



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:41 AM UTC

PDB ID : 4HG6 / pdb_00004hg6
Title : Structure of a cellulose synthase - cellulose translocation intermediate
Authors : Zimmer, J.
Deposited on : 2012-10-07
Resolution : 3.25 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 : 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

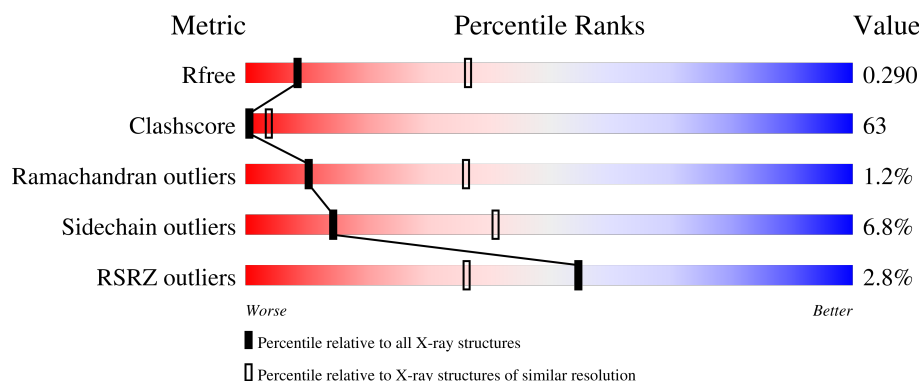
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	802	3% 37% 49% 7% 7%
2	B	707	2% 40% 46% 6% 7%
3	C	18	11% 28% 61%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BGC	C	5	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11029 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 Cellulose Synthase Subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			5893	3822	1029	1011	31			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	789	HIS	-	expression tag	UNP Q3J125
A	790	HIS	-	expression tag	UNP Q3J125
A	791	HIS	-	expression tag	UNP Q3J125
A	792	HIS	-	expression tag	UNP Q3J125
A	793	HIS	-	expression tag	UNP Q3J125
A	794	HIS	-	expression tag	UNP Q3J125
A	795	LYS	-	expression tag	UNP Q3J125
A	796	LEU	-	expression tag	UNP Q3J125
A	797	HIS	-	expression tag	UNP Q3J125
A	798	HIS	-	expression tag	UNP Q3J125
A	799	HIS	-	expression tag	UNP Q3J125
A	800	HIS	-	expression tag	UNP Q3J125
A	801	HIS	-	expression tag	UNP Q3J125
A	802	HIS	-	expression tag	UNP Q3J125

- Molecule 2 is a protein called Cellulose Synthase Subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	655	Total	C	N	O	S	0	0	0
			4887	3100	864	907	16			

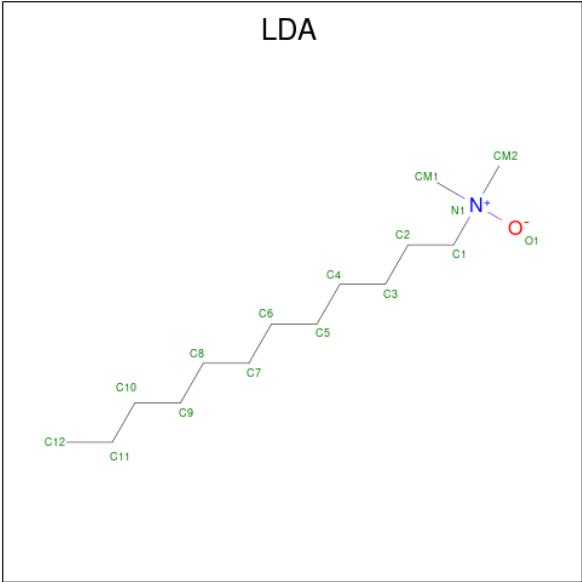
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	MET	-	expression tag	UNP Q3J126
B	20	GLY	-	expression tag	UNP Q3J126

-

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $\text{C}_9\text{H}_{14}\text{N}_2\text{O}_{12}\text{P}_2$).



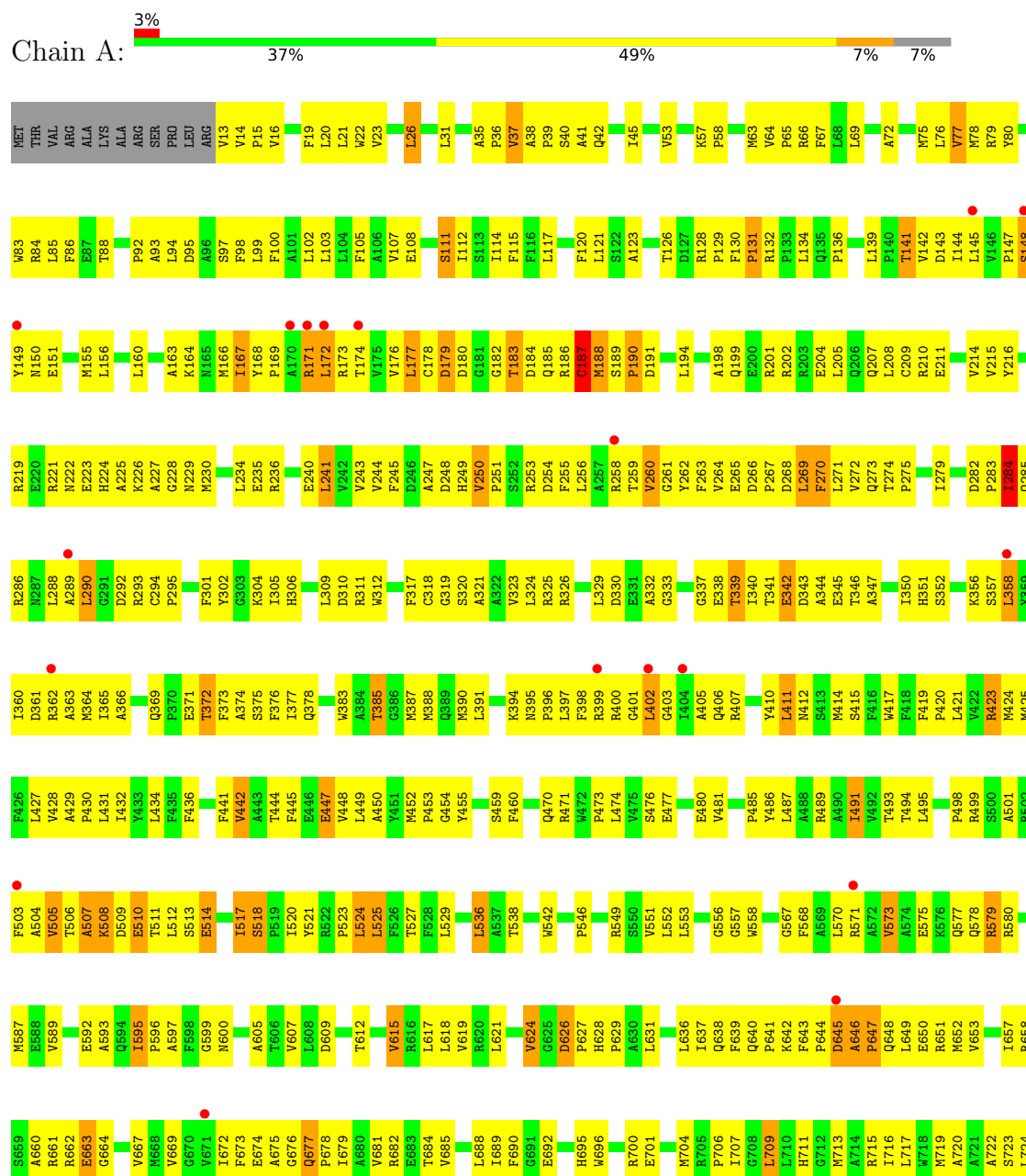


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	7	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		

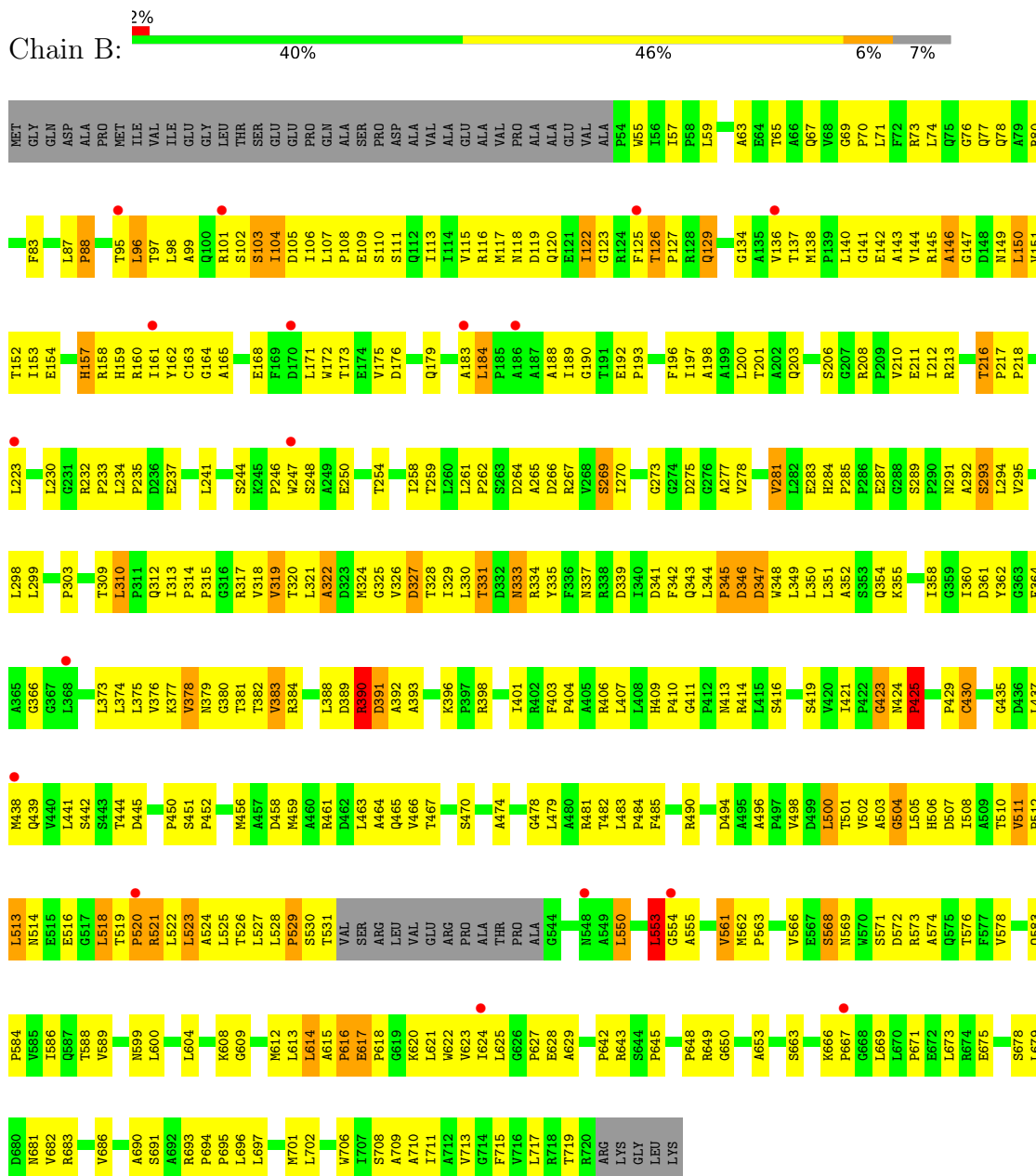
3 Residue-property plots

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: Cellulose Synthase Subunit A



- Molecule 2: Cellulose Synthase Subunit B



● Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)
-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-gluc
opyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1
-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-gl
ucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-
(1-4)-beta-D-glucopyranose

Chain C: 11% 28% 61%

B6C1	B6C2	B6C3	B6C4	B6C5	B6C6	B6C7	B6C8	B6C9	B6C10	B6C11	B6C12	B6C13	B6C14	B6C15	B6C16	B6C17	B6C18
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.12Å 103.12Å 468.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 3.25 34.81 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.81-3.25) 99.8 (34.81-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.213 , 0.282 0.229 , 0.290	Depositor DCC
R_{free} test set	2057 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	117.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 101.3	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	0.93	EDS
Total number of atoms	11029	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BGC, UDP

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	0.56	1/6044 (0.0%)	1.04	29/8217 (0.4%)
2	B	0.54	1/5006 (0.0%)	0.99	22/6865 (0.3%)
All	All	0.55	2/11050 (0.0%)	1.02	51/15082 (0.3%)

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
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	PRO	N-CD	-10.17	1.33	1.47
1	A	284	ILE	CA-CB	-5.24	1.48	1.54

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	648	GLN	N-CA-C	-10.96	99.43	112.92
1	A	179	ASP	N-CA-C	-9.62	101.23	113.16
2	B	425	PRO	N-CA-C	-9.34	99.30	110.70
1	A	645	ASP	N-CA-C	-9.28	99.61	113.72
1	A	171	ARG	N-CA-C	-9.16	102.12	113.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	390	ARG	Sidechain

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	5893	0	5996	768	0
2	B	4887	0	4966	622	0
3	C	199	0	165	28	0
4	A	25	0	11	1	0
5	A	25	0	45	7	0
All	All	11029	0	11183	1389	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 63.

The worst 5 of 1389 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)
2:B:330:LEU:CD2	2:B:439:GLN:HG3	1.33	1.58
2:B:377:LYS:CG	2:B:382:THR:HG22	1.32	1.56
1:A:643:PHE:HB3	1:A:646:ALA:CB	1.42	1.49
2:B:118:ASN:CG	2:B:144:VAL:HG11	1.42	1.42
2:B:107:LEU:CD1	2:B:160:ARG:HA	1.47	1.41

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	745/802 (93%)	674 (90%)	64 (9%)	7 (1%)	14	42
2	B	651/707 (92%)	574 (88%)	67 (10%)	10 (2%)	8	32
All	All	1396/1509 (92%)	1248 (89%)	131 (9%)	17 (1%)	10	36

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	A	514	GLU
1	A	647	PRO
2	B	146	ALA
2	B	529	PRO

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	614/661 (93%)	573 (93%)	41 (7%)	15	41
2	B	520/559 (93%)	484 (93%)	36 (7%)	14	41
All	All	1134/1220 (93%)	1057 (93%)	77 (7%)	14	41

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	374	LEU
2	B	568	SER
2	B	383	VAL
2	B	513	LEU
2	B	614	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	695	HIS

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Mol	Chain	Res	Type
1	A	711	HIS
2	B	579	GLN
2	B	343	GLN
2	B	413	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 ⓘ

18 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	$\# Z > 2$
3	BGC	C	1	3	12,12,12	0.49	0	17,17,17	1.86	3 (17%)
3	BGC	C	10	3	11,11,12	0.64	0	15,15,17	1.06	1 (6%)
3	BGC	C	11	3	11,11,12	0.85	0	15,15,17	1.34	2 (13%)
3	BGC	C	12	3	11,11,12	0.99	1 (9%)	15,15,17	1.85	3 (20%)
3	BGC	C	13	3	11,11,12	0.75	0	15,15,17	1.65	4 (26%)
3	BGC	C	14	3	11,11,12	0.62	0	15,15,17	2.77	6 (40%)
3	BGC	C	15	3	11,11,12	0.58	0	15,15,17	1.37	2 (13%)
3	BGC	C	16	3	11,11,12	0.62	0	15,15,17	1.38	3 (20%)
3	BGC	C	17	3	11,11,12	0.71	0	15,15,17	2.62	5 (33%)
3	BGC	C	18	3	11,11,12	0.70	0	15,15,17	1.94	3 (20%)
3	BGC	C	2	3	11,11,12	0.66	0	15,15,17	2.16	3 (20%)
3	BGC	C	3	3	11,11,12	0.59	0	15,15,17	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	C	4	3	11,11,12	0.62	0	15,15,17	0.80	0
3	BGC	C	5	3	11,11,12	0.64	0	15,15,17	0.81	0
3	BGC	C	6	3	11,11,12	0.81	0	15,15,17	1.92	5 (33%)
3	BGC	C	7	3	11,11,12	0.74	0	15,15,17	1.81	3 (20%)
3	BGC	C	8	3	11,11,12	0.61	0	15,15,17	1.15	2 (13%)
3	BGC	C	9	3	11,11,12	0.55	0	15,15,17	1.55	3 (20%)

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
3	BGC	C	1	3	-	2/2/22/22	0/1/1/1
3	BGC	C	10	3	-	2/2/19/22	0/1/1/1
3	BGC	C	11	3	-	0/2/19/22	0/1/1/1
3	BGC	C	12	3	-	1/2/19/22	0/1/1/1
3	BGC	C	13	3	-	1/2/19/22	0/1/1/1
3	BGC	C	14	3	-	0/2/19/22	0/1/1/1
3	BGC	C	15	3	-	0/2/19/22	0/1/1/1
3	BGC	C	16	3	-	1/2/19/22	0/1/1/1
3	BGC	C	17	3	-	1/2/19/22	0/1/1/1
3	BGC	C	18	3	-	0/2/19/22	0/1/1/1
3	BGC	C	2	3	-	2/2/19/22	0/1/1/1
3	BGC	C	3	3	-	1/2/19/22	0/1/1/1
3	BGC	C	4	3	-	2/2/19/22	0/1/1/1
3	BGC	C	5	3	-	0/2/19/22	0/1/1/1
3	BGC	C	6	3	-	0/2/19/22	0/1/1/1
3	BGC	C	7	3	-	2/2/19/22	0/1/1/1
3	BGC	C	8	3	-	2/2/19/22	0/1/1/1
3	BGC	C	9	3	-	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)
3	C	12	BGC	O5-C5	-2.02	1.39	1.43

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	17	BGC	C1-O5-C5	8.20	123.18	112.19
3	C	14	BGC	C1-O5-C5	6.97	121.52	112.19
3	C	2	BGC	C1-O5-C5	6.72	121.19	112.19
3	C	18	BGC	C1-C2-C3	5.67	117.90	109.64
3	C	1	BGC	O5-C5-C4	5.40	119.42	109.70

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

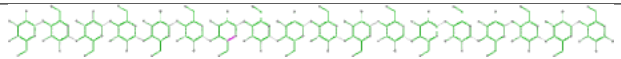
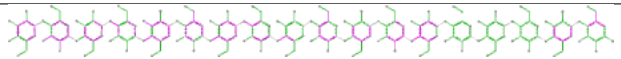
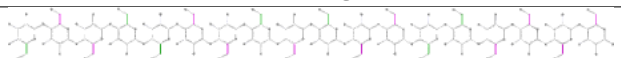
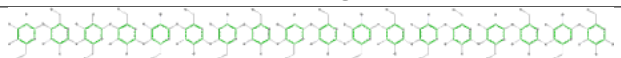
Mol	Chain	Res	Type	Atoms
3	C	7	BGC	O5-C5-C6-O6
3	C	10	BGC	O5-C5-C6-O6
3	C	7	BGC	C4-C5-C6-O6
3	C	10	BGC	C4-C5-C6-O6
3	C	2	BGC	C4-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	17	BGC	4	0
3	C	6	BGC	1	0
3	C	16	BGC	1	0
3	C	12	BGC	4	0
3	C	7	BGC	1	0
3	C	8	BGC	2	0
3	C	5	BGC	6	0
3	C	11	BGC	4	0
3	C	9	BGC	3	0
3	C	10	BGC	3	0
3	C	13	BGC	3	0
3	C	18	BGC	3	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.

Oligosaccharide Chain C	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.6 Ligand geometry

3 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
5	LDA	A	920	-	6,8,15	3.49	2 (33%)	7,10,17	0.43	0
5	LDA	A	921	-	13,15,15	2.14	2 (15%)	14,17,17	0.46	0
4	UDP	A	919	-	25,26,26	0.97	1 (4%)	38,40,40	1.58	5 (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
5	LDA	A	920	-	-	3/6/6/13	-
5	LDA	A	921	-	-	4/13/13/13	-
4	UDP	A	919	-	-	10/16/32/32	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	920	LDA	O1-N1	-6.79	1.25	1.42
5	A	921	LDA	O1-N1	-6.30	1.26	1.42
5	A	920	LDA	C1-N1	-5.15	1.46	1.51
5	A	921	LDA	C1-N1	-4.30	1.47	1.51
4	A	919	UDP	C5-C4	-2.09	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	919	UDP	C4-N3-C2	-5.58	119.69	126.61
4	A	919	UDP	N3-C2-N1	4.19	120.35	114.89
4	A	919	UDP	C5-C4-N3	3.37	119.52	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	919	UDP	O4-C4-C5	-2.68	120.54	125.16
4	A	919	UDP	O2-C2-N1	-2.67	119.33	122.80

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

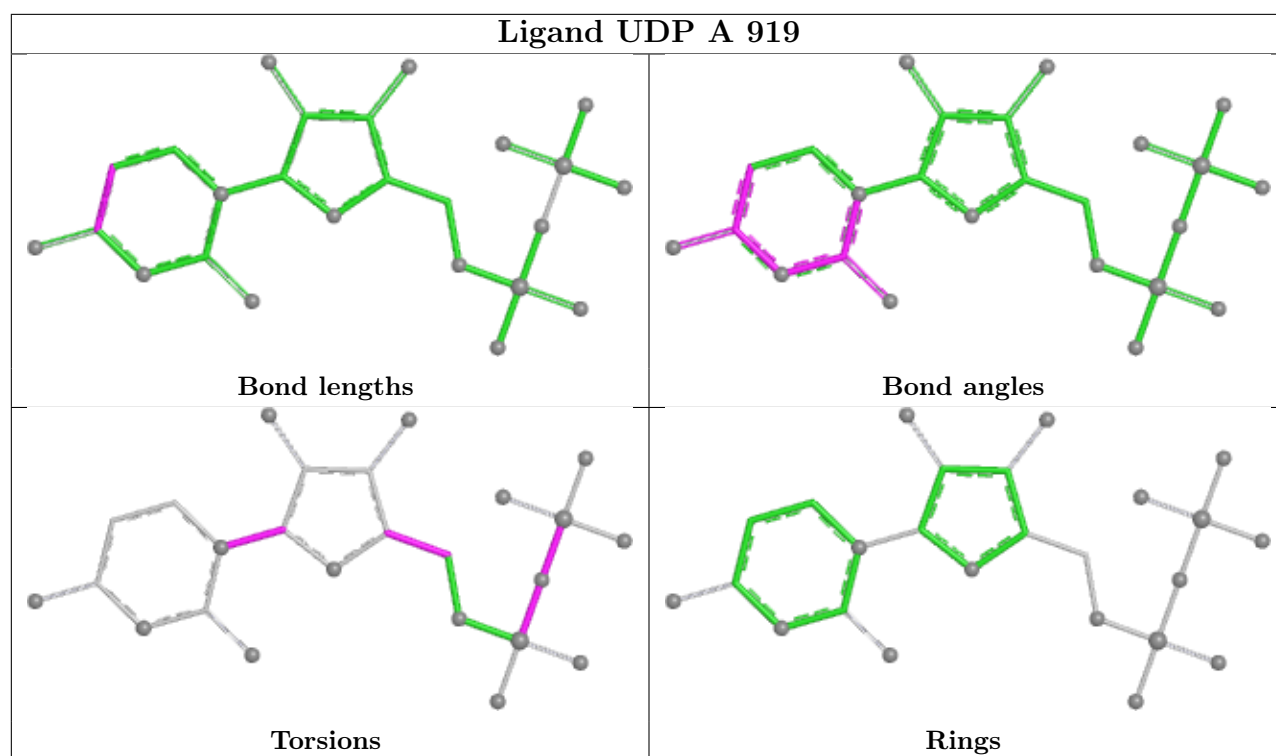
Mol	Chain	Res	Type	Atoms
5	A	920	LDA	C2-C1-N1-O1
5	A	920	LDA	C2-C1-N1-CM1
5	A	920	LDA	C2-C1-N1-CM2
4	A	919	UDP	O4'-C4'-C5'-O5'
5	A	921	LDA	C11-C10-C9-C8

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	920	LDA	5	0
5	A	921	LDA	2	0
4	A	919	UDP	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	747/802 (93%)	-0.00	22 (2%) 53 36	77, 127, 205, 236	0
2	B	655/707 (92%)	0.08	17 (2%) 57 38	82, 143, 210, 235	0
All	All	1402/1509 (92%)	0.04	39 (2%) 55 36	77, 135, 208, 236	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	ARG	6.1
2	B	183	ALA	4.2
2	B	101	ARG	4.2
2	B	125	PHE	4.0
1	A	399	ARG	3.5

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.

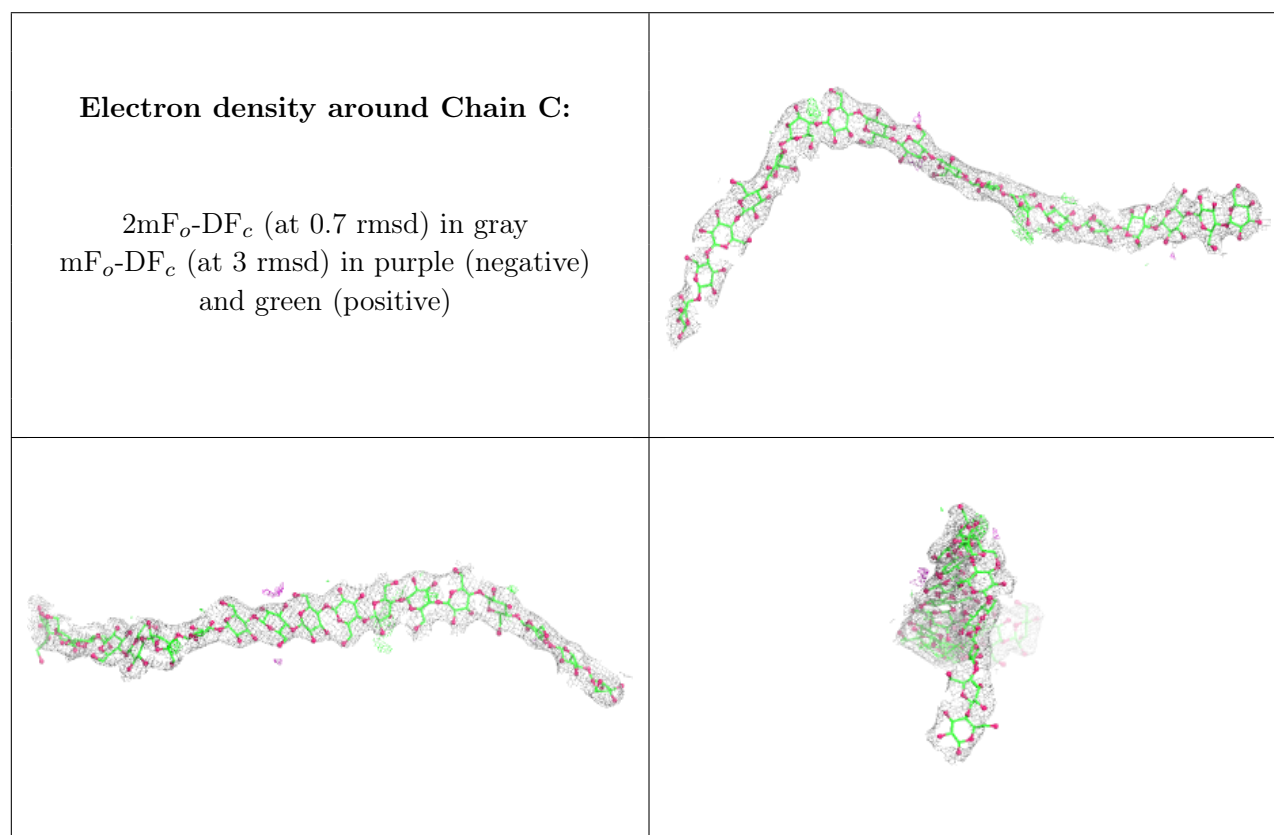
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	C	1	12/12	0.67	0.09	176,192,196,198	0
3	BGC	C	2	11/12	0.75	0.09	149,170,193,198	0
3	BGC	C	13	11/12	0.91	0.11	88,107,120,127	0
3	BGC	C	12	11/12	0.93	0.10	86,103,140,157	0
3	BGC	C	6	11/12	0.93	0.09	77,96,110,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	C	3	11/12	0.94	0.06	100,112,144,154	0
3	BGC	C	8	11/12	0.94	0.10	78,92,104,118	0
3	BGC	C	15	11/12	0.94	0.11	108,116,170,173	0
3	BGC	C	17	11/12	0.94	0.10	97,106,119,140	0
3	BGC	C	7	11/12	0.95	0.08	79,109,137,143	0
3	BGC	C	16	11/12	0.95	0.11	90,104,129,158	0
3	BGC	C	5	11/12	0.95	0.08	95,114,142,143	0
3	BGC	C	9	11/12	0.96	0.13	70,96,103,127	0
3	BGC	C	18	11/12	0.96	0.07	116,121,136,142	0
3	BGC	C	4	11/12	0.97	0.06	97,115,128,142	0
3	BGC	C	14	11/12	0.97	0.08	97,114,126,129	0
3	BGC	C	11	11/12	0.98	0.05	83,93,108,111	0
3	BGC	C	10	11/12	0.98	0.08	82,97,109,114	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,

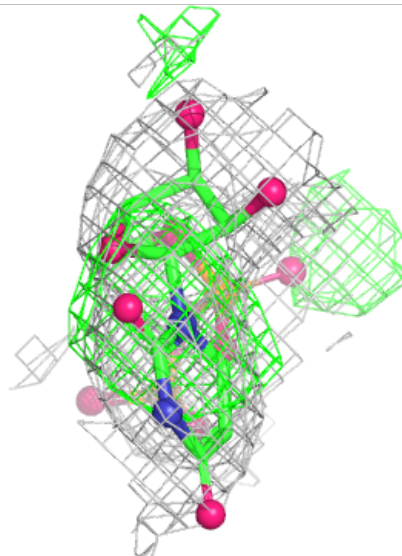
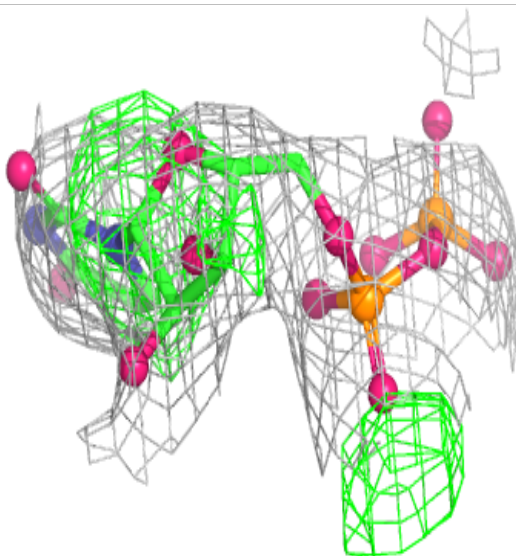
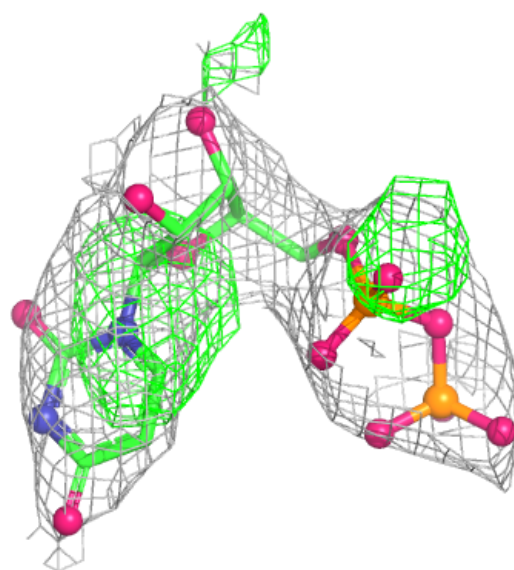
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	LDA	A	921	16/16	0.87	0.21	105,128,177,182	0
4	UDP	A	919	25/25	0.92	0.17	57,85,113,131	25
5	LDA	A	920	9/16	0.94	0.17	92,109,143,144	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 UDP A 919:

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 [i](#)

There are no such residues in this entry.