
1	B	47	ALA	C-O	5.38	1.30	1.24
1	A	329	TRP	C-O	5.37	1.30	1.24
1	A	352	ALA	C-O	5.33	1.34	1.23
1	A	371	ALA	C-O	5.10	1.30	1.24
1	B	319	TYR	N-CA	5.05	1.50	1.46
1	A	152	HIS	CE1-NE2	5.04	1.37	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	LEU	CA-C-N	7.50	131.84	120.82
1	A	286	LEU	C-N-CA	7.50	131.84	120.82
1	A	71	ASP	CA-CB-CG	5.89	118.50	112.60
1	B	153	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	42	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	114	GLY	CA-C-O	-5.17	117.81	122.57
1	B	97	GLU	N-CA-C	-5.09	105.81	111.36
1	A	296	LYS	CB-CA-C	-5.04	101.31	110.63

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	2653	0	2409	6	0
1	B	2686	0	2443	6	0
2	C	22	0	19	0	0
2	D	22	0	19	0	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
4	A	16	0	24	1	0
4	B	16	0	24	0	0
5	A	222	0	0	1	0
5	B	217	0	0	1	0
All	All	5878	0	4938	12	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 (12) 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:333:ASN:O	1:A:336[B]:MET:HB2	1.92	0.69
1:B:285:VAL:HG22	1:B:336[A]:MET:HG3	1.81	0.62
1:B:287:ASN:ND2	5:B:502:HOH:O	2.30	0.59
1:A:285:VAL:HG22	1:A:336[B]:MET:HG3	1.85	0.58
1:B:285:VAL:HG21	1:B:336[B]:MET:HG3	1.95	0.48
1:B:288:TYR:OH	1:B:296[A]:LYS:HE3	2.15	0.46
1:A:116:ASP:CG	5:A:630:HOH:O	2.59	0.45
1:A:113:TYR:CD1	4:A:405:EDO:H11	2.53	0.44
1:B:285:VAL:CG2	1:B:336[A]:MET:HG3	2.45	0.43
1:A:292:ASN:O	1:A:296:LYS:HG3	2.19	0.41
1:A:117:TRP:CE3	1:A:152:HIS:CE1	3.08	0.41
1:B:292:ASN:O	1:B:296[A]:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/362 (91%)	324 (98%)	5 (2%)	0	100	100
1	B	337/362 (93%)	333 (99%)	4 (1%)	0	100	100
All	All	666/724 (92%)	657 (99%)	9 (1%)	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	264/294 (90%)	263 (100%)	1 (0%)	84	67
1	B	264/294 (90%)	263 (100%)	1 (0%)	84	67
All	All	528/588 (90%)	526 (100%)	2 (0%)	84	67

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

Mol	Chain	Res	Type
1	A	243	TYR
1	B	243	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN

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Mol	Chain	Res	Type
1	A	278	HIS
1	B	190	GLN
1	B	278	HIS
1	B	287	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	3,2	11,11,12	0.83	0	15,15,17	1.30	2 (13%)
2	MAN	C	2	2	11,11,12	1.30	1 (9%)	15,15,17	1.00	1 (6%)
2	MAN	D	1	3,2	11,11,12	1.01	0	15,15,17	1.20	1 (6%)
2	MAN	D	2	2	11,11,12	0.40	0	15,15,17	1.02	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	3,2	-	0/2/19/22	0/1/1/1
2	MAN	C	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	D	1	3,2	-	0/2/19/22	0/1/1/1
2	MAN	D	2	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	C	2	MAN	C2-C3	-3.41	1.47	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	MAN	C2-C3-C4	-2.70	106.11	110.86
2	C	1	MAN	C2-C3-C4	-2.62	106.25	110.86
2	C	2	MAN	O2-C2-C3	2.47	115.27	110.15
2	D	2	MAN	C1-O5-C5	2.27	115.23	112.19
2	C	1	MAN	C3-C4-C5	2.22	114.25	110.23

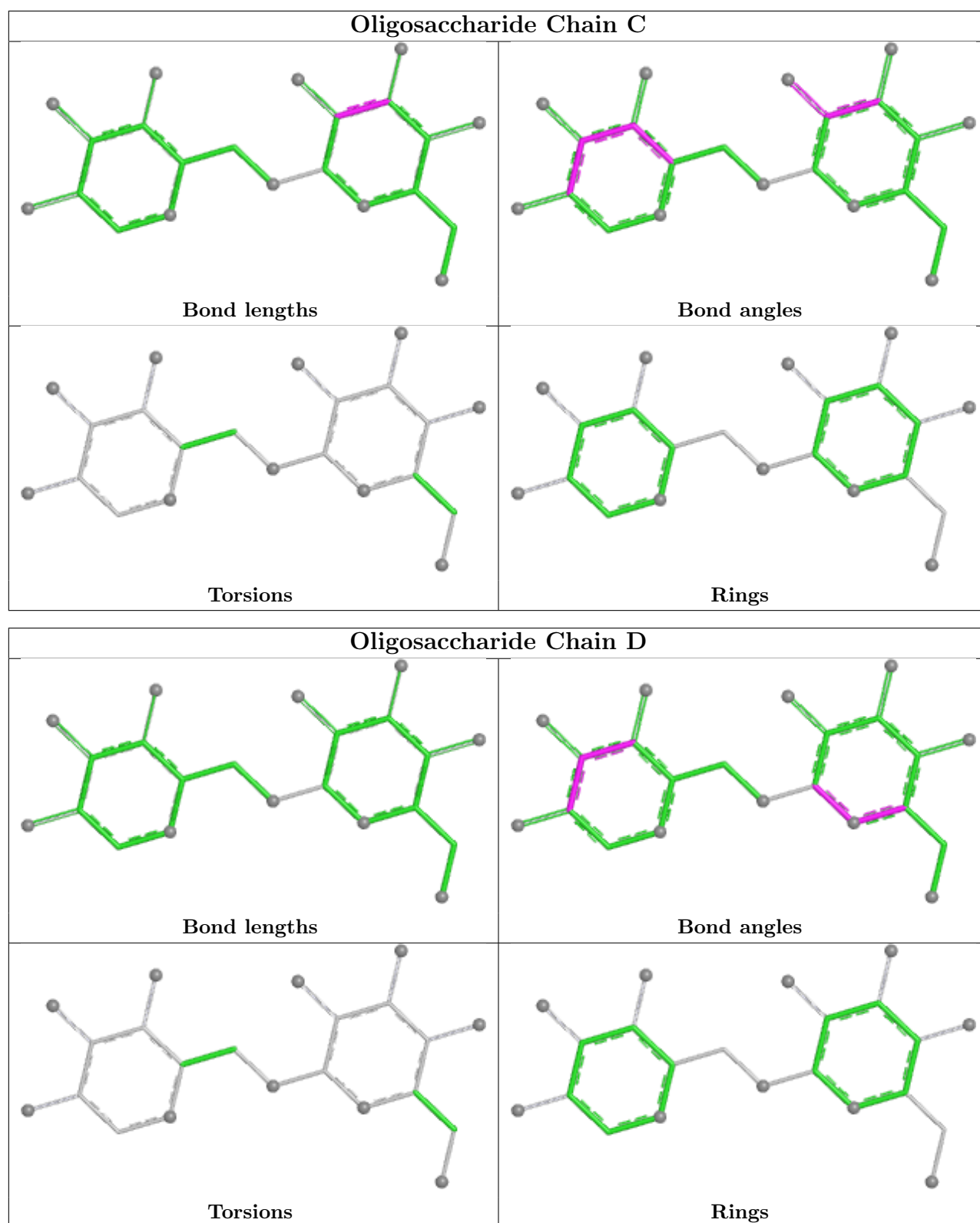
There are no chirality outliers.

There are no torsion outliers.

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](#)

10 ligands 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	$\# Z > 2$
4	EDO	A	404	-	3,3,3	0.22	0	2,2,2	0.33	0
4	EDO	A	405	-	3,3,3	0.22	0	2,2,2	0.25	0
4	EDO	B	401	-	3,3,3	0.26	0	2,2,2	0.40	0
4	EDO	A	407	-	3,3,3	0.34	0	2,2,2	0.29	0
3	PBW	B	403	2,1	12,12,13	1.44	2 (16%)	14,17,19	1.02	1 (7%)
4	EDO	B	407	-	3,3,3	0.56	0	2,2,2	0.59	0
4	EDO	A	406	-	3,3,3	0.70	0	2,2,2	0.46	0
4	EDO	B	406	-	3,3,3	0.24	0	2,2,2	0.06	0
4	EDO	B	402	-	3,3,3	0.17	0	2,2,2	0.25	0
3	PBW	A	401	2,1	12,12,13	0.90	0	14,17,19	0.94	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
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	A	405	-	-	0/1/1/1	-
4	EDO	B	401	-	-	0/1/1/1	-
4	EDO	A	407	-	-	1/1/1/1	-
3	PBW	B	403	2,1	-	0/2/22/26	0/1/1/1
4	EDO	B	407	-	-	0/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	B	406	-	-	1/1/1/1	-
4	EDO	B	402	-	-	1/1/1/1	-
3	PBW	A	401	2,1	-	0/2/22/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	PBW	C2'-C3'	2.74	1.56	1.52
3	B	403	PBW	C1'-C2'	-2.10	1.48	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	PBW	O3'-C3'-C2'	-2.04	105.90	110.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

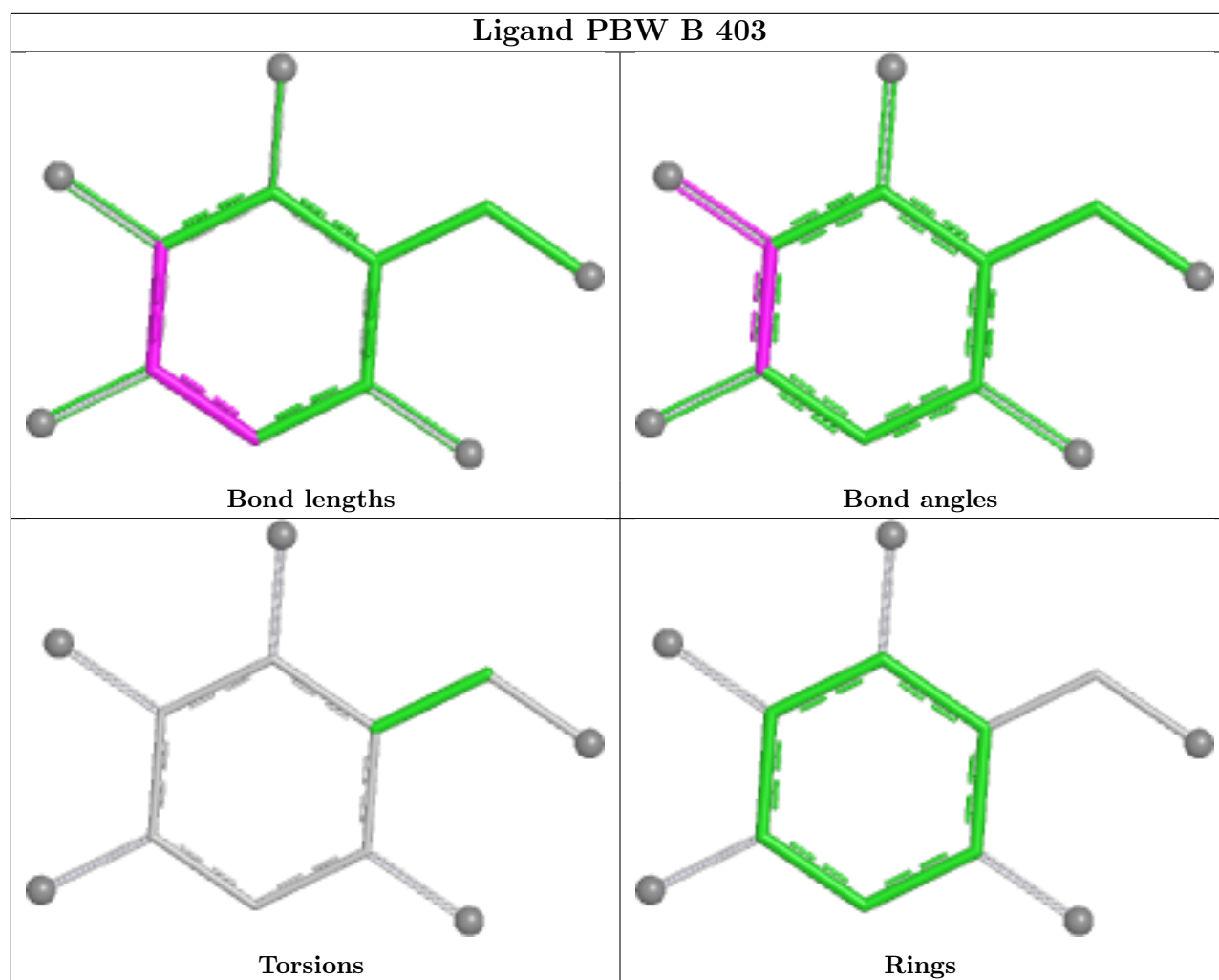
Mol	Chain	Res	Type	Atoms
4	A	407	EDO	O1-C1-C2-O2
4	B	402	EDO	O1-C1-C2-O2
4	B	406	EDO	O1-C1-C2-O2

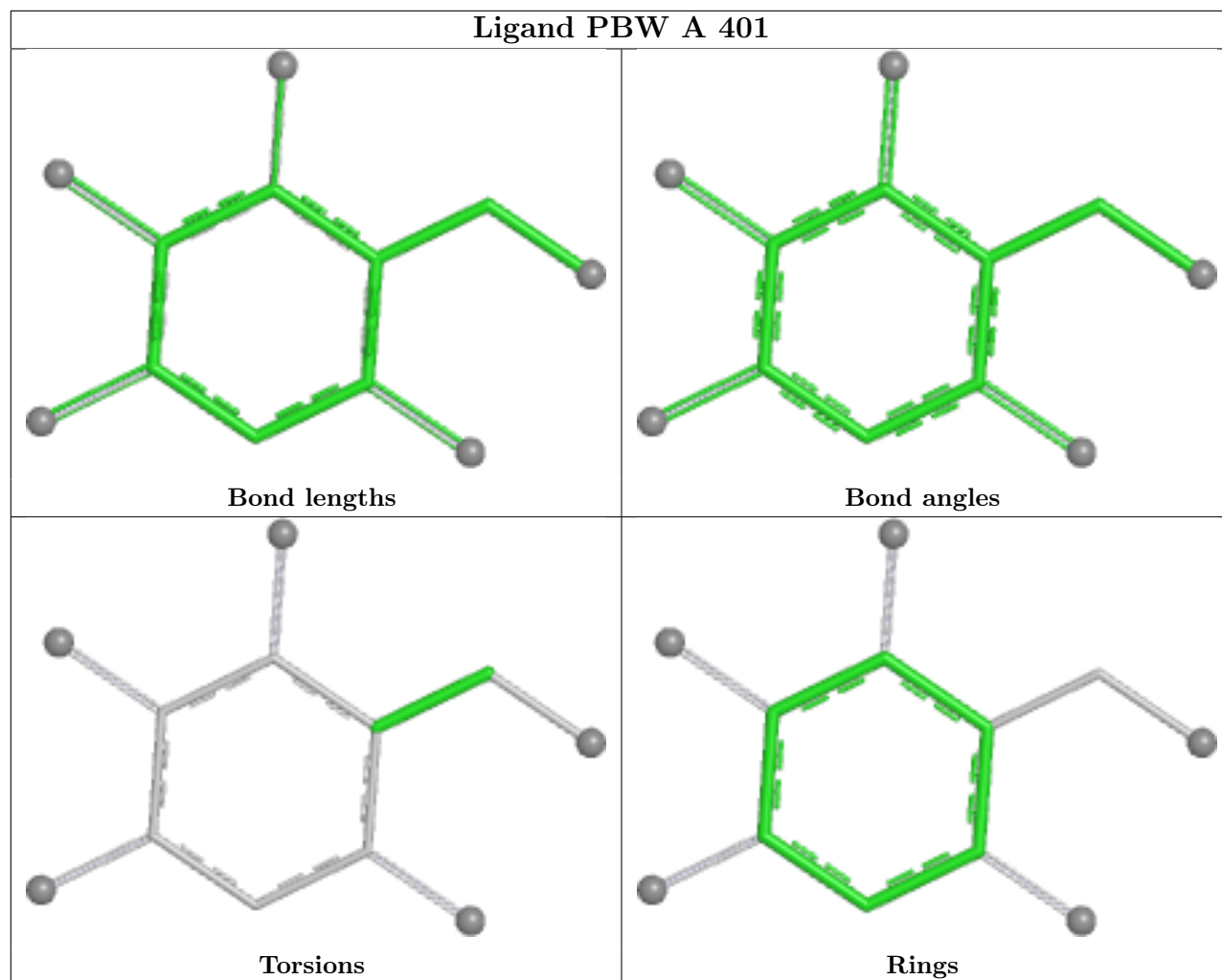
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	330/362 (91%)	-0.09	7 (2%) 63 66	13, 19, 28, 39	30 (9%)
1	B	335/362 (92%)	-0.02	12 (3%) 46 48	9, 19, 31, 43	37 (11%)
All	All	665/724 (91%)	-0.06	19 (2%) 53 56	9, 19, 30, 43	67 (10%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	LEU	7.7
1	B	355	LEU	6.6
1	A	338	TRP	5.3
1	B	358	GLY	4.9
1	B	374	GLY	4.7
1	A	352	ALA	3.3
1	B	117	TRP	3.2
1	B	354	GLN	3.1
1	B	353	GLY	3.0
1	A	234[A]	HIS	2.9
1	A	39	SER	2.7
1	B	118	THR	2.7
1	A	119	ASN	2.6
1	B	119	ASN	2.6
1	B	338	TRP	2.4
1	B	283[A]	ASN	2.2
1	A	67	GLU	2.1
1	B	115	GLN	2.0
1	A	117	TRP	2.0

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

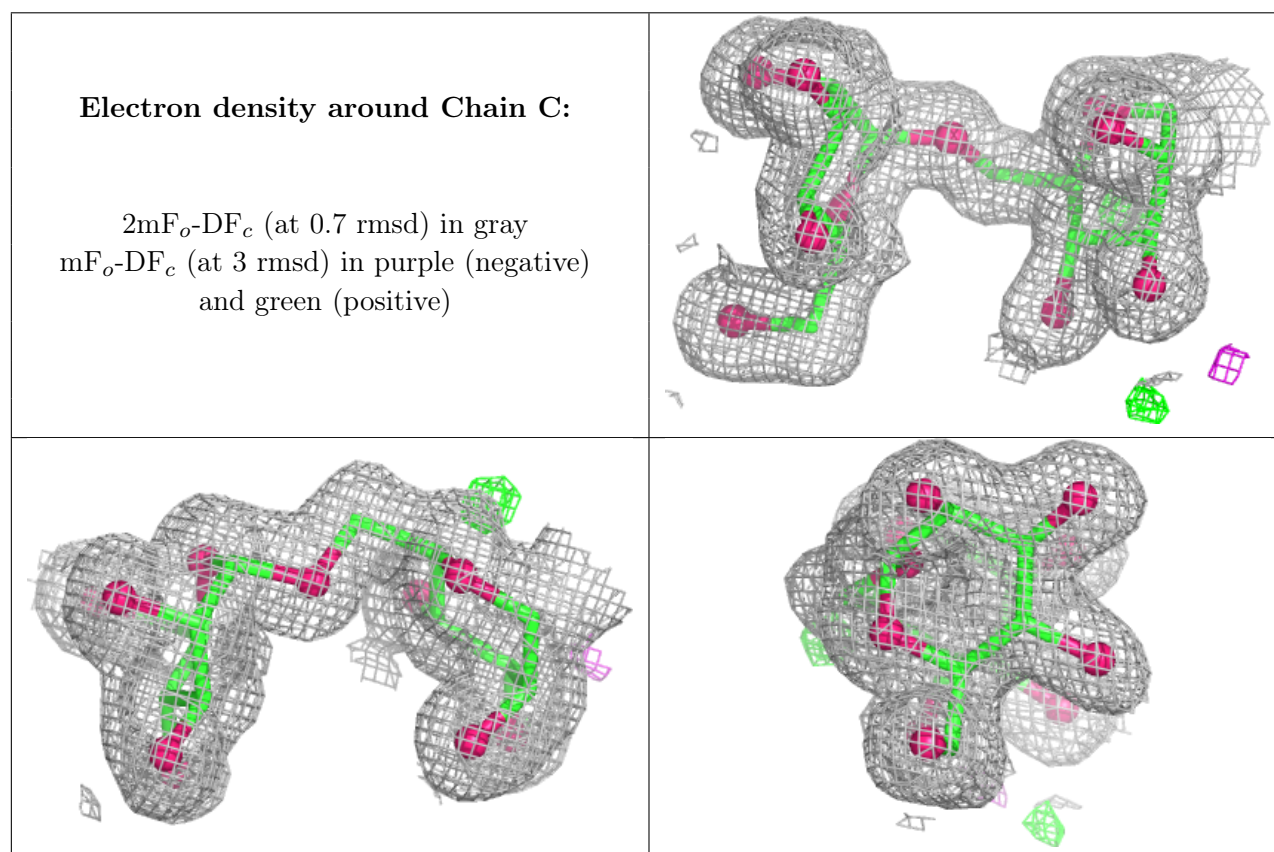
There are no non-standard protein/DNA/RNA residues in this entry.

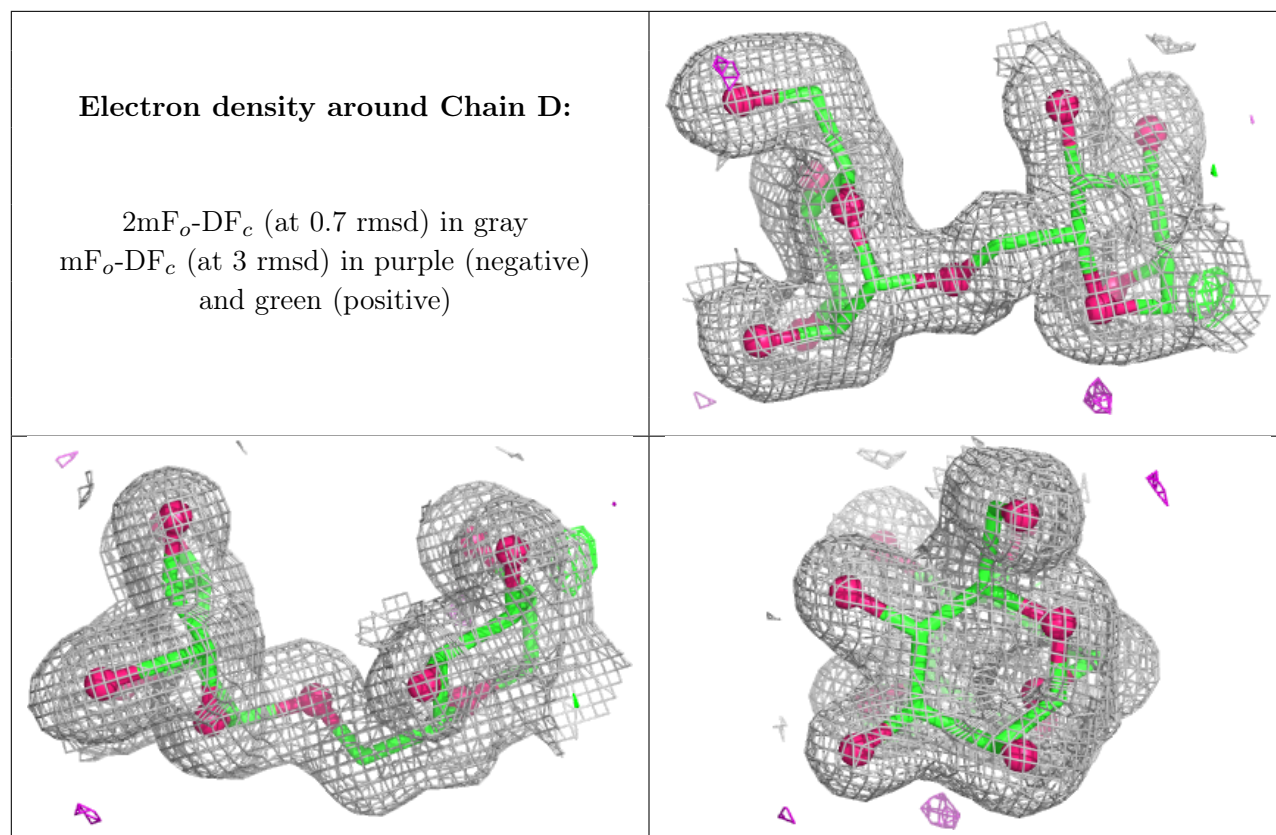
6.3 Carbohydrates ⓘ

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	MAN	D	2	11/12	0.97	0.05	16,18,22,25	0
2	MAN	C	2	11/12	0.98	0.04	17,18,23,25	0
2	MAN	D	1	11/12	0.98	0.04	14,15,16,17	0
2	MAN	C	1	11/12	0.98	0.04	13,14,16,16	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 ⓘ

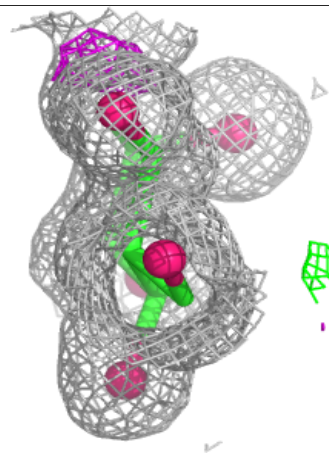
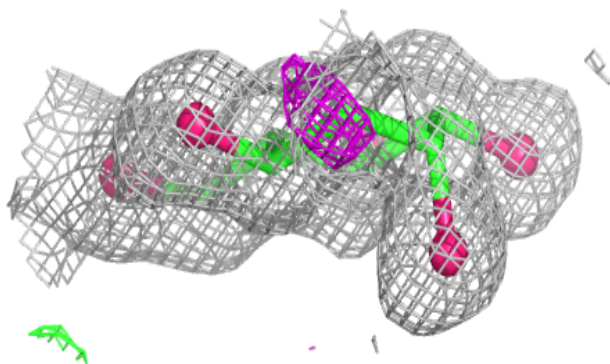
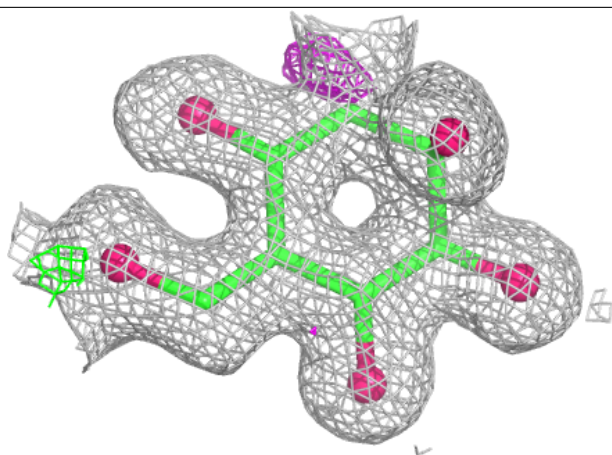
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	B	407	4/4	0.89	0.09	29,30,30,36	0
4	EDO	A	406	4/4	0.90	0.10	29,29,31,35	0
4	EDO	A	407	4/4	0.91	0.15	26,26,27,30	4
4	EDO	B	402	4/4	0.93	0.10	40,43,45,46	0
4	EDO	B	406	4/4	0.93	0.12	19,22,25,26	4
4	EDO	A	405	4/4	0.93	0.08	28,30,31,32	0
4	EDO	A	404	4/4	0.94	0.11	18,21,23,25	4
4	EDO	B	401	4/4	0.95	0.07	25,30,31,34	0
3	PBW	A	401	12/13	0.97	0.05	13,16,18,18	0
3	PBW	B	403	12/13	0.97	0.04	13,16,17,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

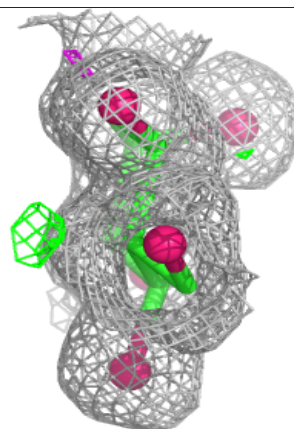
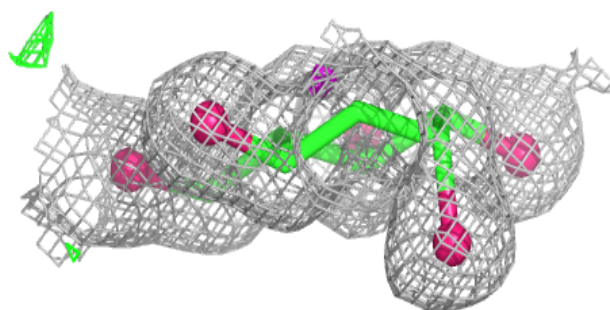
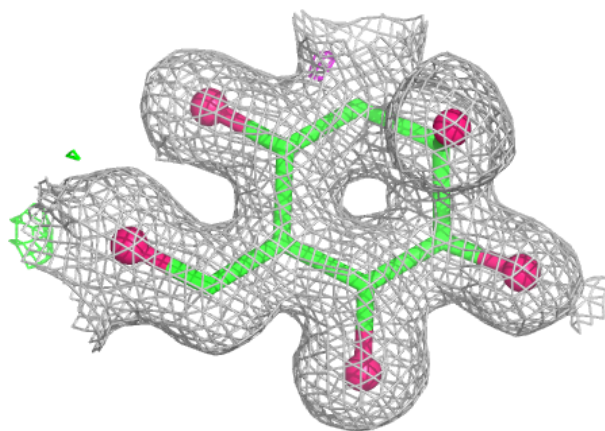
Electron density around PBW A 401:

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



Electron density around PBW B 403:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.