



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 27, 2026 – 10:15 am BST

PDB ID : 9TDJ / pdb_00009tdj
Title : Structure of an LPMO expressed in E.coli (LsAA9A) at 2.73×10^6 Gy
Authors : Huang, Z.; Lo Leggio, L.
Deposited on : 2025-11-23
Resolution : 1.86 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

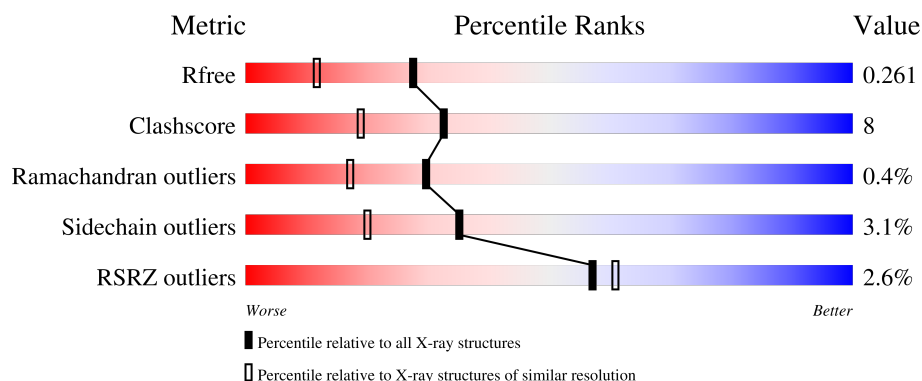
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	AAA	235	3% 88% 10%
2	DDD	3	67% 33%

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	ACT	AAA	302	-	-	X	-
3	ACT	AAA	303	-	-	X	-
6	SO4	AAA	325	-	-	X	-

2 Entry composition [i](#)

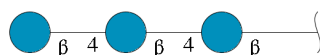
There are 7 unique types of molecules in this entry. The entry contains 2153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Auxiliary activity 9.

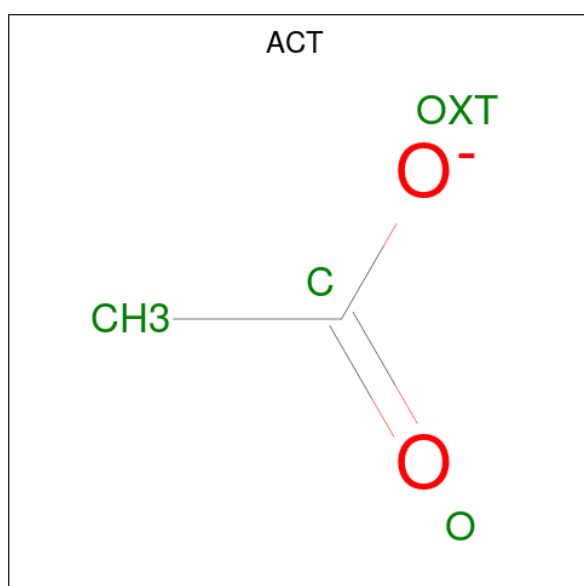
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	235	Total	C	N	O	S	0	10	0
			1870	1176	325	366	3			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	DDD	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

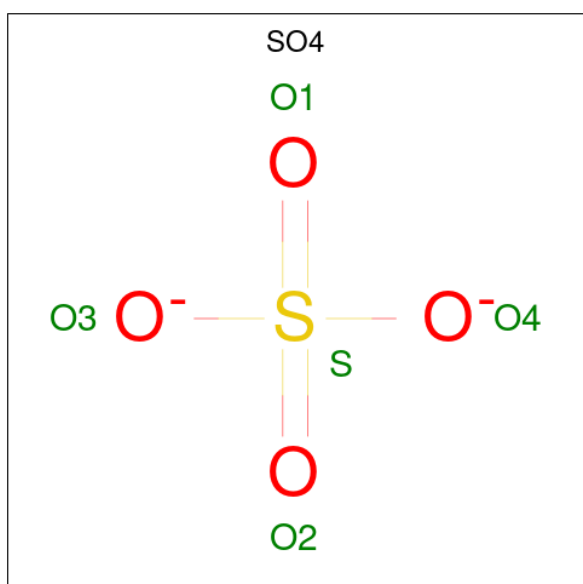
- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Cu 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	12	Total Cl 12 12	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	159	Total	O	0	8
			167	167		

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: Auxiliary activity 9

Chain AAA: 



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

Chain DDD: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	48.08Å 48.08Å 109.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.02 – 1.86 34.02 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.02-1.86) 98.7 (34.02-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.210 , 0.258 0.216 , 0.261	Depositor DCC
R_{free} test set	1055 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2153	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BGC, ACT, CL, CU

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	AAA	1.01	0/1926	1.23	0/2650

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 [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	AAA	1870	0	1757	27	0
2	DDD	34	0	30	1	0
3	AAA	24	0	18	8	0
4	AAA	1	0	0	0	0
5	AAA	12	0	0	0	0
6	AAA	45	0	0	2	0
7	AAA	167	0	0	3	0
All	All	2153	0	1805	30	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 8.

The worst 5 of 30 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:AAA:159[A]:ARG:HH11	1:AAA:159[A]:ARG:HG2	0.99	1.16
1:AAA:159[A]:ARG:HH11	1:AAA:159[A]:ARG:CG	1.79	0.95
1:AAA:159[A]:ARG:HG2	1:AAA:159[A]:ARG:NH1	1.79	0.89
1:AAA:64:TRP:HE1	1:AAA:125:HIS:HE1	1.39	0.70
1:AAA:108:VAL:HB	3:AAA:302:ACT:H3	1.83	0.59

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	AAA	243/235 (103%)	227 (93%)	15 (6%)	1 (0%)	30 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	234	LEU

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	AAA	205/195 (105%)	196 (96%)	9 (4%)	25 10

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	159[A]	ARG
1	AAA	159[B]	ARG
1	AAA	50[A]	LYS
1	AAA	50[C]	LYS
1	AAA	150[A]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

3 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	BGC	DDD	1	2	12,12,12	0.44	0	17,17,17	1.31	2 (11%)
2	BGC	DDD	2	2	11,11,12	0.74	0	15,15,17	0.98	1 (6%)
2	BGC	DDD	3	2	11,11,12	0.46	0	15,15,17	1.14	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	BGC	DDD	1	2	-	0/2/22/22	0/1/1/1
2	BGC	DDD	2	2	-	0/2/19/22	0/1/1/1
2	BGC	DDD	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	1	BGC	O4-C4-C5	-3.00	101.84	109.30
2	DDD	1	BGC	C1-O5-C5	2.82	118.98	113.66
2	DDD	3	BGC	C1-C2-C3	2.41	112.62	109.67
2	DDD	2	BGC	O5-C1-C2	-2.34	107.15	110.77

There are no chirality outliers.

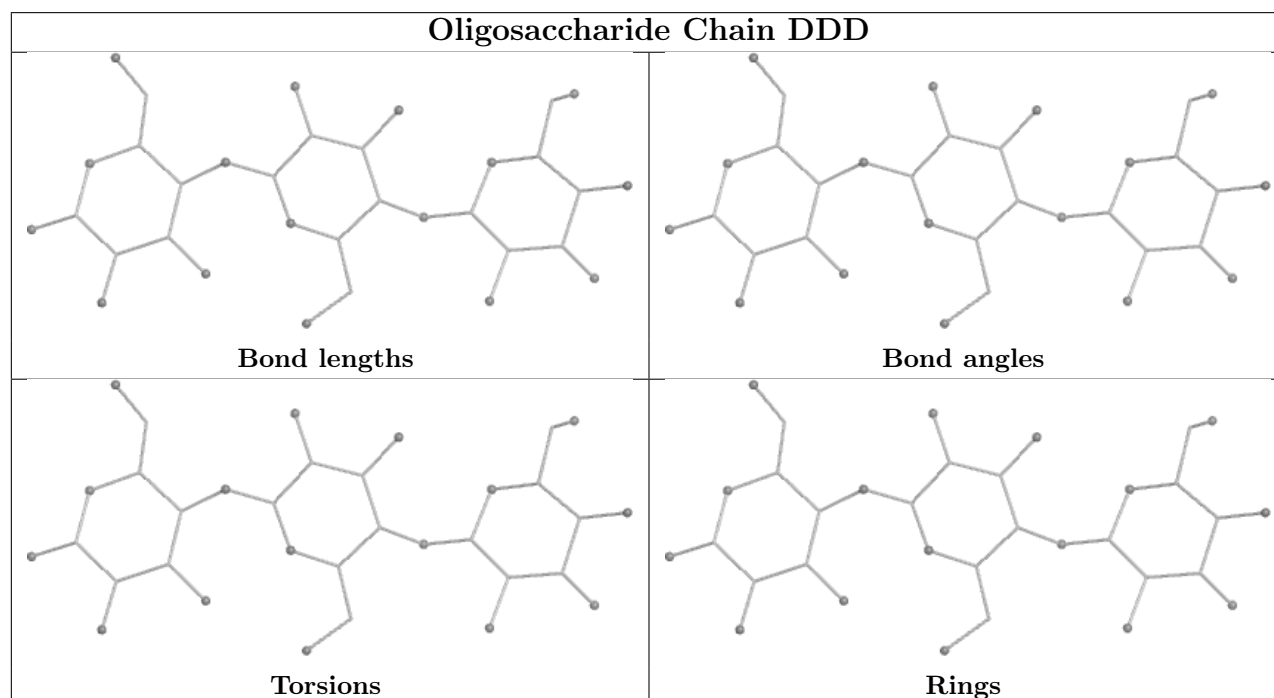
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	1	BGC	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

Of 28 ligands modelled in this entry, 13 are monoatomic - leaving 15 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	$\# Z > 2$
3	ACT	AAA	305	-	3,3,3	1.08	0	3,3,3	0.79	0
3	ACT	AAA	302	-	3,3,3	1.07	0	3,3,3	0.71	0
6	SO4	AAA	325	-	4,4,4	0.37	0	6,6,6	0.08	0
6	SO4	AAA	320	-	4,4,4	0.25	0	6,6,6	0.19	0
6	SO4	AAA	324	-	4,4,4	0.35	0	6,6,6	0.05	0
3	ACT	AAA	306	-	3,3,3	0.96	0	3,3,3	0.91	0
6	SO4	AAA	322	-	4,4,4	0.35	0	6,6,6	0.06	0
6	SO4	AAA	321	-	4,4,4	0.32	0	6,6,6	0.08	0
3	ACT	AAA	301	-	3,3,3	0.93	0	3,3,3	0.82	0
6	SO4	AAA	323	5	4,4,4	0.32	0	6,6,6	0.13	0
6	SO4	AAA	326	-	4,4,4	0.35	0	6,6,6	0.09	0
6	SO4	AAA	328	-	4,4,4	0.38	0	6,6,6	0.06	0
6	SO4	AAA	327	-	4,4,4	0.29	0	6,6,6	0.08	0
3	ACT	AAA	304	-	3,3,3	1.00	0	3,3,3	0.88	0
3	ACT	AAA	303	-	3,3,3	0.90	0	3,3,3	1.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	305	ACT	1	0
3	AAA	302	ACT	3	0
6	AAA	325	SO4	2	0
3	AAA	306	ACT	1	0
3	AAA	301	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	303	ACT	2	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, 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	AAA	235/235 (100%)	0.24	6 (2%) 57 61	9, 20, 27, 87	10 (4%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	234	LEU	6.4
1	AAA	50[A]	LYS	5.6
1	AAA	235	GLU	2.7
1	AAA	229[A]	VAL	2.5
1	AAA	231	ASP	2.2

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

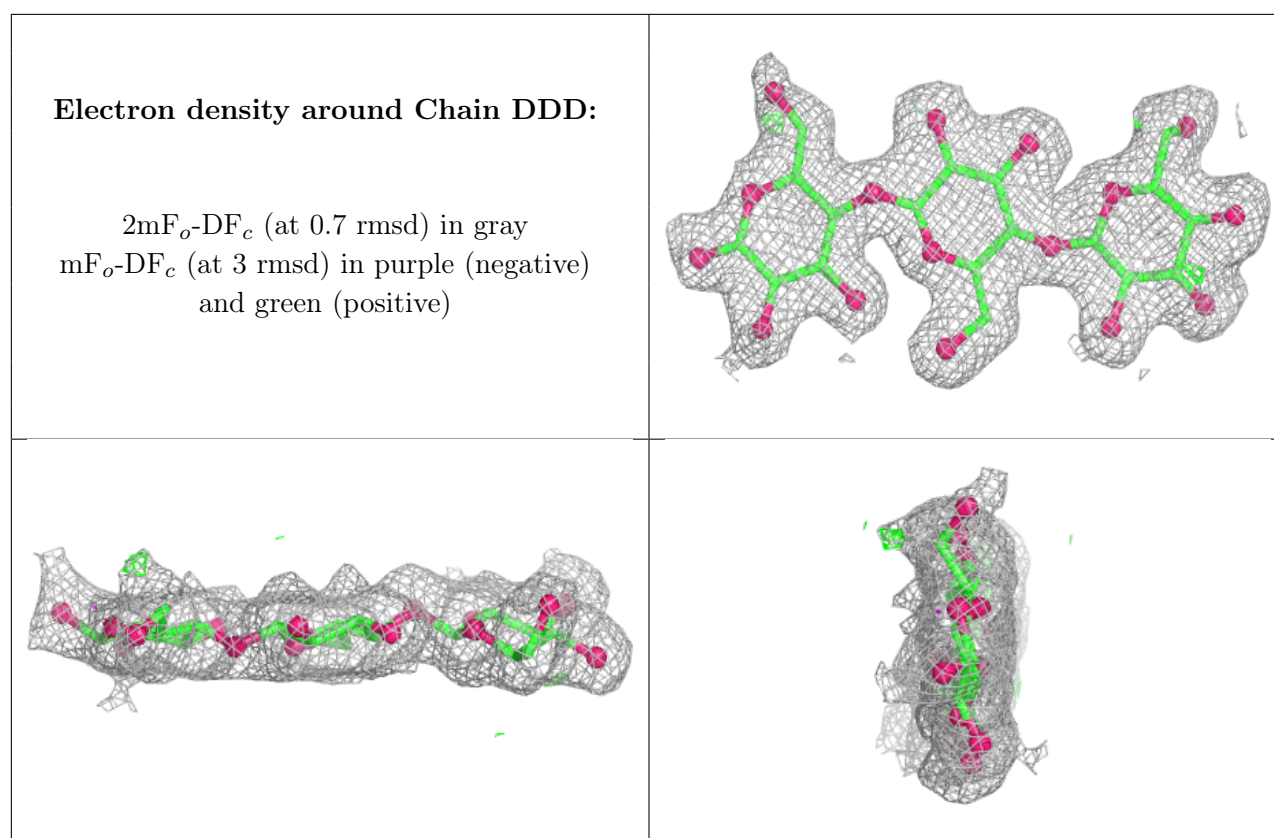
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	BGC	DDD	1	12/12	-	-	24,27,32,39	0
2	BGC	DDD	2	11/12	-	-	17,19,21,22	0
2	BGC	DDD	3	11/12	-	-	19,21,23,25	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
5	CL	AAA	319	1/1	0.40	0.20	77,77,77,77	0
6	SO4	AAA	324	5/5	0.48	0.18	109,111,112,114	0
3	ACT	AAA	302	4/4	0.59	0.24	59,60,62,67	0
6	SO4	AAA	326	5/5	0.63	0.14	76,78,83,86	0
3	ACT	AAA	305	4/4	0.65	0.22	48,49,50,51	0
6	SO4	AAA	322	5/5	0.65	0.13	76,80,81,84	0
6	SO4	AAA	321	5/5	0.66	0.14	70,79,79,83	0
3	ACT	AAA	304	4/4	0.66	0.19	47,47,48,50	0
5	CL	AAA	314	1/1	0.70	0.23	71,71,71,71	0
6	SO4	AAA	323	5/5	0.73	0.16	23,25,26,30	5
6	SO4	AAA	327	5/5	0.74	0.14	61,62,71,72	0
5	CL	AAA	318	1/1	0.77	0.17	65,65,65,65	0
5	CL	AAA	315	1/1	0.77	0.18	68,68,68,68	0
3	ACT	AAA	301	4/4	0.78	0.30	30,30,30,31	4

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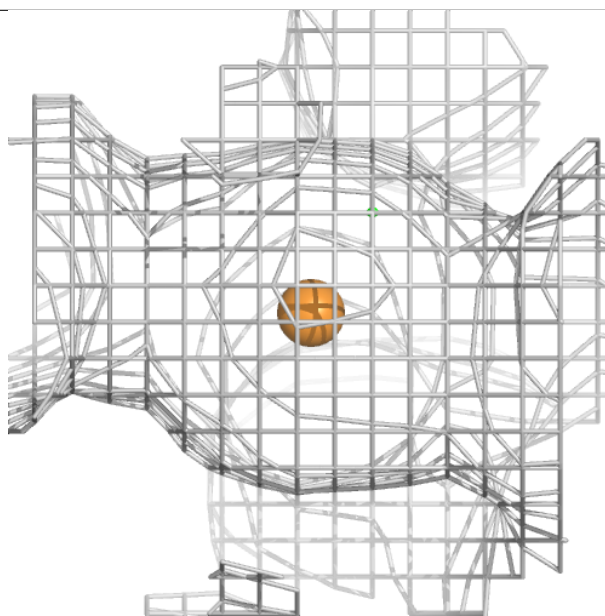
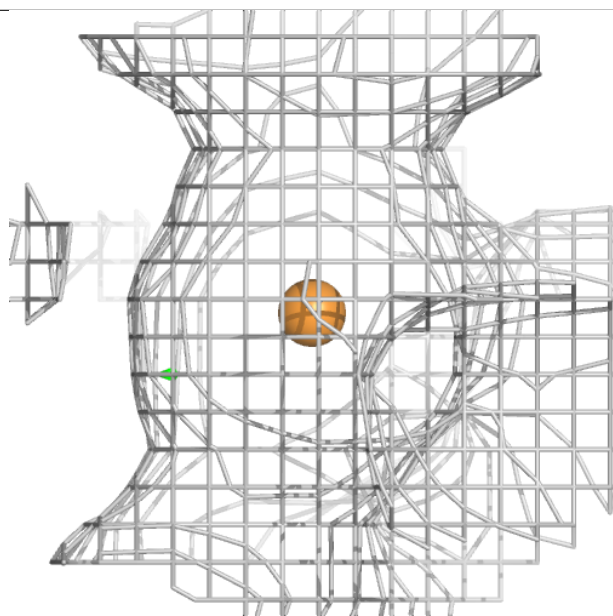
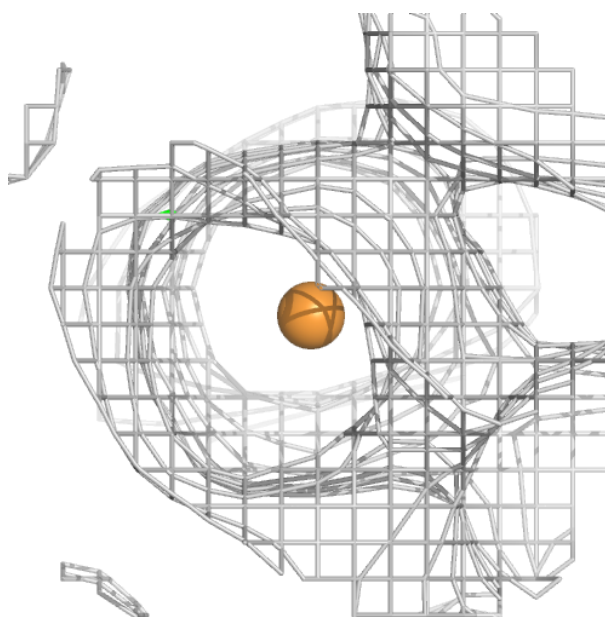
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	AAA	313	1/1	0.80	0.16	59,59,59,59	0
6	SO4	AAA	320	5/5	0.80	0.12	45,48,50,53	0
5	CL	AAA	311	1/1	0.82	0.12	62,62,62,62	0
3	ACT	AAA	303	4/4	0.82	0.13	30,34,35,39	0
5	CL	AAA	316	1/1	0.82	0.30	58,58,58,58	0
5	CL	AAA	312	1/1	0.84	0.28	59,59,59,59	0
3	ACT	AAA	306	4/4	0.84	0.15	34,35,38,42	0
5	CL	AAA	310	1/1	0.87	0.20	58,58,58,58	0
6	SO4	AAA	328	5/5	0.87	0.12	57,59,68,71	0
5	CL	AAA	308	1/1	0.88	0.10	36,36,36,36	1
5	CL	AAA	317	1/1	0.89	0.16	71,71,71,71	0
6	SO4	AAA	325	5/5	0.90	0.10	44,46,48,49	0
5	CL	AAA	309	1/1	0.91	0.23	58,58,58,58	0
4	CU	AAA	307	1/1	1.00	0.01	17,17,17,17	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 CU AAA 307:

$2mF_o-DF_c$ (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.