wwPDB X-ray Structure Validation Summary Report (i)

Oct 19, 2026 – 07:06 pm BST

PDB ID	:	32WJ / pdb_000032wj
Title	:	Structure of TRIM8 RING domain in complex with UBE2N Ub conjugate
Authors	:	Dudley-Fraser, J.; Esposito, D.; Rittinger, K.
Deposited on	:	2026-07-28
Resolution	:	2.39 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:

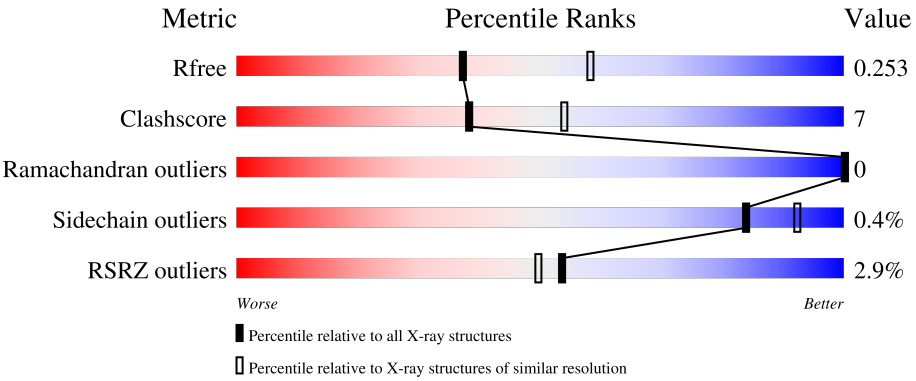
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	B	83	5% 87% 12% ·
1	C	83	4% 78% 16% 6%
1	I	83	% 81% 11% 8%
1	J	83	7% 83% 13% ·
2	D	154	% 90% 8% ··

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Mol	Chain	Length	Quality of chain
2	E	154	6% 77% 20%
2	K	154	83% 14%
2	L	154	3% 75% 23%
3	F	76	86% 14%
3	H	76	4% 86% 14%
3	M	76	3% 82% 18%
3	N	76	89% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9879 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 TRIM8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	76	Total	C	N	O	S	0	0	0
			602	382	104	108	8			
1	J	80	Total	C	N	O	S	0	0	0
			638	405	110	115	8			
1	B	82	Total	C	N	O	S	0	0	0
			649	412	112	117	8			
1	C	78	Total	C	N	O	S	0	0	0
			624	397	108	111	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLY	-	expression tag	UNP Q9BZR9
I	0	PRO	-	expression tag	UNP Q9BZR9
I	1	GLY	-	expression tag	UNP Q9BZR9
J	-1	GLY	-	expression tag	UNP Q9BZR9
J	0	PRO	-	expression tag	UNP Q9BZR9
J	1	GLY	-	expression tag	UNP Q9BZR9
B	-1	GLY	-	expression tag	UNP Q9BZR9
B	0	PRO	-	expression tag	UNP Q9BZR9
B	1	GLY	-	expression tag	UNP Q9BZR9
C	-1	GLY	-	expression tag	UNP Q9BZR9
C	0	PRO	-	expression tag	UNP Q9BZR9
C	1	GLY	-	expression tag	UNP Q9BZR9

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	149	Total	C	N	O	S	0	0	0
			1185	761	205	216	3			
2	L	151	Total	C	N	O	S	0	0	0
			1199	770	207	219	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	151	Total	C	N	O	S	0	0	0
			1198	770	207	218	3			
2	E	150	Total	C	N	O	S	0	0	0
			1194	767	206	218	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLY	-	expression tag	UNP P61088
K	0	PRO	-	expression tag	UNP P61088
K	87	LYS	CYS	engineered mutation	UNP P61088
K	92	ALA	LYS	engineered mutation	UNP P61088
L	-1	GLY	-	expression tag	UNP P61088
L	0	PRO	-	expression tag	UNP P61088
L	87	LYS	CYS	engineered mutation	UNP P61088
L	92	ALA	LYS	engineered mutation	UNP P61088
D	-1	GLY	-	expression tag	UNP P61088
D	0	PRO	-	expression tag	UNP P61088
D	87	LYS	CYS	engineered mutation	UNP P61088
D	92	ALA	LYS	engineered mutation	UNP P61088
E	-1	GLY	-	expression tag	UNP P61088
E	0	PRO	-	expression tag	UNP P61088
E	87	LYS	CYS	engineered mutation	UNP P61088
E	92	ALA	LYS	engineered mutation	UNP P61088

- Molecule 3 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
3	N	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
3	F	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
3	H	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	2	Total Zn 2 2	0	0
4	J	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0
4	C	2	Total Zn 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	16	Total O 16 16	0	0
5	J	9	Total O 9 9	0	0
5	K	27	Total O 27 27	0	0
5	L	18	Total O 18 18	0	0
5	M	8	Total O 8 8	0	0
5	N	17	Total O 17 17	0	0
5	B	12	Total O 12 12	0	0
5	C	10	Total O 10 10	0	0
5	D	19	Total O 19 19	0	0
5	E	15	Total O 15 15	0	0
5	F	11	Total O 11 11	0	0
5	H	16	Total O 16 16	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 TRIM8

Chain I:

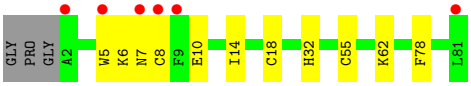




• Molecule 1: E3 ubiquitin-protein ligase TRIM8

Chain J:

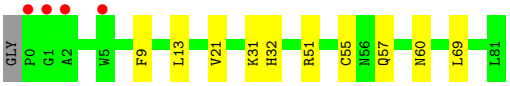




• Molecule 1: E3 ubiquitin-protein ligase TRIM8

Chain B:

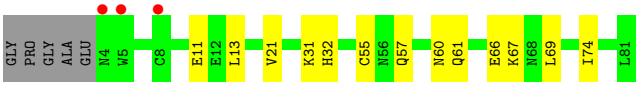




• Molecule 1: E3 ubiquitin-protein ligase TRIM8

Chain C:





• Molecule 2: Ubiquitin-conjugating enzyme E2 N

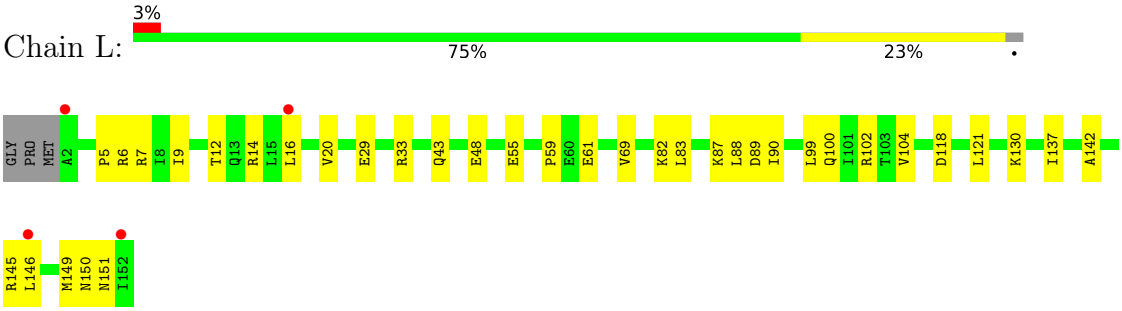
Chain K:





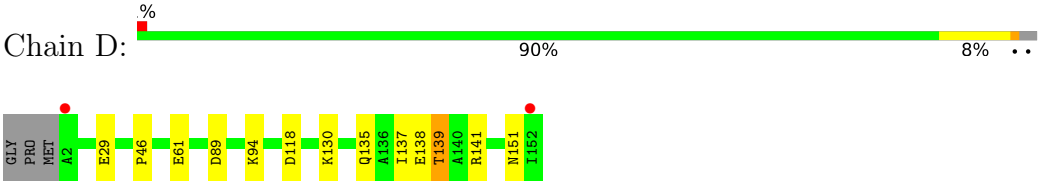
• Molecule 2: Ubiquitin-conjugating enzyme E2 N

Chain L:



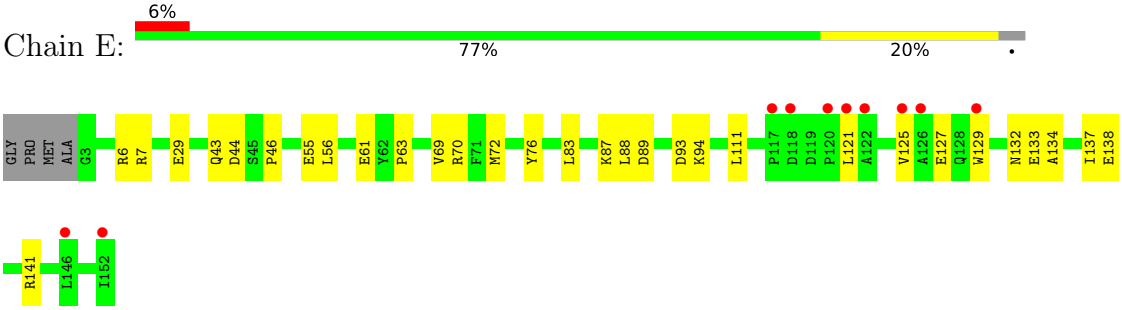
• Molecule 2: Ubiquitin-conjugating enzyme E2 N

Chain D:



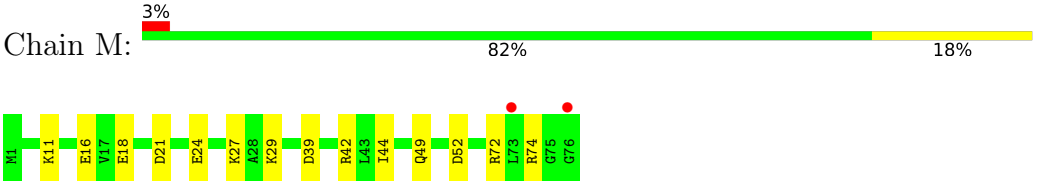
• Molecule 2: Ubiquitin-conjugating enzyme E2 N

Chain E:



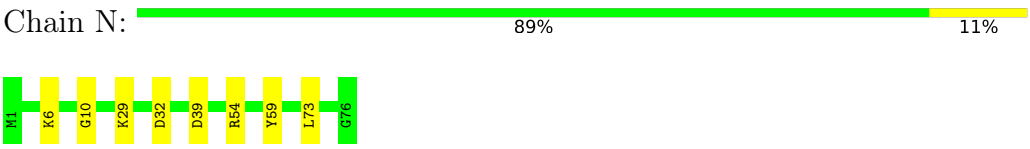
• Molecule 3: Ubiquitin

Chain M:



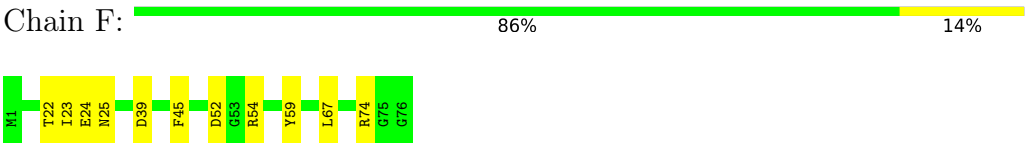
• Molecule 3: Ubiquitin

Chain N:



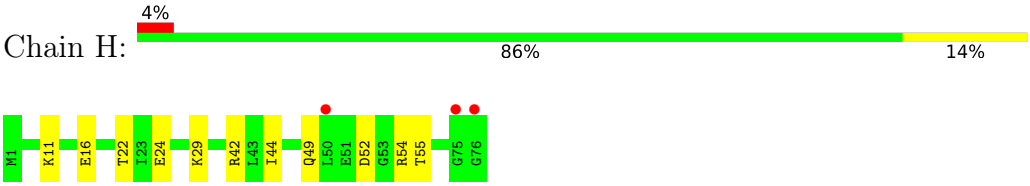
• Molecule 3: Ubiquitin

Chain F:



• Molecule 3: Ubiquitin

Chain H:


4%
86%
14%
M1
K11
E16
T22
I23
E24
K29
R42
L43
I44
Q49
L50
E51
D52
G53
R54
T55
G75
G76

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.45Å 177.44Å 75.59Å 90.00° 97.77° 90.00°	Depositor
Resolution (Å)	49.00 – 2.39 49.00 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.00-2.39) 99.6 (49.00-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.202 , 0.253 0.202 , 0.253	Depositor DCC
R_{free} test set	2612 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9879	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.37% 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	B	0.18	0/665	0.44	0/898
1	C	0.19	0/639	0.44	0/863
1	I	0.23	0/615	0.51	0/829
1	J	0.19	0/653	0.46	0/882
2	D	0.19	0/1228	0.47	0/1673
2	E	0.19	0/1224	0.45	0/1666
2	K	0.19	0/1215	0.42	0/1655
2	L	0.19	0/1229	0.44	0/1673
3	F	0.20	0/607	0.49	0/816
3	H	0.20	0/607	0.44	0/816
3	M	0.24	0/607	0.48	0/816
3	N	0.17	0/607	0.41	0/816
All	All	0.20	0/9896	0.45	0/13403

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	B	649	0	632	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	624	0	608	15	0
1	I	602	0	592	13	0
1	J	638	0	619	11	0
2	D	1198	0	1211	9	0
2	E	1194	0	1206	25	0
2	K	1185	0	1194	15	0
2	L	1199	0	1211	24	0
3	F	601	0	629	9	0
3	H	601	0	629	7	0
3	M	601	0	629	16	0
3	N	601	0	629	6	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
5	B	12	0	0	0	0
5	C	10	0	0	1	0
5	D	19	0	0	0	0
5	E	15	0	0	1	0
5	F	11	0	0	1	0
5	H	16	0	0	2	0
5	I	16	0	0	2	0
5	J	9	0	0	0	0
5	K	27	0	0	0	0
5	L	18	0	0	1	0
5	M	8	0	0	2	0
5	N	17	0	0	2	0
All	All	9879	0	9789	135	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 7.

The worst 5 of 135 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:I:77:LYS:HE3	1:J:8:CYS:SG	1.83	1.17
1:C:67:LYS:HZ2	1:C:69:LEU:HA	1.44	0.82
2:E:70:ARG:NH2	2:E:83:LEU:O	2.16	0.76
3:M:24:GLU:HG3	3:M:52:ASP:HB3	1.70	0.74
3:M:72:ARG:HB3	3:M:74:ARG:NH1	2.03	0.73

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	B	80/83 (96%)	80 (100%)	0	0	100	100
1	C	76/83 (92%)	75 (99%)	1 (1%)	0	100	100
1	I	74/83 (89%)	73 (99%)	1 (1%)	0	100	100
1	J	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
2	D	149/154 (97%)	144 (97%)	5 (3%)	0	100	100
2	E	148/154 (96%)	145 (98%)	3 (2%)	0	100	100
2	K	147/154 (96%)	142 (97%)	5 (3%)	0	100	100
2	L	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
3	F	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
3	H	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
3	M	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
3	N	74/76 (97%)	74 (100%)	0	0	100	100
All	All	1197/1252 (96%)	1174 (98%)	23 (2%)	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	B	72/72 (100%)	72 (100%)	0	100	100
1	C	70/72 (97%)	70 (100%)	0	100	100
1	I	68/72 (94%)	68 (100%)	0	100	100
1	J	71/72 (99%)	70 (99%)	1 (1%)	59	79
2	D	127/129 (98%)	126 (99%)	1 (1%)	73	86
2	E	127/129 (98%)	126 (99%)	1 (1%)	73	86
2	K	126/129 (98%)	126 (100%)	0	100	100
2	L	127/129 (98%)	126 (99%)	1 (1%)	73	86
3	F	68/68 (100%)	68 (100%)	0	100	100
3	H	68/68 (100%)	68 (100%)	0	100	100
3	M	68/68 (100%)	68 (100%)	0	100	100
3	N	68/68 (100%)	68 (100%)	0	100	100
All	All	1060/1076 (98%)	1056 (100%)	4 (0%)	84	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	62	LYS
2	L	137	ILE
2	D	139	THR
2	E	56	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	116	ASN
2	E	123	ASN
3	H	49	GLN
3	F	25	ASN
3	H	25	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 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.

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	B	82/83 (98%)	0.29	4 (4%) 35 31	39, 54, 87, 92	0
1	C	78/83 (93%)	0.32	3 (3%) 44 40	37, 53, 84, 90	0
1	I	76/83 (91%)	0.20	1 (1%) 75 71	39, 54, 84, 100	0
1	J	80/83 (96%)	0.16	6 (7%) 20 17	38, 52, 85, 92	0
2	D	151/154 (98%)	0.28	2 (1%) 75 71	39, 53, 82, 100	0
2	E	150/154 (97%)	0.42	10 (6%) 24 20	37, 57, 107, 115	0
2	K	149/154 (96%)	0.10	0 100 100	40, 53, 75, 84	0
2	L	151/154 (98%)	0.23	4 (2%) 57 53	40, 52, 83, 98	0
3	F	76/76 (100%)	0.39	0 100 100	42, 59, 80, 87	0
3	H	76/76 (100%)	0.28	3 (3%) 43 39	40, 56, 74, 102	0
3	M	76/76 (100%)	0.35	2 (2%) 57 53	42, 59, 84, 95	0
3	N	76/76 (100%)	0.16	0 100 100	38, 57, 75, 84	0
All	All	1221/1252 (97%)	0.26	35 (2%) 53 50	37, 55, 84, 115	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	76	GLY	4.8
1	C	5	TRP	4.8
1	B	5	TRP	4.5
2	L	152	ILE	3.5
1	J	2	ALA	3.5

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 (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

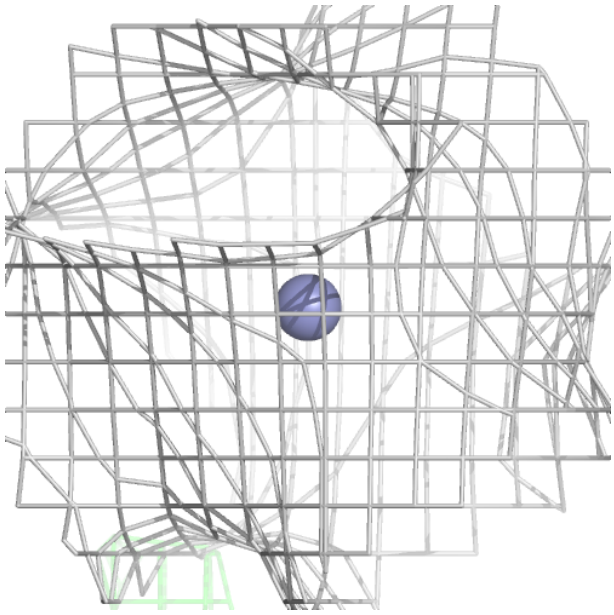
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

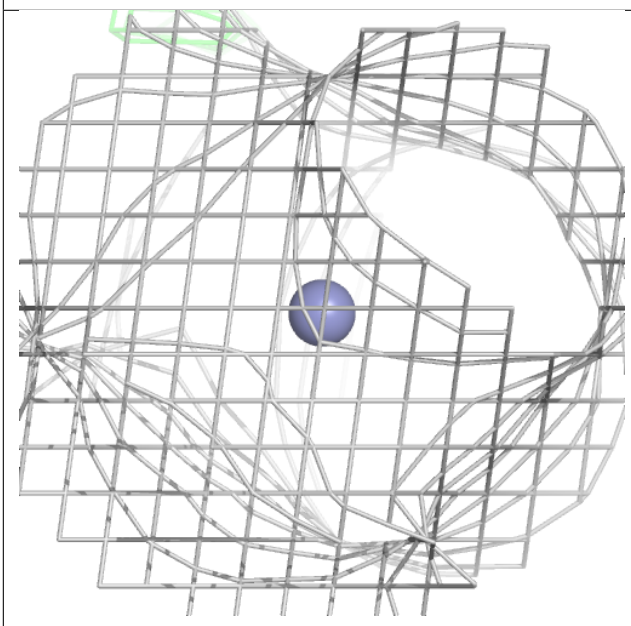
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	I	102	1/1	0.99	0.03	51,51,51,51	0
4	ZN	J	101	1/1	0.99	0.02	46,46,46,46	0
4	ZN	I	101	1/1	1.00	0.02	46,46,46,46	0
4	ZN	J	102	1/1	1.00	0.03	45,45,45,45	0
4	ZN	B	101	1/1	1.00	0.02	45,45,45,45	0
4	ZN	B	102	1/1	1.00	0.02	42,42,42,42	0
4	ZN	C	101	1/1	1.00	0.03	49,49,49,49	0
4	ZN	C	102	1/1	1.00	0.02	46,46,46,46	0

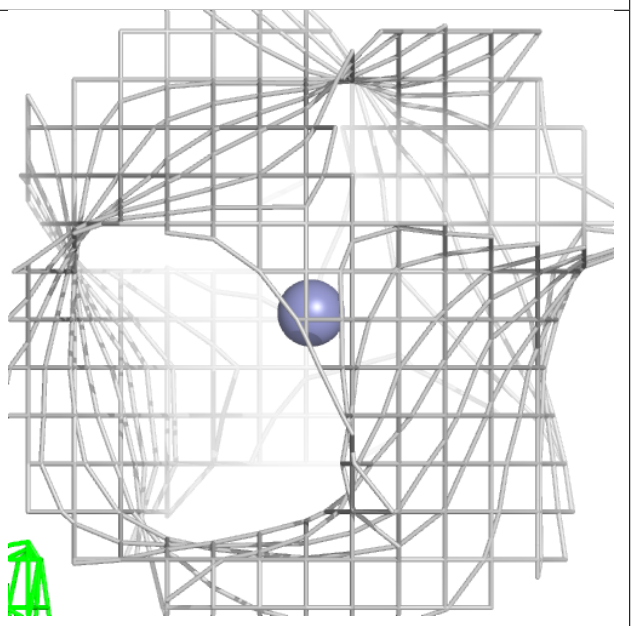
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN I 102:

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

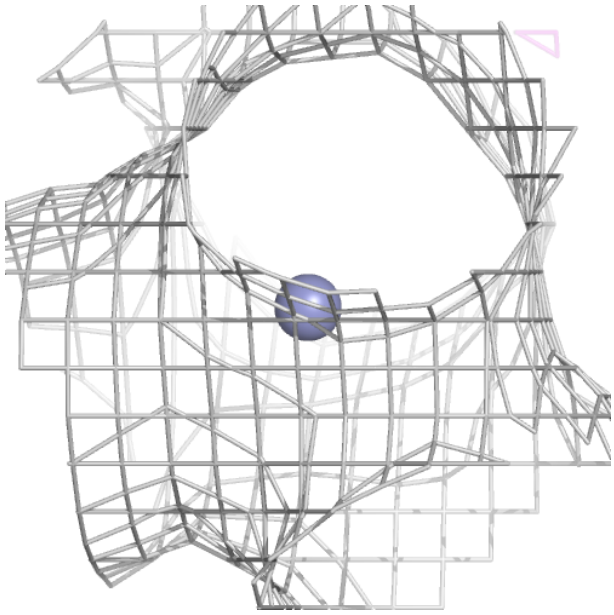


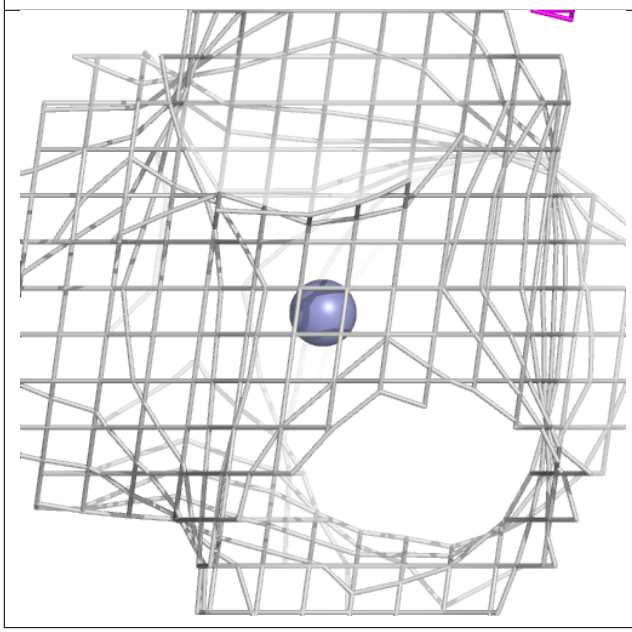


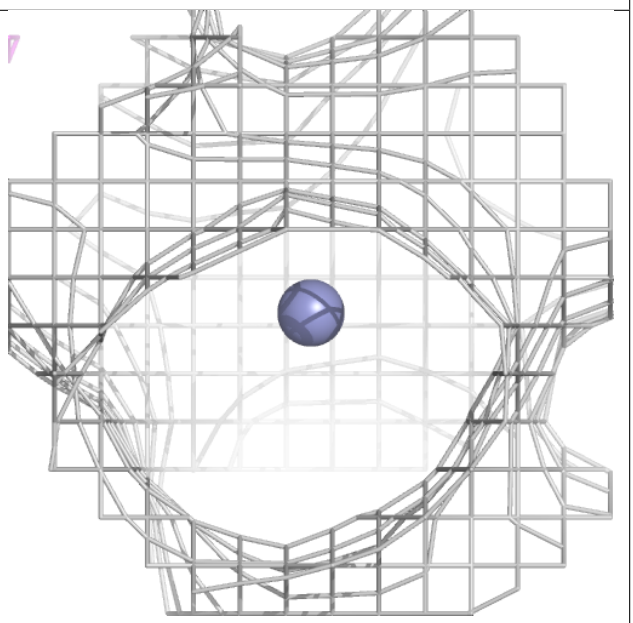


Electron density around ZN J 101:

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

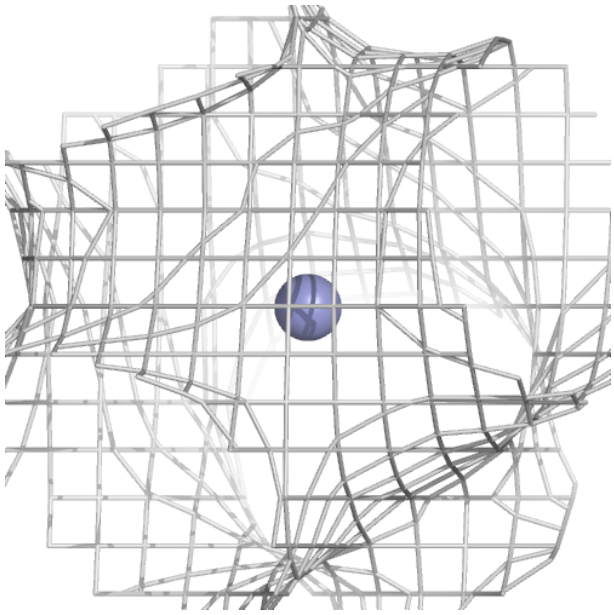


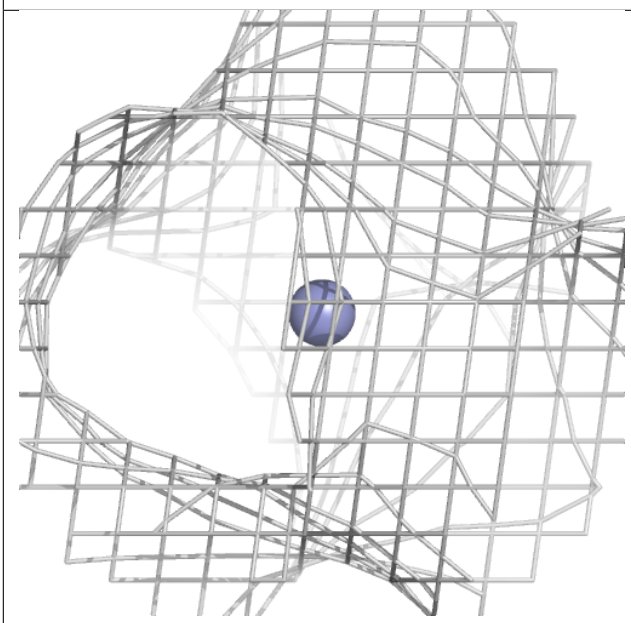


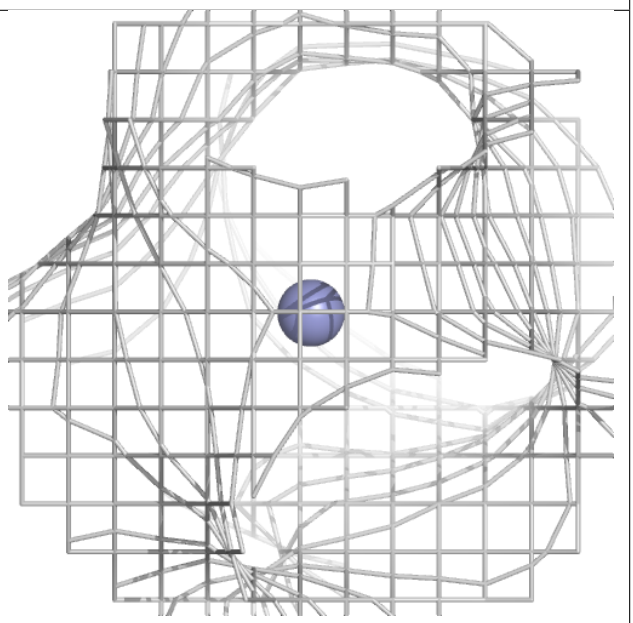


Electron density around ZN I 101:

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

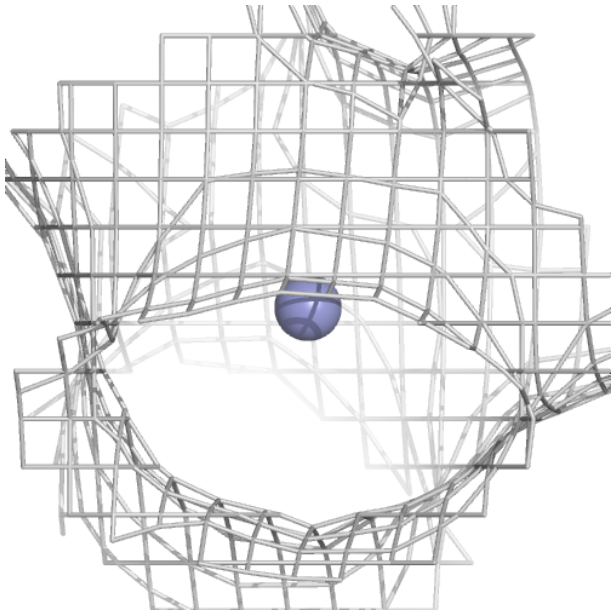


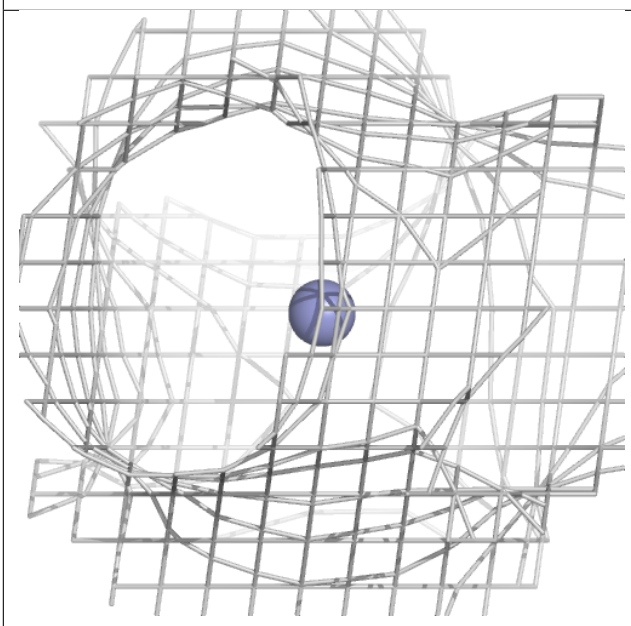


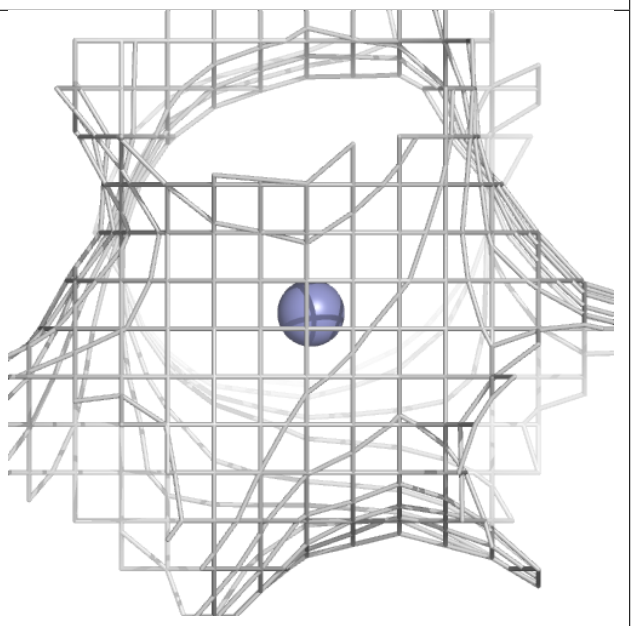


Electron density around ZN J 102:

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

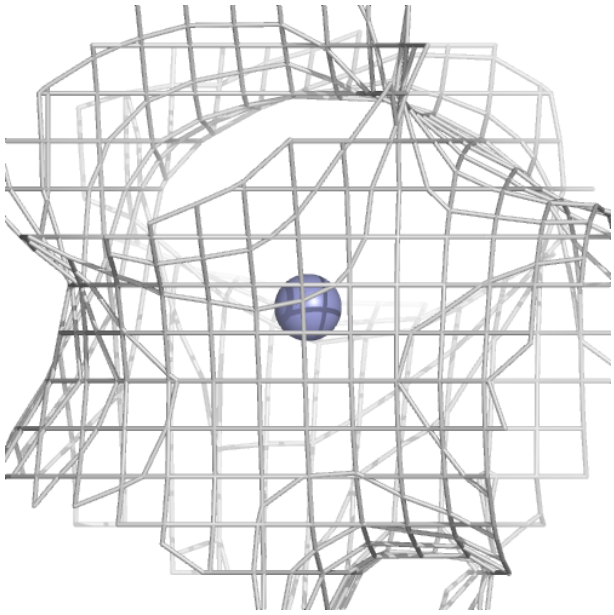


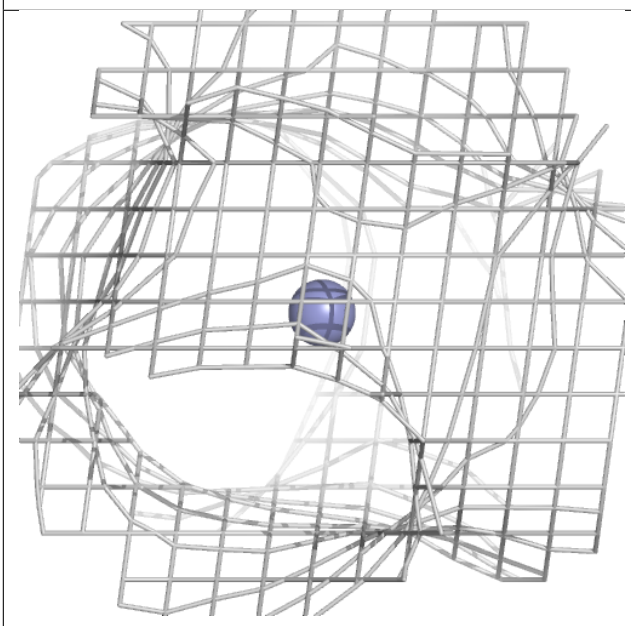


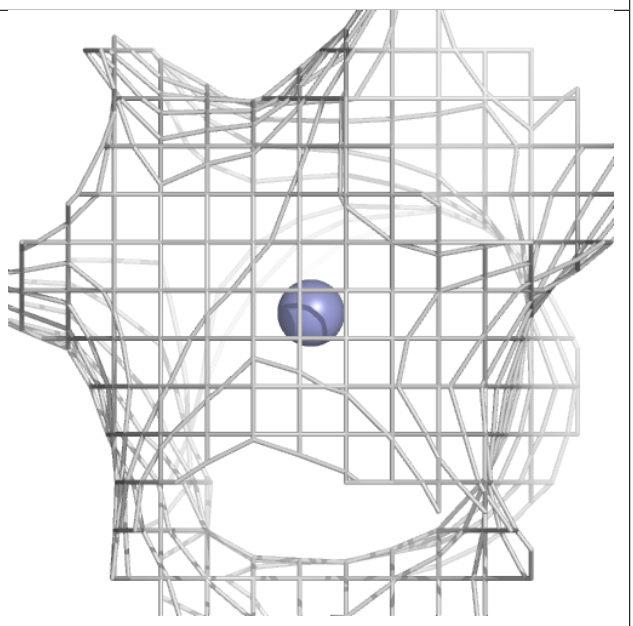


Electron density around ZN B 101:

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

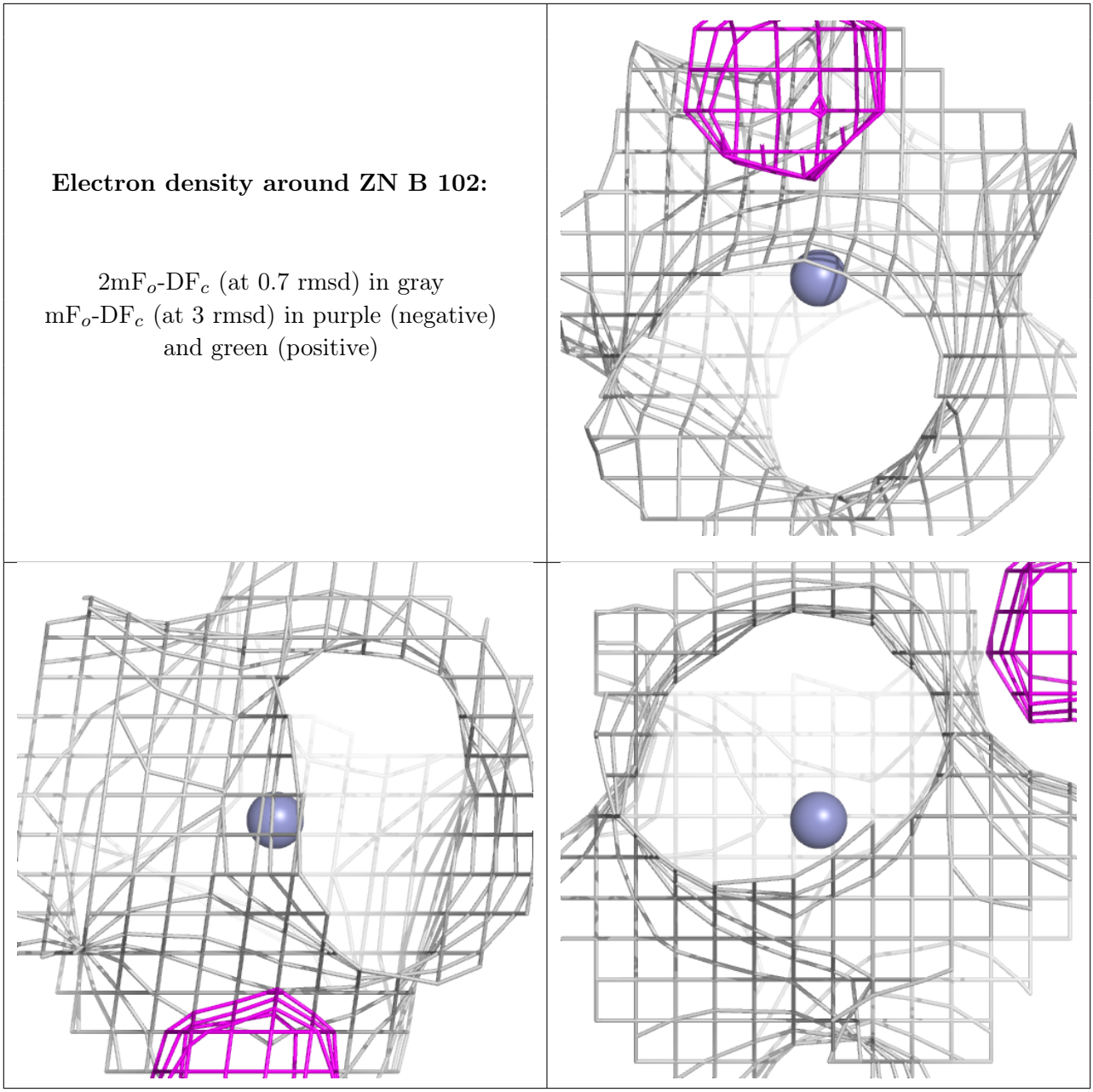






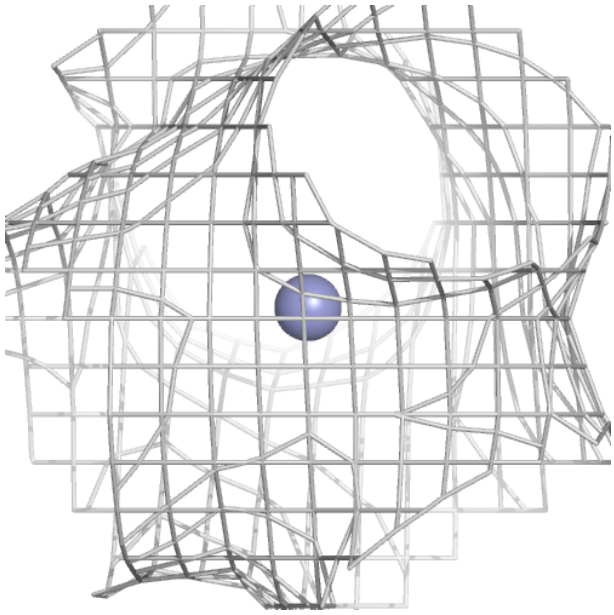
Electron density around ZN B 102:

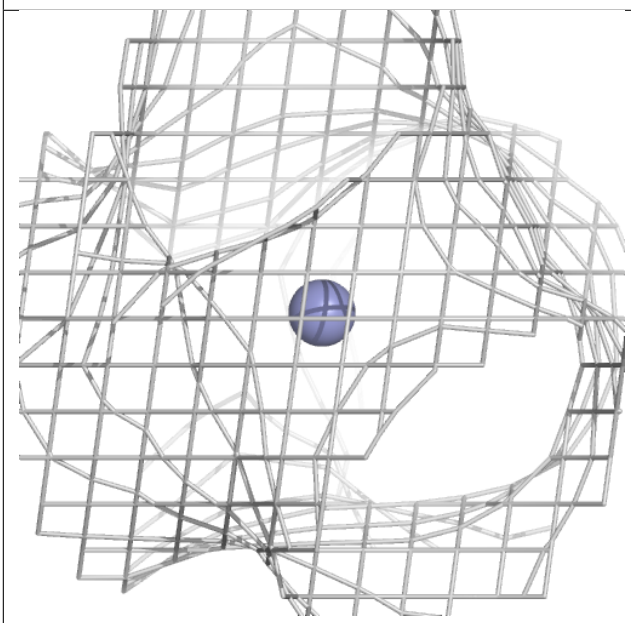
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

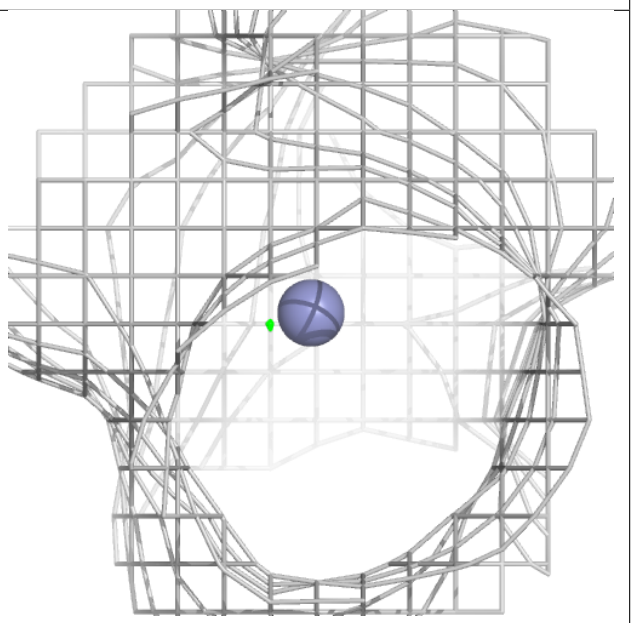


Electron density around ZN C 101:

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

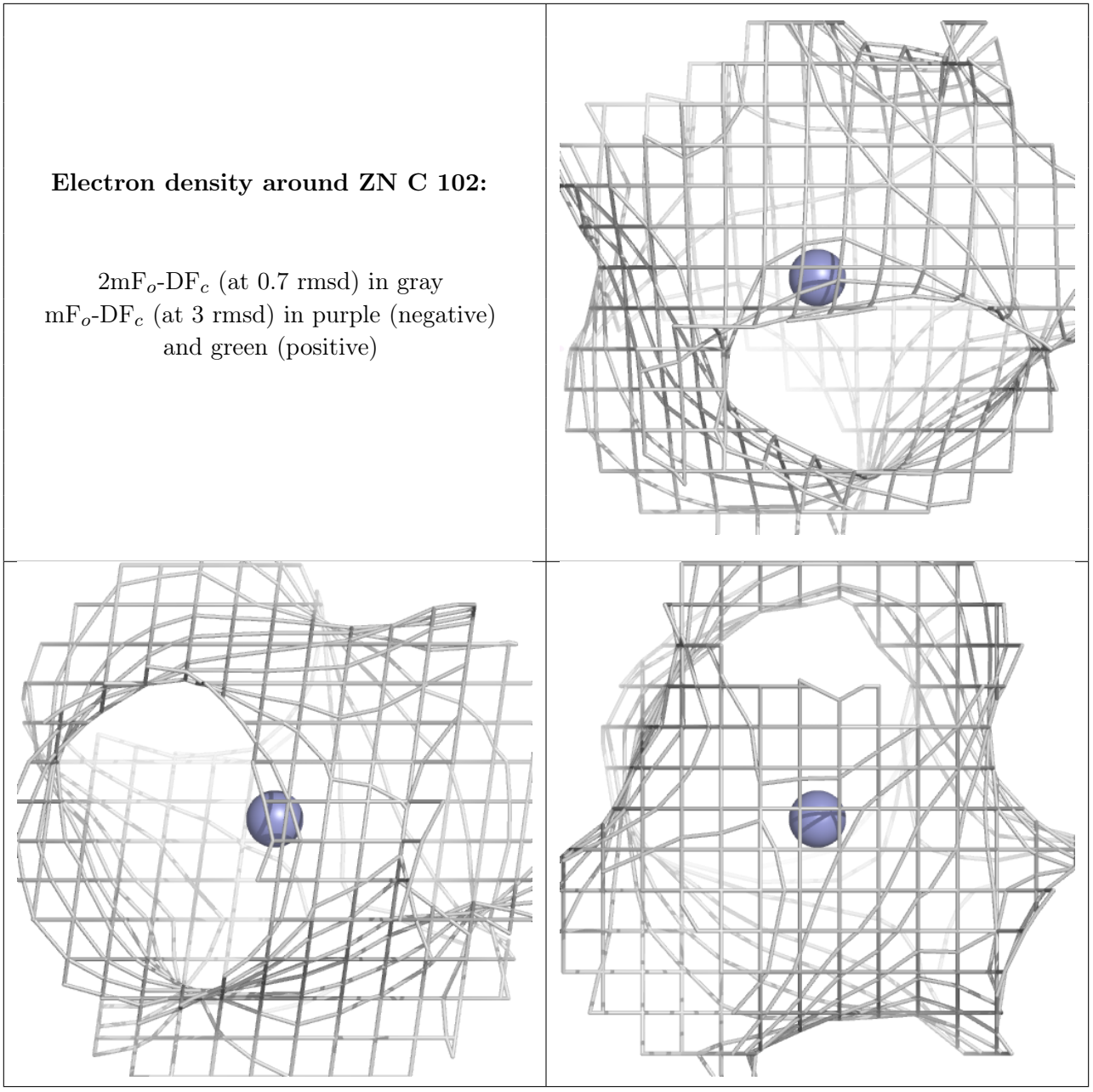






Electron density around ZN C 102:

$2mF_o$-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.