



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 03:32 AM BST

PDB ID : 7BP1
Title : Crystal structure of 2, 3-dihydroxybenzoic acid decarboxylase from *Fusarium oxysporum* in complex with Catechol
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Deposited on : 2020-03-21
Resolution : 1.97 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

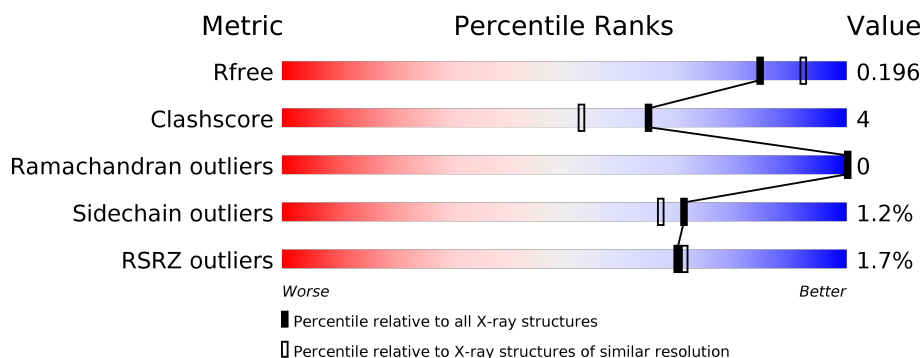
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 on 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	A	343	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 87% 10% </div> </div>
1	B	343	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, orange 0%, yellow 12%, green 88%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 86% 12% </div> </div>
1	C	343	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 11%, green 85%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 87% 11% </div> </div>
1	D	343	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 14%, green 80%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 82% 14% </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	C	402	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12008 atoms, of which 18 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 2,3-dihydroxybenzoate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2709	1746	462	492	9			
1	B	336	Total	C	N	O	S	0	0	0
			2709	1746	462	492	9			
1	C	335	Total	C	N	O	S	0	0	0
			2701	1742	461	489	9			
1	D	331	Total	C	N	O	S	0	0	0
			2665	1720	456	480	9			

There are 28 discrepancies between the modelled and reference sequences:

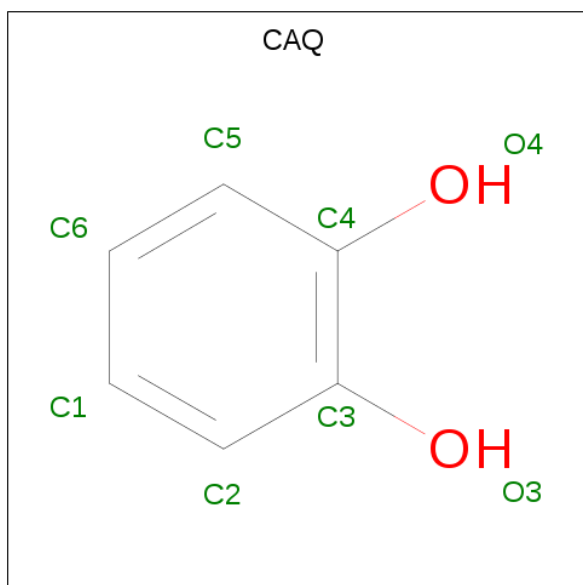
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP A0A420U2F4
A	338	HIS	-	expression tag	UNP A0A420U2F4
A	339	HIS	-	expression tag	UNP A0A420U2F4
A	340	HIS	-	expression tag	UNP A0A420U2F4
A	341	HIS	-	expression tag	UNP A0A420U2F4
A	342	HIS	-	expression tag	UNP A0A420U2F4
A	343	HIS	-	expression tag	UNP A0A420U2F4
B	1	HIS	-	expression tag	UNP A0A420U2F4
B	338	HIS	-	expression tag	UNP A0A420U2F4
B	339	HIS	-	expression tag	UNP A0A420U2F4
B	340	HIS	-	expression tag	UNP A0A420U2F4
B	341	HIS	-	expression tag	UNP A0A420U2F4
B	342	HIS	-	expression tag	UNP A0A420U2F4
B	343	HIS	-	expression tag	UNP A0A420U2F4
C	1	HIS	-	expression tag	UNP A0A420U2F4
C	338	HIS	-	expression tag	UNP A0A420U2F4
C	339	HIS	-	expression tag	UNP A0A420U2F4
C	340	HIS	-	expression tag	UNP A0A420U2F4
C	341	HIS	-	expression tag	UNP A0A420U2F4
C	342	HIS	-	expression tag	UNP A0A420U2F4
C	343	HIS	-	expression tag	UNP A0A420U2F4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	HIS	-	expression tag	UNP A0A420U2F4
D	338	HIS	-	expression tag	UNP A0A420U2F4
D	339	HIS	-	expression tag	UNP A0A420U2F4
D	340	HIS	-	expression tag	UNP A0A420U2F4
D	341	HIS	-	expression tag	UNP A0A420U2F4
D	342	HIS	-	expression tag	UNP A0A420U2F4
D	343	HIS	-	expression tag	UNP A0A420U2F4

- Molecule 2 is CATECHOL (three-letter code: CAQ) (formula: $C_6H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	6	6	2		
2	C	1	Total	C	H	O	0	0
			14	6	6	2		
2	D	1	Total	C	H	O	0	0
			14	6	6	2		

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

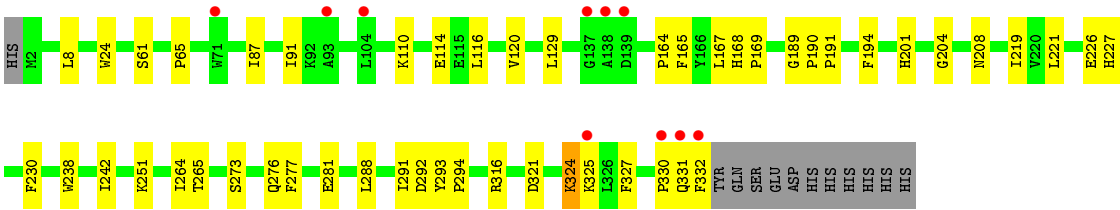
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	284	Total 284	O 284	0	0
4	B	340	Total 340	O 340	0	0
4	C	284	Total 284	O 284	0	0
4	D	273	Total 273	O 273	0	0

- Molecule 1: 2,3-dihydroxybenzoate decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.02Å 131.37Å 141.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.87 – 1.97 24.87 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.87-1.97) 99.7 (24.87-1.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.96Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.166 , 0.196 0.167 , 0.196	Depositor DCC
R_{free} test set	5072 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12008	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: ZN, CAQ

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	A	0.39	0/2790	0.52	0/3790
1	B	0.36	0/2790	0.53	0/3790
1	C	0.40	0/2782	0.53	0/3779
1	D	0.47	0/2745	0.57	0/3729
All	All	0.41	0/11107	0.54	0/15088

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	2709	0	2621	19	0
1	B	2709	0	2621	25	0
1	C	2701	0	2617	19	0
1	D	2665	0	2589	29	0
2	A	8	6	6	0	0
2	C	8	6	6	0	0
2	D	8	6	6	0	0
3	C	1	0	0	0	0
4	A	284	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	340	0	0	5	0
4	C	284	0	0	4	0
4	D	273	0	0	1	0
All	All	11990	18	10466	88	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 4.

The worst 5 of 88 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:D:164:PRO:HG2	1:D:327:PHE:CE1	2.33	0.63
1:B:74:LYS:HE3	4:B:699:HOH:O	1.99	0.61
1:C:165:PHE:HB3	1:C:219:ILE:HD13	1.84	0.59
1:B:238:TRP:CZ3	1:B:242:ILE:HD13	2.39	0.58
1:D:324:LYS:HD2	1:D:332:PHE:CE2	2.39	0.57

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	A	334/343 (97%)	321 (96%)	13 (4%)	0	100	100
1	B	334/343 (97%)	322 (96%)	12 (4%)	0	100	100
1	C	333/343 (97%)	319 (96%)	14 (4%)	0	100	100
1	D	329/343 (96%)	316 (96%)	13 (4%)	0	100	100
All	All	1330/1372 (97%)	1278 (96%)	52 (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	Outliers	Percentiles	
1	A	283/290 (98%)	280 (99%)	3 (1%)	73	70
1	B	283/290 (98%)	280 (99%)	3 (1%)	73	70
1	C	282/290 (97%)	277 (98%)	5 (2%)	59	51
1	D	278/290 (96%)	275 (99%)	3 (1%)	73	70
All	All	1126/1160 (97%)	1112 (99%)	14 (1%)	71	67

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	LEU
1	C	74	LYS
1	D	8	LEU
1	B	336	GLU
1	C	170	ARG

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

Mol	Chain	Res	Type
1	A	331	GLN
1	C	53	HIS
1	C	276	GLN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CAQ	C	401	3	8,8,8	1.03	1 (12%)	10,10,10	0.41	0
2	CAQ	D	401	-	8,8,8	1.05	1 (12%)	10,10,10	0.35	0
2	CAQ	A	401	-	8,8,8	1.04	1 (12%)	10,10,10	0.34	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	CAQ	C	401	3	-	-	0/1/1/1
2	CAQ	D	401	-	-	-	0/1/1/1
2	CAQ	A	401	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	CAQ	O3-C3	2.15	1.40	1.36
2	A	401	CAQ	O4-C4	2.12	1.40	1.36
2	C	401	CAQ	O3-C3	2.04	1.40	1.36

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	336/343 (97%)	-0.17	5 (1%) 73 75	19, 26, 38, 71	0
1	B	336/343 (97%)	-0.19	1 (0%) 94 94	20, 26, 41, 54	0
1	C	335/343 (97%)	-0.11	7 (2%) 63 65	19, 29, 42, 68	0
1	D	331/343 (96%)	0.12	10 (3%) 50 52	21, 31, 45, 73	0
All	All	1338/1372 (97%)	-0.09	23 (1%) 70 71	19, 28, 42, 73	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	ASP	6.2
1	C	138	ALA	6.0
1	C	330	PRO	4.8
1	A	331	GLN	4.7
1	D	331	GLN	4.7

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](#)

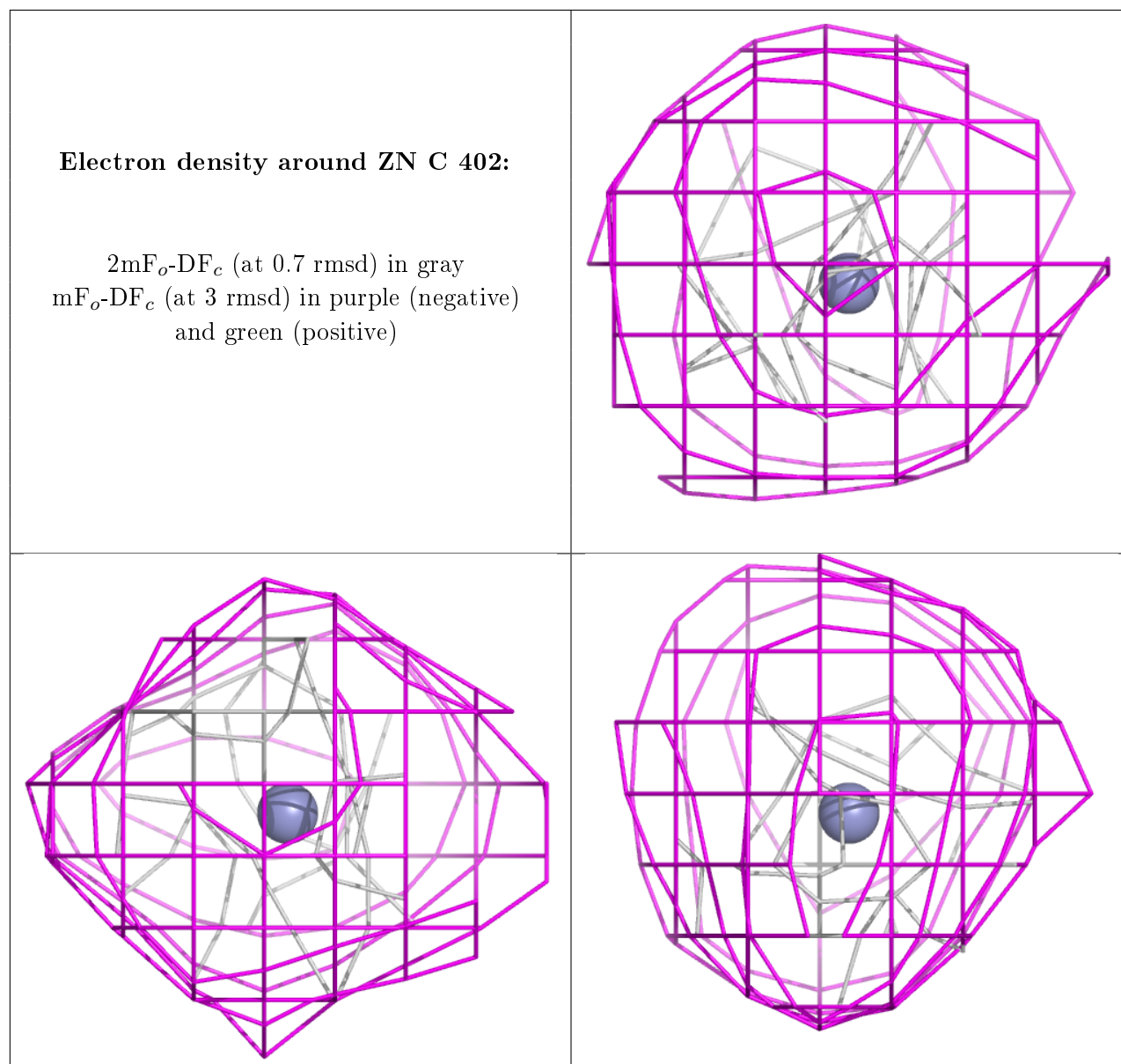
There are no monosaccharides in this entry.

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, 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(\AA^2)	Q<0.9
3	ZN	C	402	1/1	0.68	0.56	86,86,86,86	0
2	CAQ	A	401	8/8	0.94	0.10	26,29,35,39	0
2	CAQ	C	401	8/8	0.95	0.10	26,28,33,35	0
2	CAQ	D	401	8/8	0.96	0.08	29,33,38,40	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.