wwPDB X-ray Structure Validation Summary Report (i)

Nov 23, 2023 – 02:37 AM JST

PDB ID	:	7YH3
Title	:	TRAPPC3 from Thorarchaeota SMTZ1-45
Authors	:	Robinson, R.C.; Tran, L.T.
Deposited on	:	2022-07-12
Resolution	:	1.70 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:

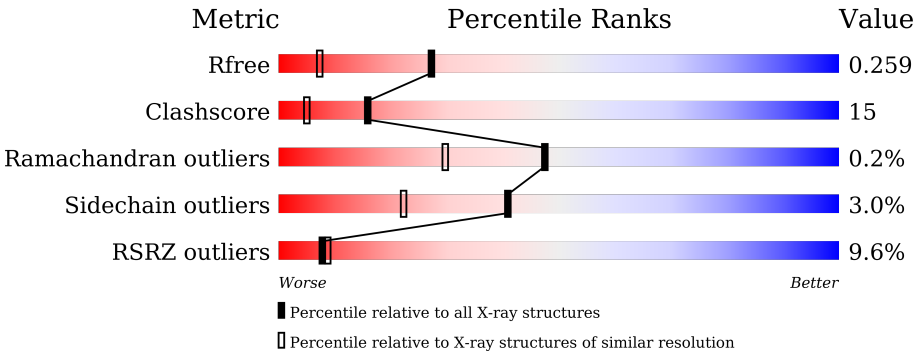
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	159	10% 77% 15% • 6%
1	B	159	4% 77% 20% •
1	C	159	13% 62% 32% • •
1	D	159	10% 71% 28% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5688 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 TRAPPC3 from Thorarchaeota SMTZ1-45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	1	0
			1203	760	200	236	7			
1	B	154	Total	C	N	O	S	0	4	0
			1258	795	207	248	8			
1	C	155	Total	C	N	O	S	0	2	0
			1249	788	207	247	7			
1	D	157	Total	C	N	O	S	0	2	0
			1264	798	209	249	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A135VRB8
A	0	PRO	-	expression tag	UNP A0A135VRB8
B	-1	GLY	-	expression tag	UNP A0A135VRB8
B	0	PRO	-	expression tag	UNP A0A135VRB8
C	-1	GLY	-	expression tag	UNP A0A135VRB8
C	0	PRO	-	expression tag	UNP A0A135VRB8
D	-1	GLY	-	expression tag	UNP A0A135VRB8
D	0	PRO	-	expression tag	UNP A0A135VRB8

- 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	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

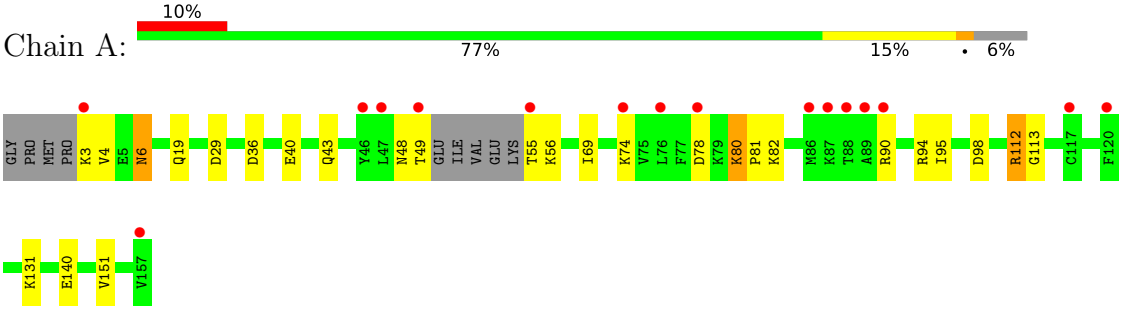
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	173	Total O 173 173	0	0
3	B	161	Total O 161 161	0	0
3	C	166	Total O 166 166	0	0
3	D	210	Total O 210 210	0	0

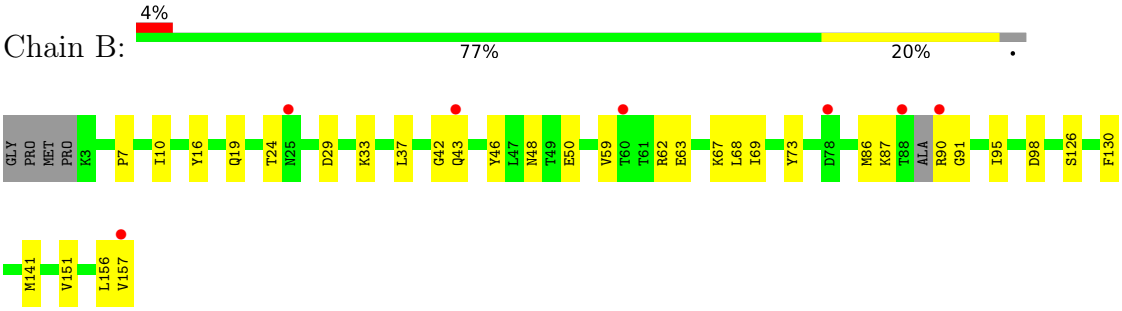
3 Residue-property plots (i)

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.

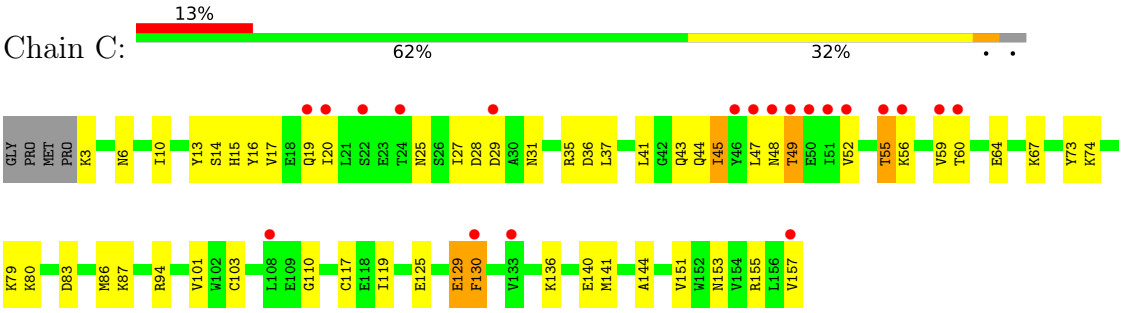
• Molecule 1: TRAPPC3 from Thorarchaeota SMTZ1-45



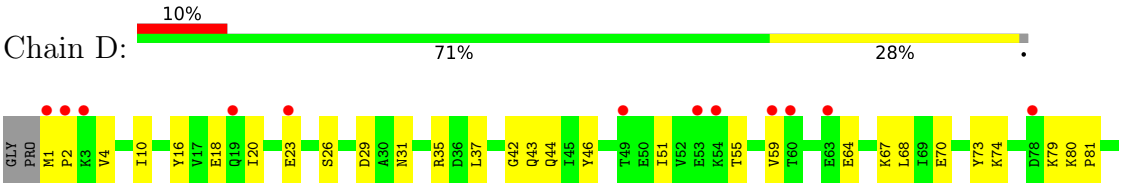
• Molecule 1: TRAPPC3 from Thorarchaeota SMTZ1-45

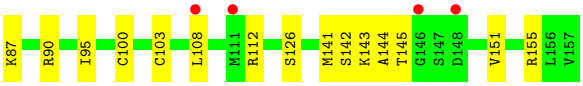


• Molecule 1: TRAPPC3 from Thorarchaeota SMTZ1-45



• Molecule 1: TRAPPC3 from Thorarchaeota SMTZ1-45




K87
R90
I95
C100
C103
L108
M111
R112
S126
M141
S142
K143
A144
T145
G146
S147
D148
V151
R155
L156
V157

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.39Å 62.06Å 69.32Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	19.48 – 1.70 19.48 – 1.70	Depositor EDS
% Data completeness (in resolution range)	81.3 (19.48-1.70) 81.3 (19.48-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.23 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.216 , 0.258 0.216 , 0.259	Depositor DCC
R_{free} test set	2486 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	13.7	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5688	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.41% 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: 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	A	0.27	0/1221	0.43	0/1643
1	B	0.28	0/1282	0.43	0/1724
1	C	0.28	0/1271	0.46	0/1711
1	D	0.28	0/1287	0.46	0/1734
All	All	0.28	0/5061	0.44	0/6812

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	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	C	49	THR	Peptide

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	1203	0	1206	20	0
1	B	1258	0	1264	27	0
1	C	1249	0	1254	58	0
1	D	1264	0	1273	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	173	0	0	14	4
3	B	161	0	0	13	2
3	C	166	0	0	40	6
3	D	210	0	0	22	9
All	All	5688	0	4997	146	14

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 15.

The worst 5 of 146 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:C:17:VAL:N	3:C:601:HOH:O	1.89	0.99
1:D:81:PRO:O	3:D:601:HOH:O	1.84	0.95
1:C:13:TYR:O	3:C:601:HOH:O	1.85	0.94
1:C:44:GLN:O	3:C:602:HOH:O	1.85	0.93
1:C:67:LYS:NZ	3:C:607:HOH:O	2.13	0.81

The worst 5 of 14 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)
3:A:710:HOH:O	3:C:663:HOH:O[2_546]	1.73	0.47
3:A:631:HOH:O	3:C:690:HOH:O[2_545]	1.89	0.31
3:A:768:HOH:O	3:C:765:HOH:O[2_545]	1.90	0.30
3:C:623:HOH:O	3:D:731:HOH:O[1_455]	1.98	0.22
3:D:643:HOH:O	3:D:739:HOH:O[2_646]	1.98	0.22

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	147/159 (92%)	142 (97%)	4 (3%)	1 (1%)	22 8
1	B	154/159 (97%)	150 (97%)	4 (3%)	0	100 100
1	C	155/159 (98%)	149 (96%)	6 (4%)	0	100 100
1	D	157/159 (99%)	152 (97%)	5 (3%)	0	100 100
All	All	613/636 (96%)	593 (97%)	19 (3%)	1 (0%)	47 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ARG

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	137/144 (95%)	130 (95%)	7 (5%)	24 8
1	B	145/144 (101%)	144 (99%)	1 (1%)	84 77
1	C	143/144 (99%)	136 (95%)	7 (5%)	25 9
1	D	145/144 (101%)	143 (99%)	2 (1%)	67 53
All	All	570/576 (99%)	553 (97%)	17 (3%)	41 22

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	130	PHE
1	D	108	LEU
1	B	73	TYR
1	C	6	ASN
1	C	45	ILE

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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 (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

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	150/159 (94%)	0.77	16 (10%) 6 7	6, 23, 43, 63	0
1	B	154/159 (96%)	0.57	7 (4%) 33 37	6, 22, 42, 53	0
1	C	155/159 (97%)	0.96	20 (12%) 3 4	9, 26, 53, 70	0
1	D	157/159 (98%)	0.80	16 (10%) 6 7	4, 22, 45, 52	0
All	All	616/636 (96%)	0.78	59 (9%) 8 9	4, 23, 46, 70	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	ALA	7.3
1	C	49	THR	6.2
1	A	117	CYS	5.7
1	A	88	THR	5.4
1	A	47	LEU	5.3

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

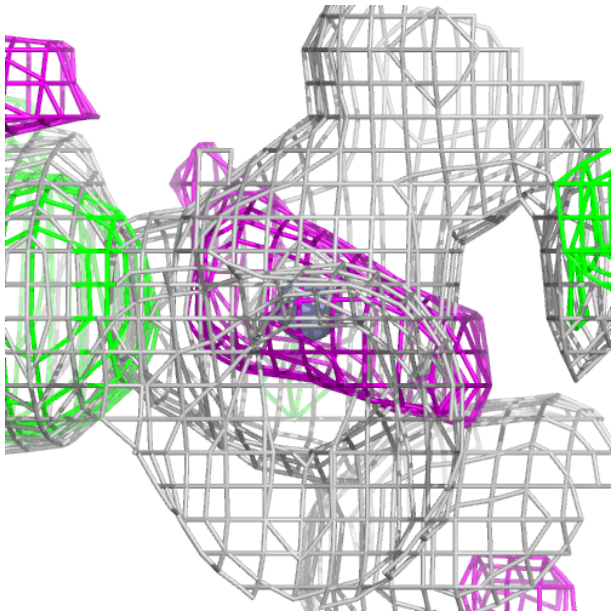
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

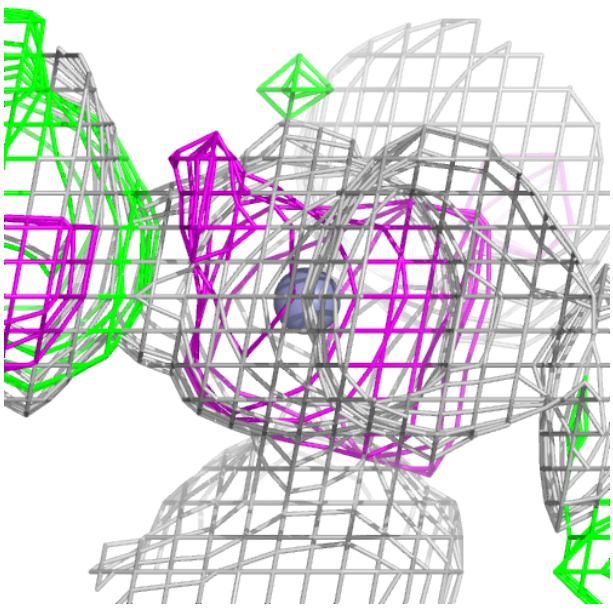
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	500	1/1	0.99	0.05	11,11,11,11	0
2	ZN	C	500	1/1	0.99	0.09	12,12,12,12	0
2	ZN	D	500	1/1	0.99	0.05	13,13,13,13	0
2	ZN	B	500	1/1	1.00	0.05	8,8,8,8	0

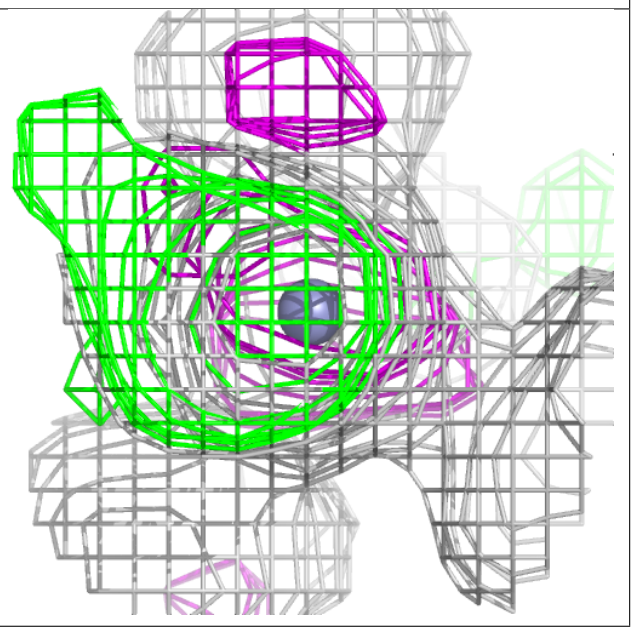
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN A 500:

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

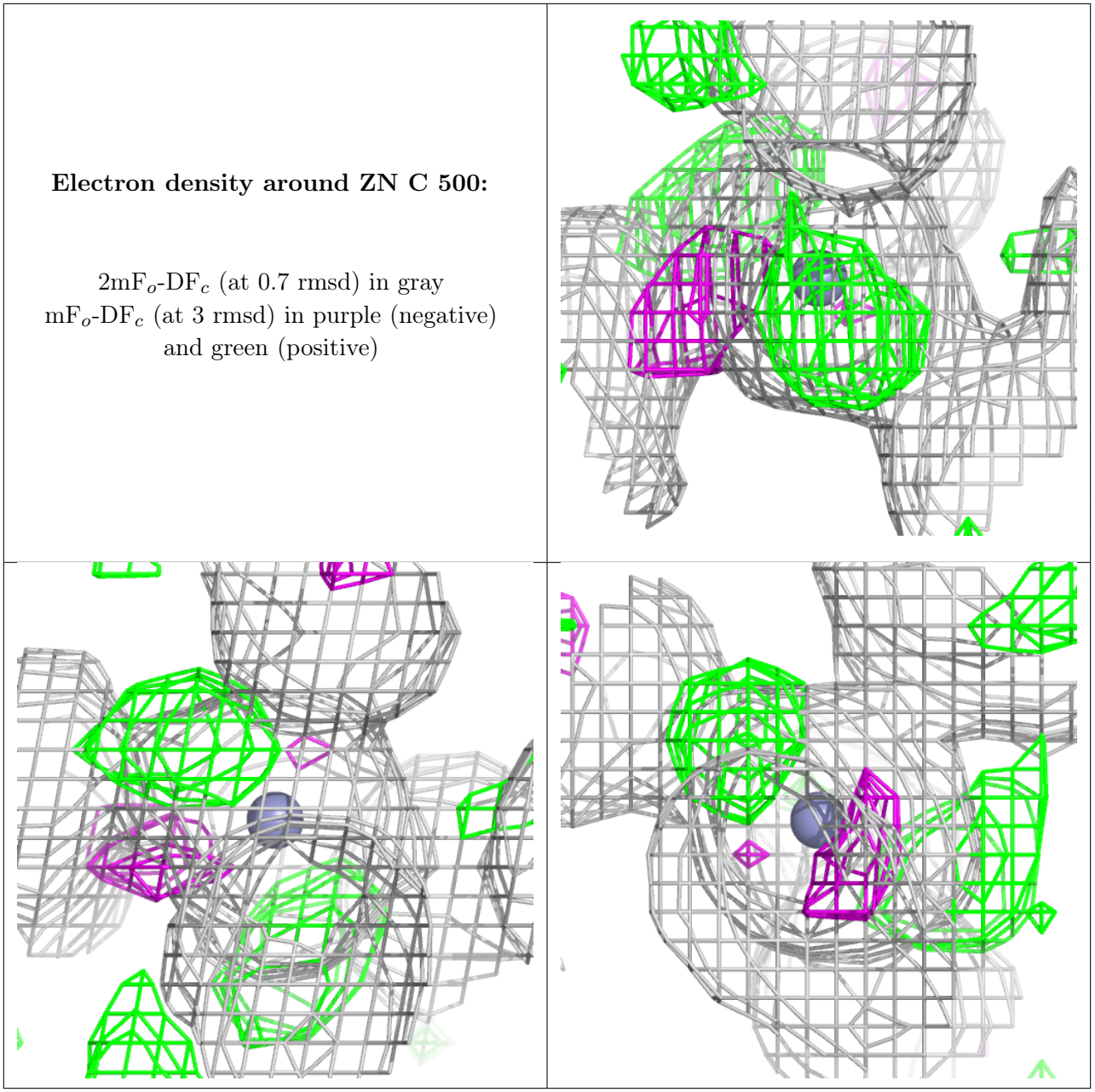






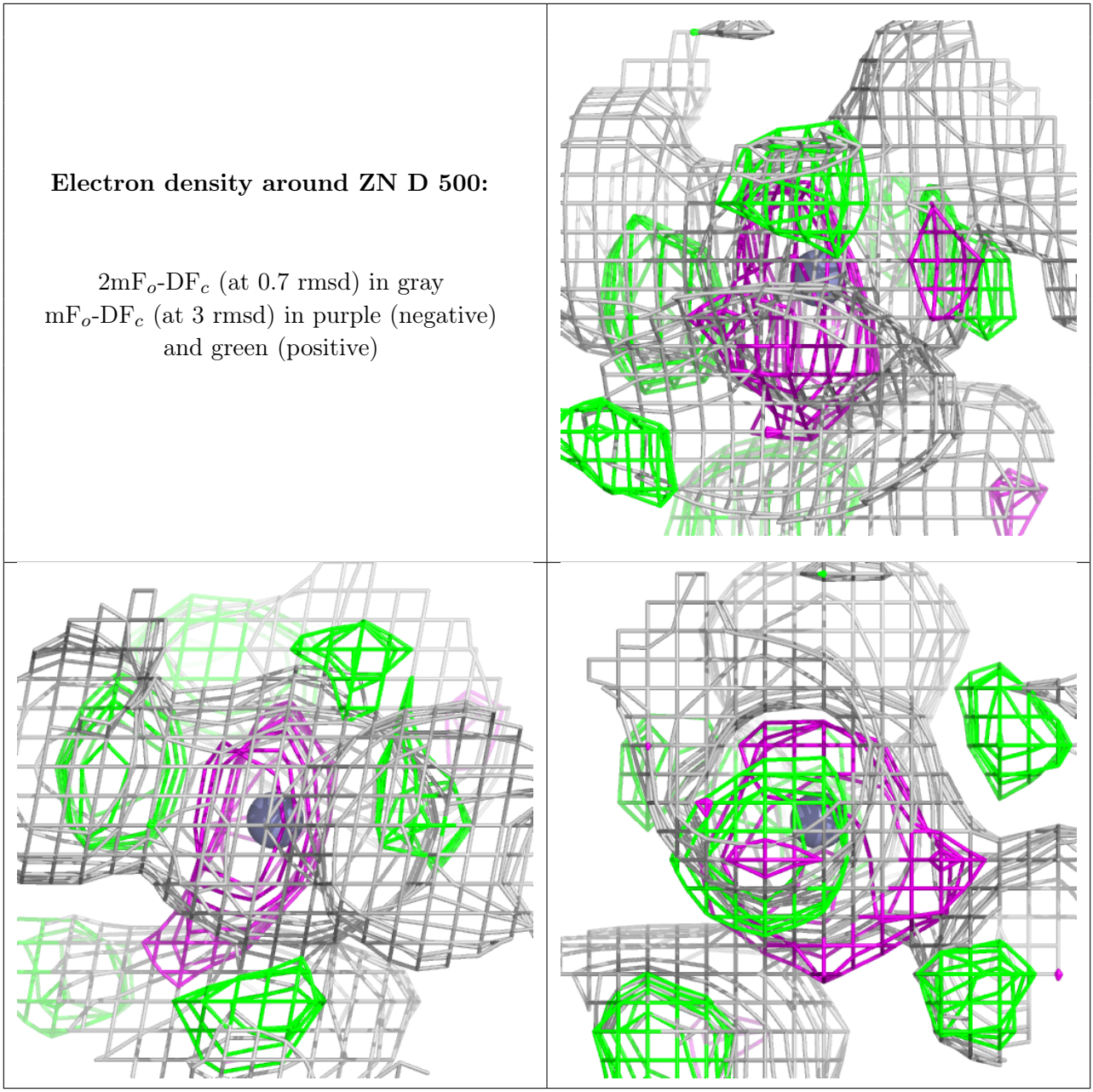
Electron density around ZN C 500:

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



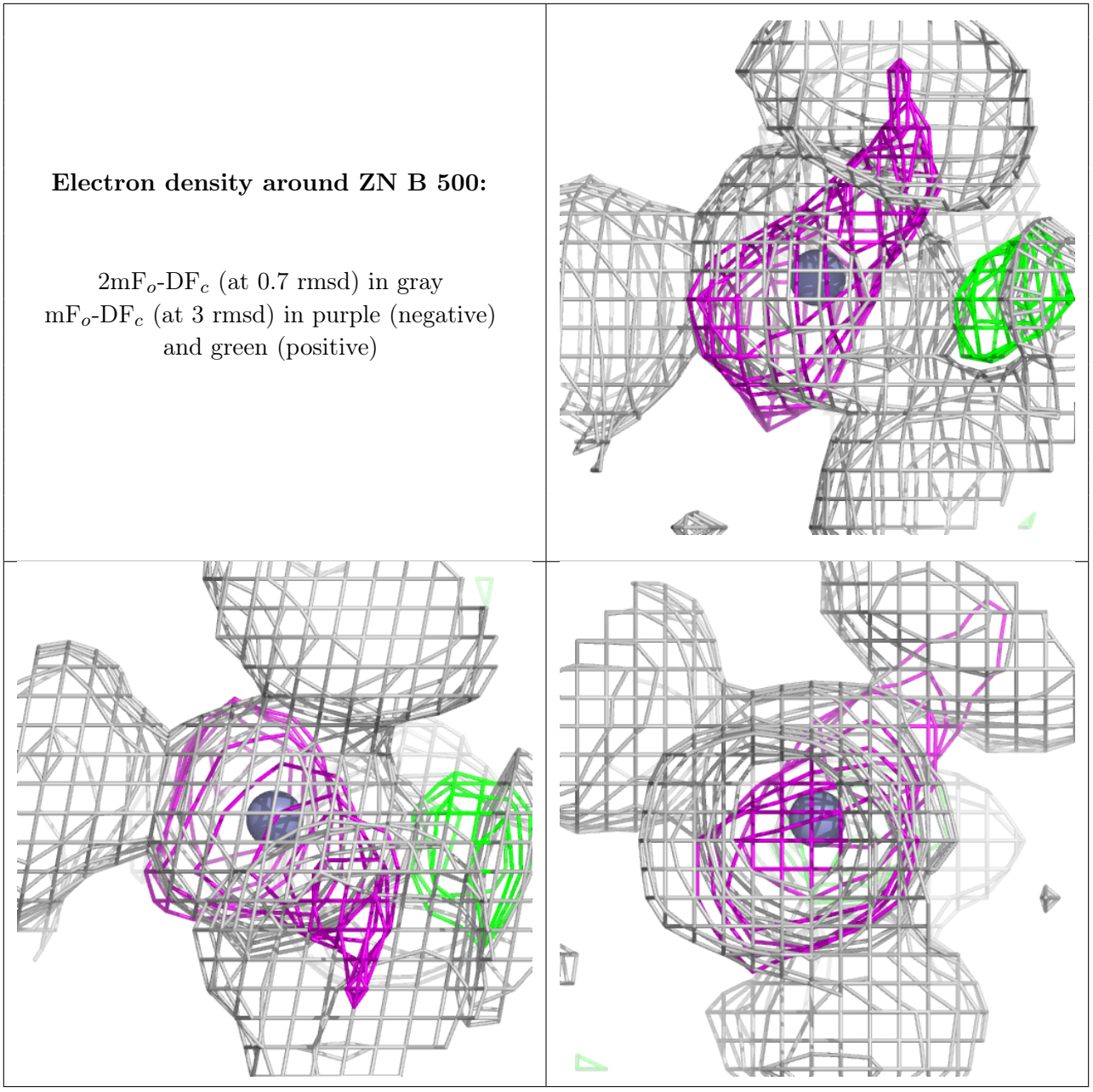
Electron density around ZN D 500:

$2mF_o$-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 500:

$2mF_o$-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.