



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 03:16 AM UTC

PDB ID : 1OGG / pdb_00001ogg
Title : chitinase b from serratia marcescens mutant d142n in complex with inhibitor allosamidin
Authors : Vaaje-Kolstad, G.; Houston, D.R.; Rao, F.V.; Peter, M.G.; Synstad, B.; van Aalten, D.M.F.; Eijsink, V.G.H.
Deposited on : 2003-04-30
Resolution : 1.97 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

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	:	FAILED
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

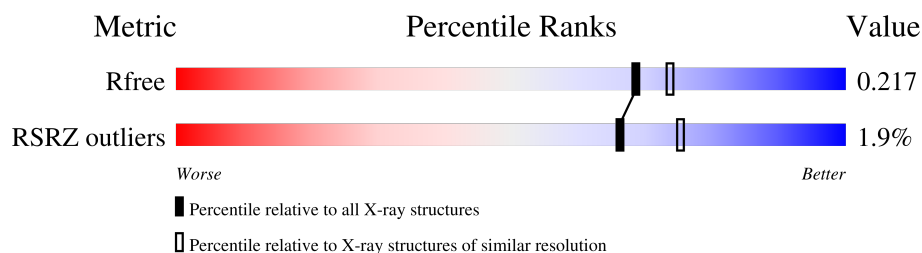
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8811 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 CHITINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	23	1	1
			3904	2497	661	732	14			
1	B	497	Total	C	N	O	S	12	2	0
			3919	2505	663	737	14			

There are 4 discrepancies between the modelled and reference sequences:

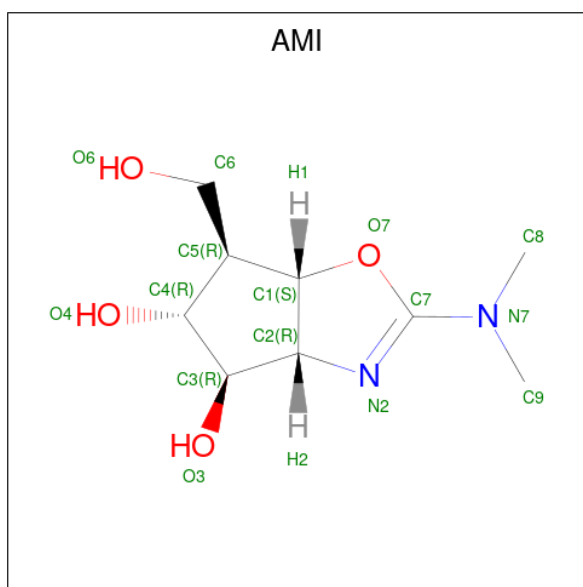
Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ASN	ASP	engineered mutation	UNP P11797
B	142	ASN	ASP	engineered mutation	UNP P11797
A	498	VAL	LEU	conflict	UNP P11797
B	498	VAL	LEU	conflict	UNP P11797

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-allopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-allopyranose.



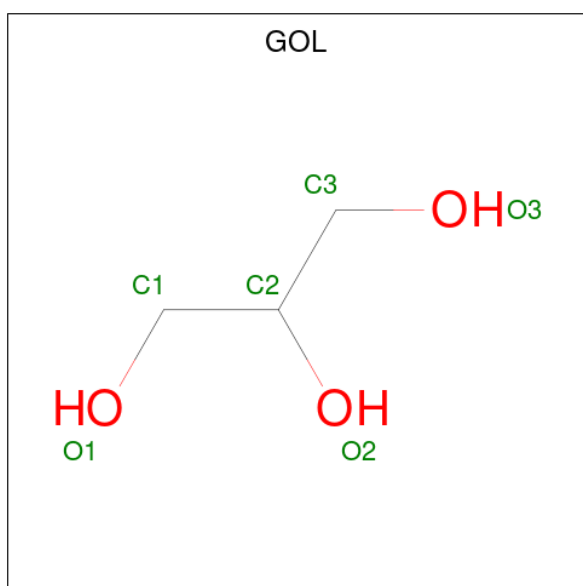
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is ALLOSAMIZOLINE (CCD ID: AMI) (formula: C₉H₁₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	9	2	4		
3	B	1	Total	C	N	O	0	0
			15	9	2	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



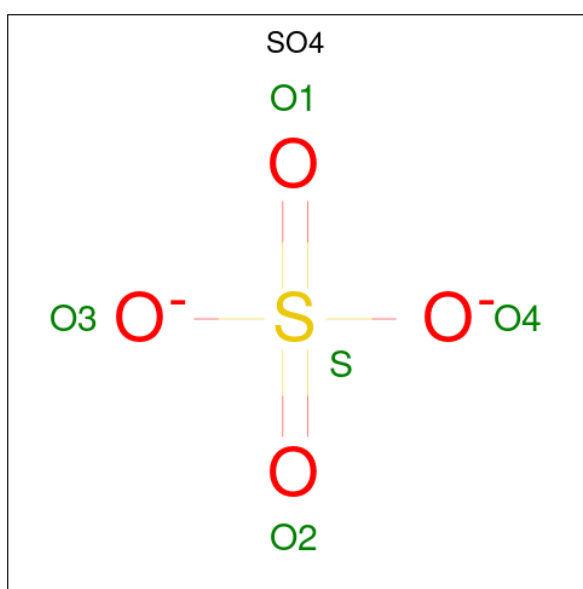
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	386	Total	O	0	0
			386	386		
6	B	475	Total	O	0	0
			475	475		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.87Å 104.74Å 186.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.76 – 1.97 24.76 – 1.97	Depositor EDS
% Data completeness (in resolution range)	95.1 (24.76-1.97) 95.2 (24.76-1.97)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.238 0.184 , 0.217	Depositor DCC
R_{free} test set	732 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8811	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 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	NAA	C	1	3,2	14,14,15	1.02	0	17,19,21	0.95	1 (5%)
2	NAA	C	2	2	14,14,15	0.96	1 (7%)	17,19,21	0.66	0
2	NAA	D	1	3,2	14,14,15	1.01	0	17,19,21	0.89	0
2	NAA	D	2	2	14,14,15	1.04	1 (7%)	17,19,21	0.84	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	NAA	C	1	3,2	-	0/6/23/26	0/1/1/1
2	NAA	C	2	2	-	0/6/23/26	0/1/1/1
2	NAA	D	1	3,2	-	0/6/23/26	0/1/1/1
2	NAA	D	2	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAA	C1-C2	2.53	1.55	1.52
2	C	2	NAA	C1-C2	2.15	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAA	C1-C2-N2	-2.58	106.37	110.43

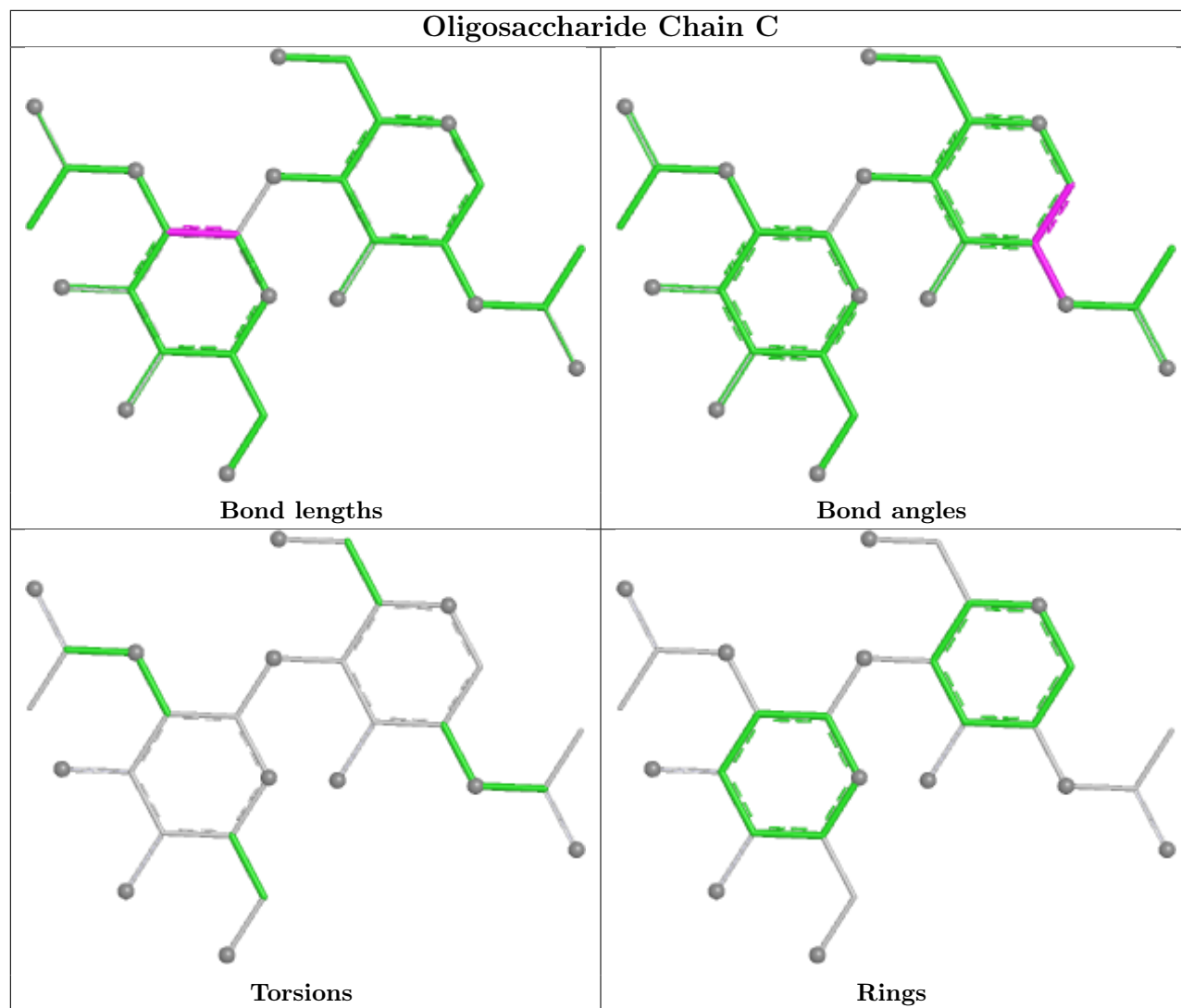
There are no chirality outliers.

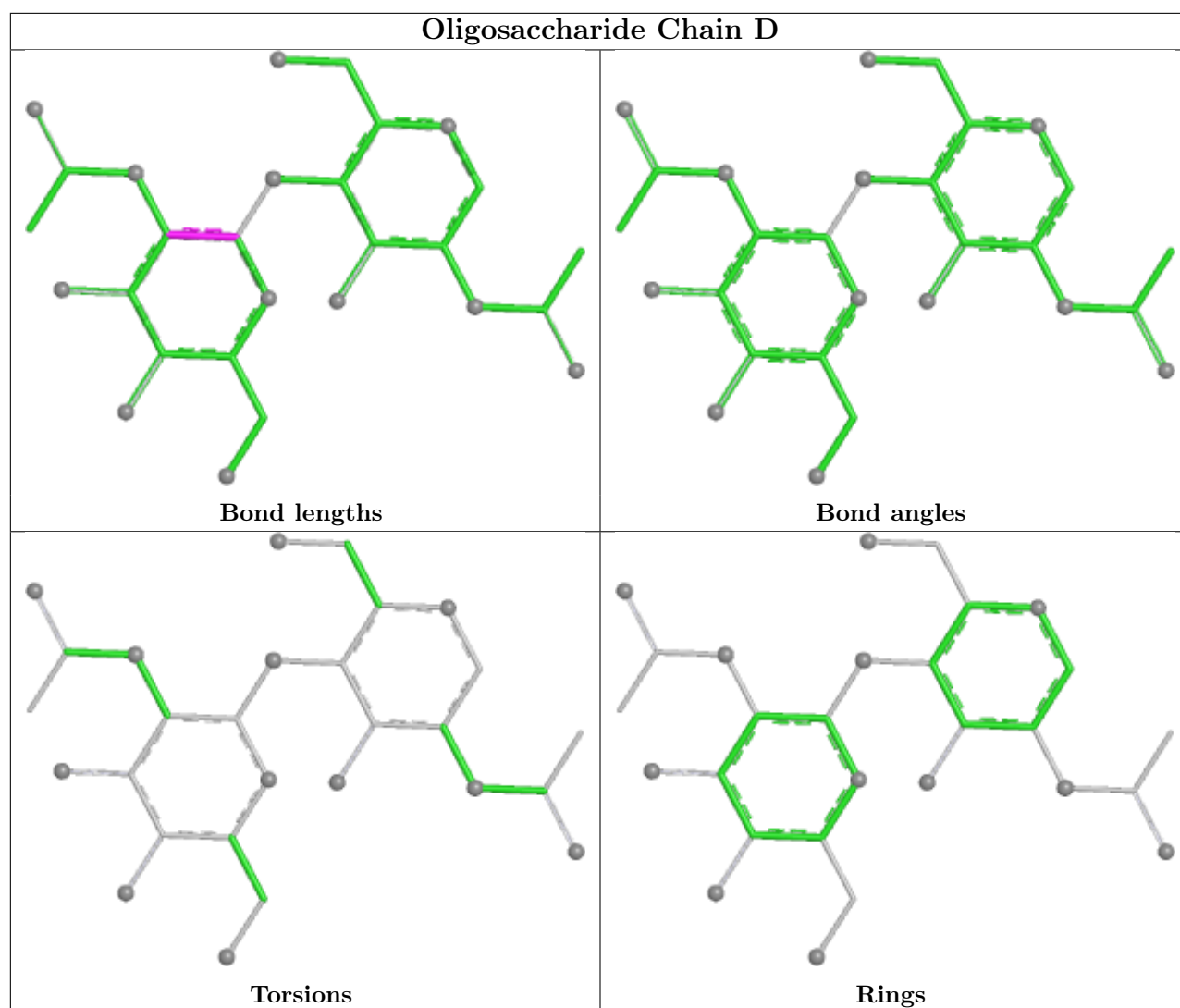
There are no torsion outliers.

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.





4.6 Ligand geometry [i](#)

9 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	GOL	B	1503	-	5,5,5	0.38	0	5,5,5	0.32	0
3	AMI	B	1502	2	15,16,16	0.96	1 (6%)	15,24,24	2.29	3 (20%)
4	GOL	A	1504	-	5,5,5	0.48	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	1503	-	5,5,5	0.50	0	5,5,5	0.14	0
4	GOL	A	1502	-	5,5,5	0.37	0	5,5,5	0.24	0
3	AMI	A	1501	2	15,16,16	1.11	2 (13%)	15,24,24	2.28	5 (33%)
5	SO4	A	1505	-	4,4,4	0.40	0	6,6,6	0.12	0
4	GOL	B	1504	-	5,5,5	0.42	0	5,5,5	0.28	0
4	GOL	B	1506	-	5,5,5	0.50	0	5,5,5	0.14	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	GOL	B	1503	-	-	0/4/4/4	-
3	AMI	B	1502	2	-	0/6/34/34	0/2/2/2
4	GOL	A	1504	-	-	0/4/4/4	-
4	GOL	A	1503	-	-	0/4/4/4	-
4	GOL	A	1502	-	-	0/4/4/4	-
3	AMI	A	1501	2	-	0/6/34/34	0/2/2/2
4	GOL	B	1504	-	-	0/4/4/4	-
4	GOL	B	1506	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1501	AMI	C1-C2	2.34	1.57	1.54
3	B	1502	AMI	C2-N2	-2.14	1.45	1.47
3	A	1501	AMI	O7-C7	2.12	1.37	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1501	AMI	O7-C7-N2	-5.90	114.73	117.78
3	B	1502	AMI	O7-C7-N2	-5.60	114.88	117.78
3	B	1502	AMI	C5-C4-C3	-4.77	97.99	103.86
3	A	1501	AMI	C5-C4-C3	-3.77	99.23	103.86
3	A	1501	AMI	C4-C5-C1	3.26	108.78	102.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

5.1 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	497/499 (99%)	0.11	14 (2%) 55 65	17, 32, 55, 71	8 (1%)
1	B	497/499 (99%)	-0.18	5 (1%) 79 86	18, 28, 47, 57	8 (1%)
All	All	994/998 (99%)	-0.04	19 (1%) 66 75	17, 29, 52, 71	16 (1%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	ALA	6.7
1	A	498	VAL	3.9
1	A	470	TYR	3.4
1	B	445	PRO	3.1
1	B	487	GLY	2.7

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

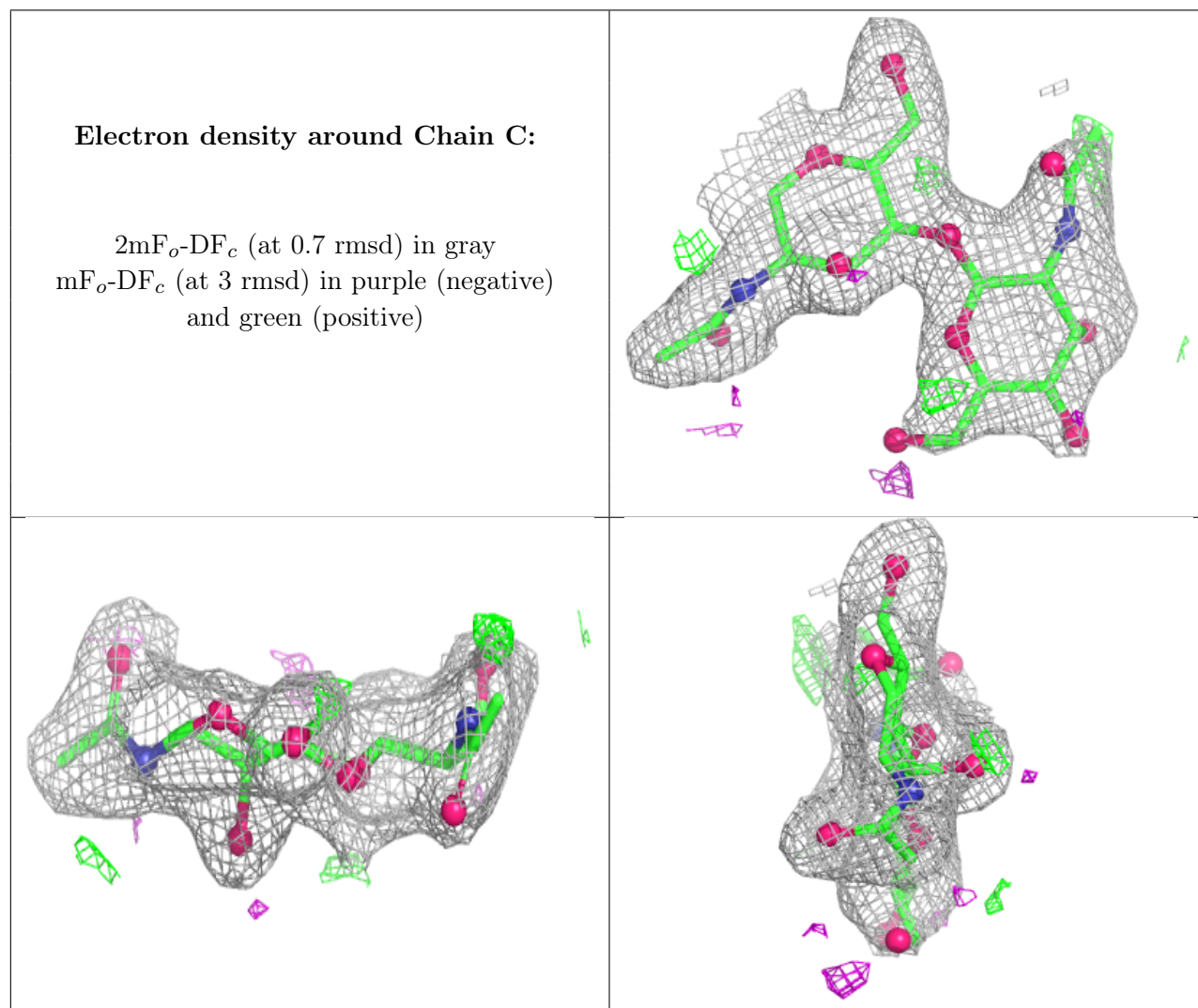
There are no non-standard protein/DNA/RNA residues in this entry.

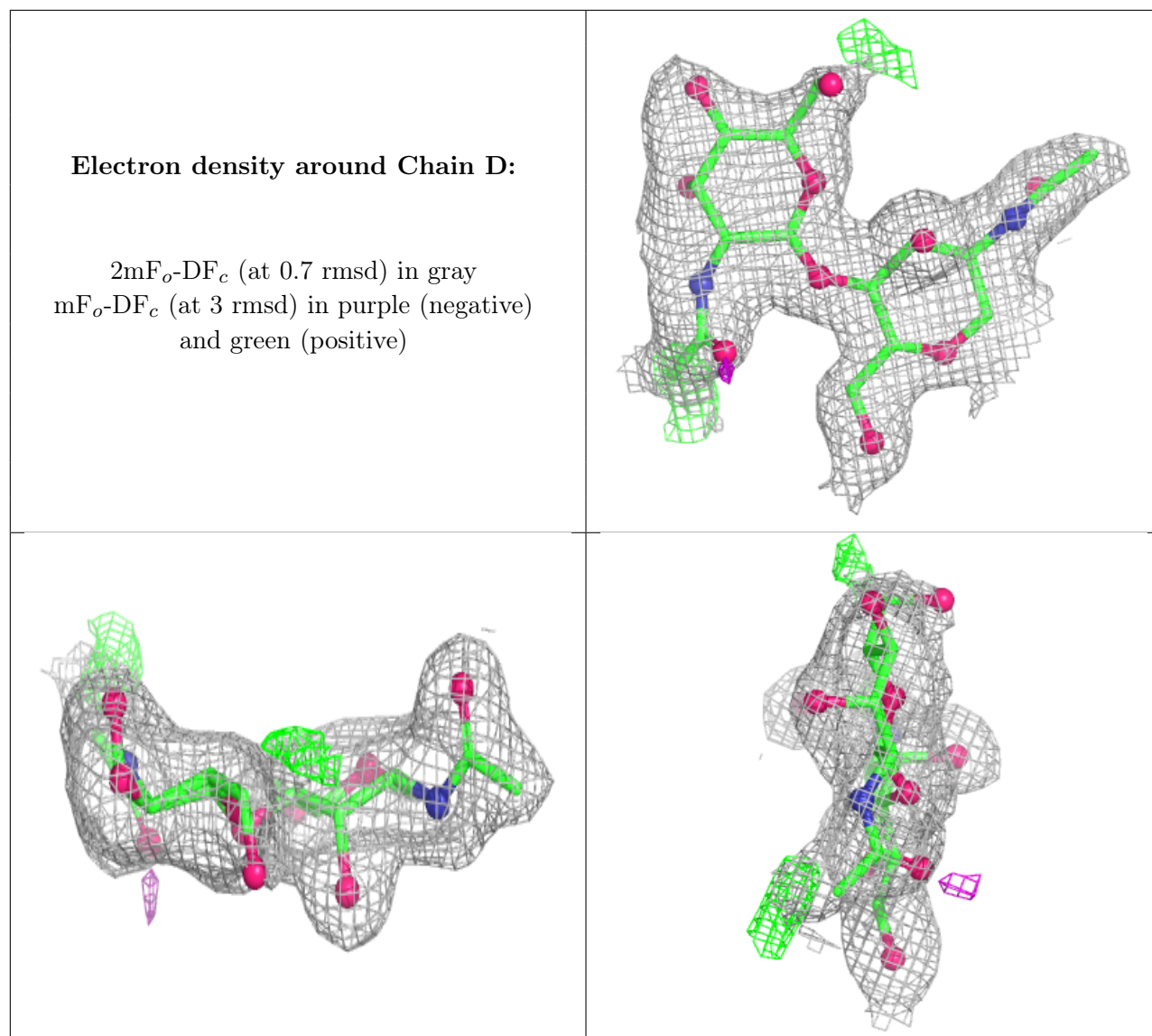
5.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAA	C	2	14/15	0.76	0.15	44,50,54,54	0
2	NAA	D	2	14/15	0.76	0.13	42,48,51,53	0
2	NAA	C	1	14/15	0.91	0.08	26,29,32,39	0
2	NAA	D	1	14/15	0.96	0.06	20,26,28,32	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.





5.4 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, 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	GOL	A	1503	6/6	0.81	0.15	57,60,61,62	0
4	GOL	B	1504	6/6	0.82	0.14	51,53,53,54	0
5	SO4	A	1505	5/5	0.86	0.13	86,87,87,87	0
4	GOL	A	1504	6/6	0.89	0.10	52,54,55,55	0
4	GOL	B	1503	6/6	0.89	0.12	41,44,46,46	0
4	GOL	B	1506	6/6	0.92	0.09	33,36,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	1502	6/6	0.93	0.10	30,38,41,42	0
3	AMI	A	1501	15/15	0.96	0.06	22,24,27,30	0
3	AMI	B	1502	15/15	0.97	0.05	18,21,25,26	0

5.5 Other polymers [i](#)

There are no such residues in this entry.