



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 10, 2026 – 07:06 pm BST

PDB ID : 30KY / pdb\_000030ky  
Title : Complex of Colletotrichum higginsianum effector protein ChEC108 with HMA domain 2 (HMA2) of HIP6 from Arabidopsis thaliana.  
Authors : Turley, E.K.; Bentham, A.R.; Banfield, M.J.; Faulkner, C.  
Deposited on : 2026-05-01  
Resolution : 2.20 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](mailto: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>.

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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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

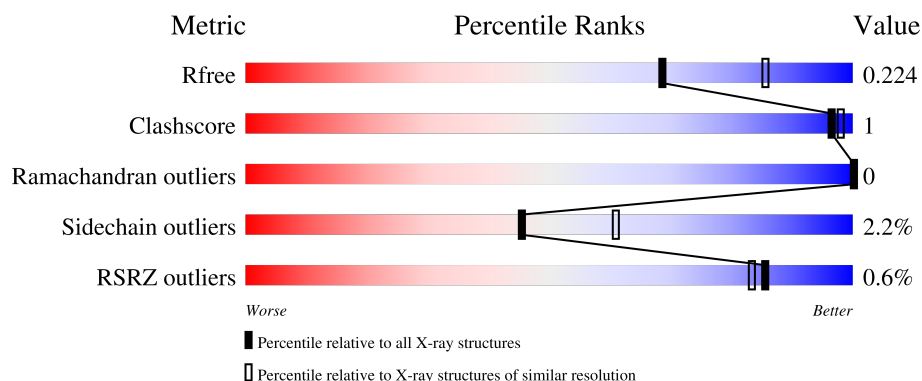
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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  $\geq 3$ , 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	C	75	 84% 8% 8%
1	D	75	 84% 9% 7%
2	B	194	 87% 6% 7%
2	E	194	 86% 7% 7%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4397 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 Heavy metal-associated isoprenylated plant protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	70	Total	C	N	O	S	0	0	0
			544	348	96	98	2			
1	C	69	Total	C	N	O	S	0	0	0
			535	342	94	97	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	149	GLY	-	expression tag	UNP Q9LZF1
D	150	PRO	-	expression tag	UNP Q9LZF1
D	151	MET	-	expression tag	UNP Q9LZF1
C	149	GLY	-	expression tag	UNP Q9LZF1
C	150	PRO	-	expression tag	UNP Q9LZF1
C	151	MET	-	expression tag	UNP Q9LZF1

- Molecule 2 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1495	956	255	278	6			
2	E	181	Total	C	N	O	S	0	0	0
			1495	956	255	278	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	MET	-	initiating methionine	UNP A0A1B7Y7K7
E	20	MET	-	initiating methionine	UNP A0A1B7Y7K7

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0
5	E	1	Total 1	Cl 1	0	0


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	28	Total 28	O 28	0	0
6	B	128	Total 128	O 128	0	0
6	E	104	Total 104	O 104	0	0
6	C	32	Total 32	O 32	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: Heavy metal-associated isoprenylated plant protein 6

Chain D: 




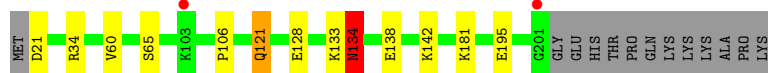
- Molecule 1: Heavy metal-associated isoprenylated plant protein 6

Chain C: 




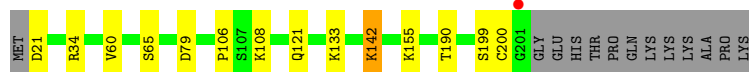
- Molecule 2: EF-hand domain-containing protein

Chain B: 



- Molecule 2: EF-hand domain-containing protein

Chain E: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.70Å 60.11Å 77.12Å 70.36° 89.72° 84.01°	Depositor
Resolution (Å)	72.60 – 2.20 72.59 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (72.60-2.20) 99.4 (72.59-2.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.172 , 0.221 0.180 , 0.224	Depositor DCC
$R_{free}$ test set	1663 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, CL, 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	C	0.70	0/539	1.26	3/725 (0.4%)
1	D	0.68	0/548	1.20	2/736 (0.3%)
2	B	0.71	0/1536	1.18	9/2065 (0.4%)
2	E	0.69	0/1536	1.19	7/2065 (0.3%)
All	All	0.70	0/4159	1.20	21/5591 (0.4%)

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	142	LYS	CB-CA-C	-8.17	94.16	110.42
1	C	179	LYS	CB-CA-C	-7.51	100.56	109.80
2	E	34	ARG	N-CA-CB	6.81	120.13	110.12
2	B	133	LYS	N-CA-CB	6.67	120.03	110.16
2	B	142	LYS	CB-CA-C	-6.63	95.70	110.21

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	C	535	0	590	1	0
1	D	544	0	603	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1495	0	1454	3	0
2	E	1495	0	1454	3	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	20	0	30	0	0
4	E	12	0	18	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	B	128	0	0	0	0
6	C	32	0	0	1	0
6	D	28	0	0	0	0
6	E	104	0	0	1	0
All	All	4397	0	4149	8	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 1.

The worst 5 of 8 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)
2:E:65:SER:HB3	2:E:106:PRO:HA	1.91	0.52
2:B:65:SER:HB3	2:B:106:PRO:HA	1.91	0.51
2:E:108:LYS:HD2	2:E:190:THR:HG21	1.96	0.46
2:E:142:LYS:HE2	6:E:429:HOH:O	2.15	0.46
1:C:170:LYS:NZ	6:C:403:HOH:O	2.50	0.44

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	C	67/75 (89%)	65 (97%)	2 (3%)	0	100	100
1	D	68/75 (91%)	66 (97%)	2 (3%)	0	100	100
2	B	179/194 (92%)	174 (97%)	5 (3%)	0	100	100
2	E	179/194 (92%)	172 (96%)	7 (4%)	0	100	100
All	All	493/538 (92%)	477 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	C	63/68 (93%)	61 (97%)	2 (3%)	34	47
1	D	64/68 (94%)	61 (95%)	3 (5%)	23	31
2	B	159/170 (94%)	157 (99%)	2 (1%)	61	76
2	E	159/170 (94%)	156 (98%)	3 (2%)	50	66
All	All	445/476 (94%)	435 (98%)	10 (2%)	45	61

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	199	SER
1	C	161	LYS
1	C	165	GLU
2	B	121	GLN
2	B	134	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	115	ASN
2	B	121	GLN
2	E	75	GLN

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Mol	Chain	Res	Type
1	C	176	ASN

### 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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z  > 2$
4	EDO	E	302	-	3,3,3	0.18	0	2,2,2	0.45	0
4	EDO	B	305	-	3,3,3	0.32	0	2,2,2	0.65	0
4	EDO	B	301	-	3,3,3	0.31	0	2,2,2	0.78	0
4	EDO	E	301	-	3,3,3	0.31	0	2,2,2	0.28	0
4	EDO	B	302	-	3,3,3	0.36	0	2,2,2	0.28	0
4	EDO	B	303	-	3,3,3	0.45	0	2,2,2	0.37	0
4	EDO	B	304	-	3,3,3	0.15	0	2,2,2	0.61	0
4	EDO	E	303	-	3,3,3	0.08	0	2,2,2	0.03	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
4	EDO	E	302	-	-	1/1/1/1	-
4	EDO	B	305	-	-	1/1/1/1	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	E	301	-	-	0/1/1/1	-
4	EDO	B	302	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	E	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	305	EDO	O1-C1-C2-O2
4	E	302	EDO	O1-C1-C2-O2
4	E	303	EDO	O1-C1-C2-O2
4	B	301	EDO	O1-C1-C2-O2
4	B	304	EDO	O1-C1-C2-O2

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	69/75 (92%)	-0.25	0 <a href="#">100</a> <a href="#">100</a>	30, 42, 60, 65	0
1	D	70/75 (93%)	-0.10	0 <a href="#">100</a> <a href="#">100</a>	33, 50, 75, 85	0
2	B	181/194 (93%)	-0.39	2 (1%) <a href="#">78</a> <a href="#">76</a>	27, 38, 63, 99	0
2	E	181/194 (93%)	-0.29	1 (0%) <a href="#">85</a> <a href="#">83</a>	29, 42, 73, 100	0
All	All	501/538 (93%)	-0.30	3 (0%) <a href="#">85</a> <a href="#">83</a>	27, 42, 70, 100	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	201	GLY	3.7
2	E	201	GLY	2.5
2	B	103	LYS	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](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

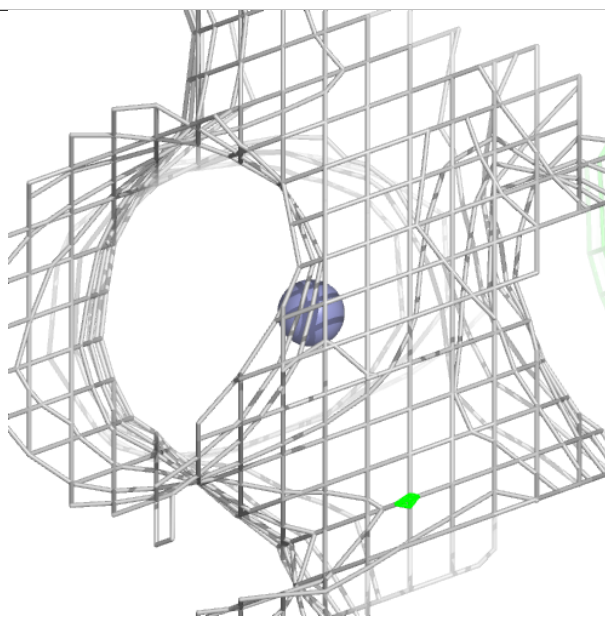
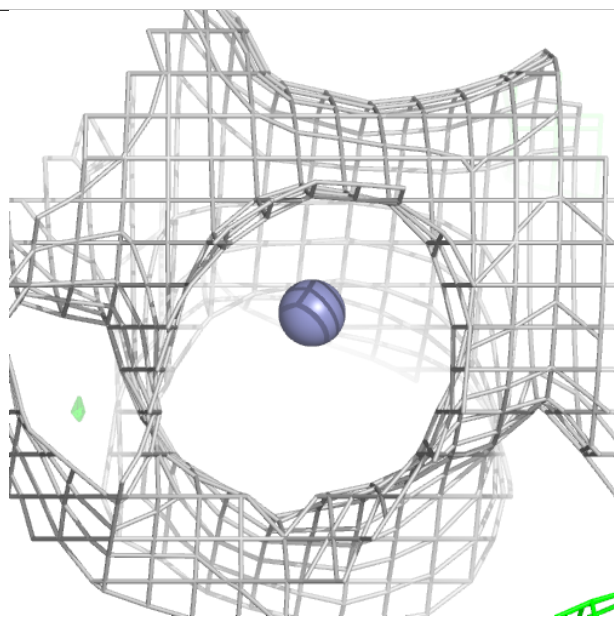
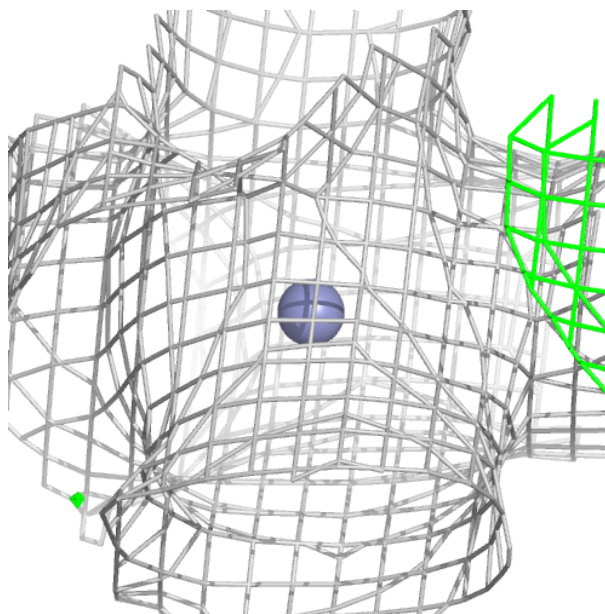
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

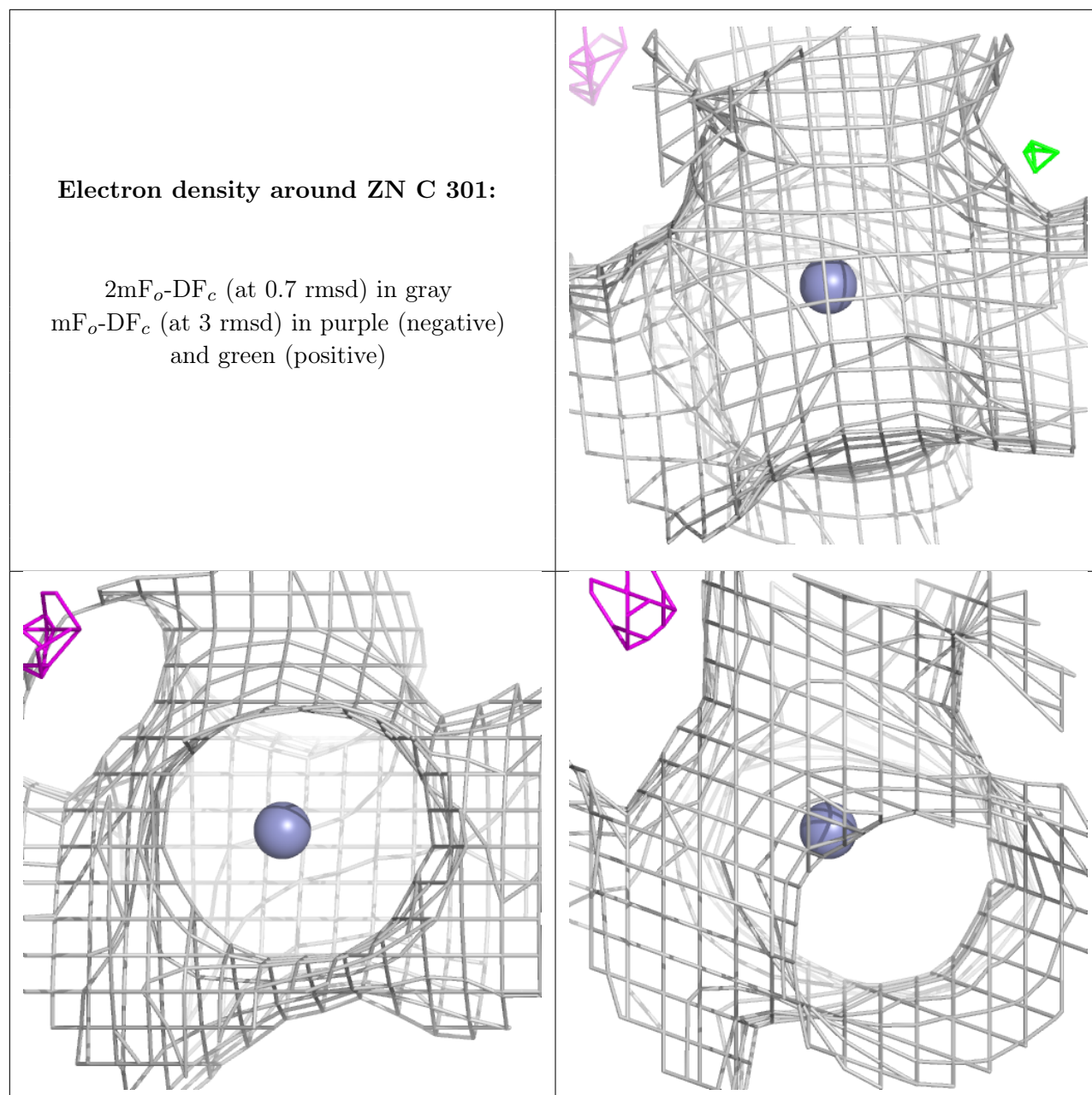
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	305	4/4	0.81	0.16	62,63,66,69	0
4	EDO	E	301	4/4	0.85	0.15	39,49,53,55	0
4	EDO	B	304	4/4	0.87	0.12	30,40,41,43	0
5	CL	E	304	1/1	0.87	0.14	75,75,75,75	0
4	EDO	E	303	4/4	0.89	0.12	43,44,46,51	0
4	EDO	E	302	4/4	0.90	0.10	54,58,58,60	0
4	EDO	B	303	4/4	0.90	0.15	51,53,57,58	0
4	EDO	B	302	4/4	0.90	0.11	41,43,44,51	0
5	CL	B	306	1/1	0.91	0.10	83,83,83,83	0
4	EDO	B	301	4/4	0.91	0.11	52,57,59,61	0
3	ZN	D	301	1/1	1.00	0.01	33,33,33,33	0
3	ZN	C	301	1/1	1.00	0.01	28,28,28,28	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 D 301:**

$2mF_o-DF_c$  (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.