



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 27, 2026 – 10:16 am BST

PDB ID : 9TDI / pdb_00009tdi
Title : Structure of an LPMO expressed in E.coli (LsAA9A) at 2.80×10^6 Gy
Authors : Huang, Z.; Lo Leggio, L.
Deposited on : 2025-11-23
Resolution : 1.06 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

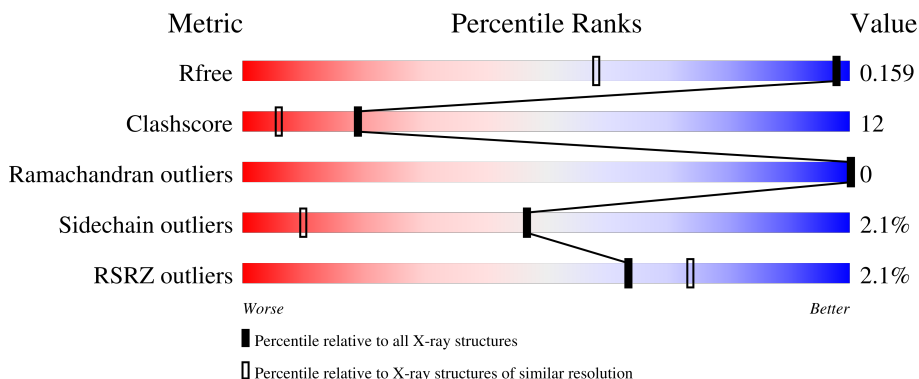
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

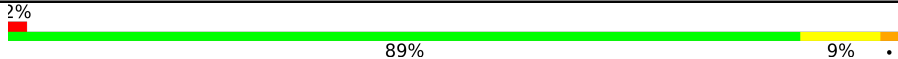
The reported resolution of this entry is 1.06 Å.

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	1182 (1.08-1.04)
Clashscore	190562	1204 (1.08-1.04)
Ramachandran outliers	187476	1175 (1.08-1.04)
Sidechain outliers	187428	1176 (1.08-1.04)
RSRZ outliers	180081	1181 (1.08-1.04)

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	

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
2	ACT	AAA	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	AAA	303	-	-	X	-
2	ACT	AAA	307	-	-	X	-
2	ACT	AAA	313	-	-	X	-
4	SO4	AAA	331	-	-	X	-

2 Entry composition [i](#)

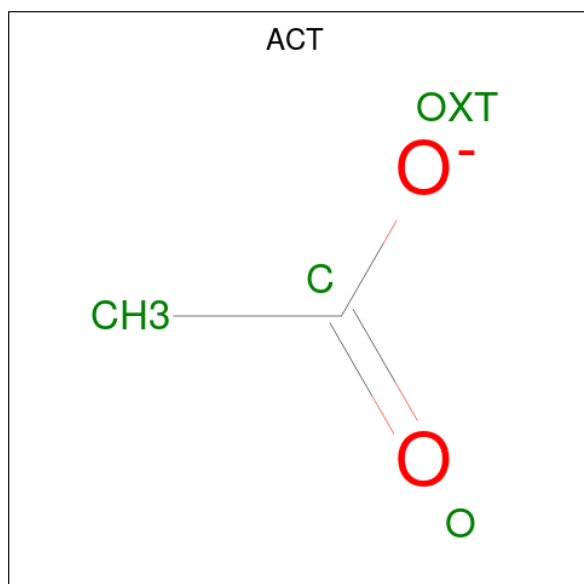
There are 6 unique types of molecules in this entry. The entry contains 2478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	12	0
			1892	1191	328	370	3			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

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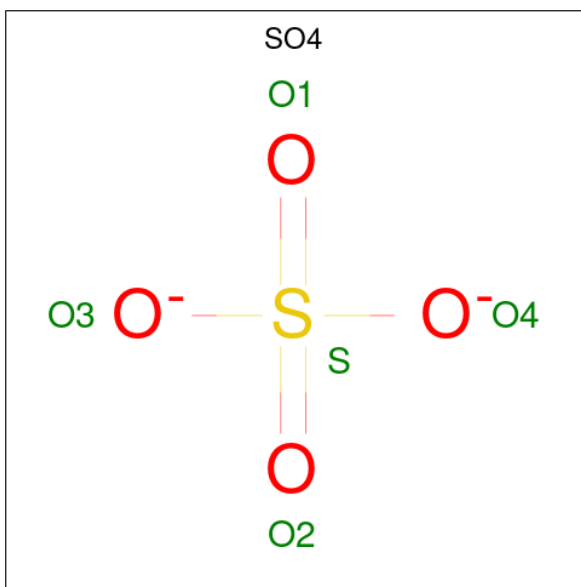
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total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

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total 1	Cl 1	0	0

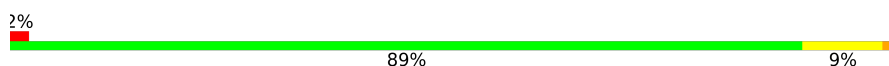
- Molecule 6 is water.

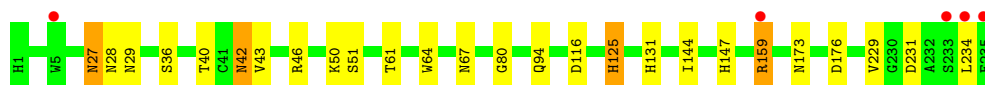
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	423	Total 442	O 442	0	19

3 Residue-property plots [i](#)

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: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	48.28Å 48.28Å 109.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 1.06 48.28 – 1.06	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.28-1.06) 99.3 (48.28-1.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.06Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.143 , 0.153 0.151 , 0.159	Depositor DCC
R_{free} test set	5596 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2478	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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: CL, CU, ACT, SO4

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	1.13	2/1949 (0.1%)	1.02	3/2680 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	36	SER	CA-CB	-5.49	1.43	1.53
1	AAA	147	HIS	CE1-NE2	5.41	1.38	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	116	ASP	CA-CB-CG	6.10	118.70	112.60
1	AAA	125	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	AAA	125	HIS	CB-CG-ND1	5.92	131.57	122.70

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	1892	0	1780	33	1
2	AAA	72	0	52	22	0
3	AAA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	70	0	0	5	0
5	AAA	1	0	0	0	0
6	AAA	442	0	0	15	0
All	All	2478	0	1832	46	1

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 12.

The worst 5 of 46 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:CG	1.38	1.32
4:AAA:331:SO4:O1	6:AAA:407[B]:HOH:O	1.57	1.21
1:AAA:159[A]:ARG:HG2	1:AAA:159[A]:ARG:NH1	1.20	1.05
1:AAA:28:ASN:HD21	2:AAA:301:ACT:H2	1.23	1.01
2:AAA:315:ACT:OXT	6:AAA:464[B]:HOH:O	1.79	0.98

All (1) 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)
1:AAA:159[A]:ARG:NH1	1:AAA:176:ASP:O[1_655]	2.09	0.11

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	246/235 (105%)	228 (93%)	18 (7%)	0	100 100

There are no Ramachandran outliers to report.

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	208/195 (107%)	203 (98%)	5 (2%)	43 8

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	27	ASN
1	AAA	42	ASN
1	AAA	46	ARG
1	AAA	159[A]	ARG
1	AAA	159[B]	ARG

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

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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	$\# Z > 2$
2	ACT	AAA	333	-	3,3,3	0.88	0	3,3,3	0.76	0
2	ACT	AAA	315	-	3,3,3	0.95	0	3,3,3	0.90	0
4	SO4	AAA	320	-	4,4,4	0.53	0	6,6,6	0.40	0
4	SO4	AAA	324	-	4,4,4	0.58	0	6,6,6	0.37	0
4	SO4	AAA	330	-	4,4,4	0.31	0	6,6,6	0.26	0
2	ACT	AAA	313	-	3,3,3	1.44	1 (33%)	3,3,3	0.96	0
4	SO4	AAA	327	-	4,4,4	0.29	0	6,6,6	0.44	0
4	SO4	AAA	329	-	4,4,4	0.30	0	6,6,6	0.13	0
2	ACT	AAA	310	-	3,3,3	0.78	0	3,3,3	0.98	0
2	ACT	AAA	302	-	3,3,3	1.04	0	3,3,3	1.15	0
2	ACT	AAA	316	-	3,3,3	0.77	0	3,3,3	0.72	0
4	SO4	AAA	325	-	4,4,4	0.36	0	6,6,6	0.12	0
2	ACT	AAA	306	-	3,3,3	1.27	0	3,3,3	1.01	0
2	ACT	AAA	304	-	3,3,3	1.12	0	3,3,3	0.77	0
2	ACT	AAA	303	-	3,3,3	0.94	0	3,3,3	0.77	0
4	SO4	AAA	331	-	4,4,4	0.93	0	6,6,6	0.37	0
2	ACT	AAA	312	-	3,3,3	1.18	0	3,3,3	0.87	0
2	ACT	AAA	308	-	3,3,3	0.88	0	3,3,3	0.89	0
4	SO4	AAA	328	-	4,4,4	1.18	1 (25%)	6,6,6	0.10	0
2	ACT	AAA	307	-	3,3,3	0.90	0	3,3,3	0.94	0
4	SO4	AAA	326	-	4,4,4	0.32	0	6,6,6	0.05	0
2	ACT	AAA	317	-	3,3,3	1.01	0	3,3,3	1.12	0
2	ACT	AAA	311	-	3,3,3	0.97	0	3,3,3	0.77	0
4	SO4	AAA	323	-	4,4,4	0.38	0	6,6,6	0.38	0
4	SO4	AAA	321	-	4,4,4	0.69	0	6,6,6	0.22	0
2	ACT	AAA	305	-	3,3,3	1.80	1 (33%)	3,3,3	0.36	0
2	ACT	AAA	314	-	3,3,3	1.13	0	3,3,3	0.96	0
4	SO4	AAA	332	-	4,4,4	0.33	0	6,6,6	0.07	0
2	ACT	AAA	309	-	3,3,3	0.96	0	3,3,3	0.85	0
4	SO4	AAA	322	-	4,4,4	0.53	0	6,6,6	0.44	0
4	SO4	AAA	319	-	4,4,4	0.38	0	6,6,6	0.37	0
2	ACT	AAA	301	-	3,3,3	2.76	2 (66%)	3,3,3	0.51	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	301	ACT	CH3-C	3.59	1.64	1.49
2	AAA	301	ACT	O-C	2.95	1.35	1.22
2	AAA	305	ACT	CH3-C	2.70	1.60	1.49
2	AAA	313	ACT	CH3-C	2.28	1.58	1.49
4	AAA	328	SO4	O1-S	-2.27	1.33	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	315	ACT	1	0
2	AAA	313	ACT	4	0
4	AAA	329	SO4	1	0
2	AAA	310	ACT	1	0
2	AAA	316	ACT	1	0
2	AAA	306	ACT	1	0
2	AAA	303	ACT	2	0
4	AAA	331	SO4	4	0
2	AAA	308	ACT	1	0
2	AAA	307	ACT	2	0
2	AAA	317	ACT	1	0
2	AAA	309	ACT	1	0
2	AAA	301	ACT	7	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%)	0.11	5 (2%) 63 74	4, 11, 16, 52	12 (5%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	234	LEU	5.0
1	AAA	233	SER	3.5
1	AAA	235	GLU	2.9
1	AAA	159[A]	ARG	2.1
1	AAA	5	TRP	2.1

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](#)

There are no oligosaccharides in this entry.

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
2	ACT	AAA	309	4/4	0.55	0.35	89,92,92,94	0
2	ACT	AAA	333	4/4	0.58	0.17	53,63,67,70	0

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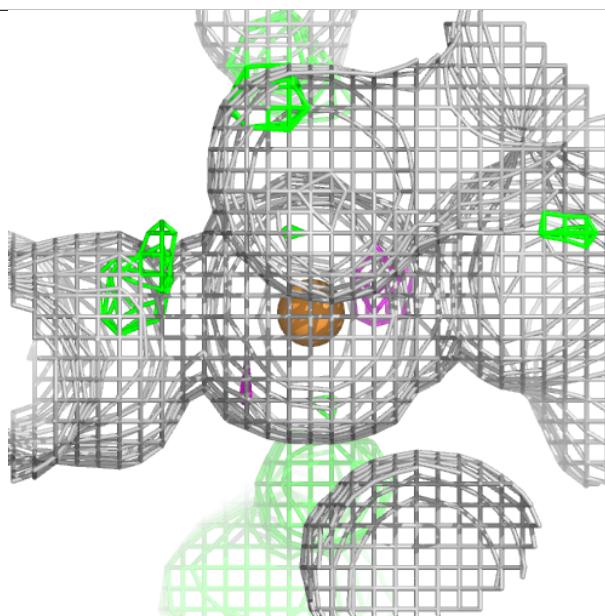
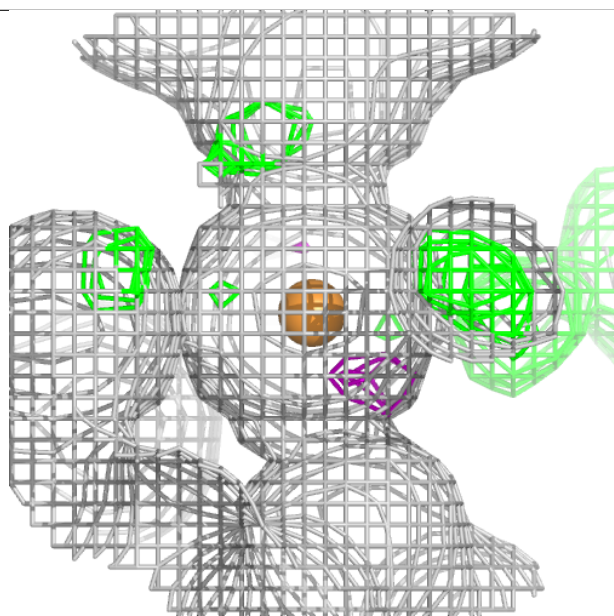
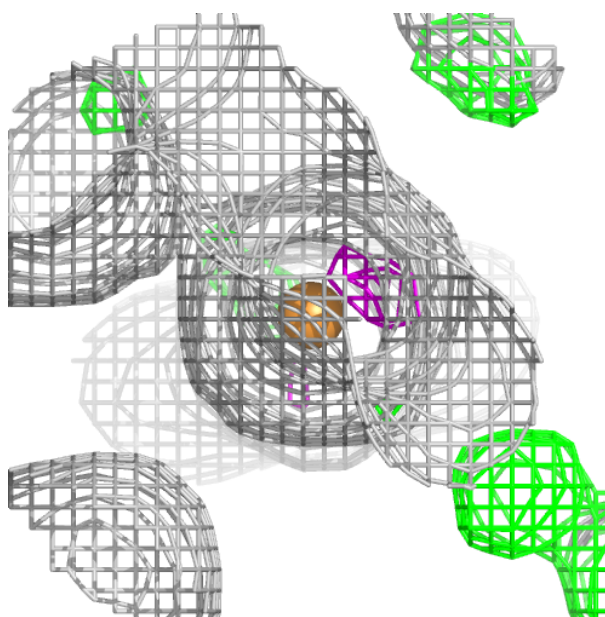
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	AAA	308	4/4	0.60	0.21	68,69,70,80	0
4	SO4	AAA	326	5/5	0.64	0.12	67,76,82,84	0
4	SO4	AAA	329	5/5	0.66	0.14	60,63,68,69	0
2	ACT	AAA	305	4/4	0.68	0.18	26,27,31,32	0
2	ACT	AAA	317	4/4	0.74	0.16	37,41,41,45	0
2	ACT	AAA	313	4/4	0.74	0.15	22,36,42,45	0
2	ACT	AAA	307	4/4	0.75	0.16	39,51,56,59	0
2	ACT	AAA	311	4/4	0.77	0.19	62,63,63,66	0
2	ACT	AAA	304	4/4	0.77	0.16	32,43,47,49	0
2	ACT	AAA	306	4/4	0.78	0.24	17,20,25,27	4
2	ACT	AAA	301	4/4	0.79	0.16	13,18,24,36	4
2	ACT	AAA	316	4/4	0.79	0.15	18,31,40,45	0
2	ACT	AAA	312	4/4	0.80	0.14	31,36,39,50	0
2	ACT	AAA	310	4/4	0.82	0.14	21,24,29,39	0
4	SO4	AAA	324	5/5	0.82	0.16	16,18,20,20	5
4	SO4	AAA	330	5/5	0.82	0.14	20,39,41,46	5
2	ACT	AAA	315	4/4	0.83	0.15	28,33,40,49	0
4	SO4	AAA	327	5/5	0.83	0.16	14,16,18,18	5
4	SO4	AAA	325	5/5	0.85	0.11	39,39,41,42	5
4	SO4	AAA	331	5/5	0.86	0.14	20,33,41,43	5
2	ACT	AAA	314	4/4	0.87	0.13	20,21,28,36	4
4	SO4	AAA	328	5/5	0.88	0.14	18,24,33,34	5
5	CL	AAA	334	1/1	0.88	0.11	59,59,59,59	0
4	SO4	AAA	321	5/5	0.89	0.13	15,23,30,32	5
4	SO4	AAA	322	5/5	0.90	0.14	15,19,24,29	5
4	SO4	AAA	332	5/5	0.90	0.11	29,34,36,38	5
2	ACT	AAA	303	4/4	0.90	0.13	18,20,32,33	0
4	SO4	AAA	323	5/5	0.91	0.11	25,25,29,31	5
4	SO4	AAA	320	5/5	0.93	0.11	15,17,18,18	5
2	ACT	AAA	302	4/4	0.97	0.07	12,13,13,15	0
4	SO4	AAA	319	5/5	0.97	0.09	15,16,18,19	0
3	CU	AAA	318	1/1	1.00	0.01	10,10,10,10	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 318:

$2mF_o-DF_c$ (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.