

Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 11:16 AM EDT

PDB ID : 8U00

Title: Crystal structure of metallo-beta-lactamase superfamily protein from

Caulobacter vibrioides

Authors: Kim, Y.; Maltseva, N.; Endres, M.; Joachimiak, A.; Center for Structural

Biology of Infectious Diseases (CSBID)

Deposited on : 2023-08-28

Resolution : 1.85 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 (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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

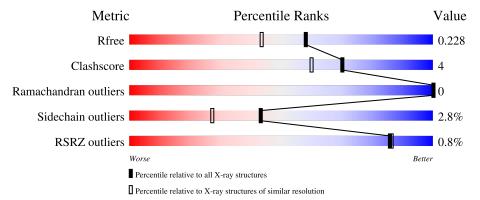
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.85 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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 <=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	271	78%	10%	• 11%
1	В	271	81%	8%	11%



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3928 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 Metallo-beta-lactamase superfamily protein.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace		
1	Δ	242	Total C	С	N	О	S	0	0	6	0
1	11	242	1887	1185	339	357	6		U		
1	P	242	Total	С	N	O	S	0	7	0	
1	. D	B 242		1189	340	359	6	0	1		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	-	expression tag	UNP Q9A6F5
A	20	ASN	-	expression tag	UNP Q9A6F5
A	77	HIS	ARG	cloning artifact	UNP Q9A6F5
A	136	THR	ILE	cloning artifact	UNP Q9A6F5
A	147	SER	PRO	cloning artifact	UNP Q9A6F5
В	19	SER	-	expression tag	UNP Q9A6F5
В	20	ASN	-	expression tag	UNP Q9A6F5
В	77	HIS	ARG	cloning artifact	UNP Q9A6F5
В	136	THR	ILE	cloning artifact	UNP Q9A6F5
В	147	SER	PRO	cloning artifact	UNP Q9A6F5

• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





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

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	3	Total Zn 3 3	0	0
3	В	3	Total Zn 3 3	0	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	В	1	Total Mg 1 1	0	0

 \bullet Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

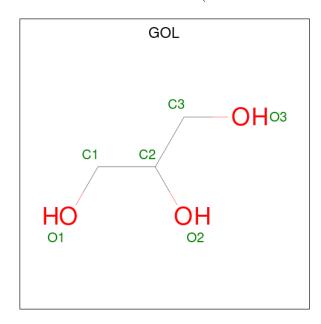
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	2	Total Cl 2 2	0	0

• Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

• Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ni 1 1	0	0
7	В	1	Total Ni 1 1	0	0

• Molecule 8 is water.

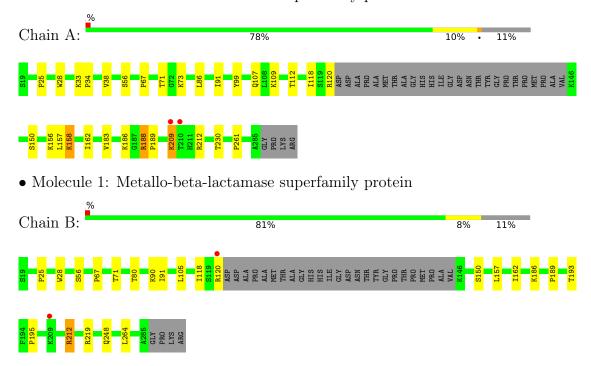
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	52	Total O 52 52	0	0
8	В	67	Total O 67 67	0	0



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: Metallo-beta-lactamase superfamily protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42	Depositor
Cell constants	85.34Å 85.34Å 78.84Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.10 - 1.85	Depositor
resolution (A)	38.17 - 1.85	EDS
% Data completeness	98.6 (24.10-1.85)	Depositor
(in resolution range)	98.7 (38.17-1.85)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.14 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.189 , 0.225	Depositor
it, it free	0.190 , 0.228	DCC
R_{free} test set	2370 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 40.9	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.489 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3928	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: MG, GOL, EDO, ZN, NI, CL

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
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.37	0/1925	0.58	0/2616
1	В	0.37	0/1932	0.58	0/2626
All	All	0.37	0/3857	0.58	0/5242

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	A	1887	0	1872	16	0
1	В	1894	0	1878	12	0
2	A	4	0	6	0	0
2	В	4	0	6	0	0
3	A	3	0	0	0	0
3	В	3	0	0	0	0
4	A	1	0	0	0	0
4	В	1	0	0	0	0
5	A	2	0	0	0	0
5	В	2	0	0	0	0
6	A	6	0	8	0	0



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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	В	1	0	0	0	0
8	A	52	0	0	0	0
8	В	67	0	0	1	0
All	All	3928	0	3770	27	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 4.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:189:PRO:HB2	1:B:189:PRO:HB2	1.57	0.83
1:B:193[B]:THR:HG23	1:B:195:PRO:HD3	1.75	0.68
1:A:91:ILE:HG21	1:A:157:LEU:HD11	1.85	0.58
1:B:91:ILE:HG21	1:B:157:LEU:HD11	1.87	0.55
1:A:156:LYS:HE3	1:A:158:LYS:NZ	2.22	0.55
1:B:67:PRO:HD2	1:B:71[A]:THR:HG21	1.93	0.50
1:A:38:VAL:HG13	1:A:183:VAL:HG21	1.92	0.50
1:B:56:SER:HB3	1:B:162:ILE:HG13	1.94	0.49
1:B:219:ARG:NE	8:B:401:HOH:O	2.24	0.47
1:A:120:ARG:HB2	1:A:150:SER:HB3	1.97	0.47
1:A:118:ILE:O	1:A:150:SER:HA	2.15	0.46
1:A:33:LYS:HG2	1:A:34:PRO:HD2	1.97	0.46
1:A:230:THR:O	1:A:261:PRO:HA	2.17	0.45
1:A:186:LYS:HZ1	1:A:188:ARG:HH22	1.65	0.45
1:A:67:PRO:HA	1:A:99:TYR:O	2.16	0.44
1:A:67:PRO:HD2	1:A:71[B]:THR:HG21	2.00	0.44
1:A:56:SER:HB3	1:A:162:ILE:HG13	2.00	0.43
1:B:193[B]:THR:HG21	1:B:264:LEU:HD22	1.99	0.43
1:B:118:ILE:O	1:B:150:SER:HA	2.19	0.42
1:B:25:PRO:HD2	1:B:28:TRP:CE2	2.55	0.42
1:A:73:LYS:HE3	1:A:107:GLN:NE2	2.35	0.41
1:B:212:ARG:H	1:B:212:ARG:HG3	1.67	0.40
1:A:25:PRO:HD2	1:A:28:TRP:CD2	2.56	0.40
1:A:209:LYS:H	1:A:209:LYS:HG2	1.59	0.40
1:A:86:LEU:HG	1:A:112:THR:HG22	2.03	0.40
1:B:25:PRO:HD2	1:B:28:TRP:CD2	2.56	0.40
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.98	0.40

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	Perce	ntiles
1	A	$244/271 \ (90\%)$	236 (97%)	8 (3%)	0	100	100
1	В	$245/271\ (90\%)$	236 (96%)	9 (4%)	0	100	100
All	All	$489/542 \ (90\%)$	472 (96%)	17 (4%)	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 Outlie		Outliers	Percentiles
1	A	200/215~(93%)	195 (98%)	5 (2%)	47 31
1	В	201/215 (94%)	194 (96%)	7 (4%)	36 18
All	All	401/430 (93%)	389 (97%)	12 (3%)	43 24

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LYS
1	A	158	LYS
1	A	188	ARG
1	A	209	LYS
1	A	212	ARG
1	В	80[A]	THR
1	В	80[B]	THR
1	В	90	LYS



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Mol	Chain	Res	Type
1	В	120	ARG
1	В	186	LYS
1	В	212	ARG
1	В	248	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 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	B	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	301	-	3,3,3	0.50	0	2,2,2	0.12	0
6	GOL	A	308	-	5,5,5	0.86	0	5,5,5	1.03	0
2	EDO	В	301	-	3,3,3	0.49	0	2,2,2	0.46	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
2	EDO	A	301	-	-	0/1/1/1	-
6	GOL	A	308	-	-	2/4/4/4	-
2	EDO	В	301	-	-	0/1/1/1	=

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	308	GOL	O1-C1-C2-O2
6	A	308	GOL	O1-C1-C2-C3

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, 95^{th} 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		$OWAB(A^2)$	Q<0.9
1	A	$242/271 \ (89\%)$	-0.30	2 (0%) 86	86	35, 50, 77, 100	3 (1%)
1	В	242/271 (89%)	-0.30	2 (0%) 86	86	34, 50, 77, 98	0
All	All	484/542 (89%)	-0.30	4 (0%) 86	86	34, 50, 77, 100	3 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	THR	2.4
1	В	209	LYS	2.4
1	A	209	LYS	2.2
1	В	120	ARG	2.0

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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	EDO	A	301	4/4	0.82	0.16	78,86,113,124	0



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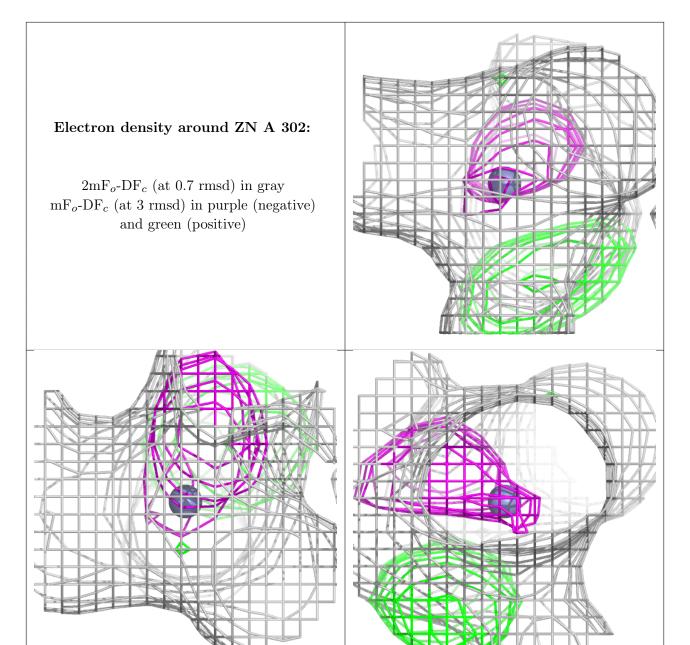
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	MG	В	305	1/1	0.88	0.15	55,55,55,55	0
2	EDO	В	301	4/4	0.90	0.10	55,57,60,62	0
6	GOL	A	308	6/6	0.93	0.09	60,65,66,69	0
4	MG	A	305	1/1	0.96	0.14	55,55,55,55	0
3	ZN	В	302	1/1	0.98	0.10	46,46,46,46	0
5	CL	A	307	1/1	0.98	0.07	39,39,39,39	0
3	ZN	A	302	1/1	0.98	0.09	47,47,47,47	0
7	NI	A	309	1/1	0.98	0.07	55,55,55,55	0
7	NI	В	308	1/1	0.98	0.08	53,53,53,53	0
3	ZN	В	304	1/1	0.99	0.12	38,38,38,38	0
5	CL	В	306	1/1	0.99	0.09	38,38,38,38	0
5	CL	В	307	1/1	0.99	0.07	39,39,39,39	0
3	ZN	A	303	1/1	0.99	0.14	39,39,39,39	0
3	ZN	В	303	1/1	0.99	0.12	40,40,40,40	0
5	CL	A	306	1/1	0.99	0.08	39,39,39,39	0
3	ZN	A	304	1/1	1.00	0.12	38,38,38,38	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 B 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





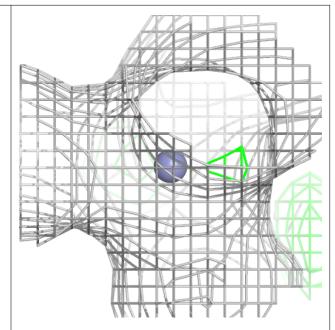


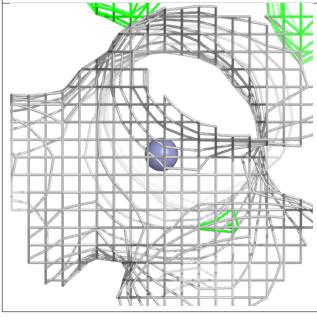
Electron density around ZN B 304: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

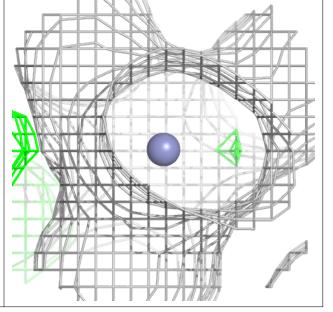


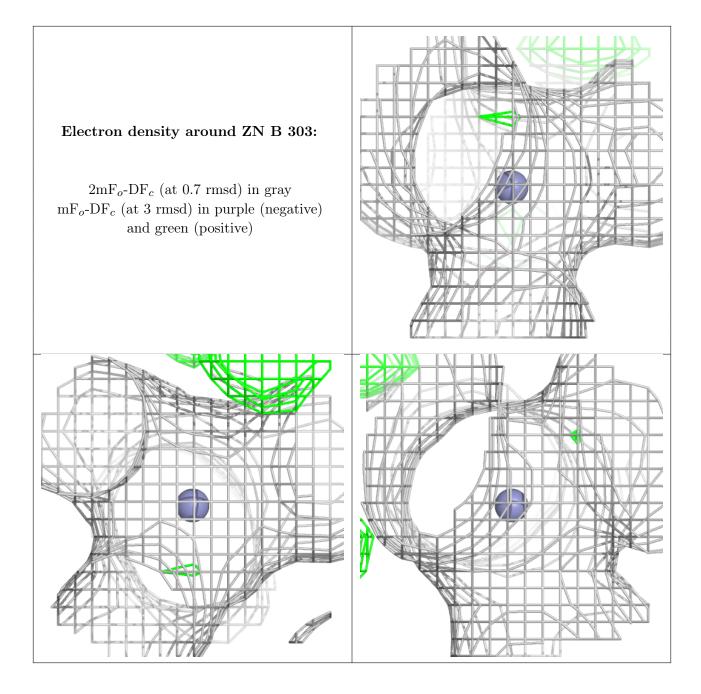
Electron density around ZN A 303:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

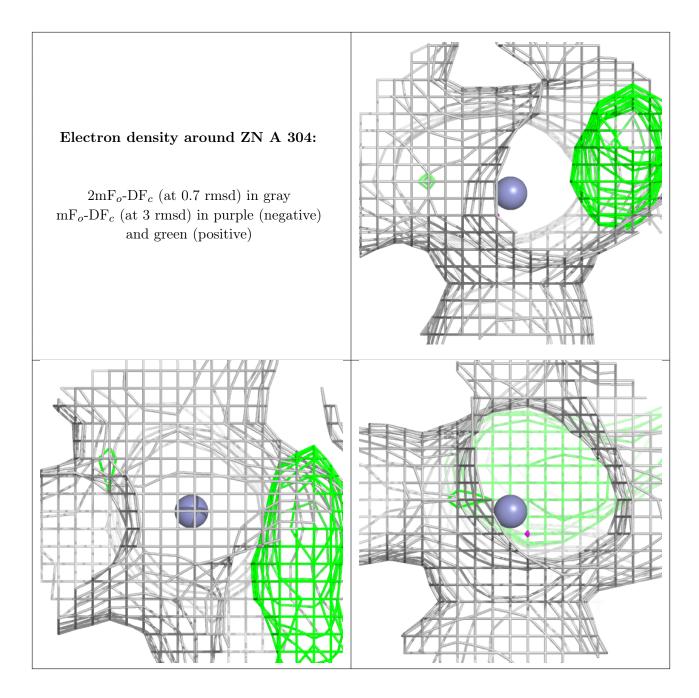












6.5 Other polymers (i)

There are no such residues in this entry.

