

wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 12:26 PM EDT

PDB ID : 8F1B

Title : Structure of zinc-bound ZrgA deletion 124-184 from Vibrio cholerae

Authors: Valencia, D.W.; Yukl, E.T.

Deposited on : 2022-11-04

Resolution : 2.41 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: 4.02b-467

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

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

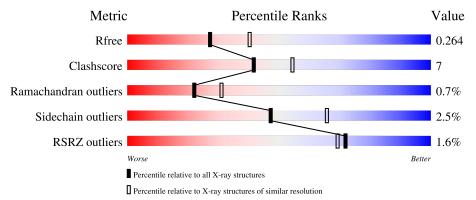
Validation Pipeline (wwPDB-VP) : 2.36

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 2.41 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	160	72%	13%	15%
	71	100	%	1370	1370
1	В	160	74%	11%	15%
1	С	160	78%	14%	9%
1	D	160	74%	17%	• 8%
1	Е	160	69%	14% •	15%

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Mol	Chain	Length	Quality of chair	1	
1	F	160	64%	19%	16%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6793 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 Zinc-binding protein.

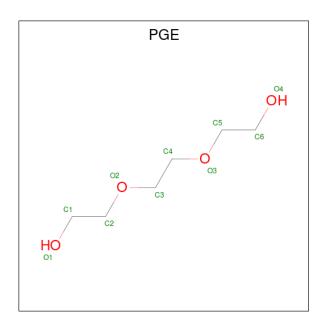
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	136	Total	С	N	О	S	0	0	0
1	Λ	150	1082	684	187	209	2	0	U	0
1	В	136	Total	С	N	О	S	0	0	0
1	Ъ	150	1082	684	187	209	2	0	U	U
1	С	146	Total	С	N	О	S	0	0	0
1		140	1164	735	202	225	2	U	O	U
1	D	147	Total	С	N	О	S	0	0	0
1	D	141	1172	739	203	228	2	0	U	0
1	Е	136	Total	С	N	O	S	0	0	0
1	ш	150	1082	684	187	209	2	0	U	U
1	F	135	Total	С	N	О	S	0	1	0
1	I.	199	1084	686	187	209	2	U	1	U

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Zn 3 3	0	0
2	В	4	Total Zn 4 4	0	0
2	С	4	Total Zn 4 4	0	0
2	D	4	Total Zn 4 4	0	0
2	E	3	Total Zn 3 3	0	0
2	F	3	Total Zn 3 3	0	0

• Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	В	1	Total 10	C 6	O 4	0	0

• Molecule 4 is water.

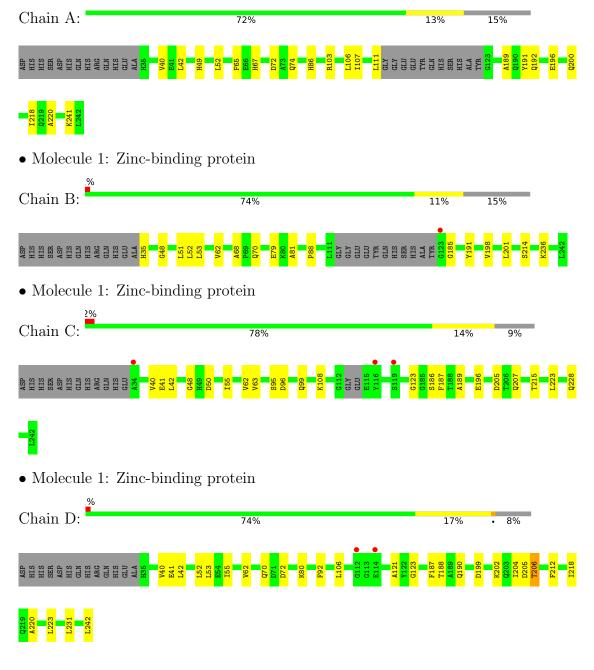
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total O 26 26	0	0
4	В	22	Total O 22 22	0	0
4	С	18	Total O 18 18	0	0
4	D	13	Total O 13 13	0	0
4	E	5	Total O 5 5	0	0
4	F	12	Total O 12 12	0	0



3 Residue-property plots (i)

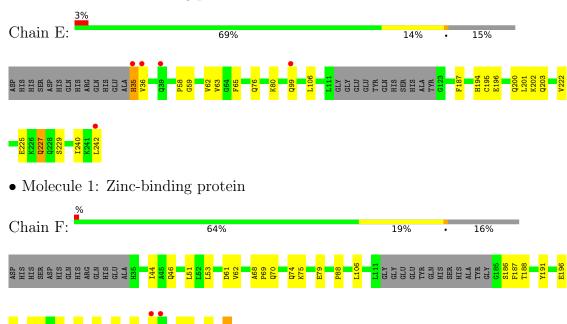
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Zinc-binding protein





• Molecule 1: Zinc-binding protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	81.99Å 66.91Å 88.24Å	Depositor
a, b, c, α , β , γ	90.00° 99.92° 90.00°	Depositor
Resolution (Å)	46.67 - 2.41	Depositor
resolution (A)	46.63 - 2.41	EDS
% Data completeness	99.2 (46.67-2.41)	Depositor
(in resolution range)	99.2 (46.63-2.41)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.32 (at 2.42Å)	Xtriage
Refinement program	REFMAC 7.1.018	Depositor
P.P.	0.218 , 0.262	Depositor
R, R_{free}	0.225 , 0.264	DCC
R_{free} test set	1734 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 34.3	EDS
L-test for twinning ²	$ < L > = 0.51, < L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6793	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.94% 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: ZN, PGE

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	0.62	0/1102	0.70	0/1488	
1	В	0.59	0/1102	0.70	0/1488	
1	С	0.62	0/1188	0.72	0/1605	
1	D	0.60	0/1197	0.70	0/1618	
1	Е	0.60	0/1102	0.71	0/1488	
1	F	0.60	0/1107	0.70	0/1495	
All	All	0.60	0/6798	0.70	0/9182	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Е	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Е	227	GLN	Peptide

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



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the ass	zmmetric	11n1t	whereas S	Symm-	Liashes	LISTS ST	vmmetry	v-related	clashes
UIIC COD	y IIIIII OUI IO	aiii o,	WITCICOD	\cup y IIIIII	CIUDIICO	110000	y IIIIIIC UI	y iciauca	CIGOTICO.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1082	0	1060	14	0
1	В	1082	0	1060	10	1
1	С	1164	0	1123	14	1
1	D	1172	0	1128	18	0
1	Ε	1082	0	1060	19	1
1	F	1084	0	1065	21	0
2	A	3	0	0	0	0
2	В	4	0	0	0	0
2	С	4	0	0	0	0
2	D	4	0	0	0	0
2	Ε	3	0	0	0	0
2	F	3	0	0	0	1
3	В	10	0	14	0	0
4	A	26	0	0	2	0
4	В	22	0	0	0	0
4	С	18	0	0	0	0
4	D	13	0	0	0	0
4	Е	5	0	0	0	0
4	F	12	0	0	1	0
All	All	6793	0	6510	92	2

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 7.

The worst 5 of 92 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\mbox{\normalfont\AA}) \end{aligned}$
1:F:210:GLN:NE2	4:F:401:HOH:O	1.86	1.03
1:F:70:GLN:N	1:F:74:GLN:OE1	2.07	0.85
1:F:226:LYS:NZ	1:F:242:LEU:OXT	2.13	0.81
1:C:62:VAL:HG23	1:C:63:VAL:HG13	1.66	0.77
1:F:62:VAL:HG21	1:F:187:PHE:CD1	2.30	0.67

All (2) 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	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:B:79:GLU:OE2	2:F:303:ZN:ZN[1_455]	1.69	0.51
1:C:50:ASP:OD2	1:E:225:GLU:OE1[2_555]	2.19	0.01



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	entiles
1	A	132/160 (82%)	130 (98%)	2 (2%)	0	100	100
1	В	132/160 (82%)	128 (97%)	3 (2%)	1 (1%)	19	27
1	С	142/160 (89%)	129 (91%)	10 (7%)	3 (2%)	7	7
1	D	145/160 (91%)	132 (91%)	11 (8%)	2 (1%)	11	14
1	E	132/160 (82%)	125 (95%)	7 (5%)	0	100	100
1	F	132/160 (82%)	127 (96%)	5 (4%)	0	100	100
All	All	815/960 (85%)	771 (95%)	38 (5%)	6 (1%)	22	31

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	206	THR
1	С	99	GLN
1	D	123	GLY
1	С	48	GLY
1	С	123	GLY

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	Analysed Rotameric Outliers		Percentiles
1	A	116/136 (85%)	113 (97%)	3 (3%)	46 64
1	В	116/136 (85%)	114 (98%)	2 (2%)	60 77
1	С	123/136 (90%)	120 (98%)	3 (2%)	49 67

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Mol	Chain	Analysed	Rotameric	Rotameric Outliers	
1	D	124/136 (91%)	121 (98%)	3 (2%)	49 67
1	E	116/136 (85%)	115 (99%)	1 (1%)	78 89
1	F	117/136 (86%)	110 (94%)	7 (6%)	19 30
All	All	712/816 (87%)	693 (97%)	19 (3%)	47 63

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	188	THR
1	F	217	LYS
1	F	242	LEU
1	F	207[B]	GLN
1	D	70	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	Е	39	GLN
1	Е	46	GLN
1	Е	49	HIS

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 22 ligands modelled in this entry, 21 are monoatomic - leaving 1 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	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PGE	В	301	-	9,9,9	0.20	0	8,8,8	0.08	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
3	PGE	В	301	-	-	2/7/7/7	-

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
3	В	301	PGE	O2-C3-C4-O3
3	В	301	PGE	C4-C3-O2-C2

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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	136/160 (85%)	-0.23	0 100 100	22, 33, 49, 66	0
1	В	136/160 (85%)	-0.19	1 (0%) 87 86	21, 35, 49, 75	0
1	С	146/160 (91%)	0.05	3 (2%) 63 60	23, 38, 72, 111	0
1	D	147/160 (91%)	0.00	2 (1%) 75 73	26, 40, 69, 88	0
1	E	136/160 (85%)	0.34	5 (3%) 41 40	28, 48, 85, 103	0
1	F	135/160 (84%)	0.02	2 (1%) 73 71	30, 48, 71, 97	0
All	All	836/960 (87%)	-0.00	13 (1%) 72 69	21, 40, 71, 111	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	35	HIS	4.5
1	С	34	ALA	4.0
1	Е	39	GLN	3.6
1	С	116	TYR	3.6
1	Е	36	VAL	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)

There are no monosaccharides in this entry.



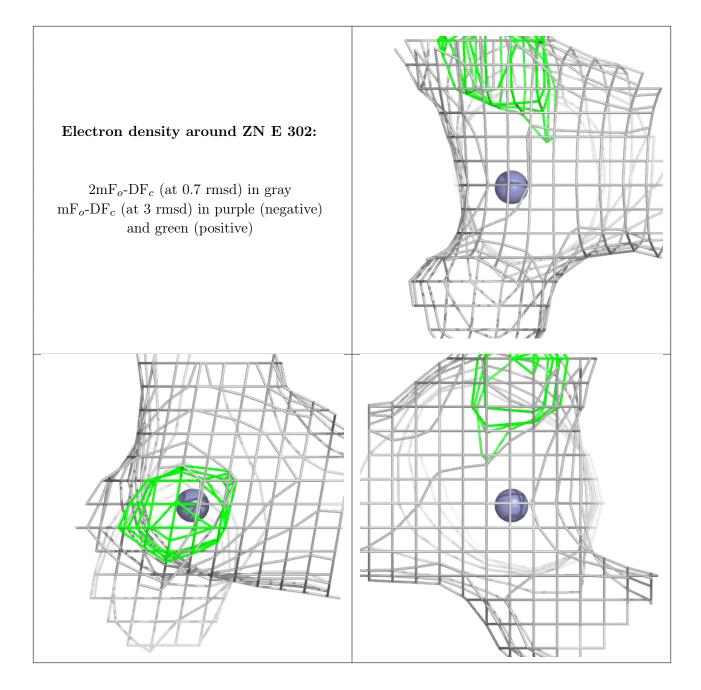
6.4 Ligands (i)

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	${f B ext{-}factors}({f \AA}^2)$	Q<0.9
3	PGE	В	301	10/10	0.72	0.18	61,80,90,93	0
2	ZN	Ε	302	1/1	0.88	0.22	80,80,80,80	1
2	ZN	С	304	1/1	0.91	0.07	55,55,55,55	1
2	ZN	С	303	1/1	0.93	0.07	54,54,54,54	1
2	ZN	D	304	1/1	0.93	0.07	52,52,52,52	1
2	ZN	D	303	1/1	0.95	0.08	51,51,51,51	1
2	ZN	Ε	303	1/1	0.97	0.08	60,60,60,60	1
2	ZN	В	305	1/1	0.97	0.05	51,51,51,51	1
2	ZN	В	303	1/1	0.98	0.09	62,62,62,62	1
2	ZN	F	301	1/1	0.98	0.07	43,43,43,43	1
2	ZN	F	302	1/1	0.98	0.06	62,62,62,62	1
2	ZN	В	304	1/1	0.98	0.08	39,39,39,39	0
2	ZN	Ε	301	1/1	0.99	0.09	33,33,33,33	0
2	ZN	В	302	1/1	0.99	0.08	40,40,40,40	0
2	ZN	A	302	1/1	0.99	0.07	34,34,34,34	0
2	ZN	D	301	1/1	0.99	0.12	43,43,43,43	0
2	ZN	С	301	1/1	0.99	0.10	31,31,31,31	0
2	ZN	F	303	1/1	0.99	0.09	49,49,49,49	0
2	ZN	С	302	1/1	0.99	0.08	38,38,38,38	0
2	ZN	A	303	1/1	1.00	0.09	33,33,33,33	0
2	ZN	A	301	1/1	1.00	0.08	32,32,32,32	0
2	ZN	D	302	1/1	1.00	0.05	33,33,33,33	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.

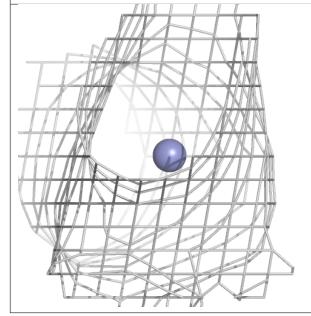


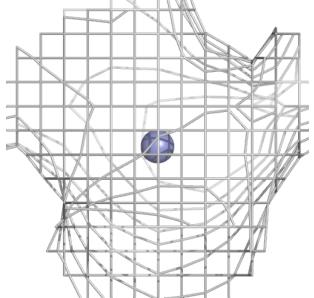




Electron density around ZN C 304:

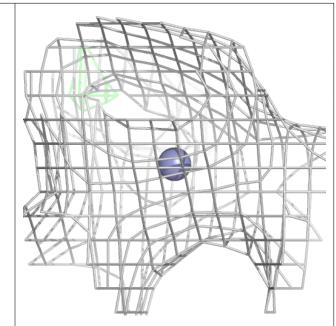


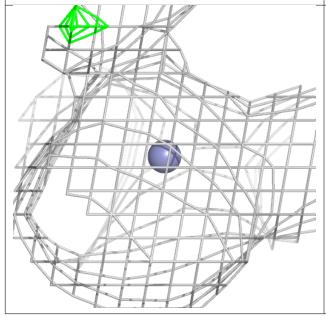


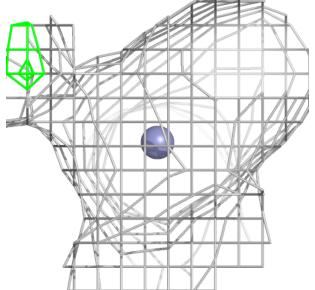




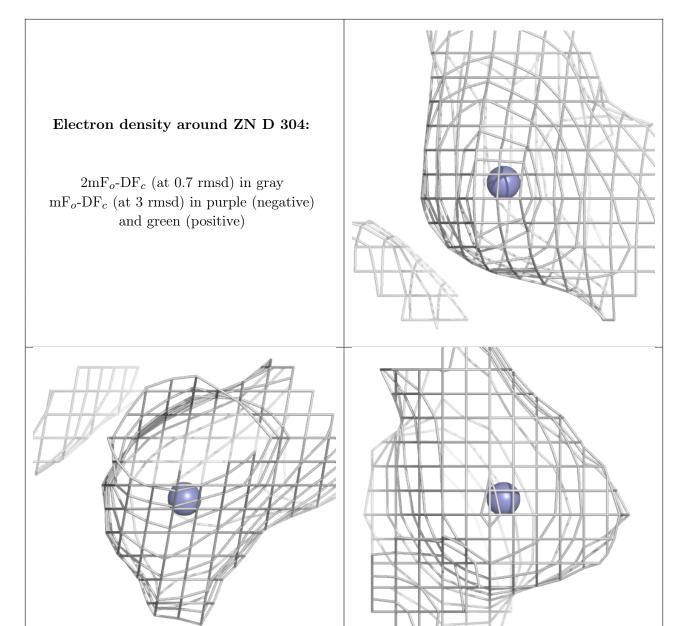
Electron density around ZN C 303:



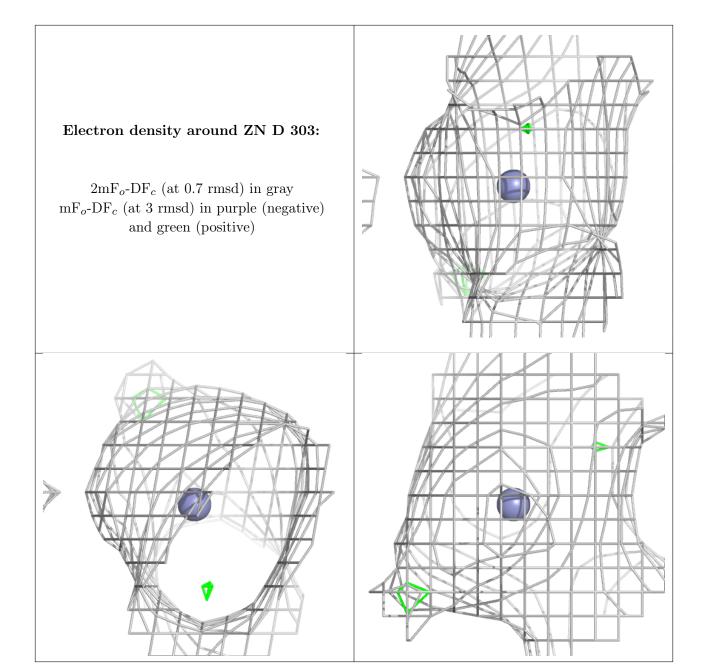






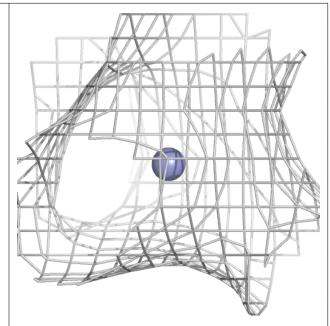


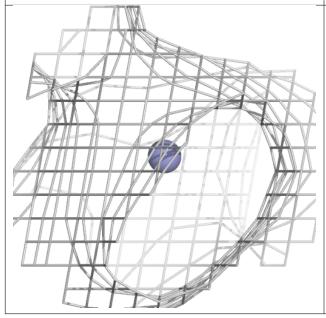


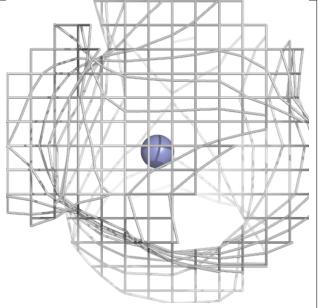




Electron density around ZN E 303:





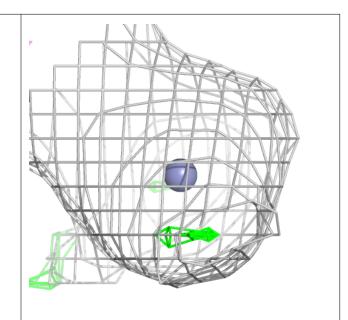


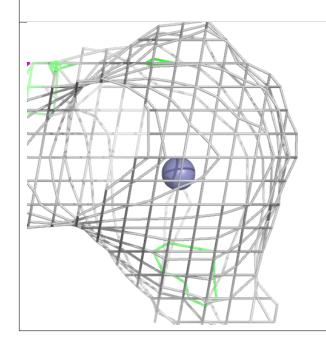


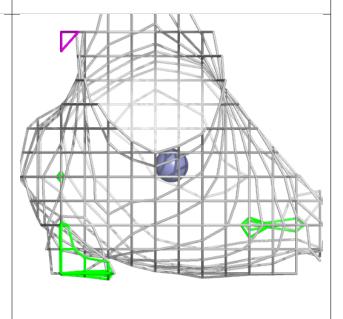
Electron density around ZN B 305: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZN B 303:









Electron density around ZN F 301: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

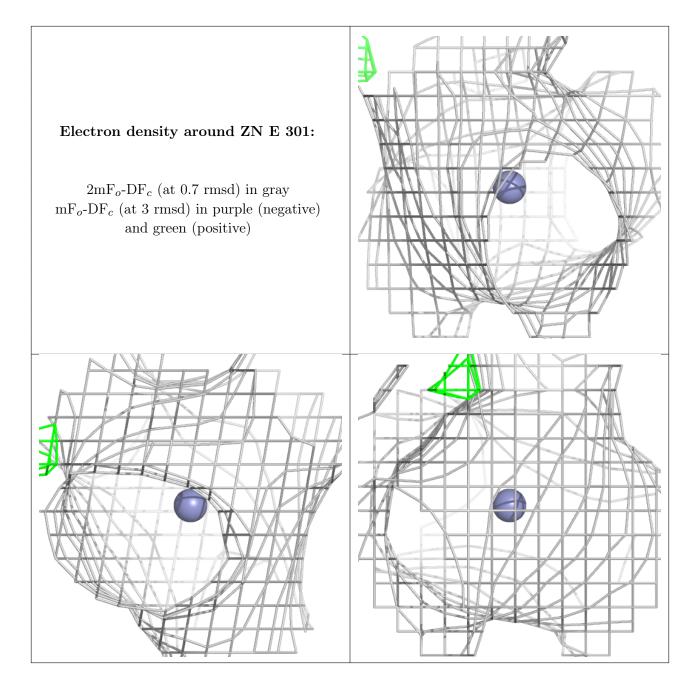


Electron density around ZN F 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



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)





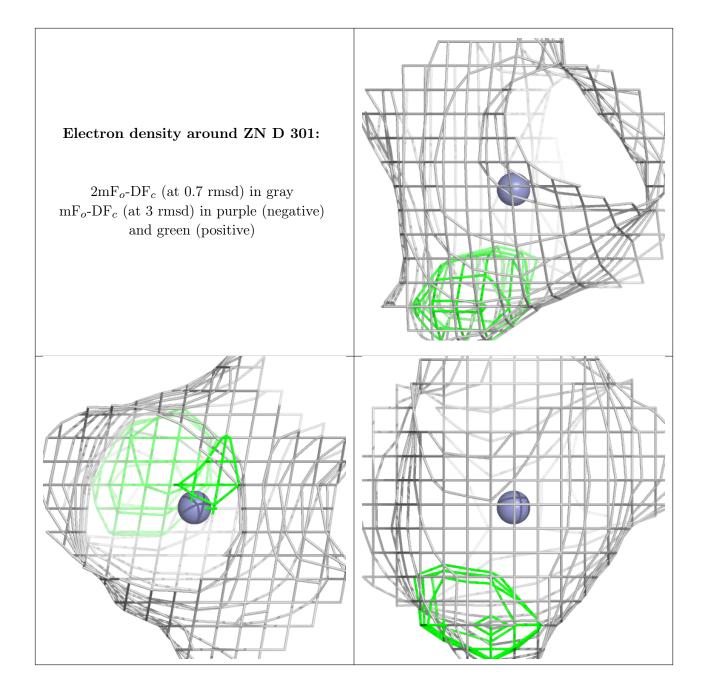


Electron density around ZN B 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZN A 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)





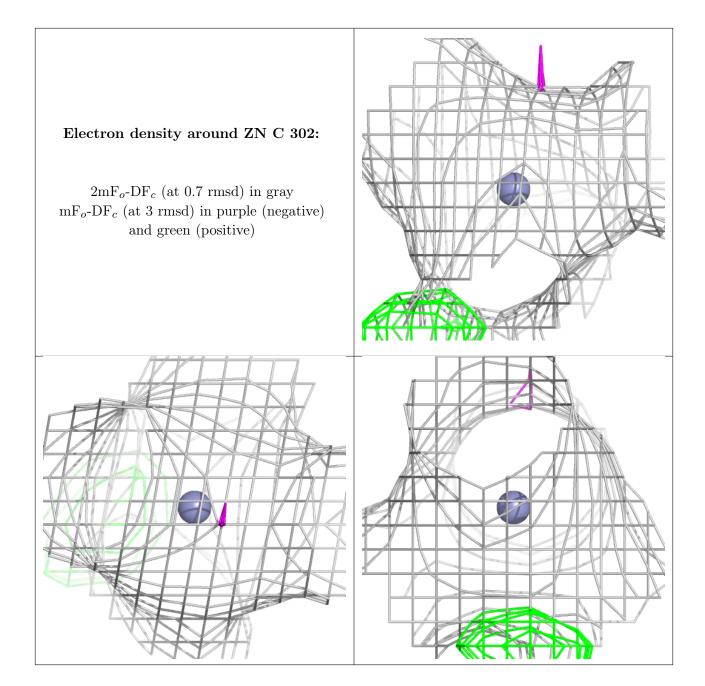


Electron density around ZN C 301: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZN F 303: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





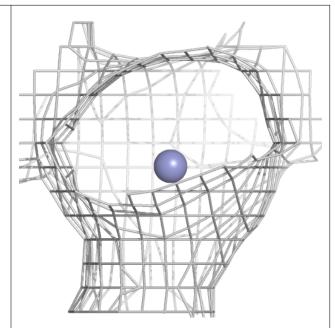


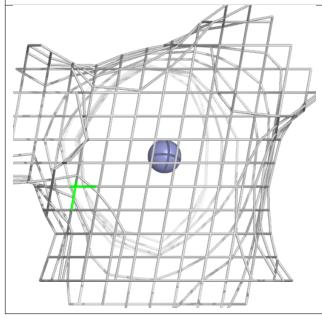
Electron density around ZN A 303: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_{o}\text{-}\mathrm{DF}_{c}$ (at 3 rmsd) in purple (negative) and green (positive)

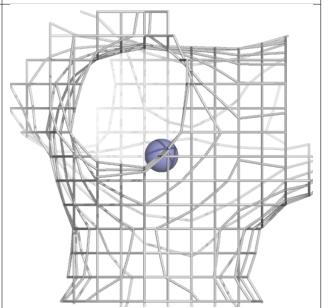


Electron density around ZN A 301:

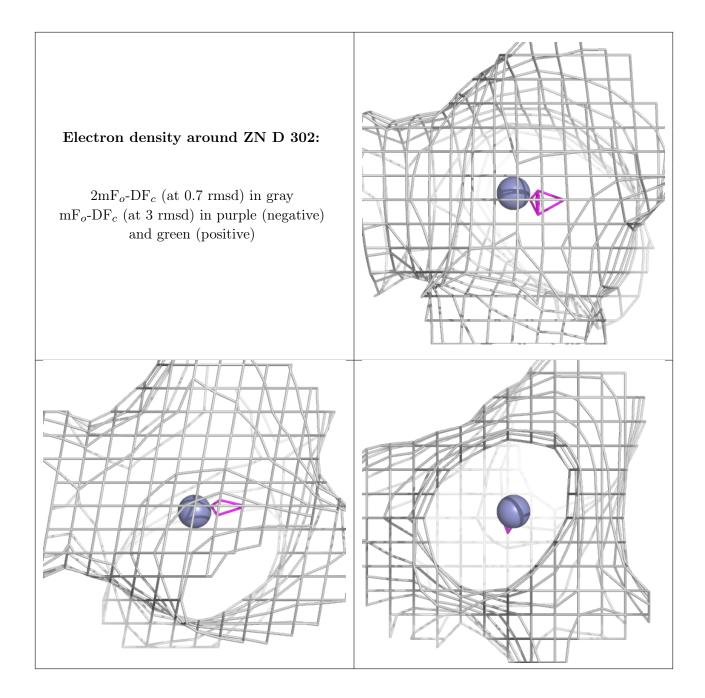
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

