wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2026 – 01:07 am BST

PDB ID	:	9SUT / pdb_00009sut
Title	:	gamma carbonic anhydrase LreCA from Limosilactobacillus reuteri in space group I222
Authors	:	Angeli, A.; Ferraroni, M.
Deposited on	:	2025-09-30
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

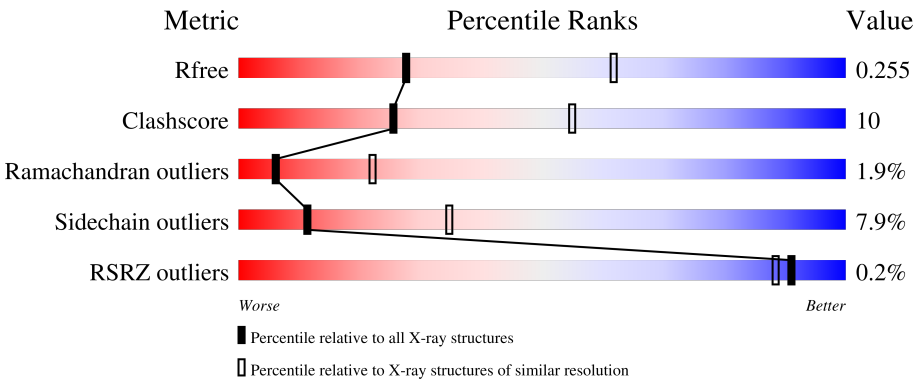
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 <=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	179	74% 22% • •
1	BBB	179	% 74% 21% • •
1	CCC	179	73% 24% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4052 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 gamma carbonic anhydrase from Limosilactobacillus reuteri.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	178	1343	847	240	250	6	0	0	0
1	BBB	178	1343	847	240	250	6	0	0	0
1	CCC	178	1343	847	240	250	6	0	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	AAA	1	1	1	0	0
2	BBB	2	2	2	0	0

- Molecule 3 is water.

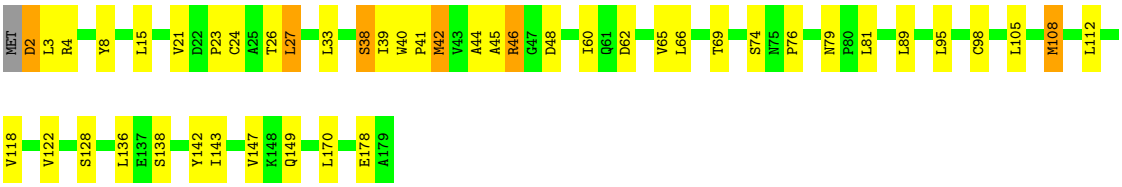
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	AAA	5	5	5	0	0
3	BBB	9	9	9	0	0
3	CCC	6	6	6	0	0

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.

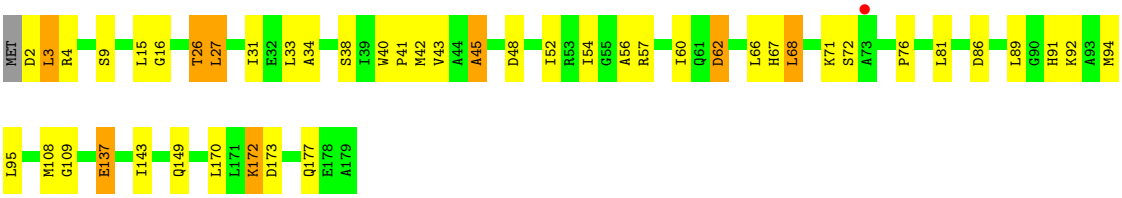
• Molecule 1: gamma carbonic anhydrase from Limosilactobacillus reuteri

Chain AAA:



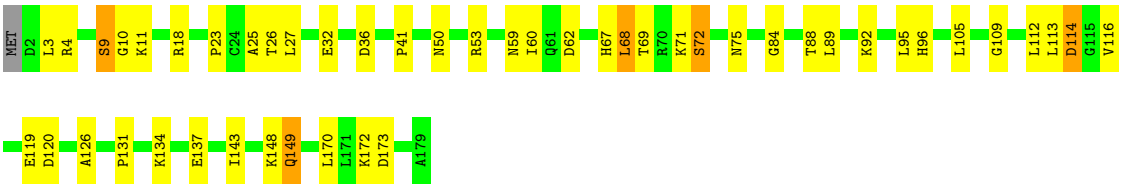
• Molecule 1: gamma carbonic anhydrase from Limosilactobacillus reuteri

Chain BBB:



• Molecule 1: gamma carbonic anhydrase from Limosilactobacillus reuteri

Chain CCC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	91.57Å 98.75Å 127.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.80 49.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.37-2.80) 97.2 (49.37-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.191 , 0.272 0.195 , 0.255	Depositor DCC
R_{free} test set	701 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	62.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4052	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	1.12	0/1366	1.47	1/1852 (0.1%)
1	BBB	1.14	1/1366 (0.1%)	1.41	1/1852 (0.1%)
1	CCC	1.12	0/1366	1.43	0/1852
All	All	1.13	1/4098 (0.0%)	1.44	2/5556 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	45	ALA	C-O	5.29	1.29	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	2	ASP	CA-CB-CG	5.67	118.27	112.60
1	BBB	48	ASP	CA-CB-CG	5.02	117.62	112.60

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	1343	0	1379	28	0
1	BBB	1343	0	1379	28	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	1343	0	1379	27	0
2	AAA	1	0	0	0	0
2	BBB	2	0	0	0	0
3	AAA	5	0	0	0	0
3	BBB	9	0	0	2	0
3	CCC	6	0	0	4	0
All	All	4052	0	4137	78	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 10.

The worst 5 of 78 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:CCC:137:GLU:OE2	3:CCC:201:HOH:O	1.56	1.23
1:CCC:119:GLU:OE1	3:CCC:201:HOH:O	1.78	1.02
1:CCC:9:SER:OG	1:CCC:10:GLY:N	2.06	0.85
1:AAA:24:CYS:SG	3:BBB:309:HOH:O	2.35	0.84
1:BBB:2:ASP:HA	3:BBB:302:HOH:O	1.85	0.76

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:BBB:137:GLU:OE2	1:BBB:137:GLU:OE2[3_555]	2.18	0.02

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	176/179 (98%)	161 (92%)	14 (8%)	1 (1%)	21 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	176/179 (98%)	158 (90%)	15 (8%)	3 (2%)	7	25
1	CCC	176/179 (98%)	151 (86%)	19 (11%)	6 (3%)	3	11
All	All	528/537 (98%)	470 (89%)	48 (9%)	10 (2%)	6	22

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	75	ASN
1	AAA	149	GLN
1	CCC	72	SER
1	CCC	84	GLY
1	CCC	149	GLN

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	144/145 (99%)	133 (92%)	11 (8%)	12	36
1	BBB	144/145 (99%)	131 (91%)	13 (9%)	9	28
1	CCC	144/145 (99%)	134 (93%)	10 (7%)	14	41
All	All	432/435 (99%)	398 (92%)	34 (8%)	11	35

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	27	LEU
1	CCC	68	LEU
1	CCC	143	ILE
1	BBB	26	THR
1	BBB	3	LEU

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	178/179 (99%)	-0.50	0 100 100	46, 68, 104, 137	0
1	BBB	178/179 (99%)	-0.40	1 (0%) 85 80	46, 70, 107, 160	0
1	CCC	178/179 (99%)	-0.50	0 100 100	46, 67, 107, 176	0
All	All	534/537 (99%)	-0.46	1 (0%) 91 88	46, 68, 106, 176	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	73	ALA	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)

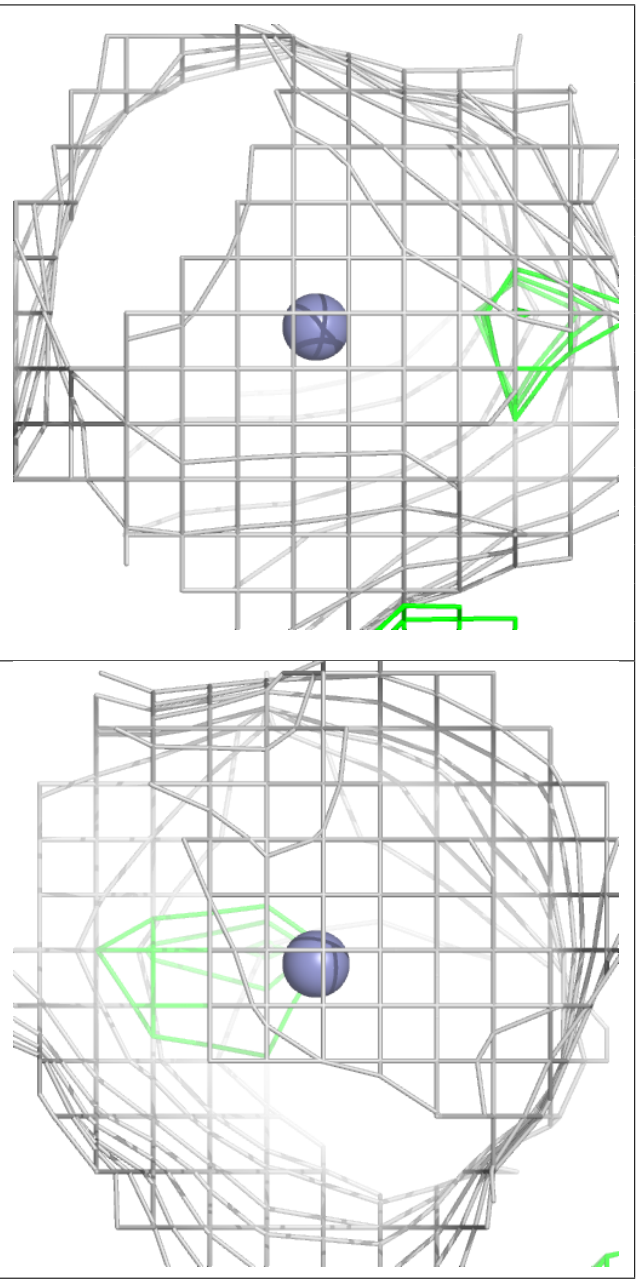
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ZN	BBB	201	1/1	0.98	0.04	72,72,72,72	0
2	ZN	AAA	201	1/1	1.00	0.01	59,59,59,59	0
2	ZN	BBB	202	1/1	1.00	0.02	69,69,69,69	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.

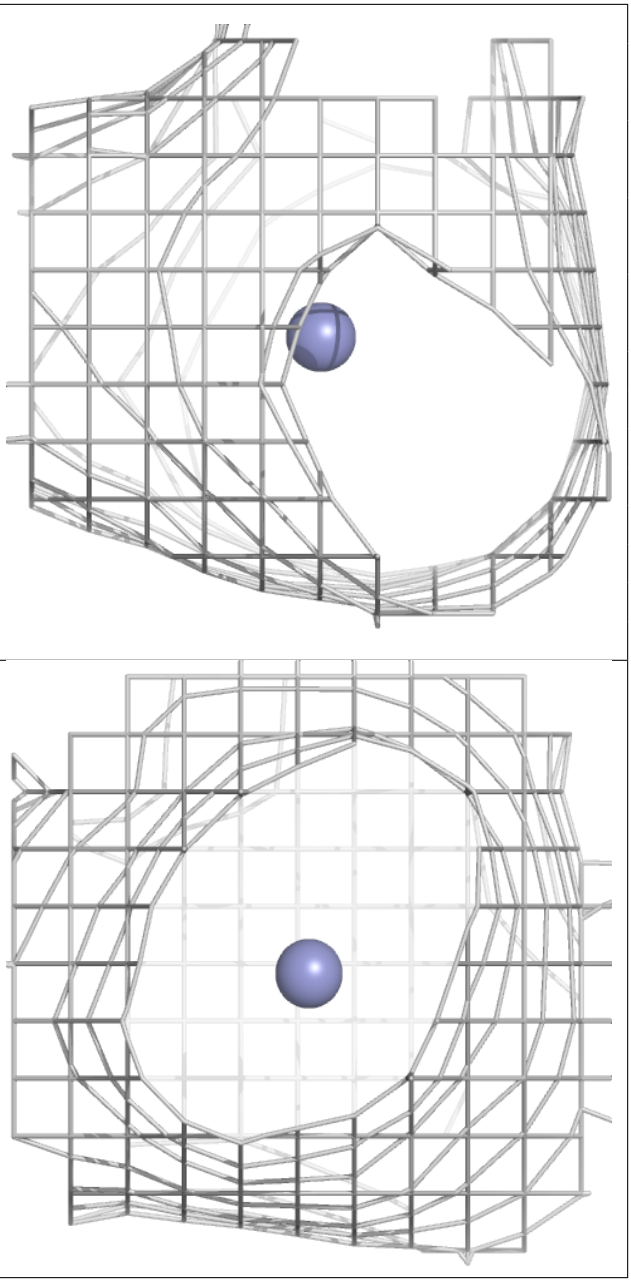
Electron density around ZN BBB 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



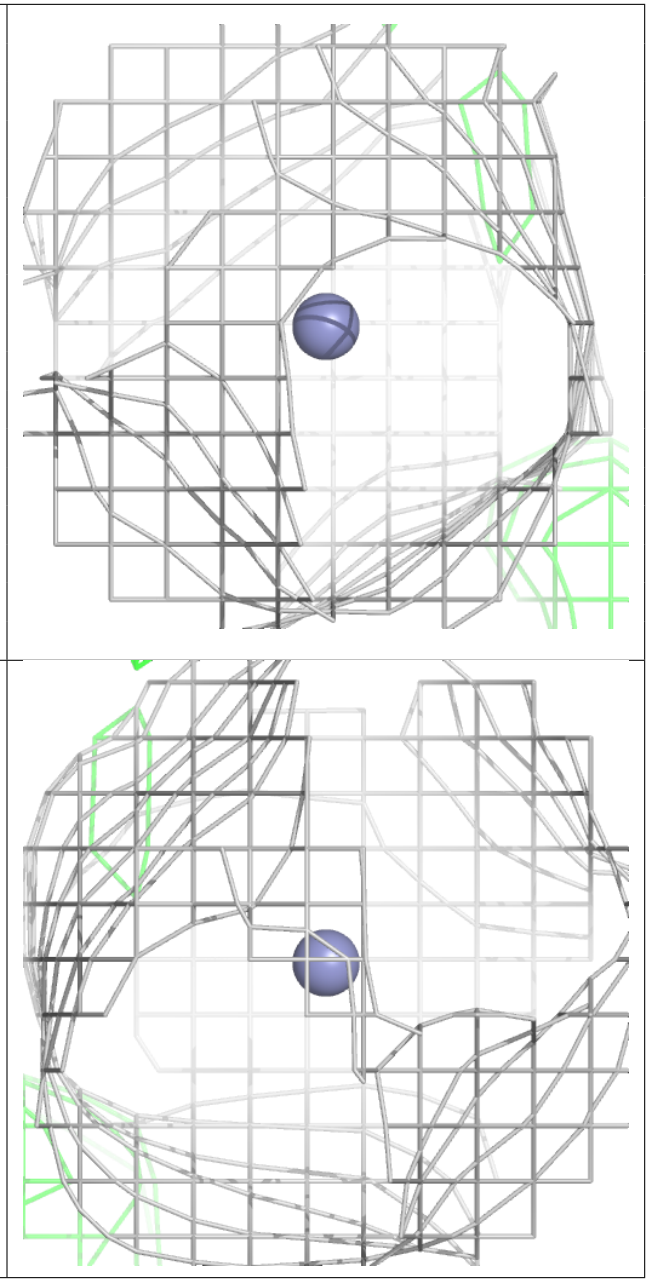
Electron density around ZN AAA 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN BBB 202:

$2mF_o$-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.