



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 05:25 PM EDT

PDB ID : 4PFT / pdb\_00004pft  
Title : Crystal structure of mannobiose bound oligopeptide ABC transporter, periplasmic oligopeptide-binding protein (TM1223) from THERMOTOGA MARITIMA at 1.75 Å resolution  
Authors : Lu, X.; Ghimire-Rijal, S.; Cuneo, M.J.  
Deposited on : 2014-04-30  
Resolution : 1.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

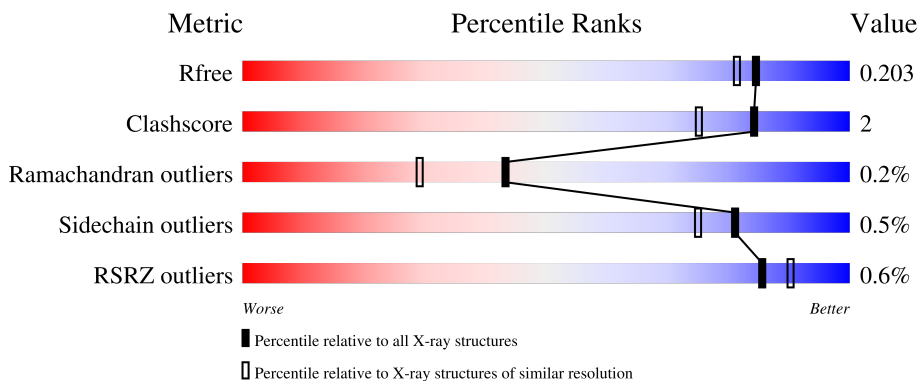
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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  $\geq 3$ , 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	544	 93% 6%
1	B	544	 94% 5%
2	C	2	 50% 50%
2	D	2	 50% 50%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10262 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 ABC transporter substrate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	4476	2936	709	819	12	0	16	0
1	B	538	4478	2933	707	827	11	0	13	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP Q9X0V0
A	558	HIS	-	expression tag	UNP Q9X0V0
A	559	HIS	-	expression tag	UNP Q9X0V0
A	560	HIS	-	expression tag	UNP Q9X0V0
A	561	HIS	-	expression tag	UNP Q9X0V0
A	562	HIS	-	expression tag	UNP Q9X0V0
A	563	HIS	-	expression tag	UNP Q9X0V0
B	20	MET	-	initiating methionine	UNP Q9X0V0
B	558	HIS	-	expression tag	UNP Q9X0V0
B	559	HIS	-	expression tag	UNP Q9X0V0
B	560	HIS	-	expression tag	UNP Q9X0V0
B	561	HIS	-	expression tag	UNP Q9X0V0
B	562	HIS	-	expression tag	UNP Q9X0V0
B	563	HIS	-	expression tag	UNP Q9X0V0

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-beta-D-mannopyranos e.

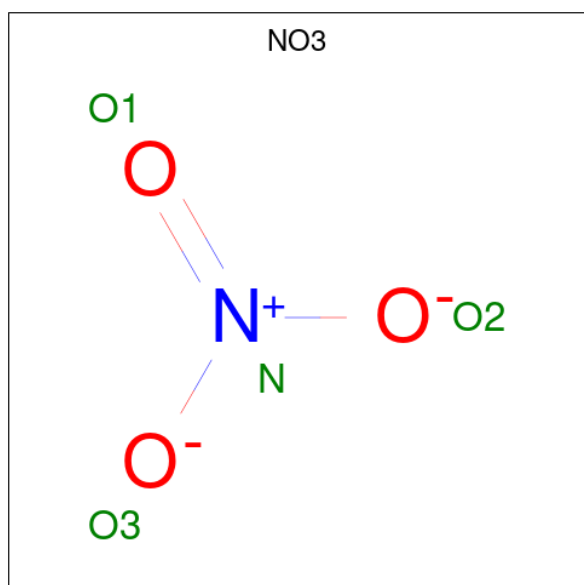


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO<sub>3</sub>).



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

- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	629	Total 629	O 629	0	0
5	B	619	Total 619	O 619	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.49Å 53.54Å 106.28Å 90.00° 110.47° 90.00°	Depositor
Resolution (Å)	46.07 – 1.75 46.07 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.07-1.75) 99.6 (46.07-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 1.75Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.152 , 0.204 0.156 , 0.203	Depositor DCC
$R_{free}$ test set	5163 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtrriage
Anisotropy	0.177	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10262	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.56 % 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 5.9310e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NO3, MG, BMA

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	0.47	0/4647	0.76	1/6353 (0.0%)
1	B	0.47	0/4636	0.76	0/6336
All	All	0.47	0/9283	0.76	1/12689 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	N-CA-C	5.05	116.19	108.42

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	A	4476	0	4298	20	0
1	B	4478	0	4290	19	0
2	C	23	0	20	1	0
2	D	23	0	20	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	1	0
4	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	629	0	0	8	1
5	B	619	0	0	7	1
All	All	10262	0	8628	40	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 40 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:232:ASN:OD1	5:B:1235:HOH:O	2.01	0.78
1:A:237:MET:SD	5:A:1329:HOH:O	2.50	0.70
1:B:139:ARG:NH2	5:B:1135:HOH:O	2.24	0.67
4:A:603:NO3:O3	5:A:1328:HOH:O	2.10	0.67
1:B:212:ARG:NE	5:B:1309:HOH:O	2.28	0.66

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:702:HOH:O	5:A:821:HOH:O[1_545]	2.15	0.05
5:B:757:HOH:O	5:B:840:HOH:O[1_565]	2.19	0.01

## 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	551/544 (101%)	533 (97%)	17 (3%)	1 (0%)	43 29
1	B	549/544 (101%)	530 (96%)	18 (3%)	1 (0%)	43 29
All	All	1100/1088 (101%)	1063 (97%)	35 (3%)	2 (0%)	43 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	TYR
1	B	451	TYR

### 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	473/472 (100%)	469 (99%)	4 (1%)	73 64
1	B	472/472 (100%)	470 (100%)	2 (0%)	84 79
All	All	945/944 (100%)	939 (99%)	6 (1%)	81 71

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	VAL
1	B	403	LYS
1	B	474	GLU
1	A	363[A]	VAL
1	A	23	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	447	ASN

### 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	BMA	C	1	2	12,12,12	1.07	0	17,17,17	3.54	5 (29%)
2	BMA	C	2	2	11,11,12	1.25	1 (9%)	15,15,17	0.63	0
2	BMA	D	1	2	12,12,12	1.10	1 (8%)	17,17,17	3.28	5 (29%)
2	BMA	D	2	2	11,11,12	1.20	1 (9%)	15,15,17	0.74	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
2	BMA	C	1	2	-	0/2/22/22	0/1/1/1
2	BMA	C	2	2	-	0/2/19/22	0/1/1/1
2	BMA	D	1	2	-	0/2/22/22	0/1/1/1
2	BMA	D	2	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	BMA	O5-C1	3.01	1.48	1.43
2	D	2	BMA	O5-C1	2.79	1.48	1.43
2	D	1	BMA	O5-C1	2.11	1.48	1.42

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	BMA	C1-O5-C5	-10.31	93.71	113.65
2	D	1	BMA	C1-O5-C5	-8.89	96.46	113.65
2	C	1	BMA	C1-C2-C3	-8.19	93.65	110.36
2	D	1	BMA	C1-C2-C3	-7.82	94.41	110.36
2	C	1	BMA	O1-C1-C2	4.08	120.83	108.98

There are no chirality outliers.

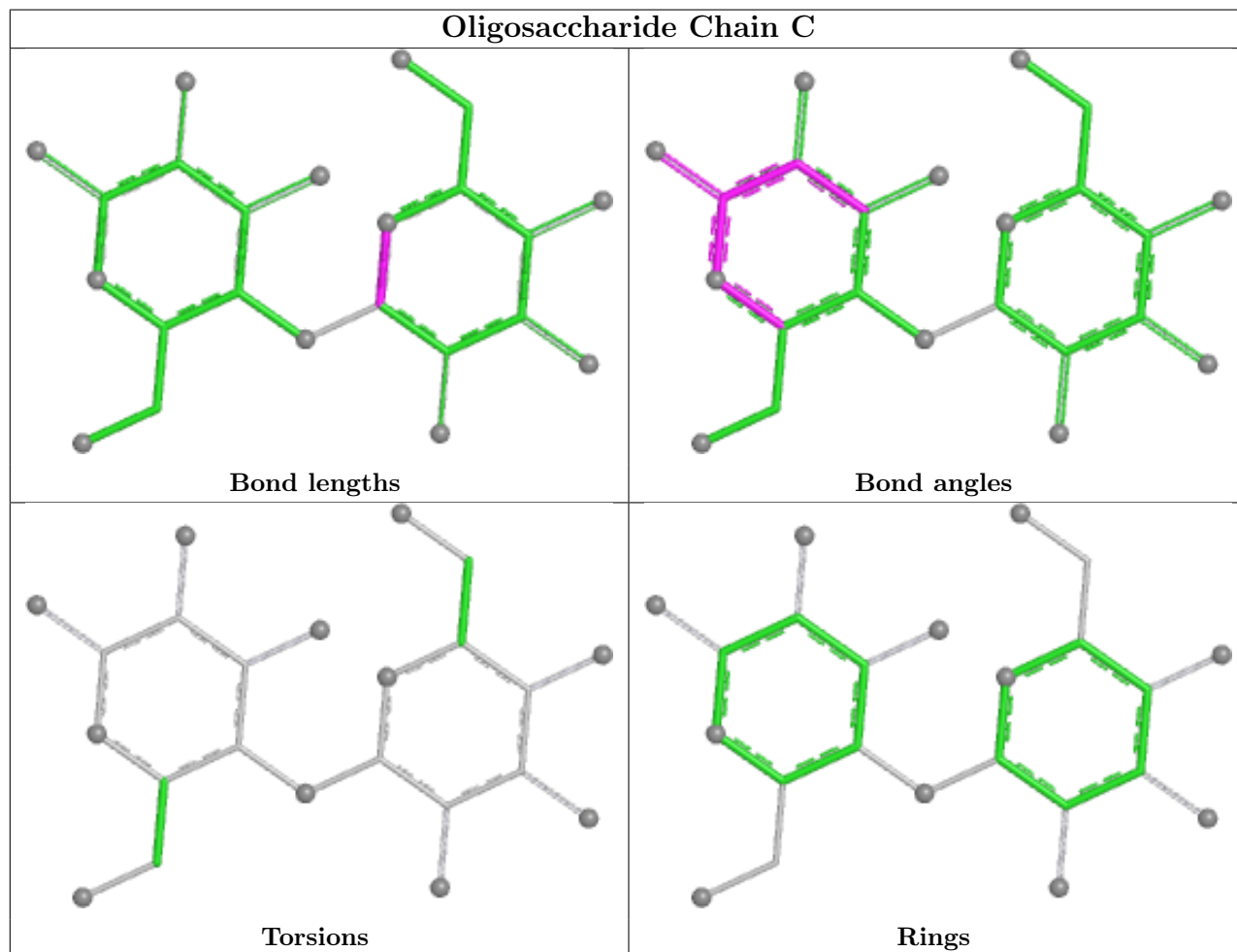
There are no torsion outliers.

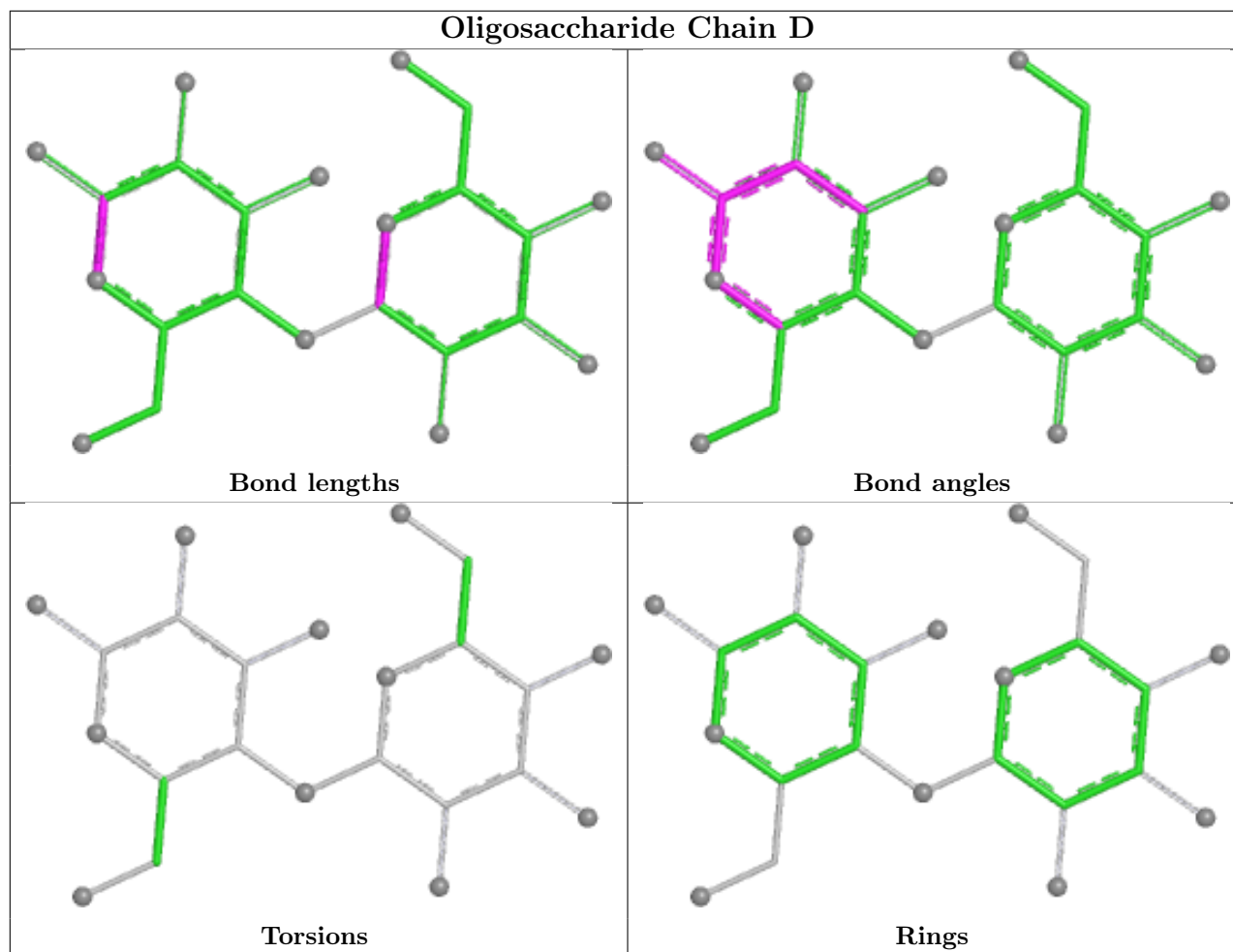
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	BMA	1	0
2	C	2	BMA	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 oligosaccharide.





## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z  > 2$
4	NO3	B	604	-	1,3,3	3.27	1 (100%)	0,3,3	-	-
4	NO3	B	603	-	1,3,3	3.20	1 (100%)	0,3,3	-	-
4	NO3	A	603	-	1,3,3	2.89	1 (100%)	0,3,3	-	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	NO3	O1-N	3.27	1.40	1.24
4	B	603	NO3	O1-N	3.20	1.40	1.24
4	A	603	NO3	O1-N	2.89	1.38	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	NO3	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	537/544 (98%)	-0.47	5 (0%) 81 87	7, 19, 36, 58	16 (2%)
1	B	538/544 (98%)	-0.47	1 (0%) 91 93	7, 19, 37, 59	13 (2%)
All	All	1075/1088 (98%)	-0.47	6 (0%) 85 90	7, 19, 37, 59	29 (2%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263[A]	VAL	6.3
1	A	350[A]	MET	4.2
1	A	558	HIS	2.5
1	A	22	PHE	2.5
1	A	327	LEU	2.3

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

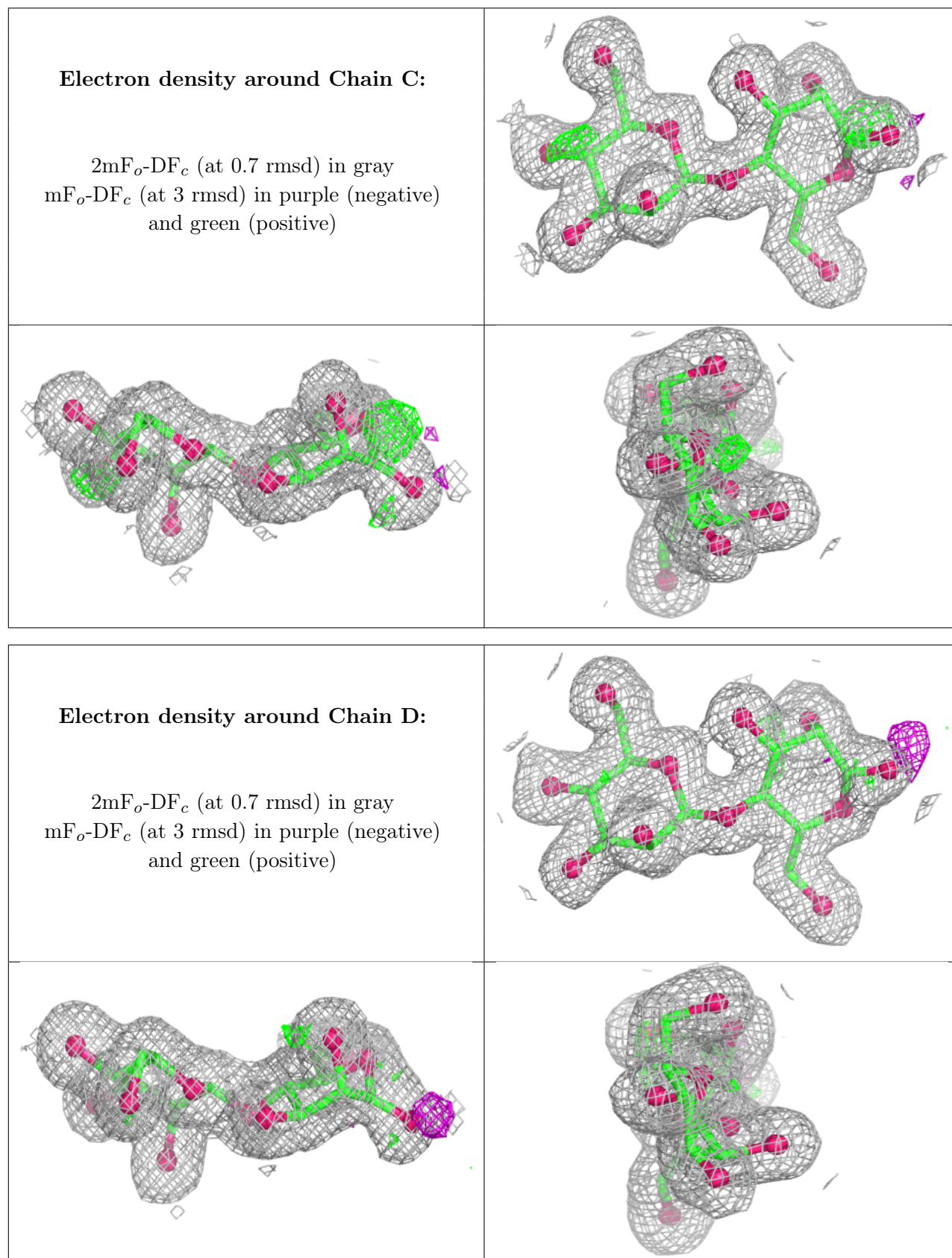
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BMA	C	1	12/12	0.96	0.05	10,13,16,20	0
2	BMA	D	1	12/12	0.96	0.05	10,11,17,20	0
2	BMA	C	2	11/12	0.98	0.03	6,11,13,13	0
2	BMA	D	2	11/12	0.98	0.04	9,11,12,14	0

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



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NO3	B	604	4/4	0.78	0.11	46,49,51,53	0
3	MG	B	602	1/1	0.89	0.10	39,39,39,39	0
4	NO3	B	603	4/4	0.90	0.11	38,39,44,44	0
4	NO3	A	603	4/4	0.91	0.13	26,29,35,40	0
3	MG	A	602	1/1	0.99	0.04	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.