



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 28, 2024 – 02:47 PM JST

PDB ID : 8XV4
Title : Crystal structure of TTD-PHD domain of UHRF1 in complex with mStella peptide (residues 85-119)
Authors : Du, X.; Gan, Q.; Xu, J.; Liu, J.
Deposited on : 2024-01-14
Resolution : 3.20 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 3.0
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

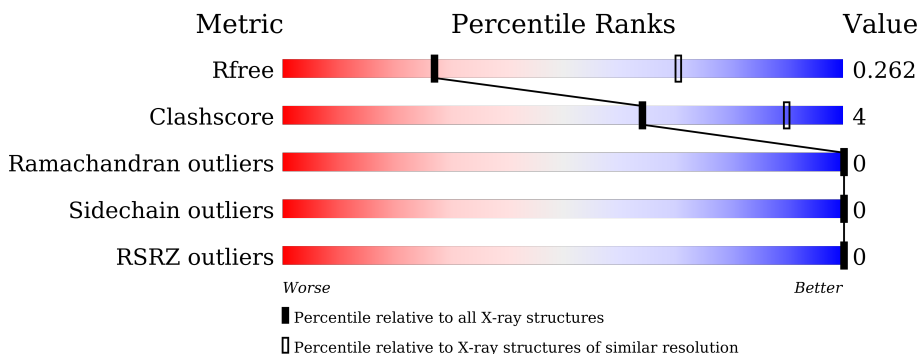
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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 ≥ 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	229	
1	B	229	
2	C	35	
2	D	35	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4029 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 E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	1800	1114	326	341	19	0	0	0
1	B	221	1792	1110	325	338	19	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	GLY	-	expression tag	UNP Q96T88
A	130	PRO	-	expression tag	UNP Q96T88
A	131	LEU	-	expression tag	UNP Q96T88
A	132	GLY	-	expression tag	UNP Q96T88
A	133	SER	-	expression tag	UNP Q96T88
A	?	-	SER	deletion	UNP Q96T88
A	?	-	ARG	deletion	UNP Q96T88
A	?	-	ASP	deletion	UNP Q96T88
A	?	-	GLU	deletion	UNP Q96T88
A	?	-	PRO	deletion	UNP Q96T88
A	?	-	CYS	deletion	UNP Q96T88
A	?	-	SER	deletion	UNP Q96T88
A	?	-	SER	deletion	UNP Q96T88
A	?	-	THR	deletion	UNP Q96T88
B	129	GLY	-	expression tag	UNP Q96T88
B	130	PRO	-	expression tag	UNP Q96T88
B	131	LEU	-	expression tag	UNP Q96T88
B	132	GLY	-	expression tag	UNP Q96T88
B	133	SER	-	expression tag	UNP Q96T88
B	?	-	SER	deletion	UNP Q96T88
B	?	-	ARG	deletion	UNP Q96T88
B	?	-	ASP	deletion	UNP Q96T88
B	?	-	GLU	deletion	UNP Q96T88
B	?	-	PRO	deletion	UNP Q96T88
B	?	-	CYS	deletion	UNP Q96T88

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP Q96T88
B	?	-	SER	deletion	UNP Q96T88
B	?	-	THR	deletion	UNP Q96T88

- Molecule 2 is a protein called Developmental pluripotency-associated protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	25	210	132	44	33	1	0	0	0
2	D	25	210	132	44	33	1	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	4	4	4	0	0
3	B	3	3	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	5	5	5	0	0
4	B	2	2	2	0	0
4	C	1	1	1	0	0
4	D	2	2	2	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: E3 ubiquitin-protein ligase UHRF1

Chain A:  87% 10%



- Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain B:  86% 10%



- Molecule 2: Developmental pluripotency-associated protein 3

Chain C:  66% 6% 29%



- Molecule 2: Developmental pluripotency-associated protein 3

Chain D:  63% 9% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.71Å 72.36Å 63.06Å 90.00° 108.05° 90.00°	Depositor
Resolution (Å)	19.99 – 3.20 19.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.3 (19.99-3.20) 95.3 (19.99-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.22Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.227 , 0.266 0.229 , 0.262	Depositor DCC
R_{free} test set	462 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtrriage
Anisotropy	0.644	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4029	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.36% 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

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	0.29	0/1839	0.66	0/2488
1	B	0.30	0/1831	0.66	1/2477 (0.0%)
2	C	0.31	0/210	0.65	0/279
2	D	0.31	0/210	0.70	0/279
All	All	0.30	0/4090	0.66	1/5523 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	LYS	CB-CA-C	8.00	126.39	110.40

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	1800	0	1717	16	0
1	B	1792	0	1713	15	0
2	C	210	0	242	2	0
2	D	210	0	242	3	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
All	All	4029	0	3914	30	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 30 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:B:207:ARG:HB3	1:B:289:MET:HE3	1.74	0.69
1:A:289:MET:O	1:A:289:MET:HG3	1.91	0.69
1:A:337:ASP:OD2	2:C:107:ARG:NE	2.32	0.60
1:A:311:ARG:HD3	1:B:314:ARG:HH22	1.72	0.54
1:B:207:ARG:NH1	1:B:294:MET:O	2.44	0.49

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	218/229 (95%)	200 (92%)	18 (8%)	0	100	100
1	B	217/229 (95%)	205 (94%)	12 (6%)	0	100	100
2	C	23/35 (66%)	21 (91%)	2 (9%)	0	100	100
2	D	23/35 (66%)	21 (91%)	2 (9%)	0	100	100
All	All	481/528 (91%)	447 (93%)	34 (7%)	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	200/205 (98%)	200 (100%)	0	100	100
1	B	199/205 (97%)	199 (100%)	0	100	100
2	C	24/33 (73%)	24 (100%)	0	100	100
2	D	24/33 (73%)	24 (100%)	0	100	100
All	All	447/476 (94%)	447 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	198	GLN
1	B	292	ASN
2	C	110	GLN
1	A	292	ASN
1	A	147	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 7 ligands modelled in this entry, 7 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 [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	222/229 (96%)	-0.15	0 100 100	41, 62, 97, 115	0
1	B	221/229 (96%)	-0.09	0 100 100	45, 67, 92, 113	0
2	C	25/35 (71%)	-0.24	0 100 100	46, 55, 76, 85	0
2	D	25/35 (71%)	-0.27	0 100 100	50, 56, 80, 108	0
All	All	493/528 (93%)	-0.14	0 100 100	41, 63, 94, 115	0

There are no RSRZ outliers to report.

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.

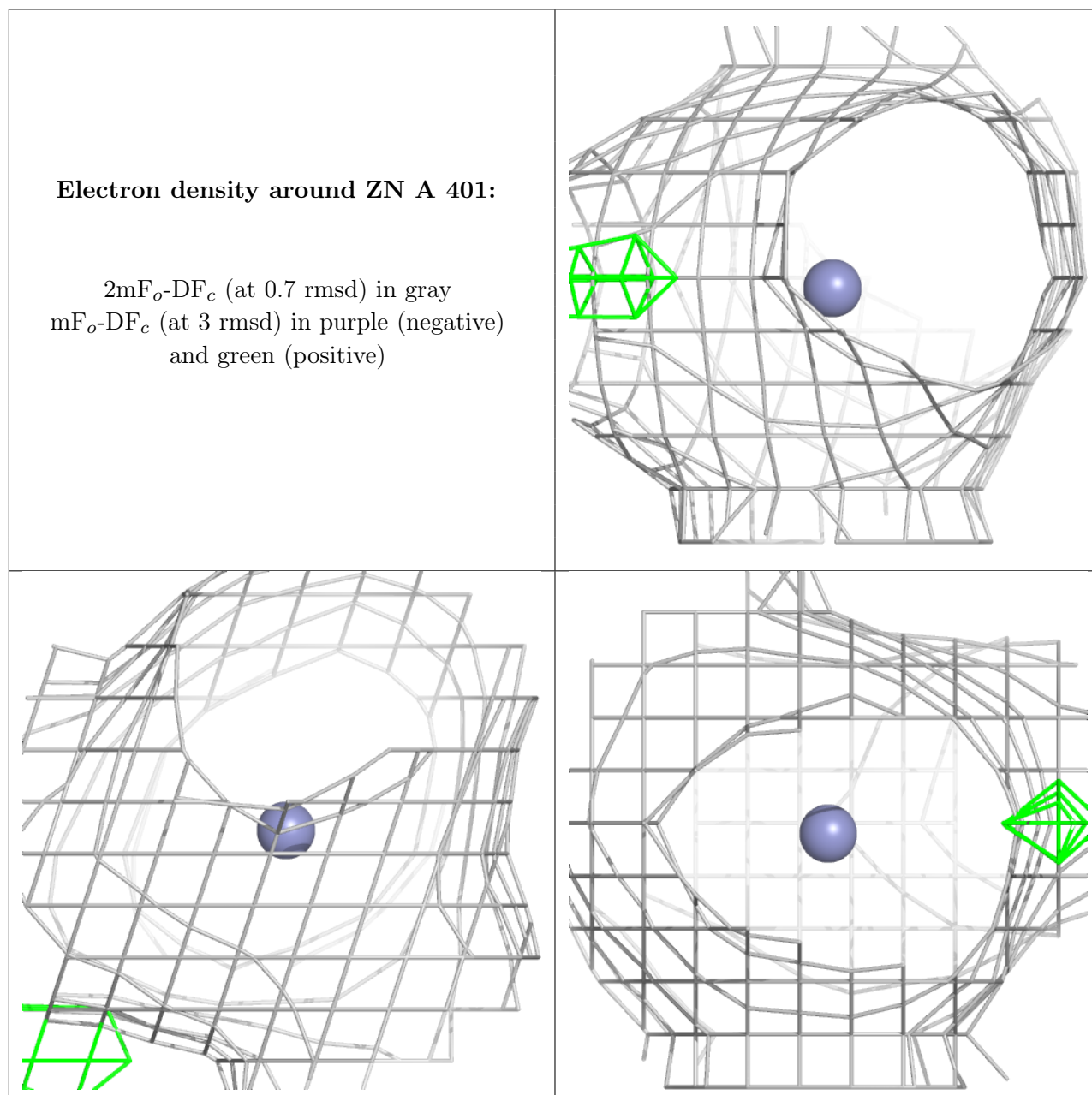
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	A	401	1/1	0.99	0.02	48,48,48,48	0
3	ZN	A	403	1/1	0.99	0.01	59,59,59,59	0
3	ZN	A	404	1/1	0.99	0.02	62,62,62,62	0
3	ZN	B	1001	1/1	0.99	0.01	54,54,54,54	0

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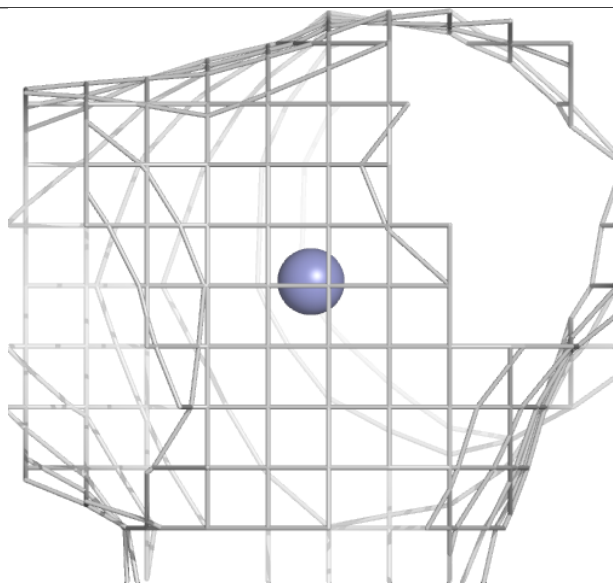
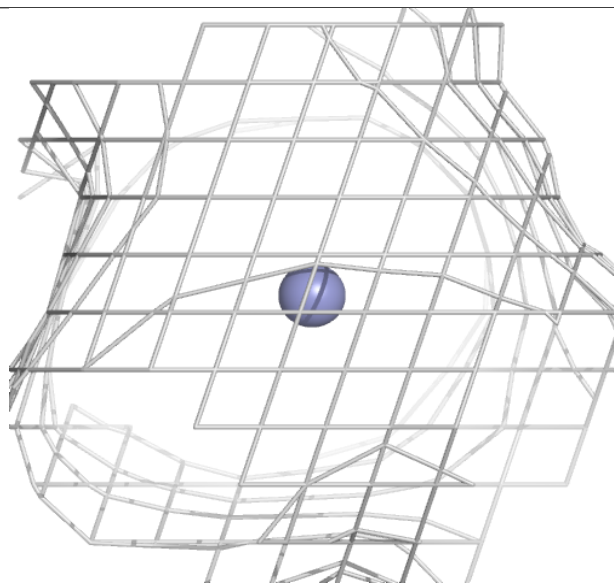
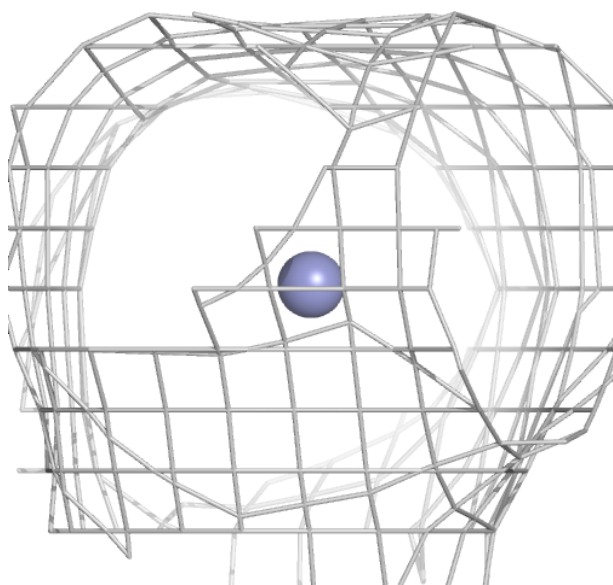
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	B	1002	1/1	0.99	0.02	50,50,50,50	0
3	ZN	B	1003	1/1	0.99	0.02	66,66,66,66	0
3	ZN	A	402	1/1	1.00	0.02	46,46,46,46	0

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.



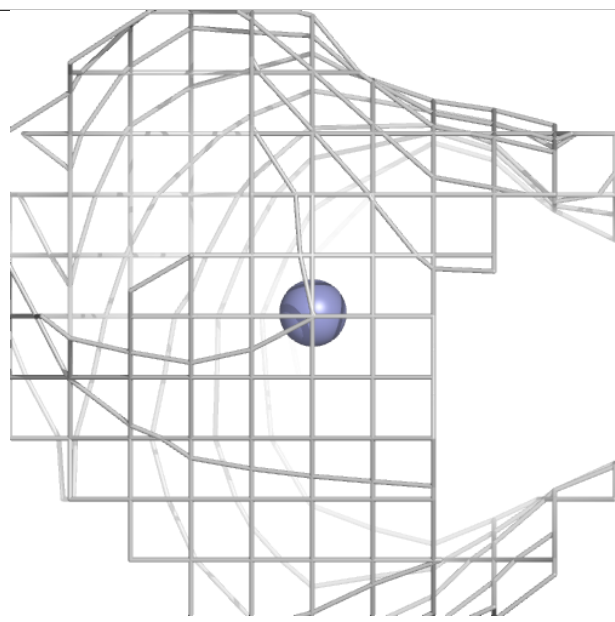
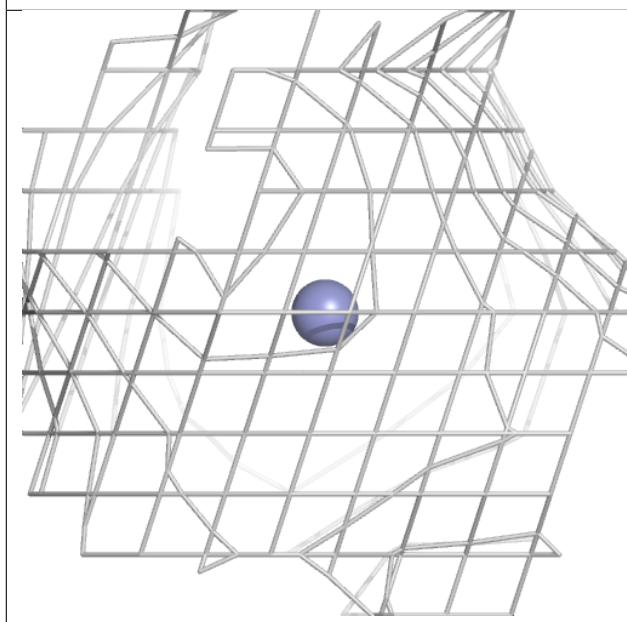
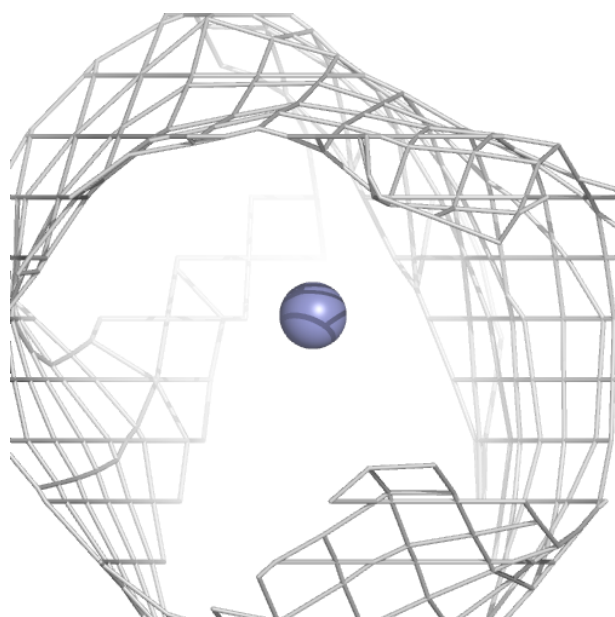
Electron density around ZN A 403:

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



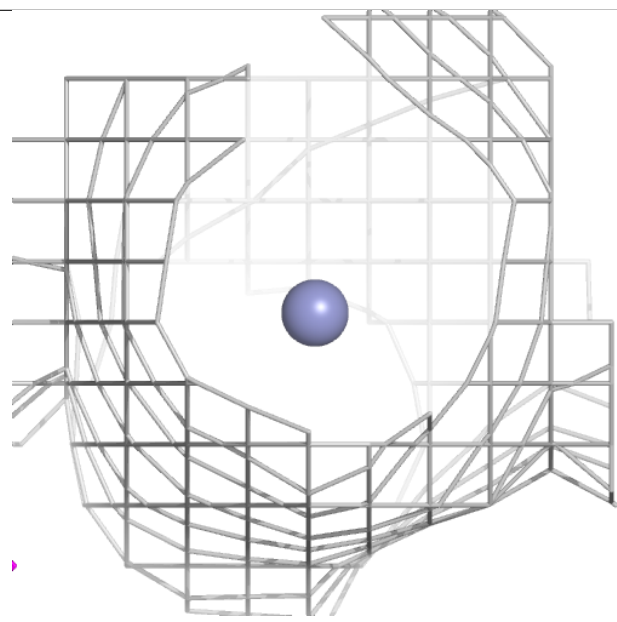
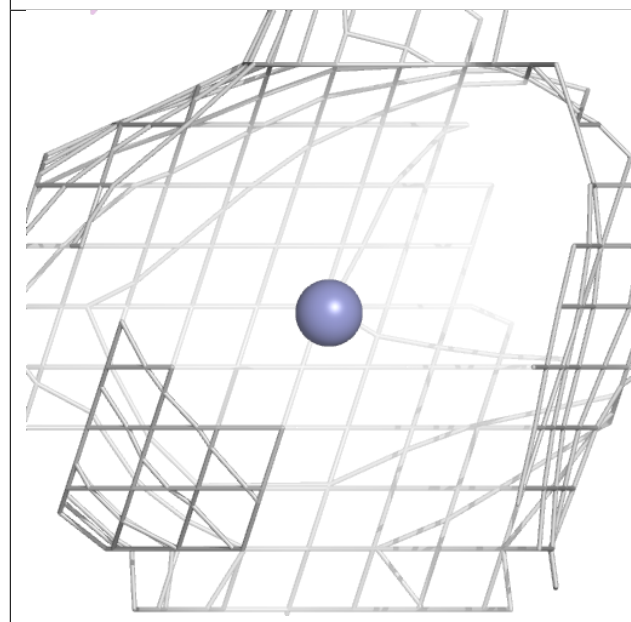
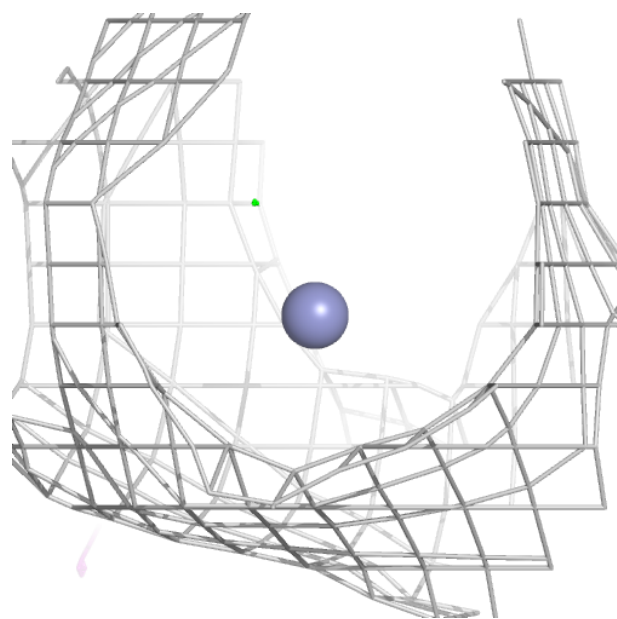
Electron density around ZN A 404:

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



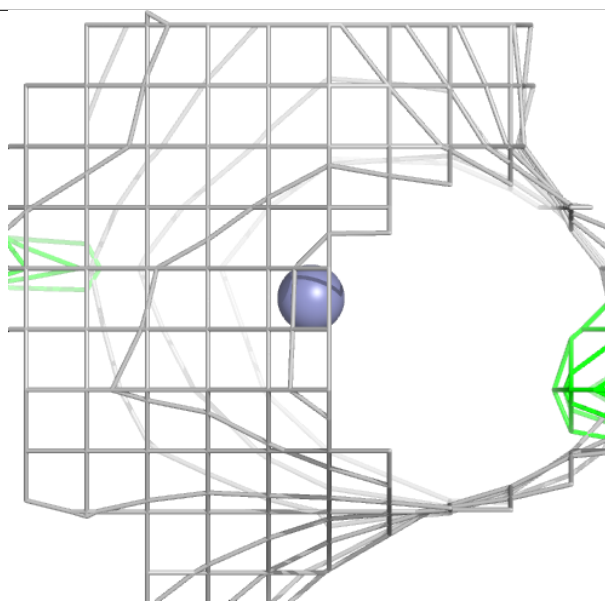
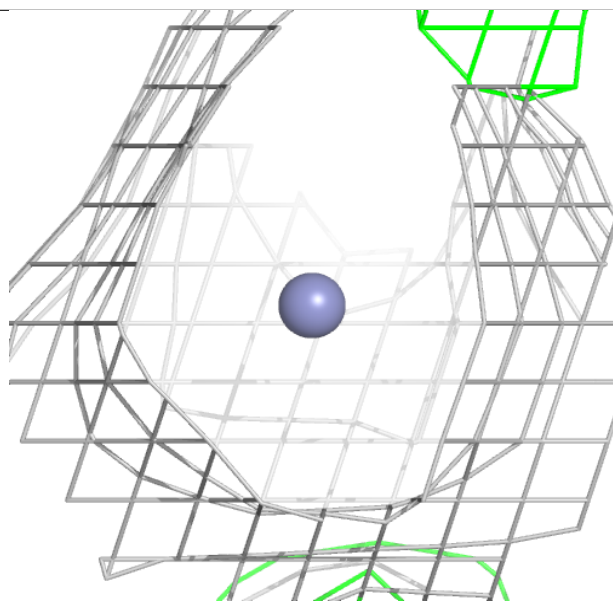
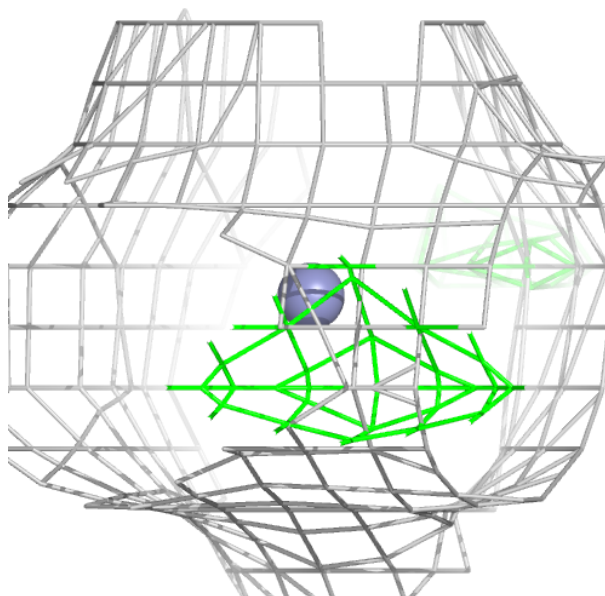
Electron density around ZN B 1001:

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



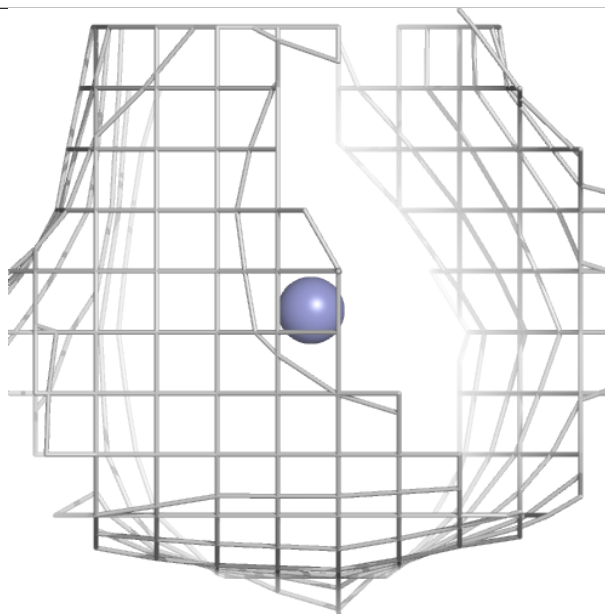
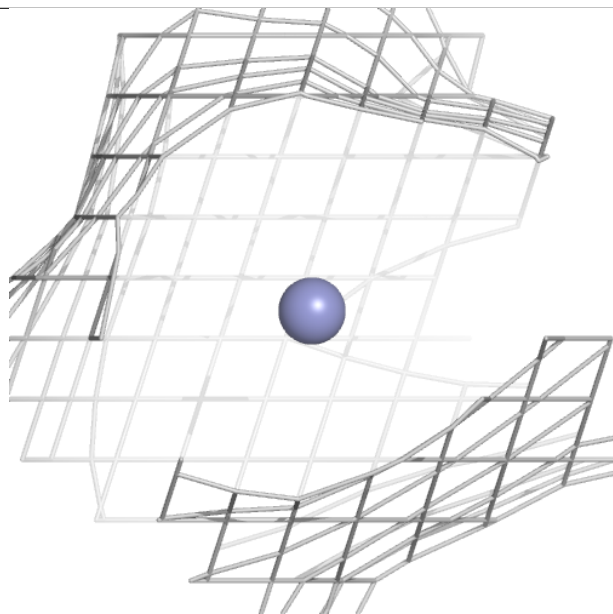
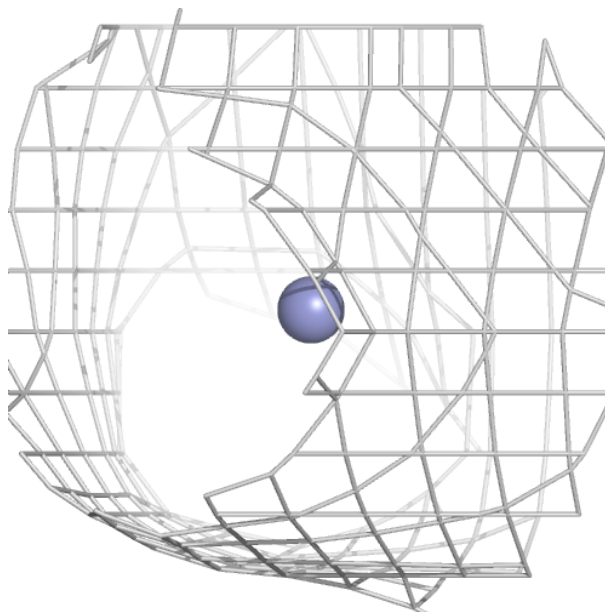
Electron density around ZN B 1002:

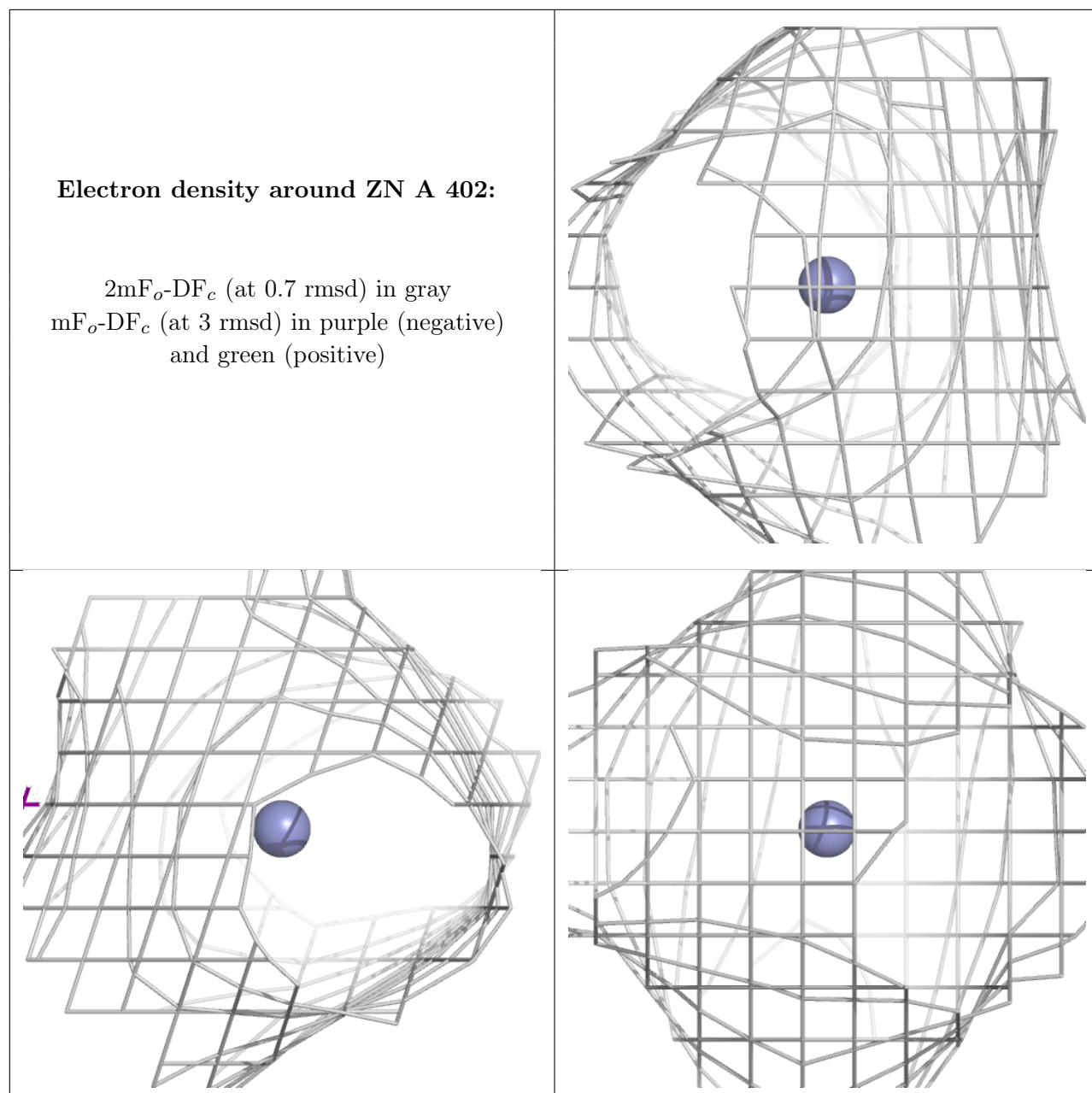
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 1003:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.