



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 01:17 AM UTC

PDB ID : 7EAX / pdb_00007eax
Title : Crystal complex of p53-V272M and antimony ion
Authors : Lu, M.; Tang, Y.
Deposited on : 2021-03-08
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	FAILED
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

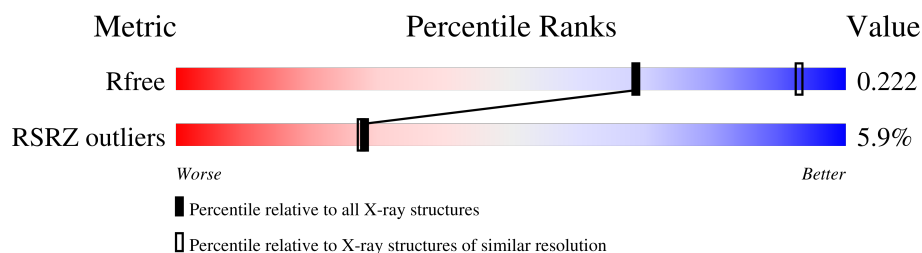
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6204 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	2	0
			1533	944	282	289	18			
1	B	193	Total	C	N	O	S	0	4	0
			1547	953	287	289	18			
1	C	194	Total	C	N	O	S	0	1	0
			1527	941	281	288	17			
1	D	193	Total	C	N	O	S	0	2	0
			1527	941	281	287	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	MET	VAL	variant	UNP P04637
B	272	MET	VAL	variant	UNP P04637
C	272	MET	VAL	variant	UNP P04637
D	272	MET	VAL	variant	UNP P04637

- Molecule 2 is ZINC ION (CCD ID: 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 ANTIMONY (III) ION (CCD ID: SB) (formula: Sb) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Sb 1	0	0
3	B	1	Total 1	Sb 1	0	0
3	C	1	Total 1	Sb 1	0	0
3	D	1	Total 1	Sb 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total 16	O 16	0	0
4	B	12	Total 12	O 12	0	0
4	C	15	Total 15	O 15	0	0
4	D	19	Total 19	O 19	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.88Å 72.55Å 85.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.53 – 2.55 42.53 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.53-2.55) 99.6 (42.53-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.206 , 0.235 0.208 , 0.222	Depositor DCC
R_{free} test set	1289 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -k,-h,-l 0.011 for k,h,-l 0.109 for h,-k,-l	Xtriage
Reported twinning fraction	0.609 for H, K, L 0.391 for -h,-k,l	Depositor
Outliers	0 of 27467 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6204	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.40% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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, 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	194/194 (100%)	0.24	5 (2%) 57 58	22, 42, 68, 76	2 (1%)
1	B	193/194 (99%)	0.36	7 (3%) 46 47	22, 45, 70, 83	4 (2%)
1	C	194/194 (100%)	0.65	12 (6%) 26 26	29, 47, 74, 92	1 (0%)
1	D	193/194 (99%)	0.74	22 (11%) 10 9	20, 48, 78, 93	2 (1%)
All	All	774/776 (99%)	0.50	46 (5%) 28 27	20, 46, 74, 93	9 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	182	CYS	4.4
1	D	147	VAL	4.1
1	D	289	LEU	3.9
1	C	182	CYS	3.8
1	D	153	PRO	3.6
1	D	149	SER	3.5
1	D	181	ARG	3.5
1	C	181	ARG	3.4
1	D	225	VAL	3.2
1	C	289	LEU	3.1
1	D	264	LEU	3.1
1	B	243	MET	2.9
1	C	153	PRO	2.9
1	A	289	LEU	2.8
1	D	183	SER	2.8
1	C	225	VAL	2.8
1	D	151	PRO	2.8
1	D	247	ASN	2.7
1	A	264	LEU	2.7
1	C	152	PRO	2.7
1	D	120	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	201	LEU	2.6
1	B	185	SER	2.6
1	D	226	GLY	2.6
1	C	243	MET	2.6
1	D	248	ARG	2.5
1	B	225	VAL	2.5
1	B	289	LEU	2.4
1	C	96	SER	2.4
1	D	243	MET	2.4
1	B	182	CYS	2.4
1	C	147	VAL	2.4
1	D	97	VAL	2.3
1	C	184	ASP	2.3
1	B	187	GLY	2.3
1	D	106[A]	SER	2.2
1	A	184	ASP	2.2
1	D	221	GLU	2.2
1	D	150	THR	2.2
1	A	182	CYS	2.2
1	C	120	LYS	2.1
1	C	183	SER	2.1
1	A	103	TYR	2.1
1	D	288	ASN	2.0
1	B	228	ASP	2.0
1	D	152	PRO	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

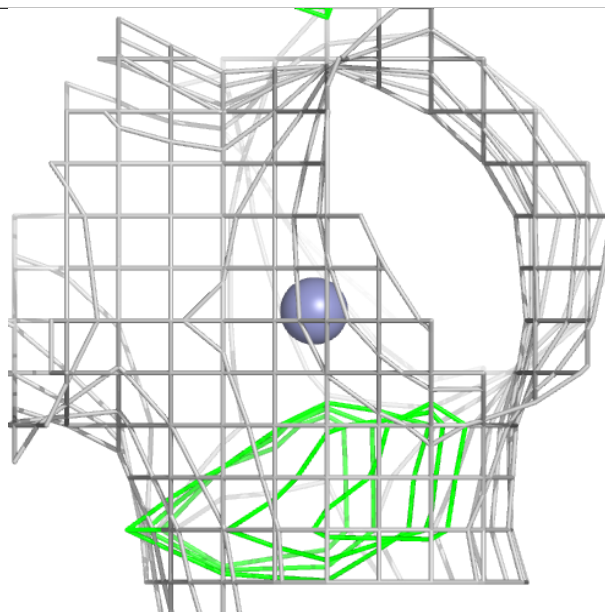
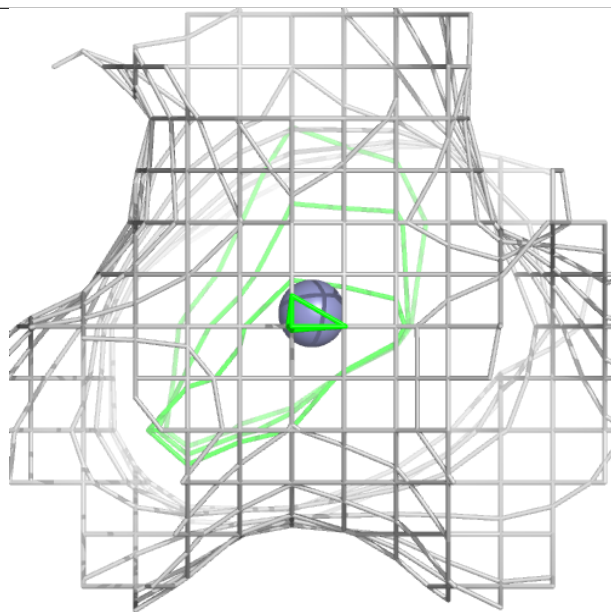
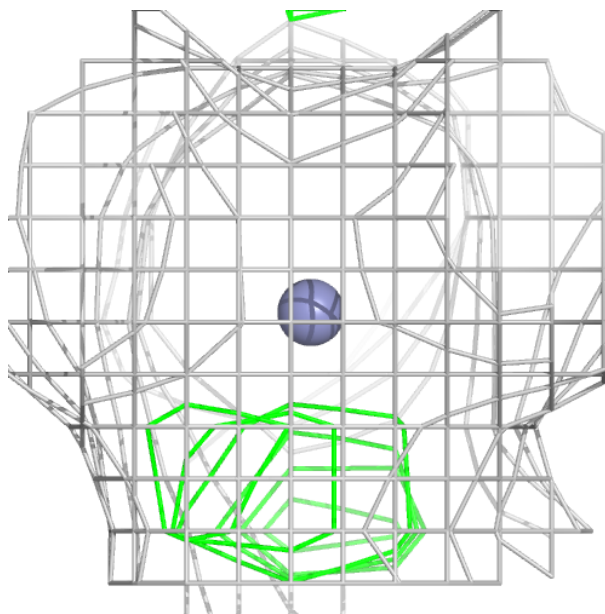
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	401	1/1	0.98	0.05	41,41,41,41	1
3	SB	A	402	1/1	0.98	0.03	56,56,56,56	0
3	SB	B	402	1/1	0.98	0.03	57,57,57,57	0
3	SB	D	402	1/1	0.98	0.03	46,46,46,46	0
2	ZN	B	401	1/1	0.99	0.04	46,46,46,46	1
2	ZN	A	401	1/1	0.99	0.07	48,48,48,48	1
3	SB	C	402	1/1	0.99	0.03	50,50,50,50	0
2	ZN	D	401	1/1	0.99	0.03	44,44,44,44	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.

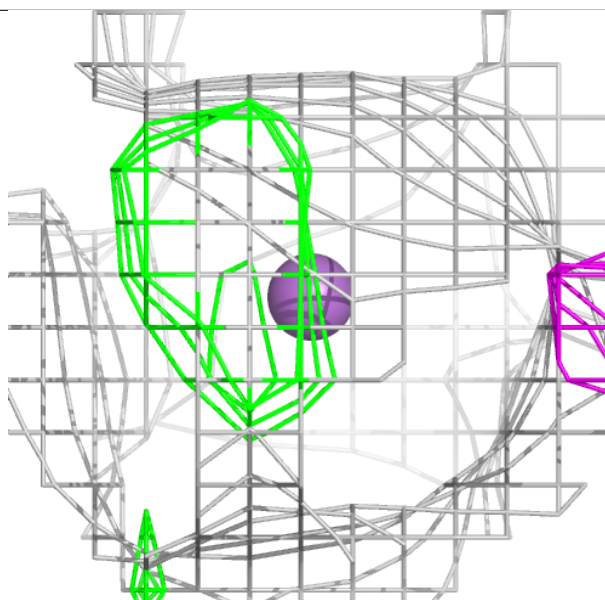
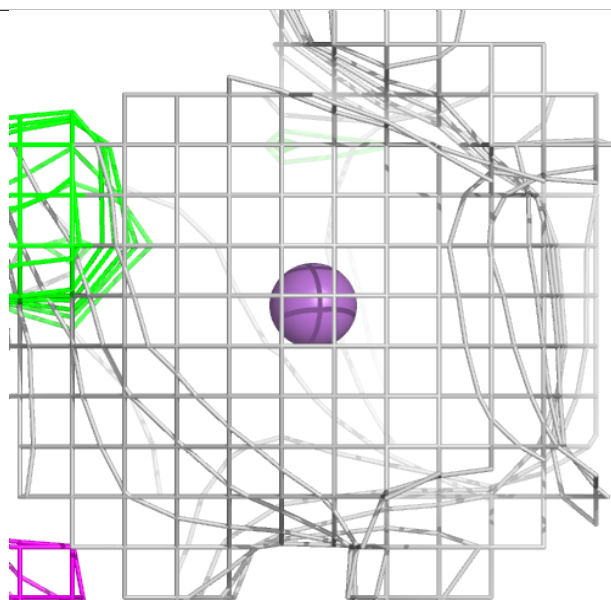
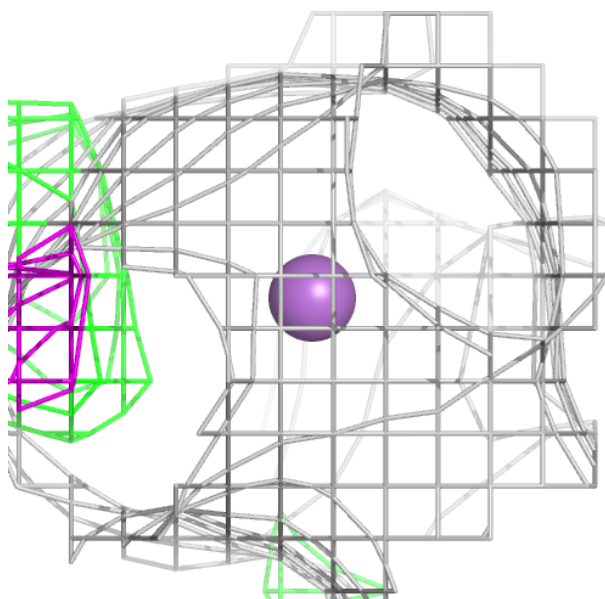
Electron density around ZN C 401:

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



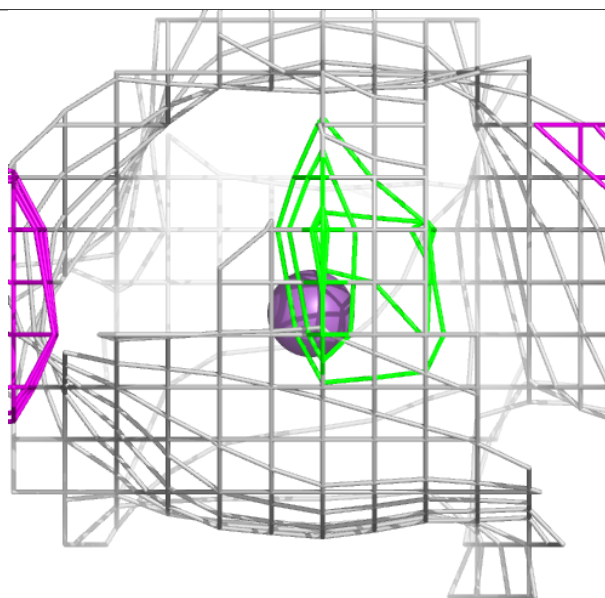
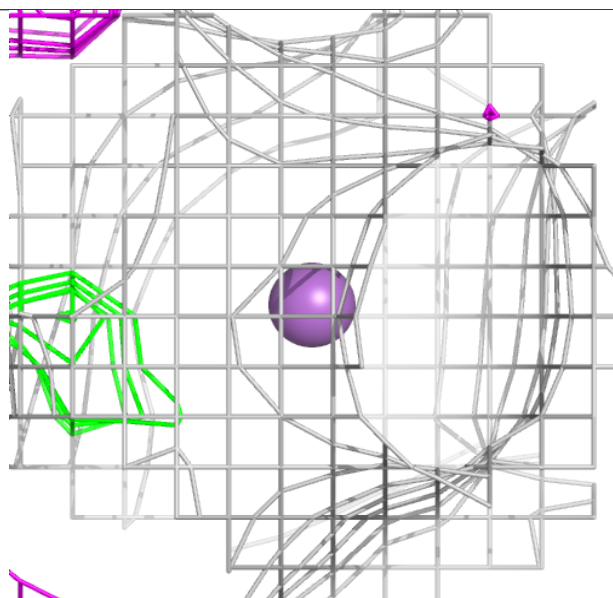
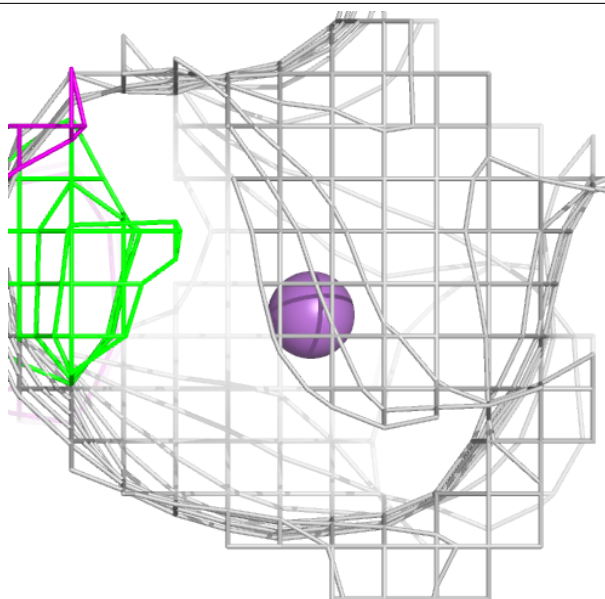
Electron density around SB A 402:

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



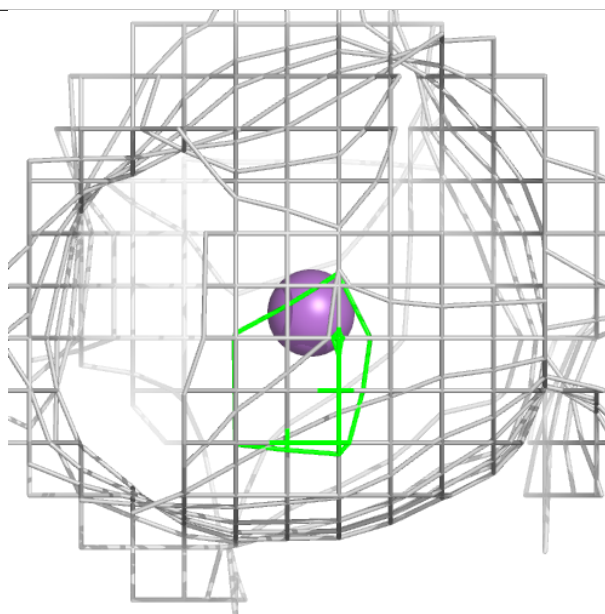
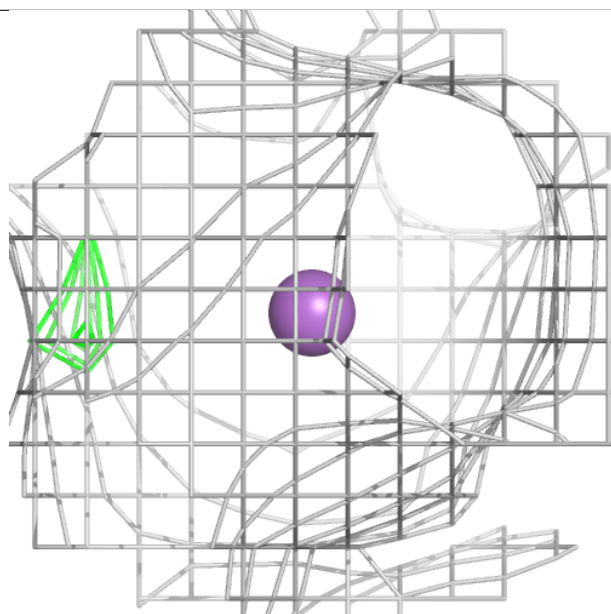
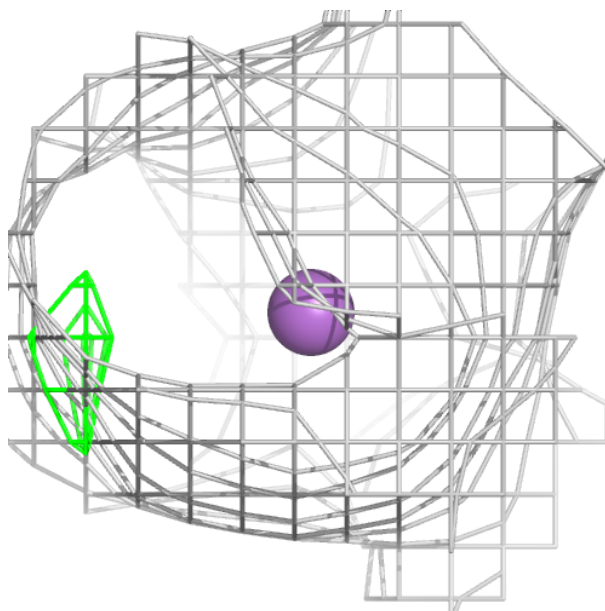
Electron density around SB B 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



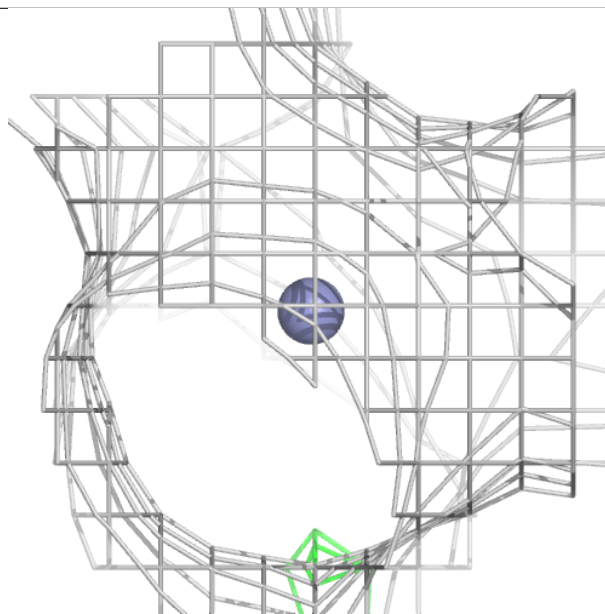
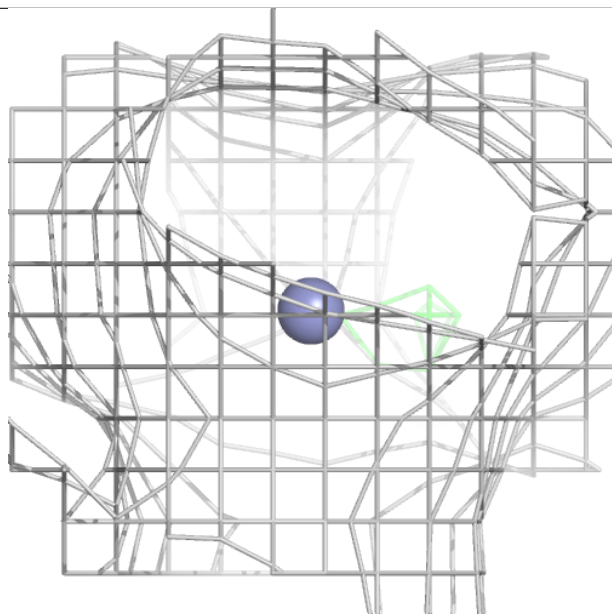
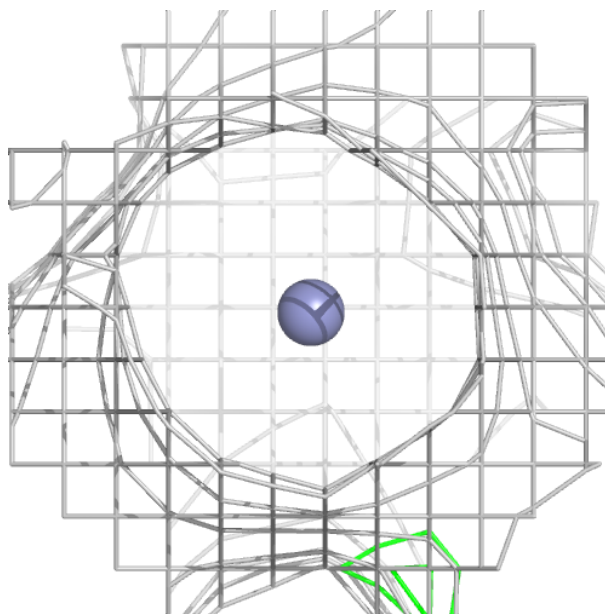
Electron density around SB D 402:

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and green (positive)



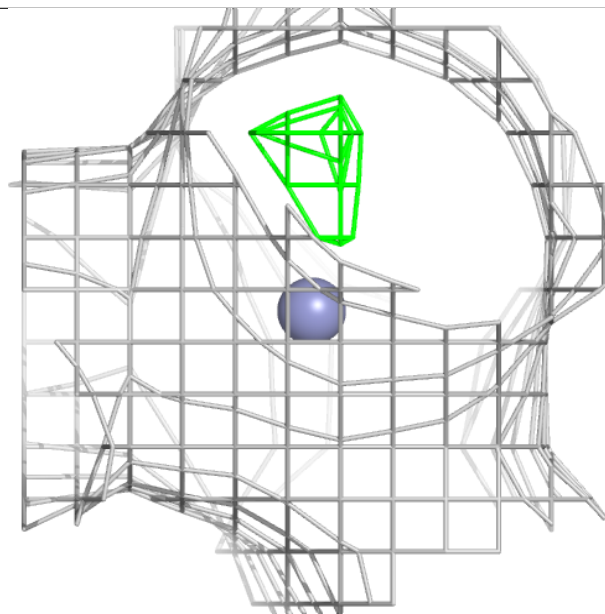
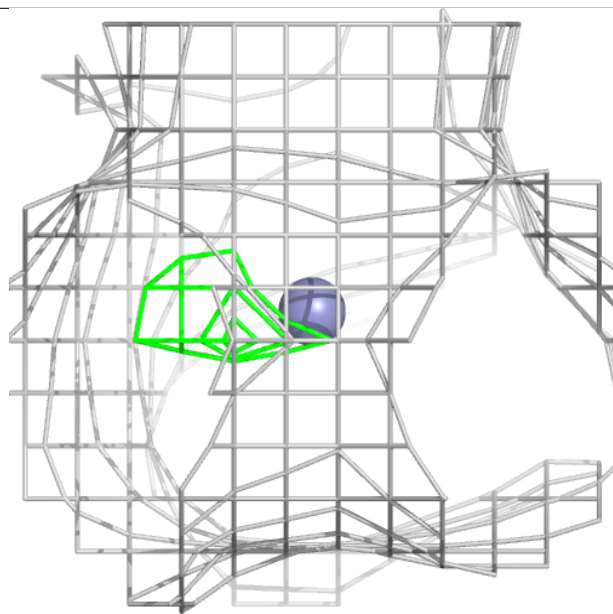
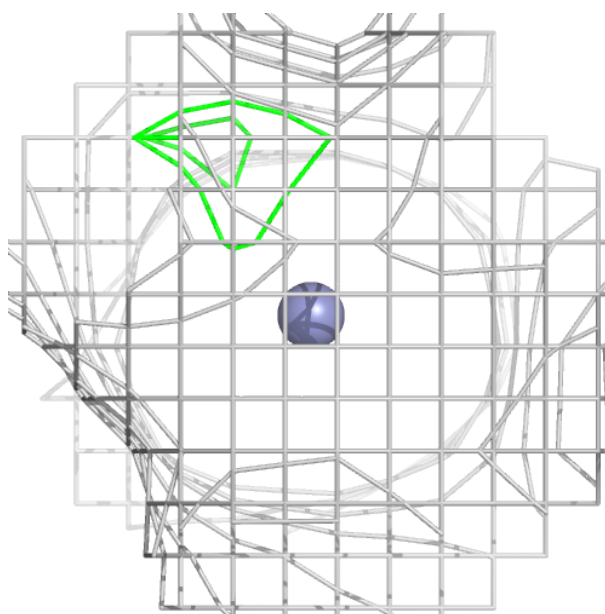
Electron density around ZN B 401:

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



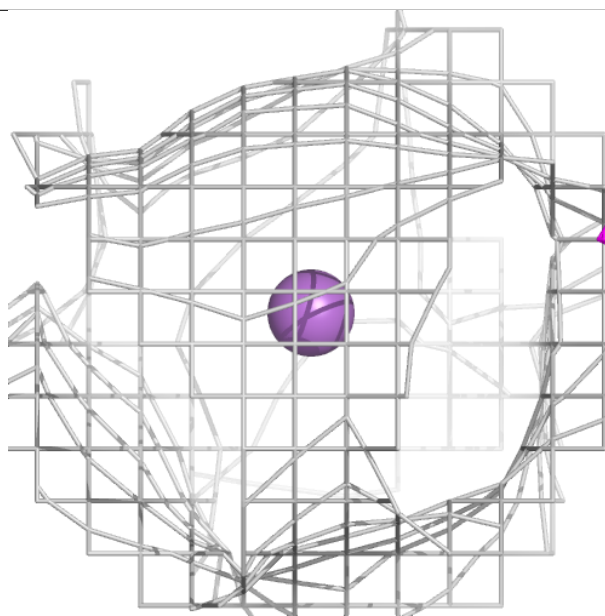
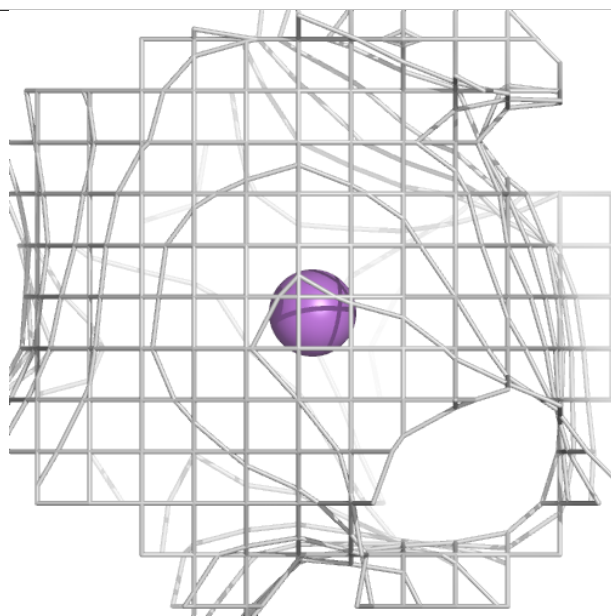
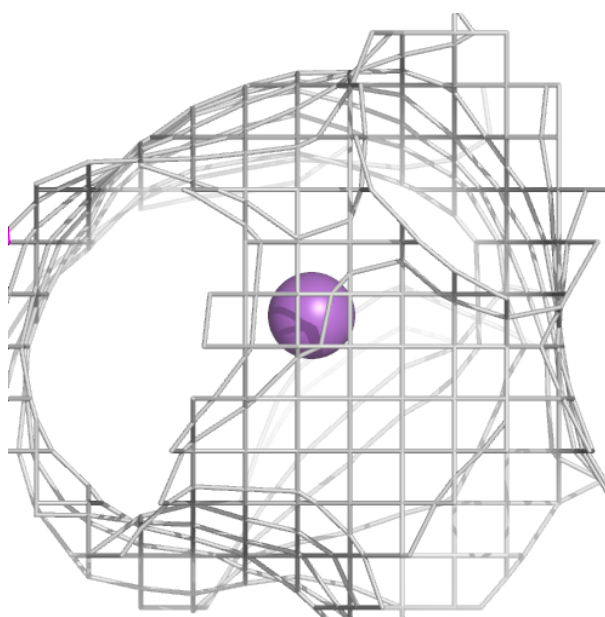
Electron density around ZN A 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



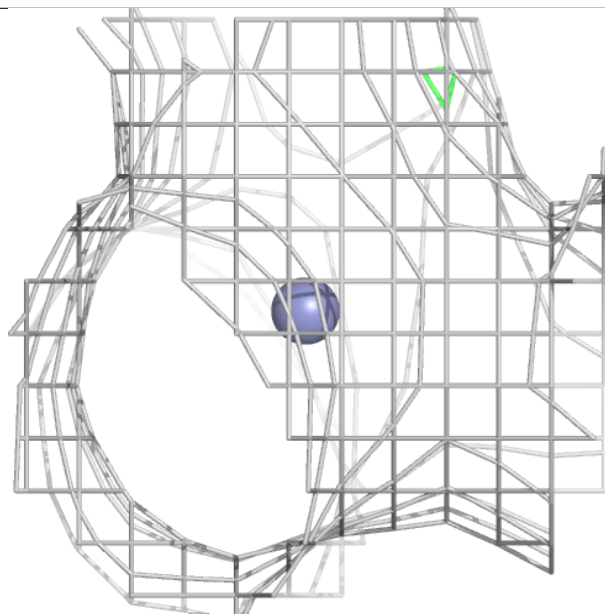
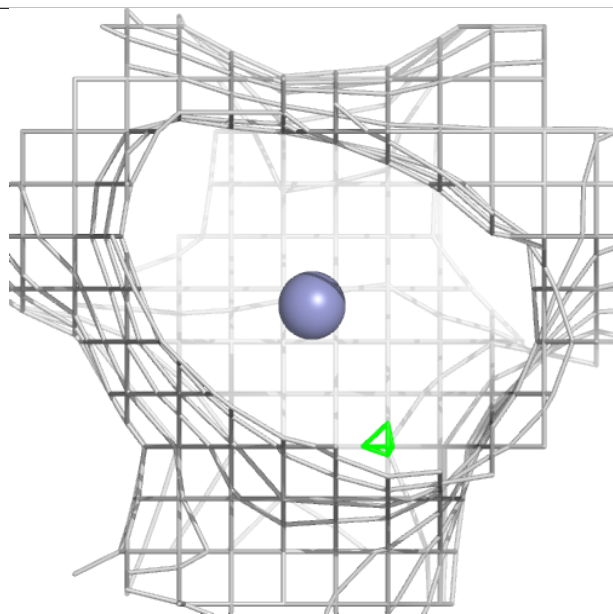
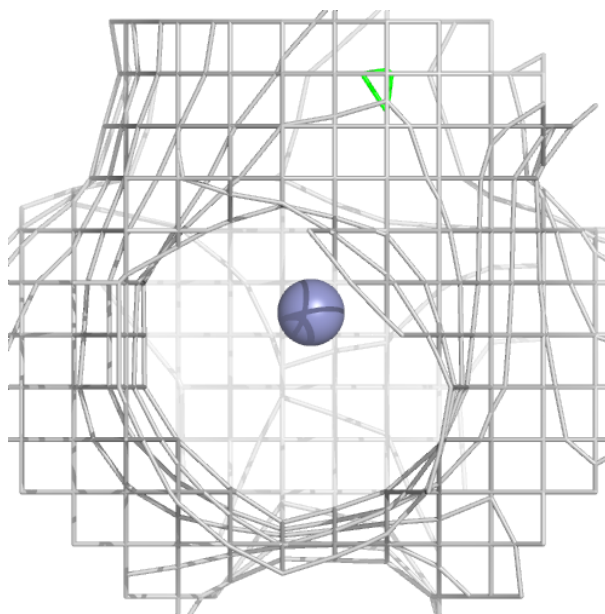
Electron density around SB C 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN D 401:

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



5.5 Other polymers ⓘ

There are no such residues in this entry.