



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:41 AM UTC

PDB ID : 4XGO / pdb_00004xgo
Title : Crystal structure of leucine-rich repeat domain of APL1B
Authors : Williams, M.; Summers, B.; Baxter, R.H.G.
Deposited on : 2015-01-01
Resolution : 1.74 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

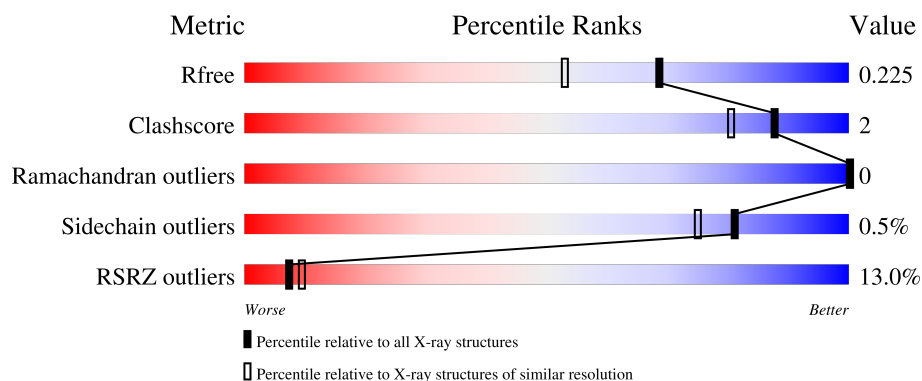
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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 ≥ 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	356	8% 90% 5%
1	B	356	16% 88% 8%
2	C	2	100%
2	D	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6299 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 Anopheles Plasmodium-responsive Leucine-rich repeat protein 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	7	0
			2746	1762	460	511	13			
1	B	328	Total	C	N	O	S	0	9	0
			2654	1698	448	493	15			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	LEU	conflict	UNP F2YBL9
A	176	ALA	VAL	conflict	UNP F2YBL9
A	225	VAL	THR	conflict	UNP F2YBL9
A	236	LYS	ILE	conflict	UNP F2YBL9
A	239	TYR	ILE	conflict	UNP F2YBL9
A	240	GLN	HIS	conflict	UNP F2YBL9
A	244	LYS	THR	conflict	UNP F2YBL9
A	245	MET	ILE	conflict	UNP F2YBL9
A	371	HIS	-	expression tag	UNP F2YBL9
A	372	HIS	-	expression tag	UNP F2YBL9
A	373	HIS	-	expression tag	UNP F2YBL9
A	374	HIS	-	expression tag	UNP F2YBL9
A	375	HIS	-	expression tag	UNP F2YBL9
A	376	HIS	-	expression tag	UNP F2YBL9
B	120	MET	LEU	conflict	UNP F2YBL9
B	176	ALA	VAL	conflict	UNP F2YBL9
B	225	VAL	THR	conflict	UNP F2YBL9
B	236	LYS	ILE	conflict	UNP F2YBL9
B	239	TYR	ILE	conflict	UNP F2YBL9
B	240	GLN	HIS	conflict	UNP F2YBL9
B	244	LYS	THR	conflict	UNP F2YBL9
B	245	MET	ILE	conflict	UNP F2YBL9
B	371	HIS	-	expression tag	UNP F2YBL9
B	372	HIS	-	expression tag	UNP F2YBL9

Continued on next page...

Continued from previous page...

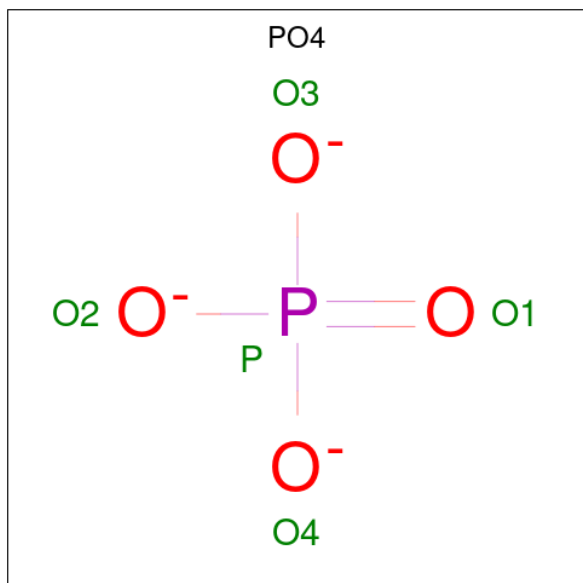
Chain	Residue	Modelled	Actual	Comment	Reference
B	373	HIS	-	expression tag	UNP F2YBL9
B	374	HIS	-	expression tag	UNP F2YBL9
B	375	HIS	-	expression tag	UNP F2YBL9
B	376	HIS	-	expression tag	UNP F2YBL9

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



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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



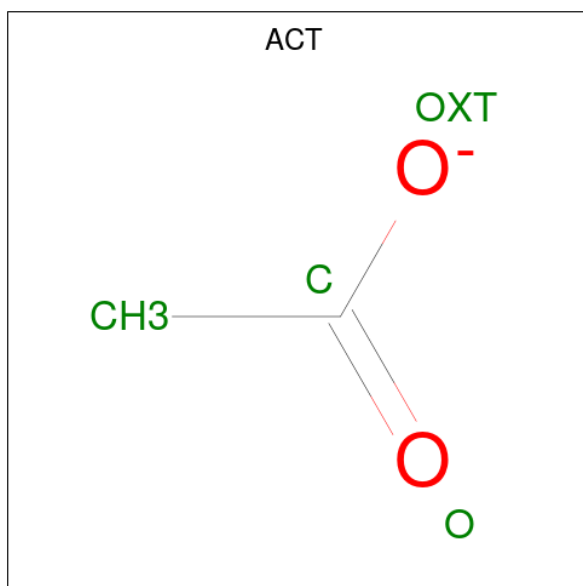
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

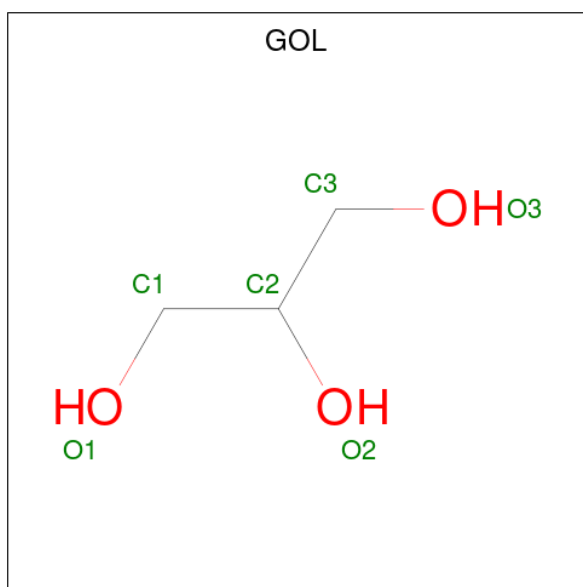
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Na 1 1	0	0

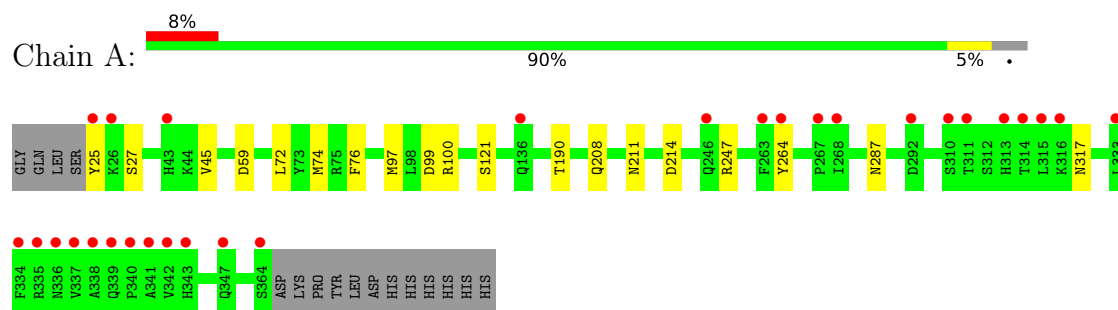
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	432	Total 438	O 438	0	6
8	B	340	Total 343	O 343	0	5

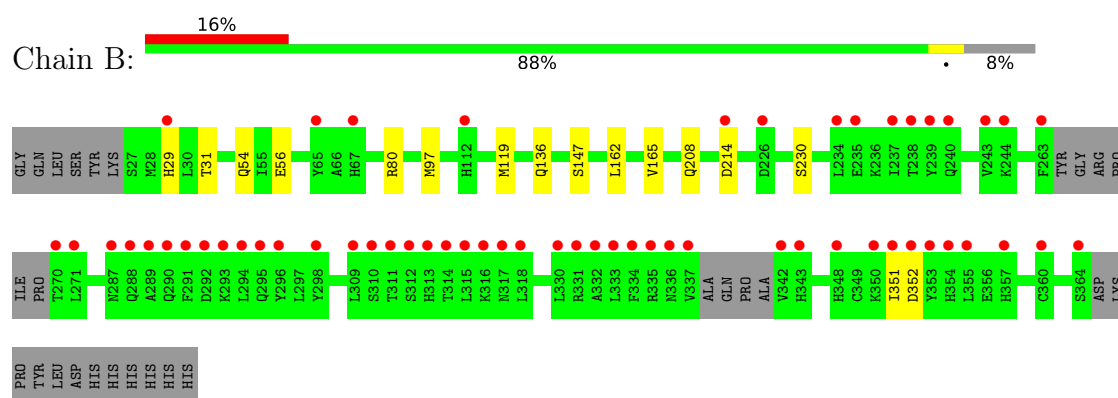
3 Residue-property plots

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.

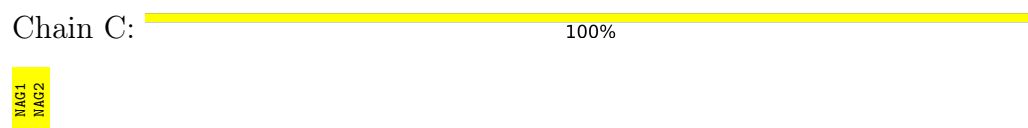
- Molecule 1: Anopheles Plasmodium-responsive Leucine-rich repeat protein 1B



- Molecule 1: Anopheles Plasmodium-responsive Leucine-rich repeat protein 1B



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.42Å 74.96Å 214.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.18 – 1.74 107.18 – 1.74	Depositor EDS
% Data completeness (in resolution range)	89.9 (107.18-1.74) 89.9 (107.18-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.187 , 0.220 0.193 , 0.225	Depositor DCC
R_{free} test set	4796 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6299	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: PO4, NAG, CL, ACT, NA, GOL

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	0.58	0/2830	0.72	0/3861
1	B	0.51	0/2728	0.68	0/3719
All	All	0.55	0/5558	0.70	0/7580

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	2746	0	2695	13	0
1	B	2654	0	2583	11	0
2	C	28	0	25	0	0
2	D	28	0	25	1	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	1	0
5	A	36	0	48	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	438	0	0	2	0
8	B	343	0	0	0	0
All	All	6299	0	5382	22	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 (22) 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:97[B]:MET:HE3	1:B:119[B]:MET:HE1	1.66	0.78
1:A:190:THR:HA	1:A:211:ASN:HD22	1.66	0.60
1:B:214:ASP:HA	4:B:1003:ACT:H3	1.83	0.59
1:A:59:ASP:OD1	1:B:29:HIS:NE2	2.40	0.54
1:B:162:LEU:HD13	1:B:165:VAL:HG21	1.91	0.53
1:A:72:LEU:CD2	1:A:74:MET:HE2	2.39	0.52
1:A:25:TYR:CD2	1:A:97[A]:MET:HE1	2.47	0.48
1:B:97[B]:MET:CE	1:B:119[B]:MET:HE1	2.38	0.48
1:A:72:LEU:HD21	1:A:74:MET:HE2	1.97	0.47
1:B:147[B]:SER:OG	2:D:1:NAG:H62	2.15	0.47
1:A:59:ASP:OD2	1:B:31:THR:HG22	2.16	0.45
1:A:27:SER:HA	1:B:54:GLN:HB3	2.00	0.42
1:B:208:GLN:HA	1:B:230:SER:O	2.20	0.42
1:A:264:TYR:O	1:A:287:ASN:ND2	2.54	0.41
1:A:99:ASP:OD1	1:A:121:SER:OG	2.32	0.41
1:B:351:ILE:O	1:B:352:ASP:CB	2.68	0.41
1:A:45:VAL:O	1:A:45:VAL:HG12	2.21	0.41
1:A:76:PHE:CE1	1:A:100:ARG:HG3	2.56	0.41
1:B:56:GLU:OE2	1:B:80:ARG:NE	2.54	0.41
1:A:317:ASN:ND2	8:A:1517:HOH:O	2.32	0.40
5:A:1010:GOL:O1	8:A:1530:HOH:O	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	345/356 (97%)	319 (92%)	26 (8%)	0	100	100
1	B	331/356 (93%)	306 (92%)	25 (8%)	0	100	100
All	All	676/712 (95%)	625 (92%)	51 (8%)	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	311/331 (94%)	309 (99%)	2 (1%)	78	71
1	B	298/331 (90%)	297 (100%)	1 (0%)	86	82
All	All	609/662 (92%)	606 (100%)	3 (0%)	81	75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ASP
1	A	247	ARG
1	B	136	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	88	GLN
1	A	287	ASN
1	A	347	GLN
1	B	124	ASN
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 ⓘ

4 non-standard protein/DNA/RNA residues 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	NAG	D	1	2,1	14,14,15	0.66	0	17,19,21	0.77	0
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	0.83	1 (5%)
2	NAG	C	1	2,1	14,14,15	0.65	0	17,19,21	1.16	1 (5%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	1.10	1 (5%)

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	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-2.69	107.13	111.29
2	D	2	NAG	C1-O5-C5	2.24	115.19	112.19
2	C	2	NAG	C3-C4-C5	2.23	114.27	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0

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	NAG	C	1	2,1	14,14,15	0.65	0	17,19,21	1.16	1 (5%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	1.10	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.66	0	17,19,21	0.77	0
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	0.83	1 (5%)

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	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-2.69	107.13	111.29
2	D	2	NAG	C1-O5-C5	2.24	115.19	112.19
2	C	2	NAG	C3-C4-C5	2.23	114.27	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

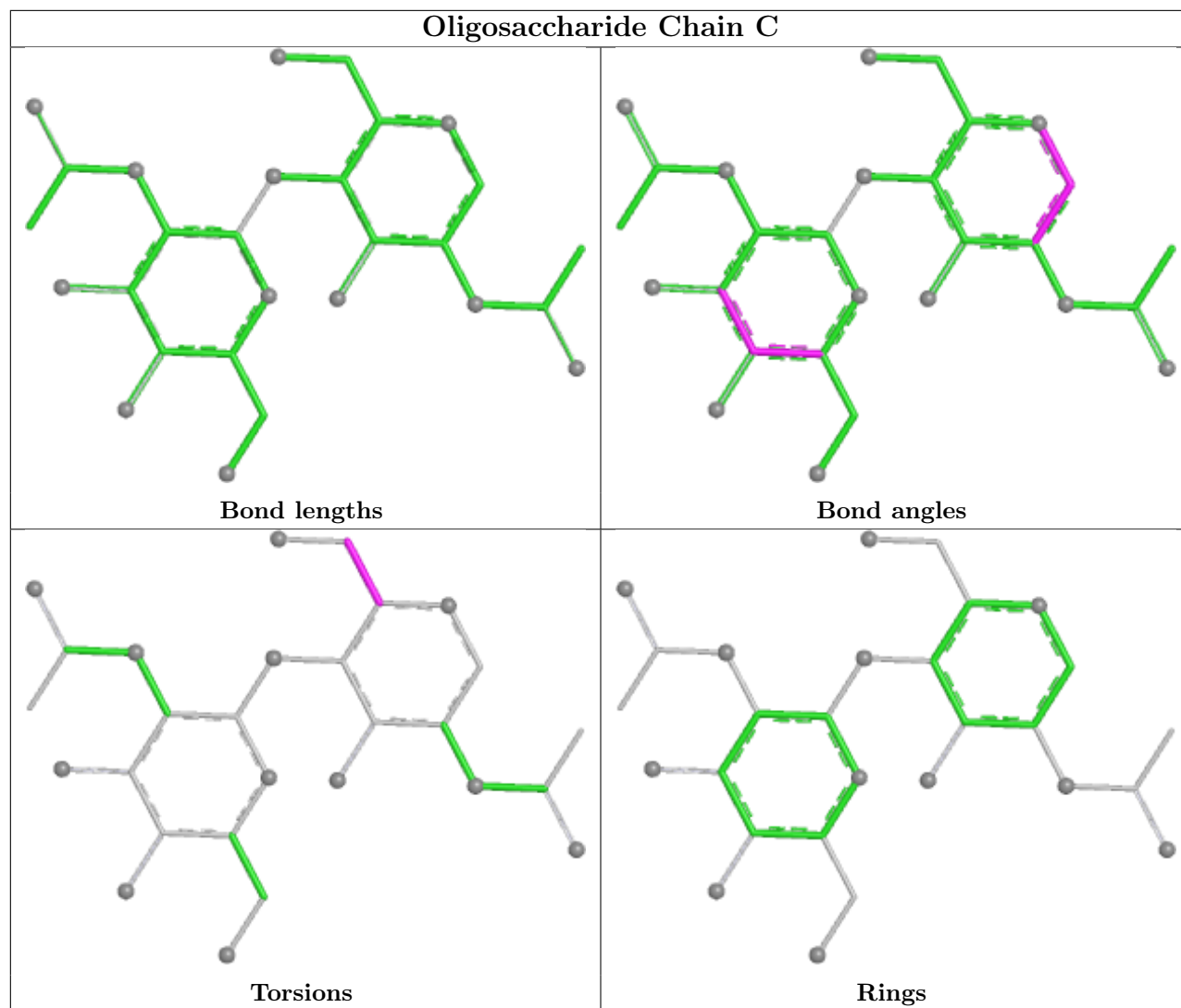
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

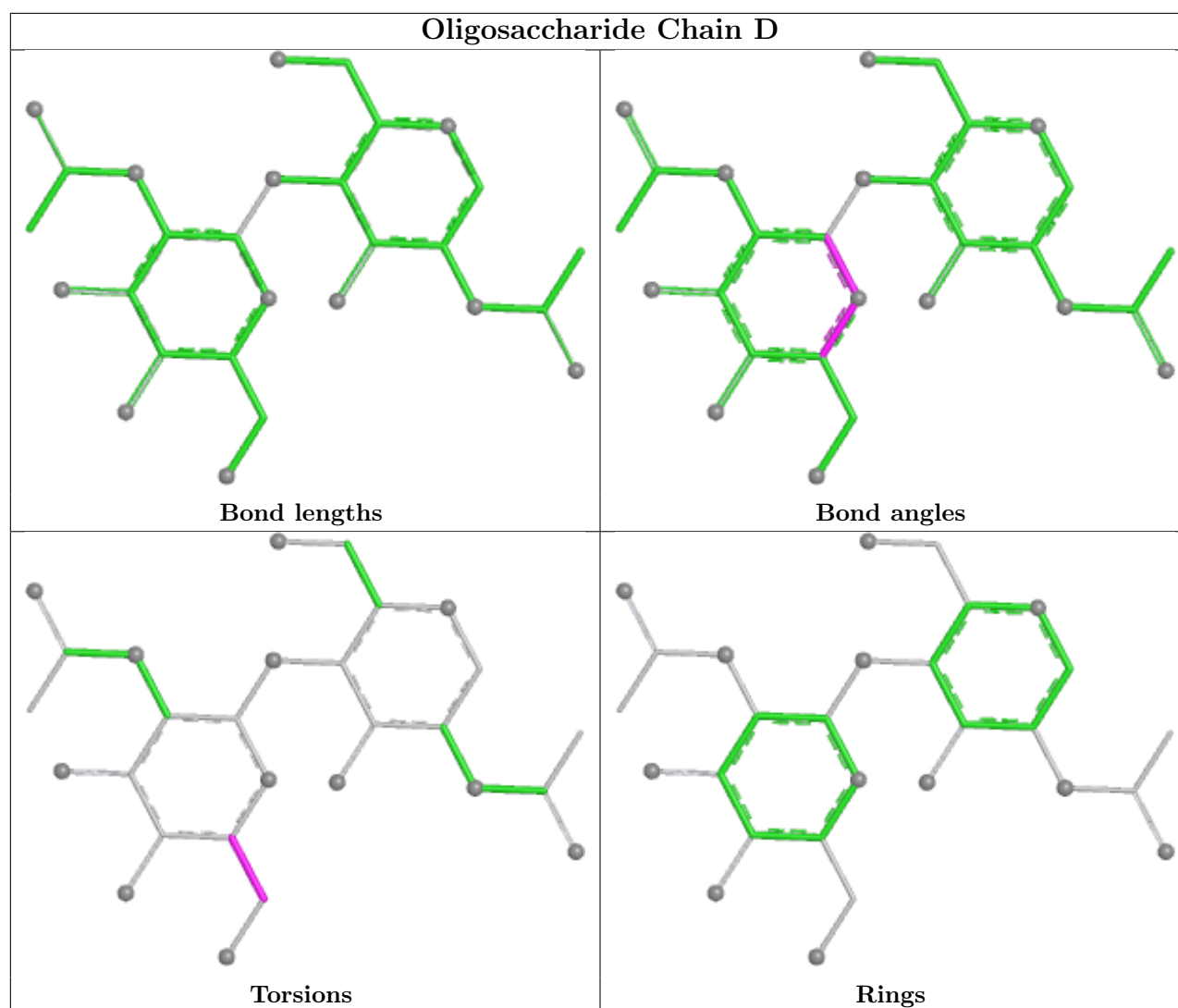
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	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 14 ligands modelled in this entry, 3 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	$\# Z > 2$
4	ACT	B	1003	-	3,3,3	0.82	0	3,3,3	0.47	0
3	PO4	B	1004	-	4,4,4	0.89	0	6,6,6	0.50	0
4	ACT	A	1004	-	3,3,3	0.73	0	3,3,3	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	B	1005	-	4,4,4	0.90	0	6,6,6	0.43	0
5	GOL	A	1008	-	5,5,5	0.35	0	5,5,5	0.33	0
5	GOL	A	1010	-	5,5,5	0.32	0	5,5,5	0.27	0
5	GOL	A	1006	-	5,5,5	0.50	0	5,5,5	0.34	0
5	GOL	A	1007	-	5,5,5	0.29	0	5,5,5	0.42	0
3	PO4	A	1003	-	4,4,4	1.00	0	6,6,6	0.74	0
5	GOL	A	1009	-	5,5,5	0.39	0	5,5,5	0.18	0
5	GOL	A	1005	-	5,5,5	0.50	0	5,5,5	0.23	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
5	GOL	A	1008	-	-	4/4/4/4	-
5	GOL	A	1010	-	-	2/4/4/4	-
5	GOL	A	1006	-	-	2/4/4/4	-
5	GOL	A	1007	-	-	2/4/4/4	-
5	GOL	A	1009	-	-	4/4/4/4	-
5	GOL	A	1005	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1006	GOL	O1-C1-C2-O2
5	A	1006	GOL	O1-C1-C2-C3
5	A	1007	GOL	C1-C2-C3-O3
5	A	1008	GOL	O1-C1-C2-C3
5	A	1009	GOL	O1-C1-C2-C3
5	A	1009	GOL	C1-C2-C3-O3
5	A	1009	GOL	O2-C2-C3-O3
5	A	1010	GOL	O1-C1-C2-C3
5	A	1010	GOL	O1-C1-C2-O2
5	A	1008	GOL	C1-C2-C3-O3
5	A	1008	GOL	O2-C2-C3-O3
5	A	1009	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1008	GOL	O1-C1-C2-O2
5	A	1007	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1003	ACT	1	0
5	A	1010	GOL	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	340/356 (95%)	0.29	29 (8%) 16 21	6, 20, 41, 57	7 (2%)
1	B	328/356 (92%)	0.87	58 (17%) 4 4	8, 27, 70, 93	9 (2%)
All	All	668/712 (93%)	0.57	87 (13%) 7 9	6, 23, 60, 93	16 (2%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	342	VAL	7.1
1	B	337	VAL	6.9
1	B	315	LEU	6.1
1	B	270	THR	5.7
1	A	25	TYR	5.6
1	B	334	PHE	5.5
1	B	311	THR	5.5
1	B	314	THR	5.2
1	B	343	HIS	4.6
1	A	338	ALA	4.6
1	B	263	PHE	4.6
1	B	291	PHE	4.6
1	B	287	ASN	4.4
1	A	336	ASN	4.2
1	B	289	ALA	4.2
1	B	351	ILE	4.1
1	B	294	LEU	3.9
1	A	334	PHE	3.8
1	A	337	VAL	3.8
1	B	290	GLN	3.7
1	B	312	SER	3.7
1	B	318	LEU	3.6
1	A	342	VAL	3.6
1	B	333	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	311	THR	3.5
1	B	243	VAL	3.5
1	B	288	GLN	3.5
1	B	357	HIS	3.5
1	B	239	TYR	3.4
1	A	313	HIS	3.4
1	A	341	ALA	3.4
1	B	335	ARG	3.4
1	B	355	LEU	3.3
1	B	336	ASN	3.3
1	B	316	LYS	3.3
1	B	332	ALA	3.2
1	B	348	HIS	3.1
1	B	271	LEU	3.1
1	B	240	GLN	3.0
1	B	238	THR	3.0
1	B	310	SER	3.0
1	B	364	SER	3.0
1	B	313	HIS	3.0
1	B	237	ILE	3.0
1	A	335	ARG	2.9
1	B	350	LYS	2.9
1	A	314	THR	2.8
1	B	293	LYS	2.8
1	B	353	TYR	2.8
1	A	267	PRO	2.8
1	A	340	PRO	2.8
1	B	360	CYS	2.8
1	B	317	ASN	2.8
1	A	364	SER	2.8
1	B	295	GLN	2.8
1	A	264	TYR	2.7
1	B	214	ASP	2.7
1	A	43	HIS	2.6
1	A	292	ASP	2.6
1	A	343	HIS	2.6
1	B	354	HIS	2.6
1	A	136	GLN	2.5
1	B	67	HIS	2.5
1	A	26	LYS	2.5
1	B	352	ASP	2.5
1	B	112[A]	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	315	LEU	2.5
1	B	296	TYR	2.5
1	B	292	ASP	2.4
1	B	226	ASP	2.4
1	B	309	LEU	2.4
1	A	310	SER	2.4
1	B	235	GLU	2.4
1	B	244	LYS	2.4
1	B	29	HIS	2.3
1	A	263	PHE	2.3
1	B	65	TYR	2.3
1	B	298	TYR	2.3
1	B	234	LEU	2.2
1	A	246	GLN	2.1
1	A	268	ILE	2.1
1	B	330	LEU	2.1
1	A	339	GLN	2.1
1	A	347	GLN	2.0
1	B	331	ARG	2.0
1	A	333	LEU	2.0
1	A	316	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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.

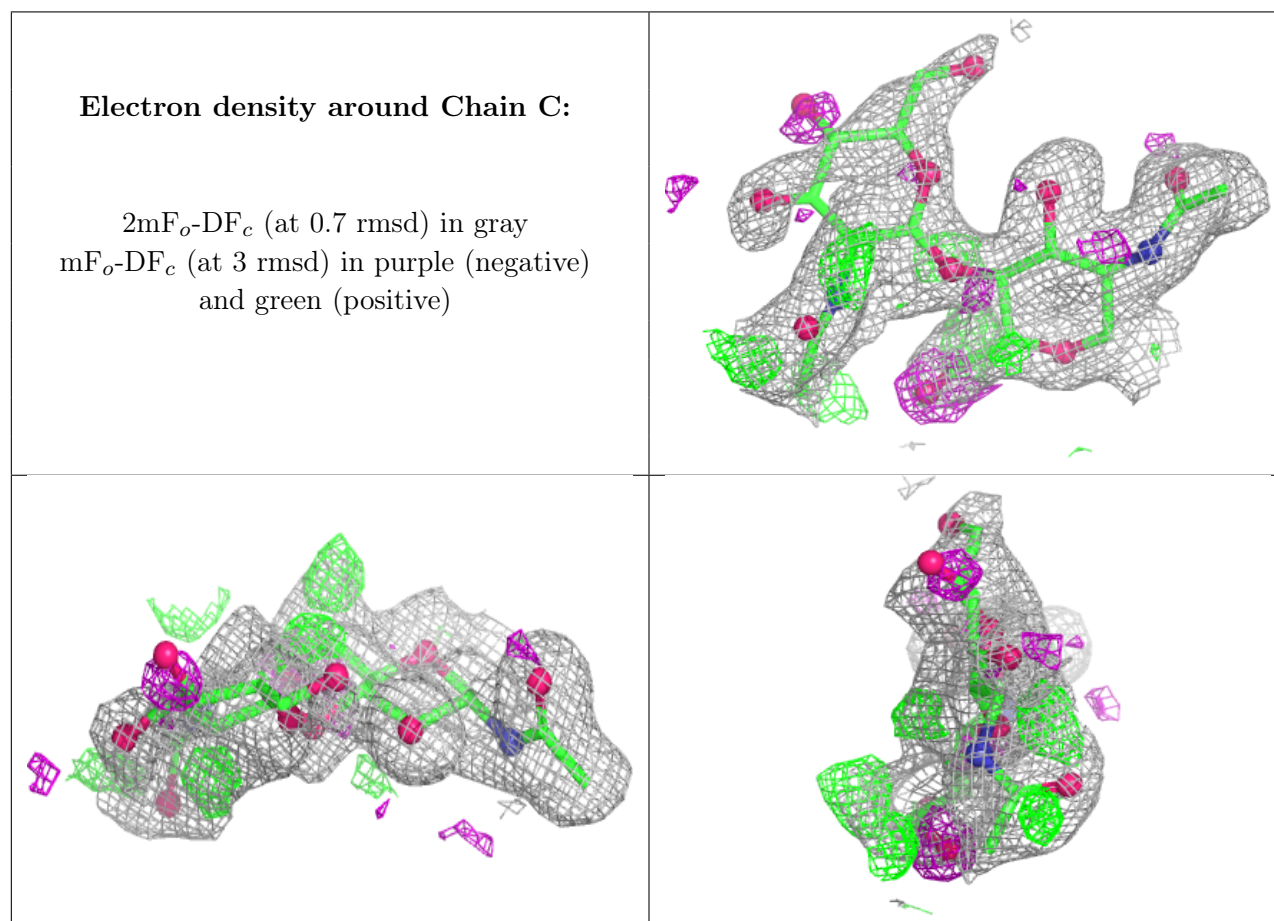
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.75	0.17	42,49,57,58	0
2	NAG	D	2	14/15	0.80	0.14	41,47,51,55	0
2	NAG	C	1	14/15	0.90	0.11	17,21,33,37	0
2	NAG	D	1	14/15	0.94	0.08	19,25,28,32	0

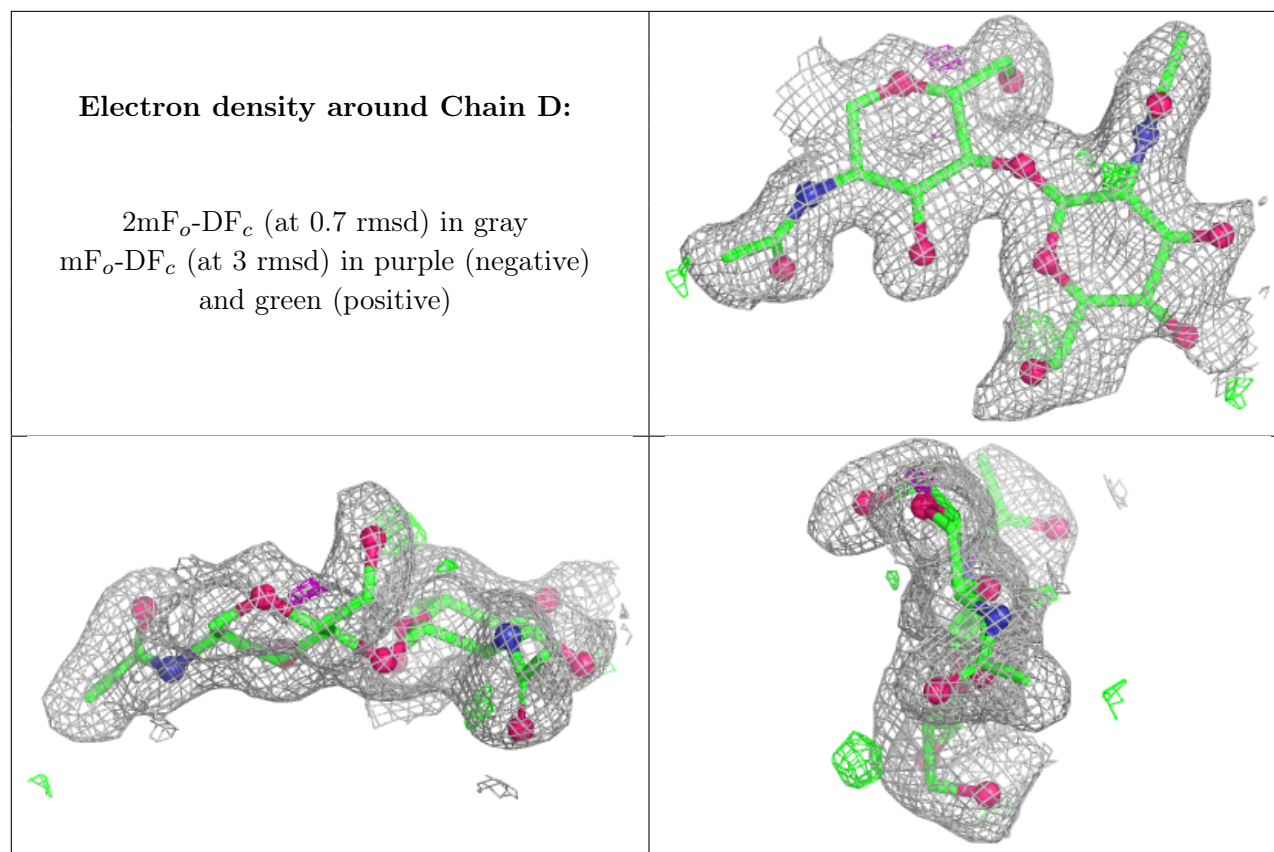
6.3 Carbohydrates [i](#)

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	NAG	C	2	14/15	0.75	0.17	42,49,57,58	0
2	NAG	D	2	14/15	0.80	0.14	41,47,51,55	0
2	NAG	C	1	14/15	0.90	0.11	17,21,33,37	0
2	NAG	D	1	14/15	0.94	0.08	19,25,28,32	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.





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, 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
5	GOL	A	1008	6/6	0.61	0.25	53,55,56,56	0
4	ACT	B	1003	4/4	0.70	0.21	41,41,41,44	0
4	ACT	A	1004	4/4	0.77	0.23	42,44,45,46	0
5	GOL	A	1007	6/6	0.79	0.16	35,42,45,46	0
5	GOL	A	1009	6/6	0.79	0.21	50,50,51,52	0
7	NA	B	1007	1/1	0.79	0.16	27,27,27,27	0
3	PO4	B	1004	5/5	0.81	0.14	69,71,73,75	0
3	PO4	B	1005	5/5	0.83	0.13	57,59,62,63	0
5	GOL	A	1006	6/6	0.84	0.18	38,41,42,44	0
5	GOL	A	1010	6/6	0.85	0.14	36,39,43,47	0
6	CL	A	1011	1/1	0.88	0.14	54,54,54,54	0
5	GOL	A	1005	6/6	0.89	0.13	30,34,34,34	0
6	CL	B	1006	1/1	0.95	0.20	64,64,64,64	0
3	PO4	A	1003	5/5	0.97	0.07	23,23,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.