wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2024 – 12:27 pm GMT

PDB ID	:	9GKW
Title	:	Crystal Structure of Dimethoate hydrolase (DmhA) of Rhizorhabdus wittichii in complex with octanoic acid
Authors	:	Graf, L.G.; Schulze, S.; Palm, G.J.; Lammers, M.
Deposited on	:	2024-08-26
Resolution	:	2.10 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 (i)) were used in the production of this report:

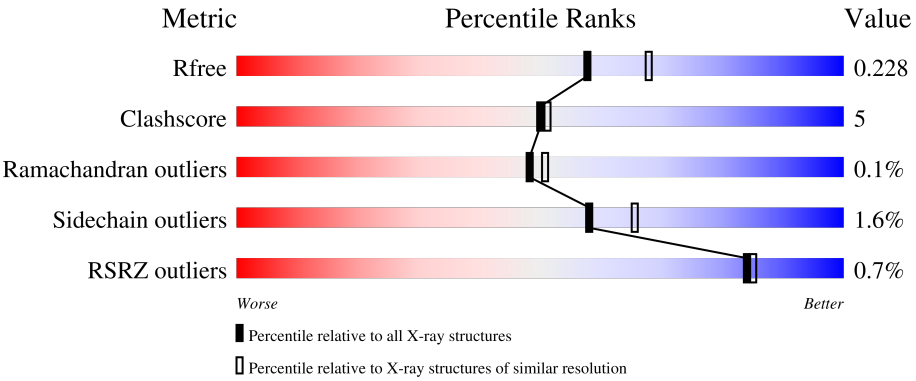
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	380	85% 11%
1	B	380	88% 9%
1	C	380	88% 9%
1	D	380	84% 12%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OCA	D	403	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12378 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 Dimethoate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	4	0
			2792	1763	494	521	14			
1	B	366	Total	C	N	O	S	0	3	0
			2785	1759	491	521	14			
1	C	369	Total	C	N	O	S	0	1	0
			2782	1758	490	519	15			
1	D	368	Total	C	N	O	S	1	5	0
			2817	1778	499	523	17			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP A0A067XIQ6
A	-9	ALA	-	expression tag	UNP A0A067XIQ6
A	-8	HIS	-	expression tag	UNP A0A067XIQ6
A	-7	HIS	-	expression tag	UNP A0A067XIQ6
A	-6	HIS	-	expression tag	UNP A0A067XIQ6
A	-5	HIS	-	expression tag	UNP A0A067XIQ6
A	-4	HIS	-	expression tag	UNP A0A067XIQ6
A	-3	HIS	-	expression tag	UNP A0A067XIQ6
A	-2	VAL	-	expression tag	UNP A0A067XIQ6
A	-1	GLY	-	expression tag	UNP A0A067XIQ6
A	0	THR	-	expression tag	UNP A0A067XIQ6
B	-10	MET	-	initiating methionine	UNP A0A067XIQ6
B	-9	ALA	-	expression tag	UNP A0A067XIQ6
B	-8	HIS	-	expression tag	UNP A0A067XIQ6
B	-7	HIS	-	expression tag	UNP A0A067XIQ6
B	-6	HIS	-	expression tag	UNP A0A067XIQ6
B	-5	HIS	-	expression tag	UNP A0A067XIQ6
B	-4	HIS	-	expression tag	UNP A0A067XIQ6
B	-3	HIS	-	expression tag	UNP A0A067XIQ6
B	-2	VAL	-	expression tag	UNP A0A067XIQ6
B	-1	GLY	-	expression tag	UNP A0A067XIQ6

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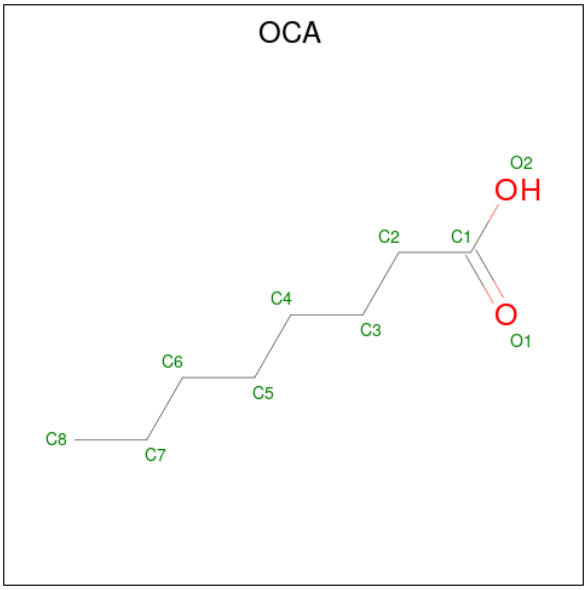
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	THR	-	expression tag	UNP A0A067XIQ6
C	-10	MET	-	initiating methionine	UNP A0A067XIQ6
C	-9	ALA	-	expression tag	UNP A0A067XIQ6
C	-8	HIS	-	expression tag	UNP A0A067XIQ6
C	-7	HIS	-	expression tag	UNP A0A067XIQ6
C	-6	HIS	-	expression tag	UNP A0A067XIQ6
C	-5	HIS	-	expression tag	UNP A0A067XIQ6
C	-4	HIS	-	expression tag	UNP A0A067XIQ6
C	-3	HIS	-	expression tag	UNP A0A067XIQ6
C	-2	VAL	-	expression tag	UNP A0A067XIQ6
C	-1	GLY	-	expression tag	UNP A0A067XIQ6
C	0	THR	-	expression tag	UNP A0A067XIQ6
D	-10	MET	-	initiating methionine	UNP A0A067XIQ6
D	-9	ALA	-	expression tag	UNP A0A067XIQ6
D	-8	HIS	-	expression tag	UNP A0A067XIQ6
D	-7	HIS	-	expression tag	UNP A0A067XIQ6
D	-6	HIS	-	expression tag	UNP A0A067XIQ6
D	-5	HIS	-	expression tag	UNP A0A067XIQ6
D	-4	HIS	-	expression tag	UNP A0A067XIQ6
D	-3	HIS	-	expression tag	UNP A0A067XIQ6
D	-2	VAL	-	expression tag	UNP A0A067XIQ6
D	-1	GLY	-	expression tag	UNP A0A067XIQ6
D	0	THR	-	expression tag	UNP A0A067XIQ6

- Molecule 2 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula: $C_8H_{16}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 8 2	0	0
2	B	1	Total C O 10 8 2	0	0
2	C	1	Total C O 10 8 2	0	0
2	D	1	Total C O 10 8 2	0	0

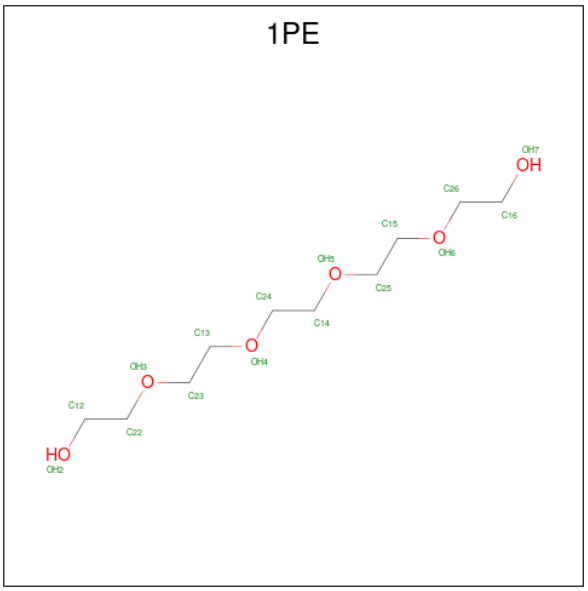
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total K 3 3	0	0
3	B	3	Total K 3 3	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 16 10 6	0	0
5	D	1	Total C O 16 10 6	0	0
5	D	1	Total C O 16 10 6	0	0

- Molecule 6 is water.

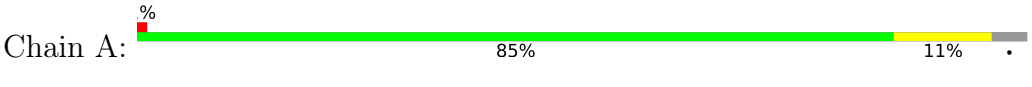
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	261	Total O 261 261	0	0
6	B	254	Total O 254 254	0	0
6	C	275	Total O 275 275	0	0
6	D	310	Total O 310 310	0	0

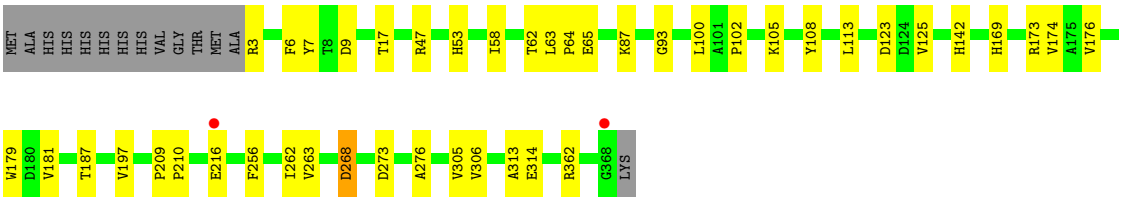
3 Residue-property plots (i)

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: Dimethoate hydrolase

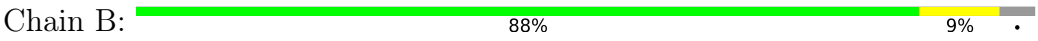
Chain A:

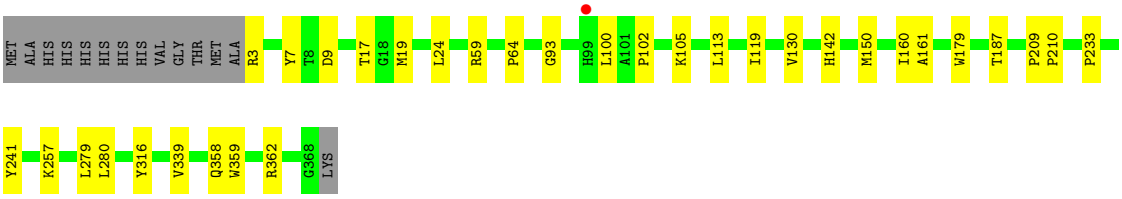




• Molecule 1: Dimethoate hydrolase

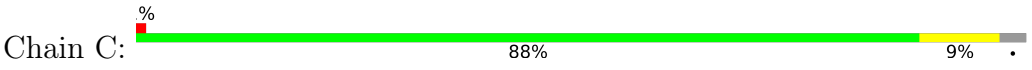
Chain B:

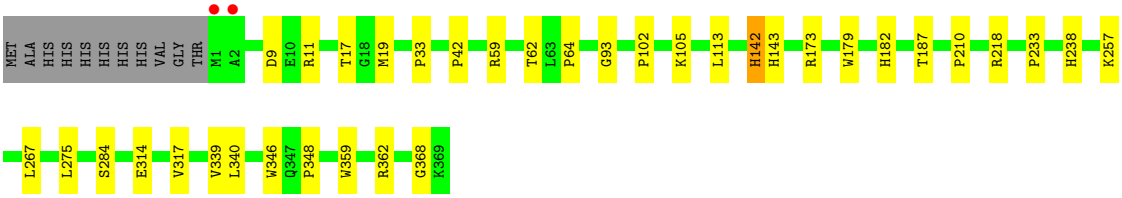




• Molecule 1: Dimethoate hydrolase

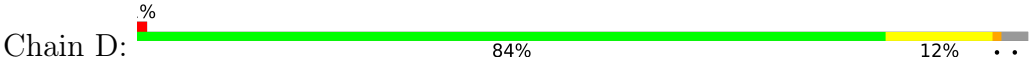
Chain C:

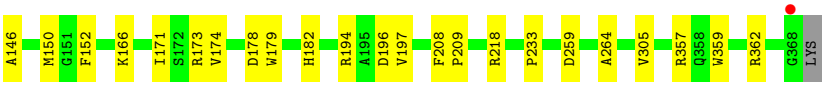




• Molecule 1: Dimethoate hydrolase

Chain D:




A146
M150
G151
F152
K166
I171
S172
R173
V174
D178
W179
H182
R194
A195
D196
V197
F208
P209
R218
P233
D259
A264
V305
R357
Q358
W359
R362
G368
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.62Å 144.03Å 92.96Å 90.00° 92.12° 90.00°	Depositor
Resolution (Å)	45.10 – 2.10 45.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.4 (45.10-2.10) 84.4 (45.10-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.169 , 0.224 0.176 , 0.228	Depositor DCC
R_{free} test set	5392 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12378	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, ZN, OCA, K

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	0.41	0/2865	0.64	0/3905
1	B	0.41	0/2855	0.62	0/3892
1	C	0.42	0/2851	0.64	0/3887
1	D	0.41	0/2886	0.66	0/3930
All	All	0.41	0/11457	0.64	0/15614

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

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	2792	0	2705	24	0
1	B	2785	0	2695	21	0
1	C	2782	0	2704	28	0
1	D	2817	0	2741	46	0
2	A	10	0	15	0	0
2	B	10	0	15	1	0
2	C	10	0	15	4	0
2	D	10	0	15	6	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	16	0	22	1	0
5	D	32	0	44	3	0
6	A	261	0	0	5	2
6	B	254	0	0	1	1
6	C	275	0	0	8	1
6	D	310	0	0	13	2
All	All	12378	0	10971	116	3

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 5.

The worst 5 of 116 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:357[A]:ARG:NH2	6:D:501:HOH:O	1.95	0.99
1:B:362:ARG:NH2	6:B:501:HOH:O	1.96	0.99
1:D:20:GLN:NE2	6:D:502:HOH:O	1.95	0.95
1:D:173:ARG:NH2	6:D:503:HOH:O	2.05	0.89
1:D:17:THR:O	6:D:502:HOH:O	1.99	0.80

All (3) 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)
6:A:708:HOH:O	6:B:713:HOH:O[1_556]	2.09	0.11
6:A:666:HOH:O	6:D:771:HOH:O[4_555]	2.16	0.04
6:C:1327:HOH:O	6:D:624:HOH:O[2_655]	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	A	368/380 (97%)	356 (97%)	12 (3%)	0	100	100
1	B	367/380 (97%)	353 (96%)	14 (4%)	0	100	100
1	C	368/380 (97%)	352 (96%)	15 (4%)	1 (0%)	37	37
1	D	371/380 (98%)	356 (96%)	14 (4%)	1 (0%)	37	37
All	All	1474/1520 (97%)	1417 (96%)	55 (4%)	2 (0%)	48	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	368	GLY
1	D	2	ALA

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	284/291 (98%)	278 (98%)	6 (2%)	48	55
1	B	283/291 (97%)	278 (98%)	5 (2%)	54	61
1	C	282/291 (97%)	278 (99%)	4 (1%)	62	70
1	D	286/291 (98%)	283 (99%)	3 (1%)	73	79
All	All	1135/1164 (98%)	1117 (98%)	18 (2%)	58	65

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	340	LEU
1	D	179	TRP
1	D	142	HIS
1	B	187	THR
1	C	187	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	D	99	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 14 are monoatomic - leaving 7 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	OCA	D	403	4	9,9,9	0.93	0	9,9,9	1.12	1 (11%)
5	1PE	D	401	-	15,15,15	0.28	0	14,14,14	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	1PE	C	402	-	15,15,15	0.29	0	14,14,14	0.20	0
5	1PE	D	402	-	15,15,15	0.30	0	14,14,14	0.43	0
2	OCA	C	401	4	9,9,9	1.04	1 (11%)	9,9,9	1.46	1 (11%)
2	OCA	A	401	4	9,9,9	1.01	1 (11%)	9,9,9	1.08	1 (11%)
2	OCA	B	401	4	9,9,9	0.88	0	9,9,9	0.76	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	OCA	D	403	4	-	6/7/7/7	-
5	1PE	D	401	-	-	7/13/13/13	-
5	1PE	C	402	-	-	8/13/13/13	-
5	1PE	D	402	-	-	6/13/13/13	-
2	OCA	C	401	4	-	5/7/7/7	-
2	OCA	A	401	4	-	4/7/7/7	-
2	OCA	B	401	4	-	4/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	OCA	C2-C1	2.35	1.56	1.50
2	A	401	OCA	C2-C1	2.24	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	OCA	C3-C2-C1	3.72	123.86	114.47
2	D	403	OCA	C3-C2-C1	2.64	121.12	114.47
2	A	401	OCA	C3-C2-C1	2.39	120.51	114.47

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	402	1PE	OH4-C13-C23-OH3
5	D	401	1PE	OH4-C13-C23-OH3

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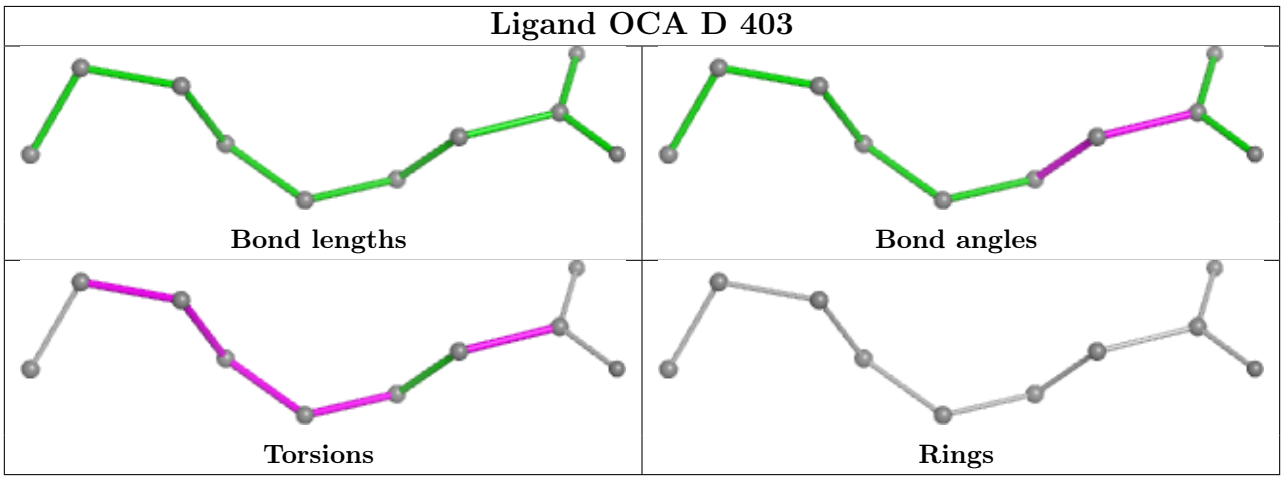
Mol	Chain	Res	Type	Atoms
5	C	402	1PE	OH7-C16-C26-OH6
2	A	401	OCA	C2-C3-C4-C5
2	A	401	OCA	C3-C4-C5-C6

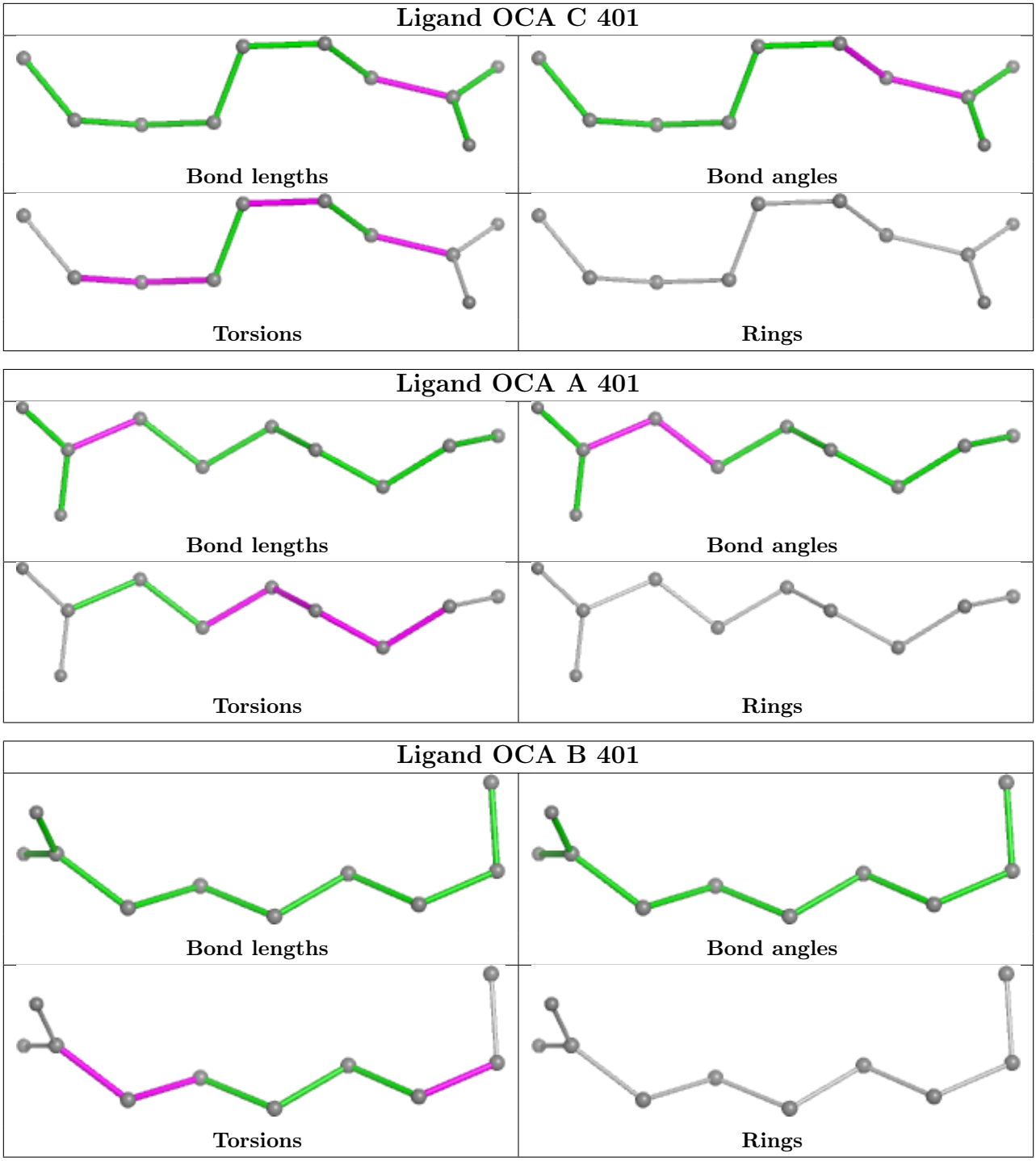
There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	403	OCA	6	0
5	D	401	1PE	1	0
5	C	402	1PE	1	0
5	D	402	1PE	3	0
2	C	401	OCA	4	0
2	B	401	OCA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

6.1 Protein, DNA and RNA chains

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(Å^2)	Q<0.9
1	A	366/380 (96%)	-0.45	2 (0%)	87	88	12, 21, 32, 50	4 (1%)
1	B	366/380 (96%)	-0.39	1 (0%)	90	91	10, 23, 36, 52	3 (0%)
1	C	369/380 (97%)	-0.42	2 (0%)	87	88	12, 22, 35, 77	1 (0%)
1	D	368/380 (96%)	-0.43	5 (1%)	73	74	10, 21, 33, 58	6 (1%)
All	All	1469/1520 (96%)	-0.42	10 (0%)	84	85	10, 22, 34, 77	14 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	4.6
1	D	2	ALA	4.4
1	D	368	GLY	3.7
1	A	368	GLY	3.4
1	D	3[A]	ARG	3.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

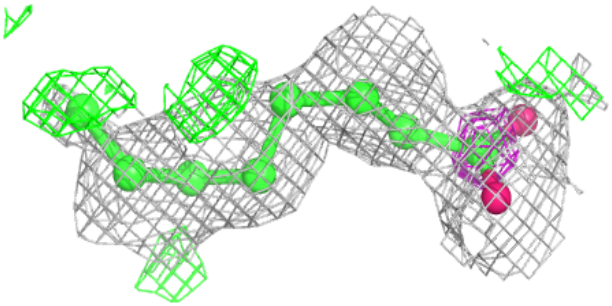
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

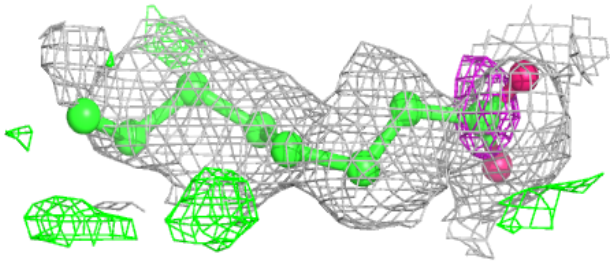
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	1PE	C	402	16/16	0.72	0.18	44,58,80,83	0
5	1PE	D	401	16/16	0.75	0.16	47,62,73,84	0
5	1PE	D	402	16/16	0.80	0.17	35,61,80,82	0
2	OCA	C	401	10/10	0.84	0.15	19,29,33,37	0
2	OCA	D	403	10/10	0.87	0.13	25,27,33,35	0
2	OCA	A	401	10/10	0.89	0.15	17,27,37,42	0
2	OCA	B	401	10/10	0.90	0.12	25,29,37,41	0
3	K	A	404	1/1	0.96	0.19	50,50,50,50	0
3	K	B	404	1/1	0.96	0.22	50,50,50,50	0
4	ZN	A	405	1/1	0.96	0.06	19,19,19,19	1
4	ZN	C	405	1/1	0.97	0.05	22,22,22,22	1
4	ZN	D	406	1/1	0.98	0.03	22,22,22,22	1
3	K	B	402	1/1	0.99	0.04	23,23,23,23	0
4	ZN	B	405	1/1	0.99	0.03	17,17,17,17	1
3	K	A	403	1/1	0.99	0.06	16,16,16,16	0
3	K	C	403	1/1	0.99	0.03	23,23,23,23	0
3	K	C	404	1/1	0.99	0.05	19,19,19,19	0
3	K	D	404	1/1	0.99	0.02	20,20,20,20	0
3	K	D	405	1/1	0.99	0.03	17,17,17,17	0
3	K	A	402	1/1	1.00	0.02	20,20,20,20	0
3	K	B	403	1/1	1.00	0.02	20,20,20,20	0

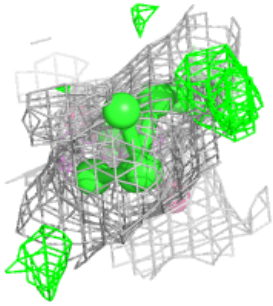
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OCA C 401:

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

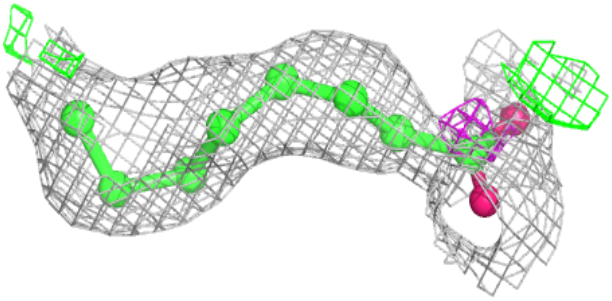


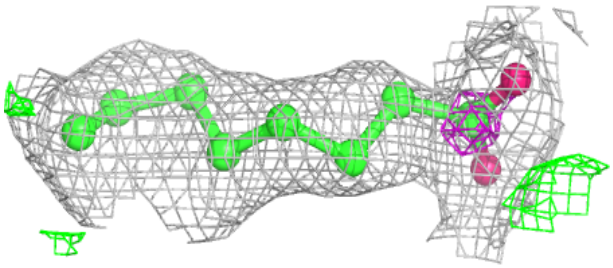


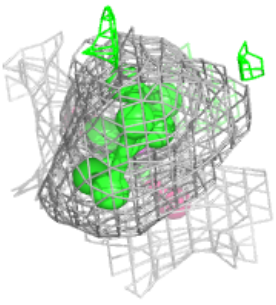


Electron density around OCA D 403:

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

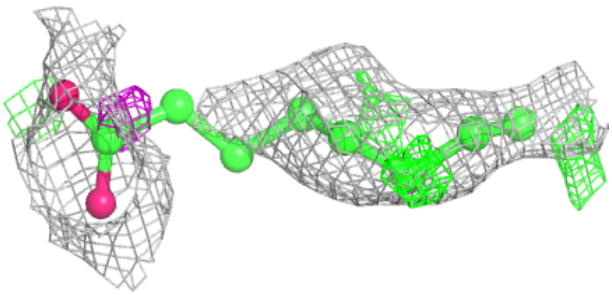


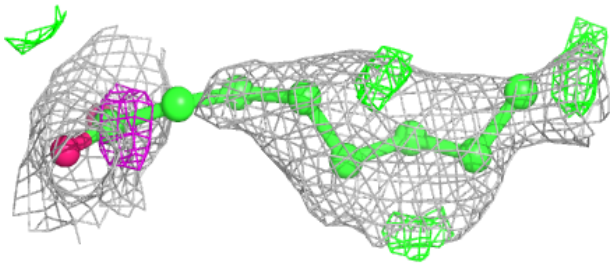


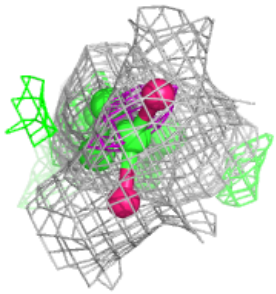


Electron density around OCA A 401:

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

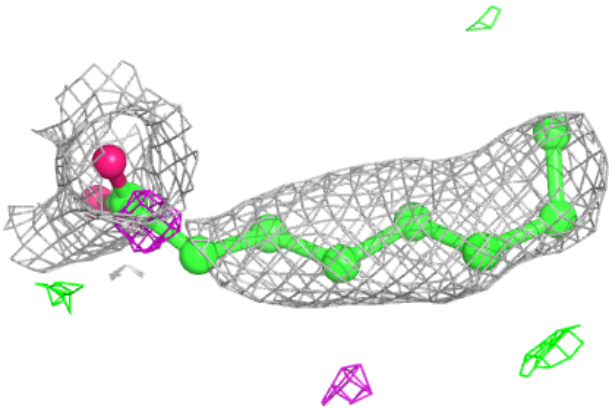


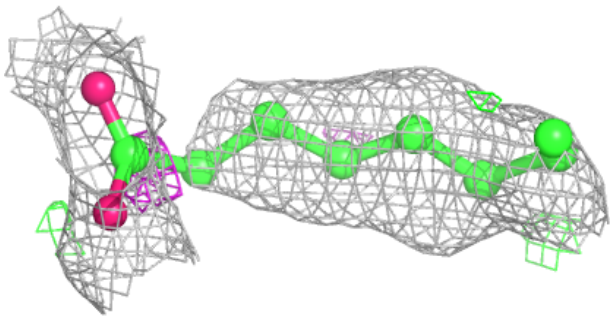


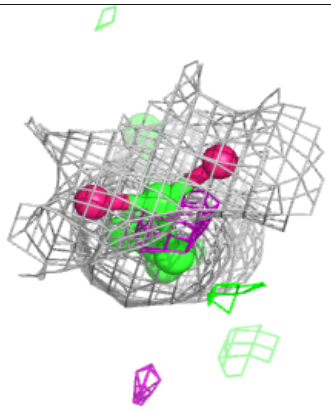


Electron density around OCA B 401:

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

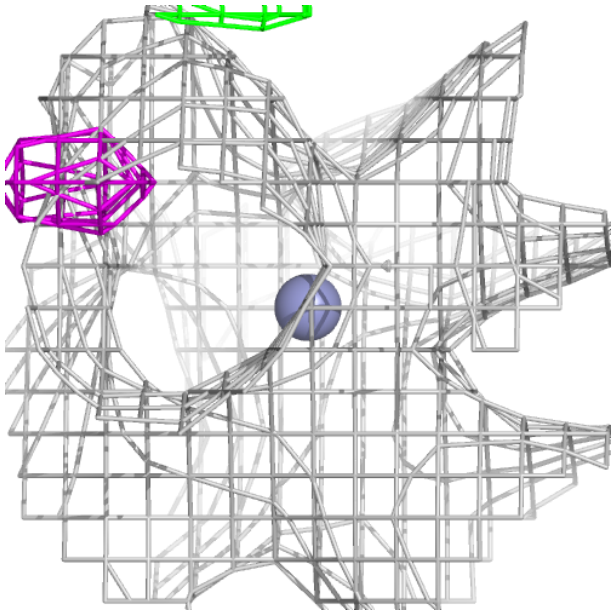


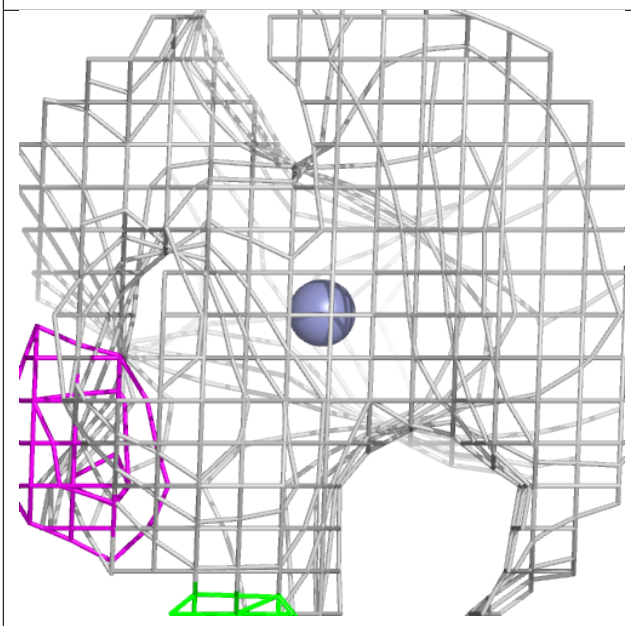


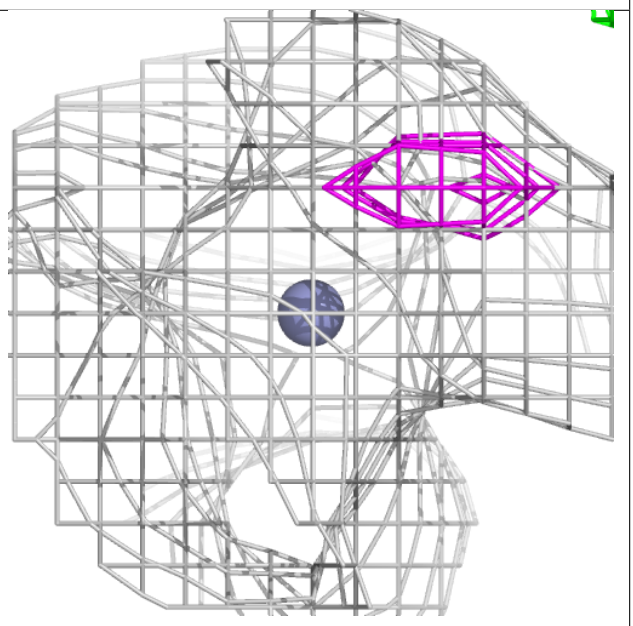


Electron density around ZN A 405:

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

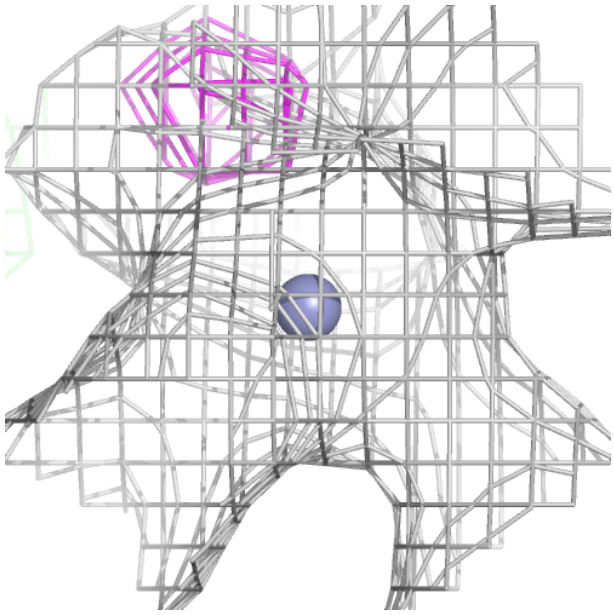


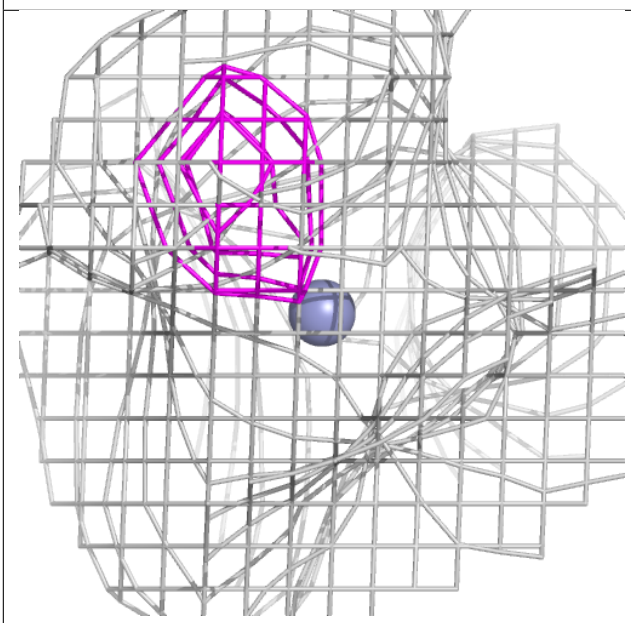


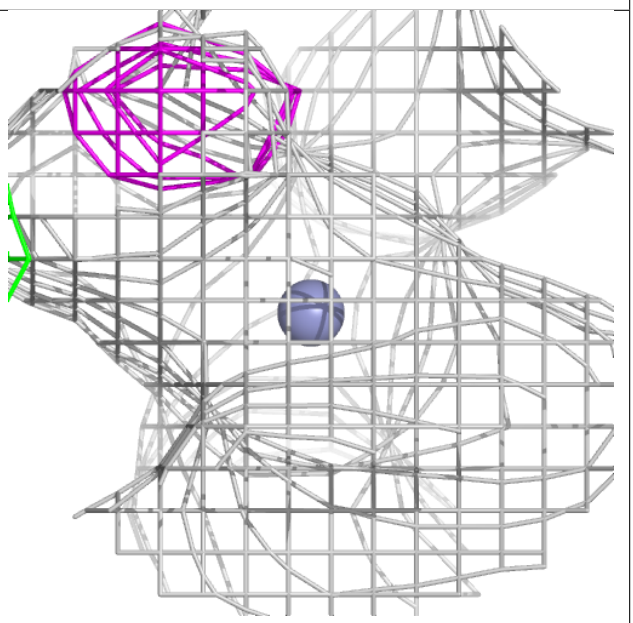


Electron density around ZN C 405:

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

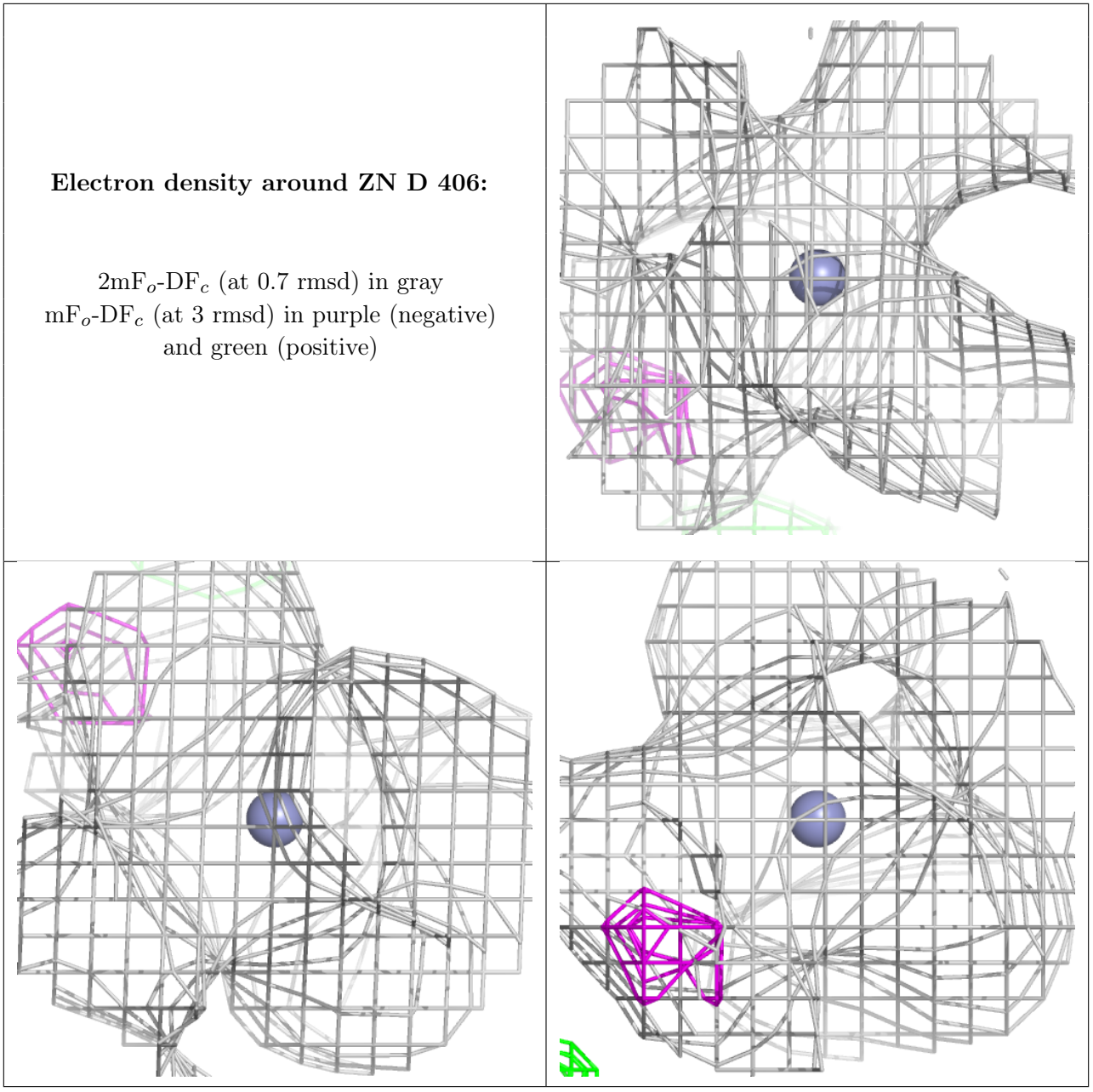






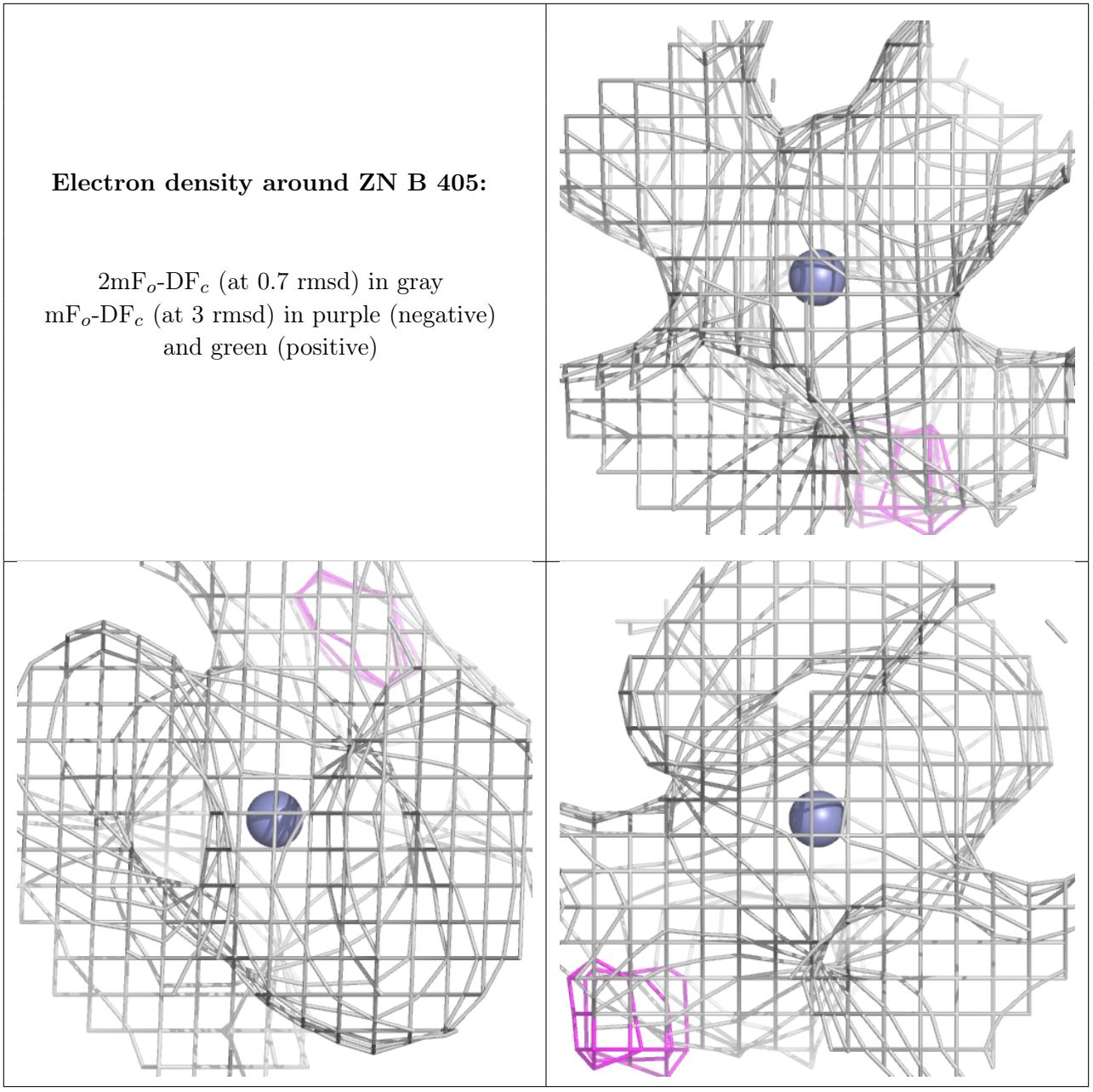
Electron density around ZN D 406:

$2mF_o$-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 405:

$2mF_o$-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.