



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:34 PM UTC

PDB ID : 7C07 / pdb_00007c07
Title : Crystal structure of yeast U2AF1 complex bound to 5'-AAGGU RNA.
Authors : Yoshida, H.; Park, S.Y.; Urano, T.; Obayashi, E.
Deposited on : 2020-04-30
Resolution : 3.20 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	:	4-5-2 with Phenix2.0
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

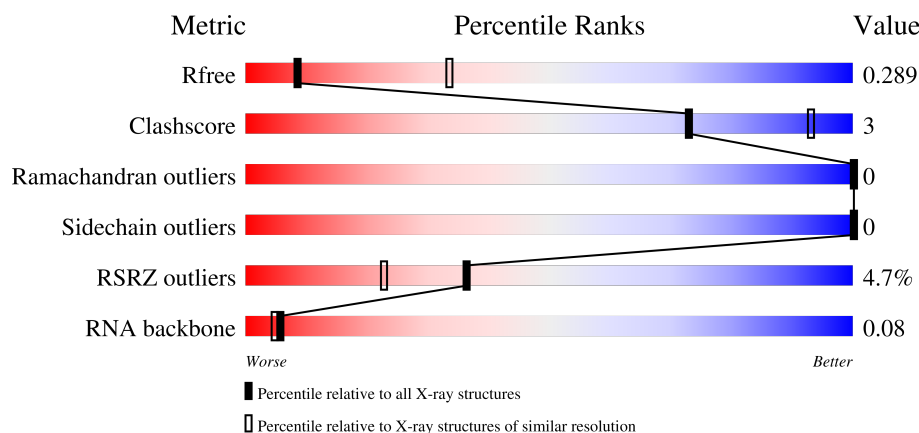
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	216	2% 84% 5% 11%
1	D	216	% 81% 6% 13%
1	G	216	2% 81% 8% 11%
1	J	216	4% 82% 7% 11%

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Mol	Chain	Length	Quality of chain
1	M	216	
1	P	216	
1	S	216	
1	V	216	
1	Y	216	
2	B	69	
2	E	69	
2	H	69	
2	K	69	
2	N	69	
2	Q	69	
2	T	69	
2	W	69	
2	Z	69	
3	1	6	
3	C	6	
3	F	6	
3	I	6	
3	L	6	
3	O	6	
3	R	6	
3	U	6	
3	X	6	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18390 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 Splicing factor U2AF 23 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1567	981	278	295	13			
1	D	187	Total	C	N	O	S	0	0	0
			1524	955	270	286	13			
1	G	193	Total	C	N	O	S	0	0	0
			1567	981	278	295	13			
1	J	193	Total	C	N	O	S	0	0	0
			1567	981	278	295	13			
1	M	179	Total	C	N	O	S	0	0	0
			1461	916	260	272	13			
1	P	189	Total	C	N	O	S	0	0	0
			1534	962	273	286	13			
1	S	188	Total	C	N	O	S	0	1	0
			1539	964	274	288	13			
1	V	174	Total	C	N	O	S	0	0	0
			1424	895	254	262	13			
1	Y	179	Total	C	N	O	S	0	0	0
			1461	916	260	272	13			

- Molecule 2 is a protein called Splicing factor U2AF 59 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	56	Total	C	N	O	S	0	0	0
			455	288	82	84	1			
2	E	51	Total	C	N	O	S	0	0	0
			417	266	74	76	1			
2	H	53	Total	C	N	O	S	0	0	0
			430	274	76	79	1			
2	K	54	Total	C	N	O	S	0	0	0
			435	277	77	80	1			
2	N	52	Total	C	N	O	S	0	0	0
			426	272	75	78	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	53	Total	C	N	O	S	0	0	0
			430	274	76	79	1			
2	T	47	Total	C	N	O	S	0	0	0
			383	246	67	69	1			
2	W	53	Total	C	N	O	S	0	0	0
			430	274	76	79	1			
2	Z	44	Total	C	N	O	S	0	0	0
			359	232	63	63	1			

- Molecule 3 is a RNA chain called RNA (5'-R(*U*AP*AP*GP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	F	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	I	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	L	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	O	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	R	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	U	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	X	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	1	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	G	2	Total	Zn	0	0
			2	2		
4	J	2	Total	Zn	0	0
			2	2		

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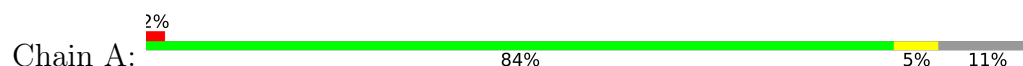
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	2	Total 2	Zn 2	0	0
4	P	2	Total 2	Zn 2	0	0
4	S	2	Total 2	Zn 2	0	0
4	V	2	Total 2	Zn 2	0	0
4	Y	2	Total 2	Zn 2	0	0

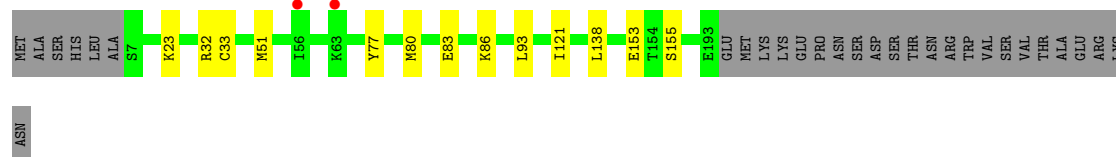
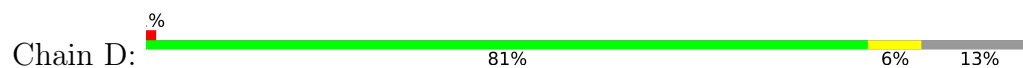
3 Residue-property plots [i](#)

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.

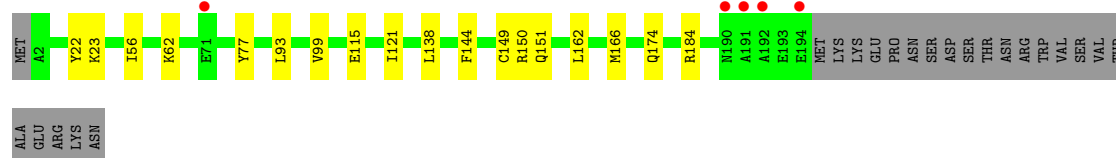
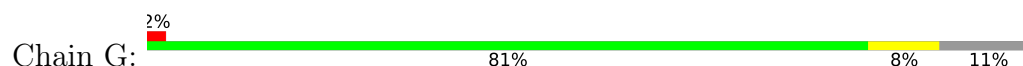
- Molecule 1: Splicing factor U2AF 23 kDa subunit



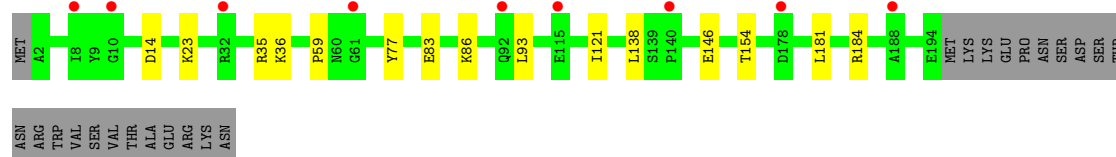
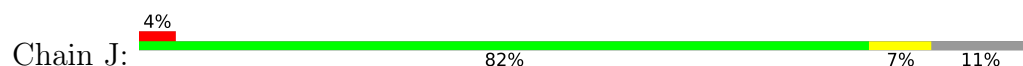
- Molecule 1: Splicing factor U2AF 23 kDa subunit



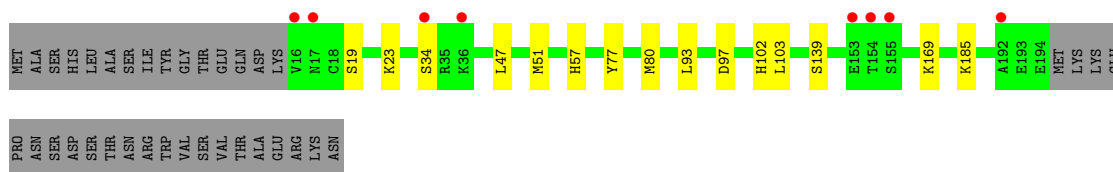
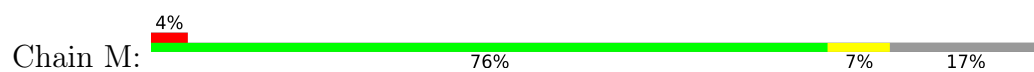
- Molecule 1: Splicing factor U2AF 23 kDa subunit



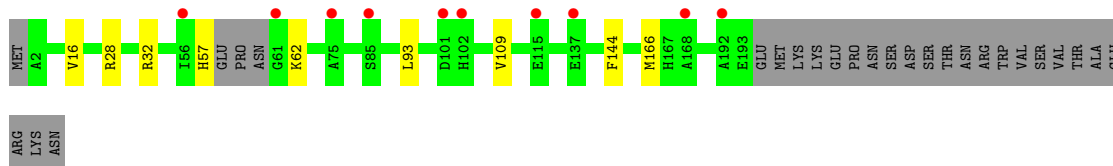
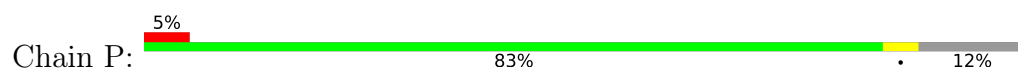
- Molecule 1: Splicing factor U2AF 23 kDa subunit



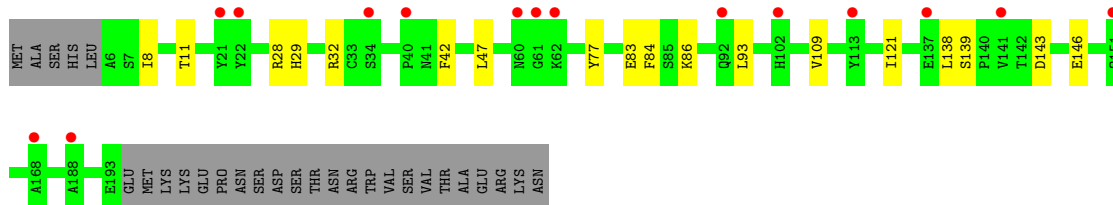
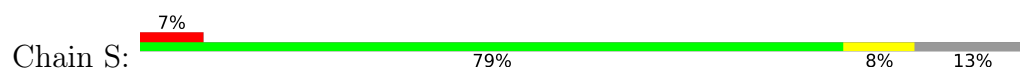
- Molecule 1: Splicing factor U2AF 23 kDa subunit



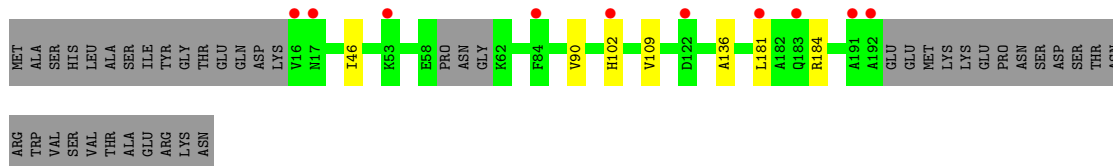
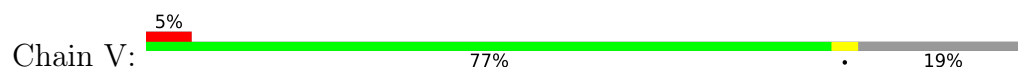
- Molecule 1: Splicing factor U2AF 23 kDa subunit



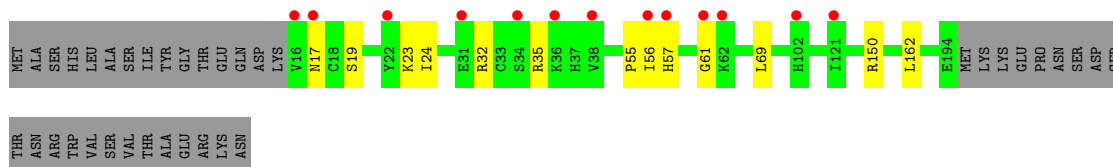
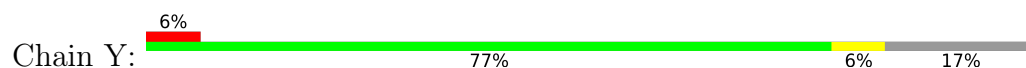
- Molecule 1: Splicing factor U2AF 23 kDa subunit



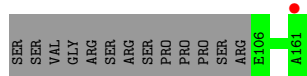
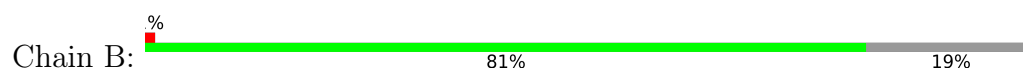
- Molecule 1: Splicing factor U2AF 23 kDa subunit



- Molecule 1: Splicing factor U2AF 23 kDa subunit



- Molecule 2: Splicing factor U2AF 59 kDa subunit



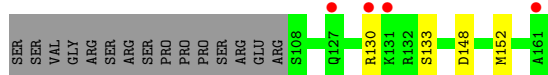
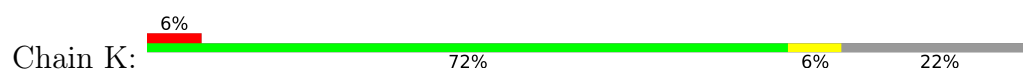
- Molecule 2: Splicing factor U2AF 59 kDa subunit



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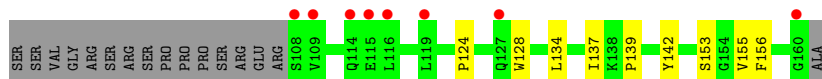
- Molecule 2: Splicing factor U2AF 59 kDa subunit



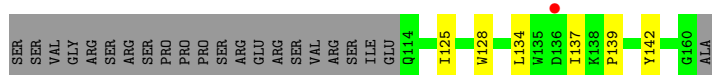
- Molecule 2: Splicing factor U2AF 59 kDa subunit



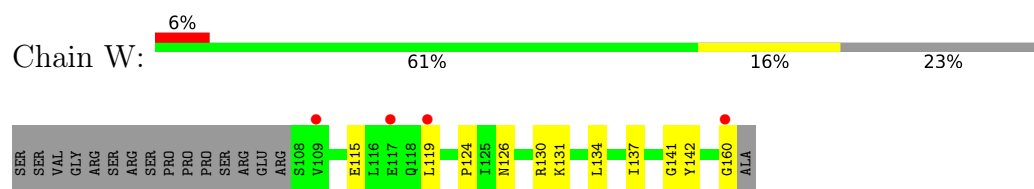
- Molecule 2: Splicing factor U2AF 59 kDa subunit



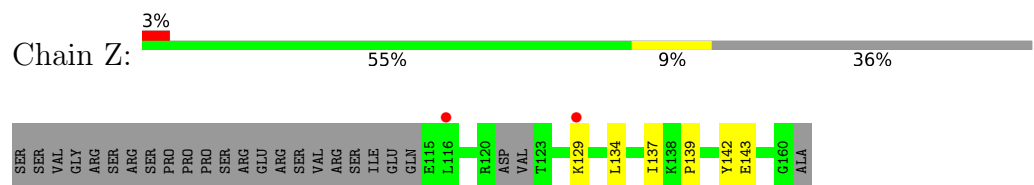
- Molecule 2: Splicing factor U2AF 59 kDa subunit



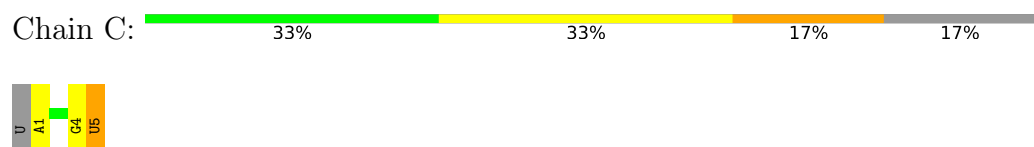
- Molecule 2: Splicing factor U2AF 59 kDa subunit



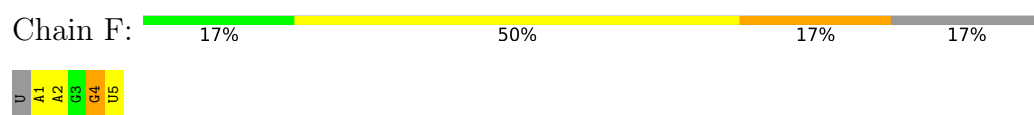
- Molecule 2: Splicing factor U2AF 59 kDa subunit



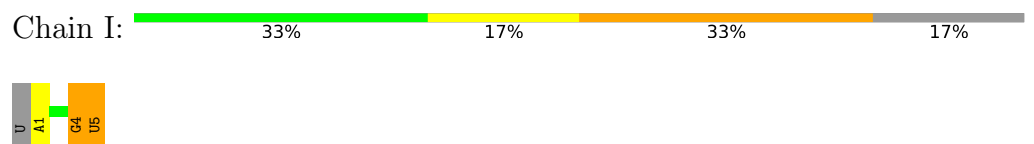
- Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')



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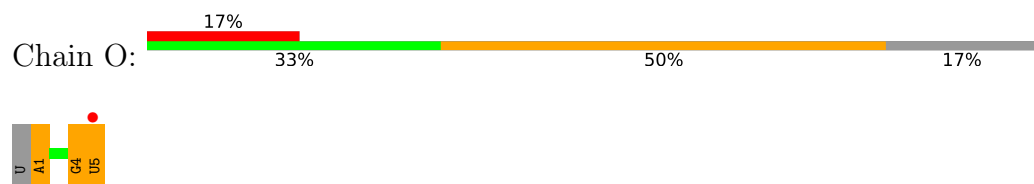
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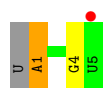
- Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')



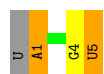
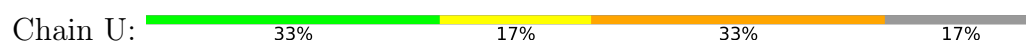
- Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')



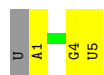
- Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')



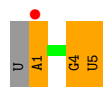
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.49Å 256.95Å 94.59Å 90.00° 100.75° 90.00°	Depositor
Resolution (Å)	48.17 – 3.20 48.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.17-3.20) 99.9 (48.17-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.255 , 0.285 0.259 , 0.289	Depositor DCC
R_{free} test set	3656 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	73.6	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.039 for l,-k,h	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18390	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.49% 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

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	0.07	0/1604	0.26	0/2163
1	D	0.08	0/1560	0.26	0/2103
1	G	0.08	0/1604	0.27	0/2163
1	J	0.08	0/1604	0.28	0/2163
1	M	0.08	0/1496	0.27	0/2017
1	P	0.08	0/1569	0.25	0/2113
1	S	0.08	0/1576	0.27	0/2125
1	V	0.08	0/1457	0.26	0/1962
1	Y	0.08	0/1496	0.27	0/2017
2	B	0.09	0/465	0.28	0/629
2	E	0.11	0/427	0.32	0/578
2	H	0.10	0/440	0.31	0/596
2	K	0.09	0/445	0.30	0/603
2	N	0.10	0/436	0.32	0/591
2	Q	0.09	0/440	0.30	0/596
2	T	0.09	0/393	0.26	0/533
2	W	0.10	0/440	0.31	0/596
2	Z	0.09	0/368	0.28	0/497
3	1	0.17	0/120	0.55	0/186
3	C	0.14	0/120	0.44	0/186
3	F	0.14	0/120	0.49	0/186
3	I	0.17	0/120	0.55	0/186
3	L	0.15	0/120	0.57	0/186
3	O	0.16	0/120	0.55	0/186
3	R	0.16	0/120	0.59	0/186
3	U	0.15	0/120	0.56	0/186
3	X	0.16	0/120	0.58	0/186
All	All	0.09	0/18900	0.30	0/25719

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	1567	0	1487	7	0
1	D	1524	0	1448	9	0
1	G	1567	0	1487	16	0
1	J	1567	0	1488	9	0
1	M	1461	0	1389	11	0
1	P	1534	0	1461	8	0
1	S	1539	0	1459	13	0
1	V	1424	0	1360	5	0
1	Y	1461	0	1389	11	0
2	B	455	0	460	0	0
2	E	417	0	422	7	0
2	H	430	0	436	6	0
2	K	435	0	441	3	0
2	N	426	0	433	7	0
2	Q	430	0	436	5	0
2	T	383	0	387	4	0
2	W	430	0	436	10	0
2	Z	359	0	365	5	0
3	1	107	0	56	4	0
3	C	107	0	56	1	0
3	F	107	0	56	3	0
3	I	107	0	56	3	0
3	L	107	0	56	0	0
3	O	107	0	56	4	0
3	R	107	0	56	1	0
3	U	107	0	56	2	0
3	X	107	0	56	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
4	M	2	0	0	0	0
4	P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	2	0	0	0	0
4	V	2	0	0	0	0
4	Y	2	0	0	0	0
All	All	18390	0	17288	114	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 3.

All (114) 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:A:22:TYR:OH	1:G:184:ARG:NH2	2.22	0.71
1:D:33:CYS:HA	3:F:1:A:H62	1.57	0.70
2:W:131:LYS:HD3	2:W:131:LYS:H	1.57	0.69
1:D:23:LYS:NZ	3:F:4:G:O2'	2.31	0.64
1:J:14:ASP:O	1:J:35:ARG:NH2	2.29	0.64
1:D:153:GLU:OE1	1:D:153:GLU:N	2.32	0.62
1:Y:23:LYS:HG3	1:Y:24:ILE:HG12	1.83	0.60
1:G:150:ARG:NH1	3:I:5:U:O4	2.34	0.59
2:W:141:GLY:HA2	1:Y:57:HIS:HB3	1.85	0.58
1:Y:55:PRO:O	1:Y:61:GLY:HA3	2.04	0.58
1:G:144:PHE:HD1	1:G:166:MET:HE1	1.69	0.58
1:P:144:PHE:HD1	1:P:166:MET:HE1	1.69	0.58
2:Q:153:SER:O	1:S:28:ARG:NH2	2.37	0.57
1:D:32:ARG:O	3:F:1:A:N6	2.38	0.56
1:Y:23:LYS:NZ	3:I:4:G:O2'	2.25	0.56
1:M:34:SER:N	3:O:1:A:H62	2.04	0.56
1:G:62:LYS:HB3	1:P:16:VAL:HG22	1.90	0.53
2:H:139:PRO:HG2	2:H:142:TYR:CD1	2.44	0.53
1:Y:17:ASN:O	1:Y:35:ARG:NH2	2.42	0.53
1:G:149:CYS:SG	1:G:151:GLN:HG2	2.49	0.52
1:J:23:LYS:NZ	1:J:146:GLU:OE1	2.42	0.52
1:P:32:ARG:O	3:R:1:A:N6	2.43	0.52
2:E:153:SER:O	1:P:28:ARG:NH1	2.43	0.51
2:K:152:MET:HG3	1:S:8:ILE:HB	1.92	0.51
1:P:93:LEU:HD13	1:P:109:VAL:HG22	1.92	0.51
1:M:185:LYS:HB2	2:N:119:LEU:HD12	1.93	0.51
1:A:121:ILE:HD13	1:A:138:LEU:HG	1.94	0.50
1:G:23:LYS:NZ	3:I:4:G:O2'	2.44	0.50
1:G:121:ILE:HD13	1:G:138:LEU:HG	1.94	0.50
1:G:115:GLU:OE1	1:G:115:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:184:ARG:HH21	2:W:115:GLU:HG3	1.77	0.49
1:Y:56:ILE:HD11	1:Y:69:LEU:HD13	1.95	0.49
1:Y:19:SER:O	1:Y:23:LYS:HG2	2.13	0.48
1:A:7:SER:HB3	2:H:122:VAL:HG22	1.96	0.48
1:S:47:LEU:HB2	1:S:139:SER:HB2	1.95	0.48
1:J:154:THR:O	1:J:154:THR:OG1	2.31	0.48
1:Y:150:ARG:HG3	3:1:4:G:N1	2.29	0.48
1:S:29:HIS:O	1:S:32:ARG:HG2	2.14	0.48
1:D:51:MET:HE2	1:D:80:MET:HE1	1.96	0.47
2:E:139:PRO:HG2	2:E:142:TYR:CG	2.48	0.47
2:Z:139:PRO:HG2	2:Z:142:TYR:CG	2.49	0.47
2:T:125:ILE:HA	2:T:128:TRP:CD1	2.48	0.47
3:C:5:U:O2'	1:G:174:GLN:HG3	2.14	0.47
1:J:121:ILE:HD13	1:J:138:LEU:HG	1.96	0.47
1:G:77:TYR:CZ	1:G:93:LEU:HD22	2.49	0.47
1:M:57:HIS:ND1	2:Z:143:GLU:OE1	2.47	0.47
2:Z:139:PRO:HG2	2:Z:142:TYR:CD1	2.50	0.47
2:Q:134:LEU:HA	2:Q:137:ILE:HD12	1.97	0.47
2:E:141:GLY:HA2	1:P:57:HIS:HB3	1.96	0.47
1:Y:32:ARG:O	3:1:1:A:N6	2.48	0.46
1:A:149:CYS:SG	1:A:151:GLN:HG2	2.54	0.46
1:D:83:GLU:O	1:D:86:LYS:HG2	2.15	0.46
2:K:148:ASP:OD2	1:S:8:ILE:HG13	2.15	0.46
2:T:139:PRO:HG2	2:T:142:TYR:CG	2.50	0.46
1:S:77:TYR:CE1	1:S:93:LEU:HD23	2.50	0.46
1:A:55:PRO:O	1:A:61:GLY:HA3	2.15	0.45
1:G:62:LYS:O	1:P:16:VAL:HG13	2.15	0.45
1:S:83:GLU:O	1:S:86:LYS:HG2	2.16	0.45
2:E:155:VAL:HG23	2:E:156:PHE:CD2	2.52	0.45
2:Z:129:LYS:HD3	2:Z:129:LYS:HA	1.74	0.45
1:M:102:HIS:CD2	1:M:103:LEU:HG	2.51	0.45
2:Z:134:LEU:HA	2:Z:137:ILE:HD12	1.98	0.45
1:A:184:ARG:NH2	1:G:22:TYR:OH	2.49	0.45
1:S:32:ARG:O	3:U:1:A:N6	2.50	0.45
1:G:150:ARG:HD3	3:I:4:G:N1	2.32	0.45
2:H:155:VAL:HG23	2:H:156:PHE:CD2	2.52	0.45
1:P:62:LYS:HB3	1:P:62:LYS:HE2	1.72	0.45
1:M:19:SER:HB3	3:O:5:U:H1'	1.98	0.45
2:Q:155:VAL:HG23	2:Q:156:PHE:CD2	2.52	0.44
2:Q:139:PRO:HG2	2:Q:142:TYR:CG	2.52	0.44
2:W:134:LEU:HA	2:W:137:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ILE:HD13	1:D:138:LEU:HG	1.99	0.44
1:M:77:TYR:CE1	1:M:93:LEU:HD23	2.52	0.44
1:J:181:LEU:HD23	1:J:184:ARG:HH21	1.83	0.44
1:S:121:ILE:HD13	1:S:138:LEU:HG	2.00	0.43
1:J:36:LYS:HD3	1:S:42:PHE:CG	2.53	0.43
2:E:117:GLU:O	2:E:120:ARG:HG3	2.19	0.43
2:H:120:ARG:O	2:H:122:VAL:HG23	2.19	0.43
1:M:97:ASP:HB2	1:M:169:LYS:HB2	2.01	0.43
2:T:134:LEU:HD23	2:T:137:ILE:HD12	2.00	0.42
2:K:130:ARG:NH2	2:K:133:SER:OG	2.49	0.42
1:D:77:TYR:CE1	1:D:93:LEU:HD23	2.55	0.42
1:G:99:VAL:HG21	2:N:145:VAL:HG21	2.02	0.42
1:A:84:PHE:HE1	1:A:124:LEU:HD11	1.84	0.42
1:D:155:SER:HA	1:J:59:PRO:HB3	2.01	0.42
2:N:139:PRO:HG2	2:N:142:TYR:CG	2.54	0.42
1:V:90:VAL:HG13	1:V:109:VAL:HG23	2.02	0.42
1:J:83:GLU:O	1:J:86:LYS:HG2	2.20	0.42
2:N:134:LEU:HA	2:N:137:ILE:HD12	2.01	0.42
1:M:34:SER:H	3:O:1:A:H62	1.66	0.42
2:E:111:SER:O	2:E:114:GLN:NE2	2.52	0.42
2:T:134:LEU:HA	2:T:137:ILE:HD12	2.02	0.41
1:G:162:LEU:HD11	2:N:142:TYR:HE2	1.85	0.41
1:S:143:ASP:HB3	1:S:146:GLU:HG2	2.01	0.41
2:W:141:GLY:HA2	1:Y:57:HIS:CB	2.47	0.41
1:G:56:ILE:HD13	2:N:144:LEU:HD11	2.02	0.41
2:Q:124:PRO:O	2:Q:128:TRP:HD1	2.04	0.41
1:V:102:HIS:NE2	2:W:160:GLY:HA3	2.36	0.41
1:V:181:LEU:HD22	2:W:119:LEU:HD21	2.02	0.41
1:S:84:PHE:CD2	1:S:109:VAL:HG21	2.55	0.41
2:E:134:LEU:HA	2:E:137:ILE:HD12	2.02	0.41
2:W:142:TYR:HE2	1:Y:162:LEU:HD21	1.86	0.41
1:J:77:TYR:CE1	1:J:93:LEU:HD23	2.55	0.41
1:S:11:THR:HG22	3:U:5:U:H5'	2.02	0.41
2:H:134:LEU:HA	2:H:137:ILE:HD12	2.02	0.41
2:W:130:ARG:H	2:W:130:ARG:HG2	1.62	0.41
1:M:51:MET:HE3	1:M:80:MET:HE1	2.02	0.41
2:H:139:PRO:HG2	2:H:142:TYR:CG	2.57	0.40
2:N:124:PRO:HB2	2:N:126:ASN:OD1	2.21	0.40
1:V:46:ILE:HD11	1:V:136:ALA:HB1	2.03	0.40
2:W:124:PRO:HB2	2:W:126:ASN:OD1	2.21	0.40
3:1:4:G:H3'	3:1:5:U:H5'	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:23:LYS:NZ	3:O:4:G:O2'	2.53	0.40
1:M:47:LEU:HB2	1:M:139:SER:HB2	2.04	0.40

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	191/216 (88%)	185 (97%)	6 (3%)	0	100	100
1	D	185/216 (86%)	181 (98%)	4 (2%)	0	100	100
1	G	191/216 (88%)	186 (97%)	5 (3%)	0	100	100
1	J	191/216 (88%)	183 (96%)	8 (4%)	0	100	100
1	M	177/216 (82%)	171 (97%)	6 (3%)	0	100	100
1	P	185/216 (86%)	179 (97%)	6 (3%)	0	100	100
1	S	187/216 (87%)	182 (97%)	5 (3%)	0	100	100
1	V	170/216 (79%)	167 (98%)	3 (2%)	0	100	100
1	Y	177/216 (82%)	171 (97%)	6 (3%)	0	100	100
2	B	54/69 (78%)	52 (96%)	2 (4%)	0	100	100
2	E	49/69 (71%)	47 (96%)	2 (4%)	0	100	100
2	H	51/69 (74%)	48 (94%)	3 (6%)	0	100	100
2	K	52/69 (75%)	48 (92%)	4 (8%)	0	100	100
2	N	50/69 (72%)	47 (94%)	3 (6%)	0	100	100
2	Q	51/69 (74%)	49 (96%)	2 (4%)	0	100	100
2	T	45/69 (65%)	41 (91%)	4 (9%)	0	100	100
2	W	51/69 (74%)	48 (94%)	3 (6%)	0	100	100
2	Z	40/69 (58%)	36 (90%)	4 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2097/2565 (82%)	2021 (96%)	76 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	170/192 (88%)	170 (100%)	0	100	100
1	D	166/192 (86%)	166 (100%)	0	100	100
1	G	170/192 (88%)	170 (100%)	0	100	100
1	J	170/192 (88%)	170 (100%)	0	100	100
1	M	159/192 (83%)	159 (100%)	0	100	100
1	P	166/192 (86%)	166 (100%)	0	100	100
1	S	167/192 (87%)	167 (100%)	0	100	100
1	V	155/192 (81%)	155 (100%)	0	100	100
1	Y	159/192 (83%)	159 (100%)	0	100	100
2	B	50/62 (81%)	50 (100%)	0	100	100
2	E	46/62 (74%)	46 (100%)	0	100	100
2	H	48/62 (77%)	48 (100%)	0	100	100
2	K	48/62 (77%)	48 (100%)	0	100	100
2	N	48/62 (77%)	48 (100%)	0	100	100
2	Q	48/62 (77%)	48 (100%)	0	100	100
2	T	42/62 (68%)	42 (100%)	0	100	100
2	W	48/62 (77%)	48 (100%)	0	100	100
2	Z	39/62 (63%)	39 (100%)	0	100	100
All	All	1899/2286 (83%)	1899 (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. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	106	ASN
1	D	44	GLN
1	G	17	ASN
1	G	106	ASN
1	G	118	GLN
1	J	131	GLN
1	M	60	ASN
1	M	164	ASN
1	P	17	ASN
1	P	44	GLN
1	P	102	HIS
1	P	131	GLN
1	S	50	ASN
1	S	106	ASN
2	T	127	GLN
1	V	131	GLN
1	V	183	GLN
1	Y	131	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	1	5/6 (83%)	2 (40%)	1 (20%)
3	C	5/6 (83%)	2 (40%)	1 (20%)
3	F	4/6 (66%)	3 (75%)	0
3	I	5/6 (83%)	2 (40%)	1 (20%)
3	L	5/6 (83%)	2 (40%)	1 (20%)
3	O	5/6 (83%)	2 (40%)	1 (20%)
3	R	5/6 (83%)	1 (20%)	1 (20%)
3	U	5/6 (83%)	2 (40%)	1 (20%)
3	X	5/6 (83%)	2 (40%)	1 (20%)
All	All	44/54 (81%)	18 (40%)	8 (18%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	4	G
3	C	5	U
3	F	2	A

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Mol	Chain	Res	Type
3	F	4	G
3	F	5	U
3	I	4	G
3	I	5	U
3	L	4	G
3	L	5	U
3	O	4	G
3	O	5	U
3	R	4	G
3	U	4	G
3	U	5	U
3	X	4	G
3	X	5	U
3	1	4	G
3	1	5	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	1	A
3	I	1	A
3	L	1	A
3	O	1	A
3	R	1	A
3	U	1	A
3	X	1	A
3	1	1	A

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 18 ligands modelled in this entry, 18 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, 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	193/216 (89%)	0.38	4 (2%) 63 43	45, 68, 108, 136	0
1	D	187/216 (86%)	0.35	2 (1%) 78 61	42, 62, 102, 125	0
1	G	193/216 (89%)	0.28	5 (2%) 57 37	33, 56, 99, 131	0
1	J	193/216 (89%)	0.85	9 (4%) 36 23	43, 72, 106, 130	0
1	M	179/216 (82%)	0.56	8 (4%) 38 24	49, 81, 121, 138	0
1	P	189/216 (87%)	0.75	10 (5%) 32 20	42, 67, 92, 122	0
1	S	188/216 (87%)	0.89	15 (7%) 18 12	33, 84, 125, 141	1 (0%)
1	V	174/216 (80%)	0.68	10 (5%) 29 19	70, 94, 119, 129	0
1	Y	179/216 (82%)	0.70	13 (7%) 21 13	43, 91, 128, 142	0
2	B	56/69 (81%)	0.53	1 (1%) 67 48	48, 72, 111, 119	0
2	E	51/69 (73%)	0.45	1 (1%) 65 45	48, 65, 144, 148	0
2	H	53/69 (76%)	0.42	0 100 100	26, 60, 115, 120	0
2	K	54/69 (78%)	0.85	4 (7%) 20 13	40, 69, 112, 136	0
2	N	52/69 (75%)	0.66	2 (3%) 44 27	52, 78, 139, 148	0
2	Q	53/69 (76%)	0.99	8 (15%) 5 4	45, 69, 128, 145	0
2	T	47/69 (68%)	0.77	1 (2%) 63 43	66, 89, 150, 156	0
2	W	53/69 (76%)	0.77	4 (7%) 20 13	69, 94, 144, 148	0
2	Z	44/69 (63%)	0.56	2 (4%) 38 24	48, 71, 124, 137	0
3	I	5/6 (83%)	1.17	1 (20%) 3 2	105, 115, 126, 146	0
3	C	5/6 (83%)	0.21	0 100 100	65, 80, 90, 93	0
3	F	5/6 (83%)	0.30	0 100 100	66, 68, 83, 118	0
3	I	5/6 (83%)	0.21	0 100 100	55, 60, 82, 95	0
3	L	5/6 (83%)	0.57	0 100 100	66, 87, 92, 101	0
3	O	5/6 (83%)	1.07	1 (20%) 3 2	100, 108, 130, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	R	5/6 (83%)	0.67	1 (20%) 3 2	58, 60, 83, 90	0
3	U	5/6 (83%)	0.36	0 100 100	71, 72, 83, 145	0
3	X	5/6 (83%)	0.63	0 100 100	105, 107, 112, 118	0
All	All	2183/2619 (83%)	0.62	102 (4%) 36 23	26, 76, 125, 156	1 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	114	GLN	5.1
1	J	8	ILE	4.8
1	S	102[A]	HIS	3.9
1	Y	16	VAL	3.8
2	K	127	GLN	3.7
1	S	34	SER	3.5
2	W	109	VAL	3.5
1	A	38	VAL	3.5
1	M	16	VAL	3.4
1	S	137	GLU	3.3
1	V	16	VAL	3.1
1	G	192	ALA	2.9
1	Y	61	GLY	2.9
1	S	62	LYS	2.9
1	G	191	ALA	2.9
2	Q	116	LEU	2.9
1	P	61	GLY	2.9
1	J	61	GLY	2.8
2	T	136	ASP	2.8
1	S	92	GLN	2.8
1	M	154	THR	2.8
3	R	5	U	2.7
2	E	160	GLY	2.7
1	Y	17	ASN	2.7
2	W	119	LEU	2.7
1	Y	62	LYS	2.7
3	O	5	U	2.7
2	Q	115	GLU	2.6
1	J	188	ALA	2.6
1	P	85	SER	2.6
1	D	63	LYS	2.6
1	Y	34	SER	2.6
1	S	113	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	Y	102	HIS	2.6
2	K	161	ALA	2.6
1	A	61	GLY	2.6
1	P	56	ILE	2.5
1	Y	57	HIS	2.5
1	M	192	ALA	2.5
1	Y	38	VAL	2.5
1	P	101	ASP	2.5
1	J	10	GLY	2.5
1	V	192	ALA	2.5
1	P	115	GLU	2.5
2	N	109	VAL	2.5
1	P	192	ALA	2.4
1	S	40	PRO	2.4
1	S	22	TYR	2.4
1	M	34	SER	2.4
2	Z	116	LEU	2.4
1	J	140	PRO	2.4
1	D	56	ILE	2.4
1	V	84	PHE	2.4
1	S	151	GLN	2.4
1	V	183	GLN	2.4
1	Y	31	GLU	2.4
2	Q	160	GLY	2.4
1	J	32	ARG	2.4
1	V	191	ALA	2.3
1	Y	56	ILE	2.3
1	A	39	LYS	2.3
1	Y	121	ILE	2.3
2	Q	119	LEU	2.3
1	V	53	LYS	2.3
1	Y	36	LYS	2.3
1	V	102	HIS	2.3
1	M	17	ASN	2.3
2	B	161	ALA	2.3
1	P	102	HIS	2.3
2	K	131	LYS	2.3
1	P	137	GLU	2.2
1	V	122	ASP	2.2
1	S	21	TYR	2.2
1	S	141	VAL	2.2
2	Q	109	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	60	ASN	2.2
3	1	1	A	2.2
2	W	160	GLY	2.2
2	N	122	VAL	2.2
1	A	31	GLU	2.2
1	P	168	ALA	2.2
1	V	181	LEU	2.1
1	G	71	GLU	2.1
2	Q	127	GLN	2.1
1	M	155	SER	2.1
1	P	75	ALA	2.1
1	S	168	ALA	2.1
1	M	153	GLU	2.1
1	G	190	ASN	2.1
2	K	130	ARG	2.1
2	Q	108	SER	2.1
1	M	36	LYS	2.1
1	V	17	ASN	2.1
1	J	115	GLU	2.1
2	W	117	GLU	2.1
1	J	178	ASP	2.0
1	S	188	ALA	2.0
1	Y	22	TYR	2.0
1	J	92	GLN	2.0
1	S	61	GLY	2.0
2	Z	129	LYS	2.0
1	G	194	GLU	2.0

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 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,

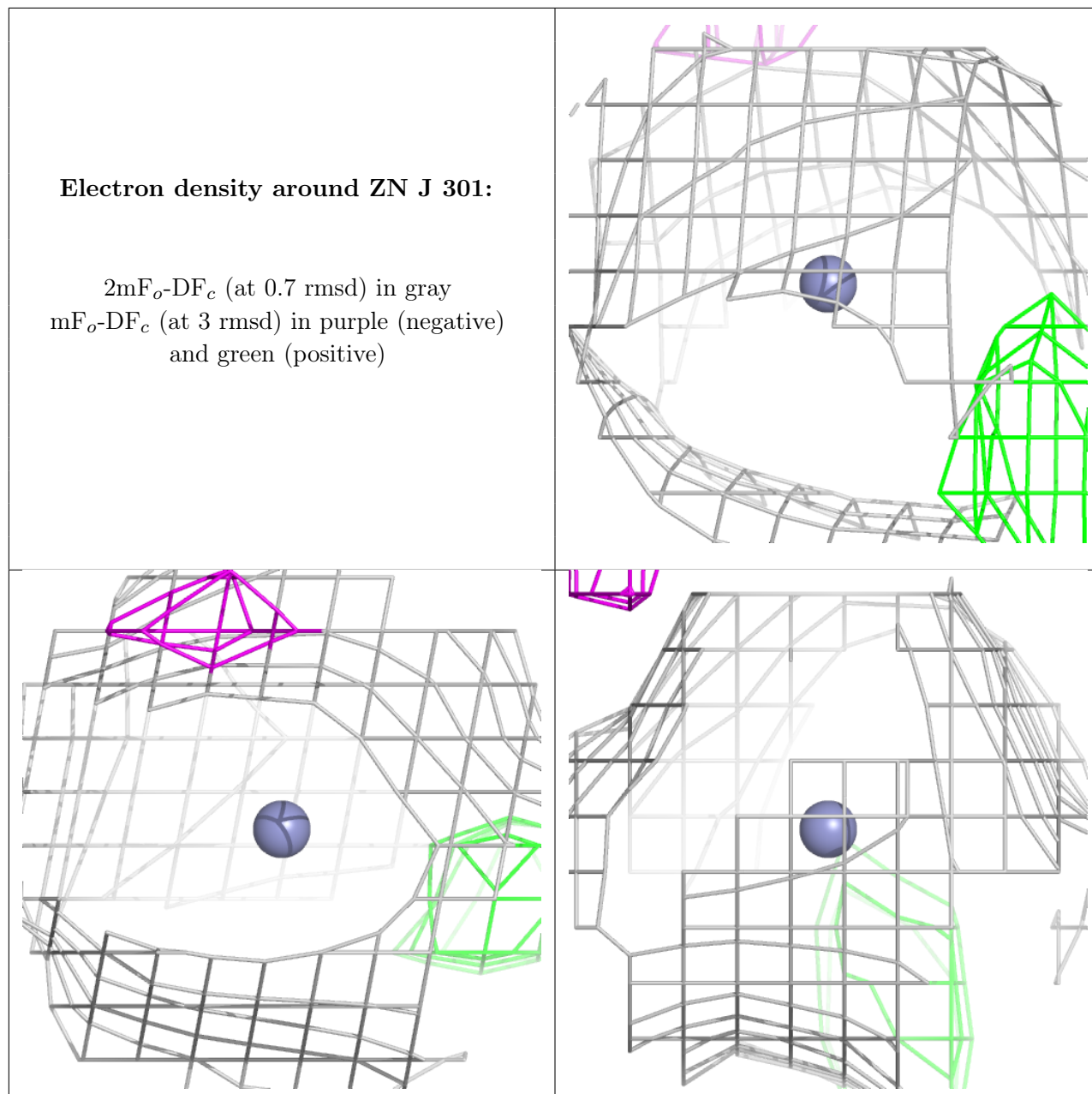
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ZN	J	301	1/1	0.98	0.04	67,67,67,67	0
4	ZN	A	302	1/1	0.99	0.04	55,55,55,55	0
4	ZN	G	301	1/1	0.99	0.05	48,48,48,48	0
4	ZN	G	302	1/1	0.99	0.04	54,54,54,54	0
4	ZN	A	301	1/1	0.99	0.03	60,60,60,60	0
4	ZN	J	302	1/1	0.99	0.04	54,54,54,54	0
4	ZN	M	301	1/1	0.99	0.03	70,70,70,70	0
4	ZN	M	302	1/1	0.99	0.03	65,65,65,65	0
4	ZN	P	302	1/1	0.99	0.04	45,45,45,45	0
4	ZN	S	301	1/1	0.99	0.05	59,59,59,59	0
4	ZN	S	302	1/1	0.99	0.05	73,73,73,73	0
4	ZN	V	301	1/1	0.99	0.05	72,72,72,72	0
4	ZN	V	302	1/1	0.99	0.02	71,71,71,71	0
4	ZN	Y	301	1/1	0.99	0.05	80,80,80,80	0
4	ZN	Y	302	1/1	0.99	0.03	70,70,70,70	0
4	ZN	D	302	1/1	1.00	0.02	49,49,49,49	0
4	ZN	P	301	1/1	1.00	0.04	44,44,44,44	0
4	ZN	D	301	1/1	1.00	0.04	45,45,45,45	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.

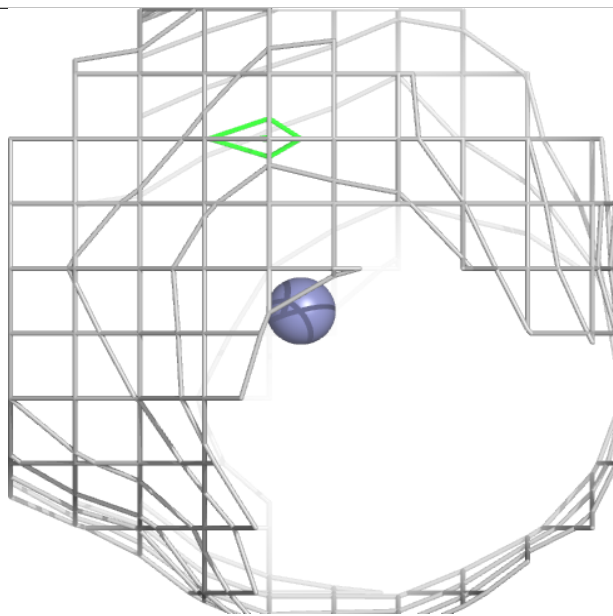
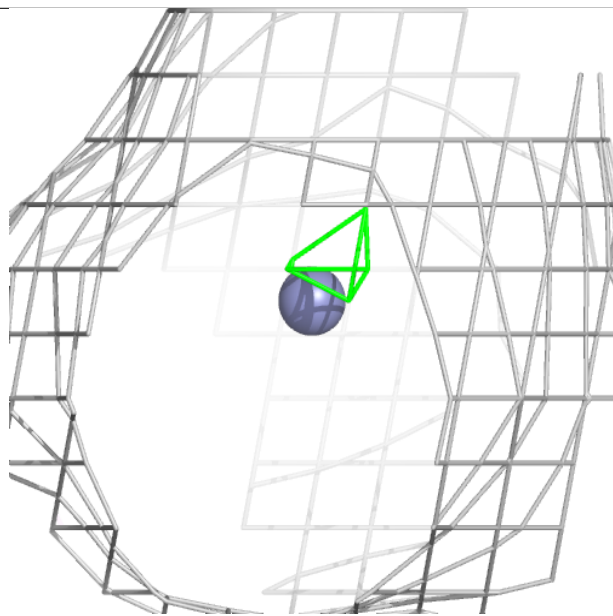
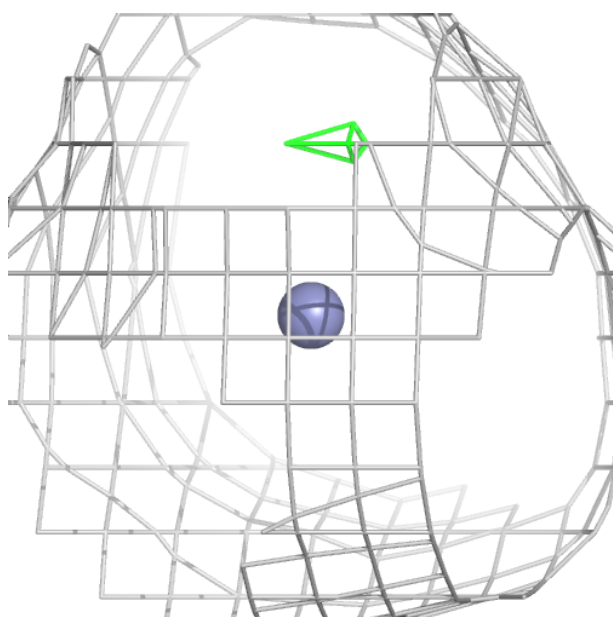
Electron density around ZN J 301:

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



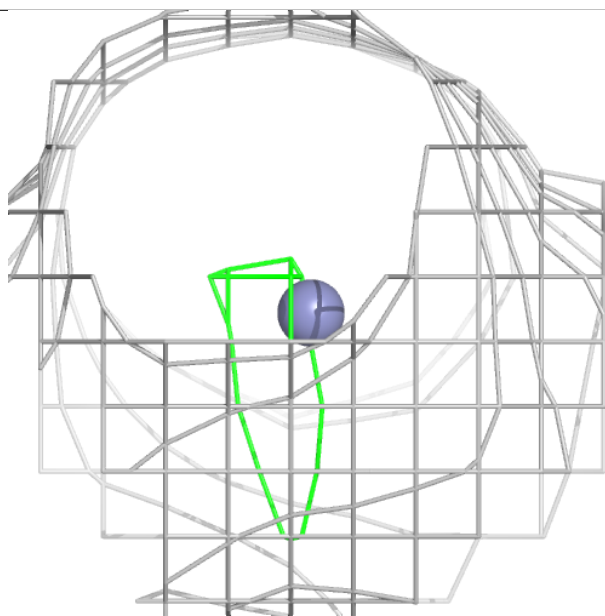
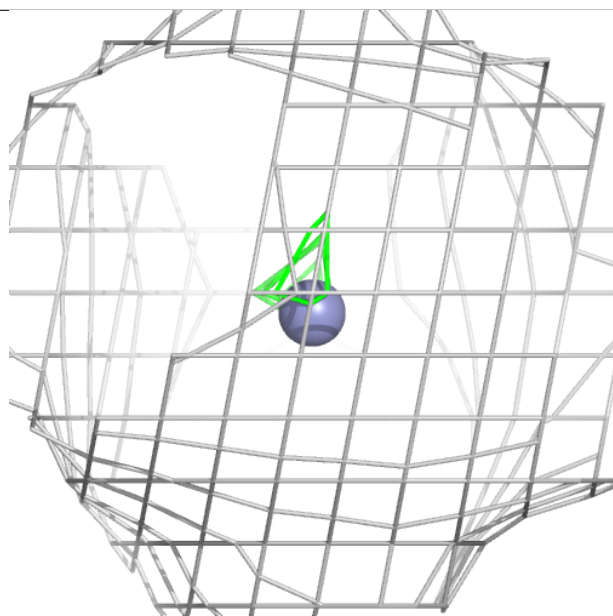
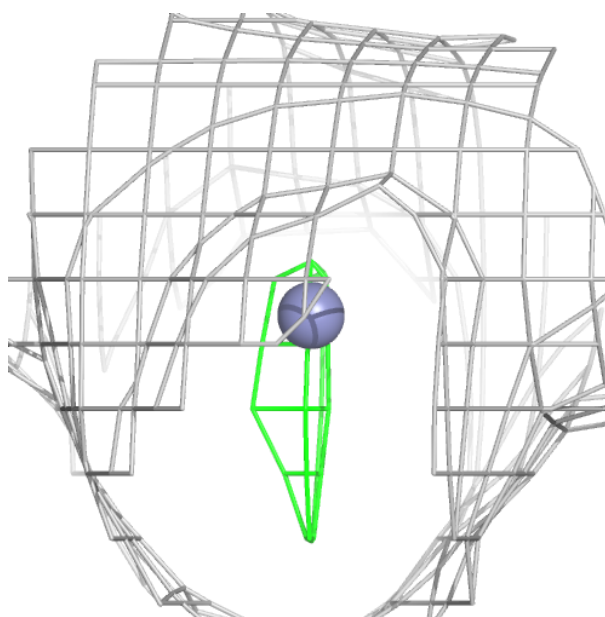
Electron density around ZN A 302:

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



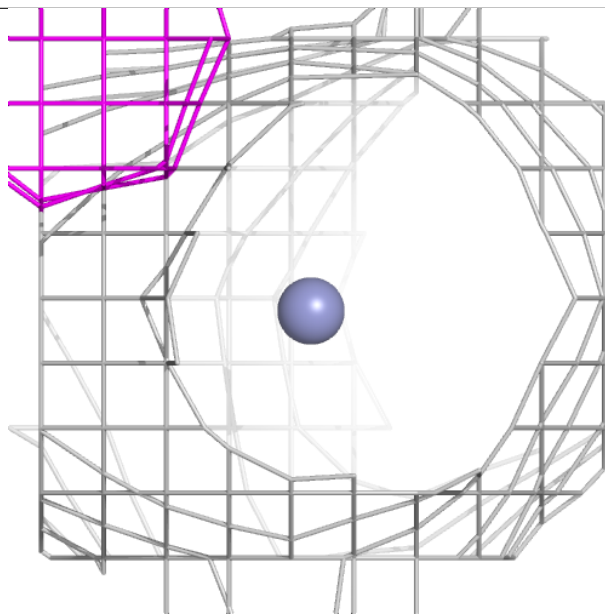
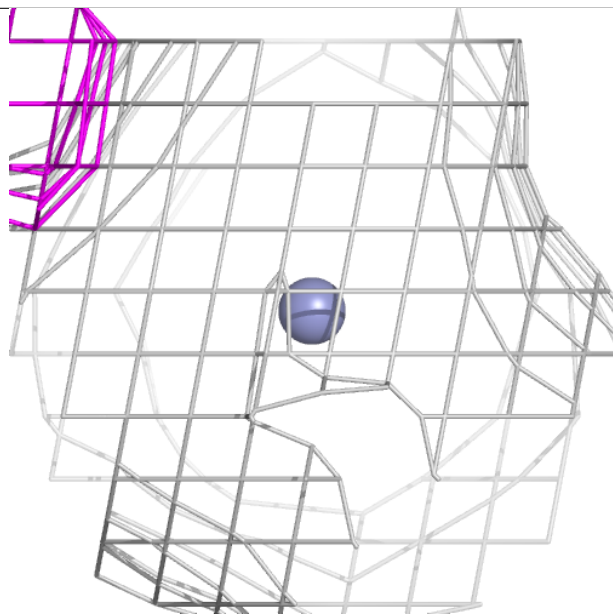
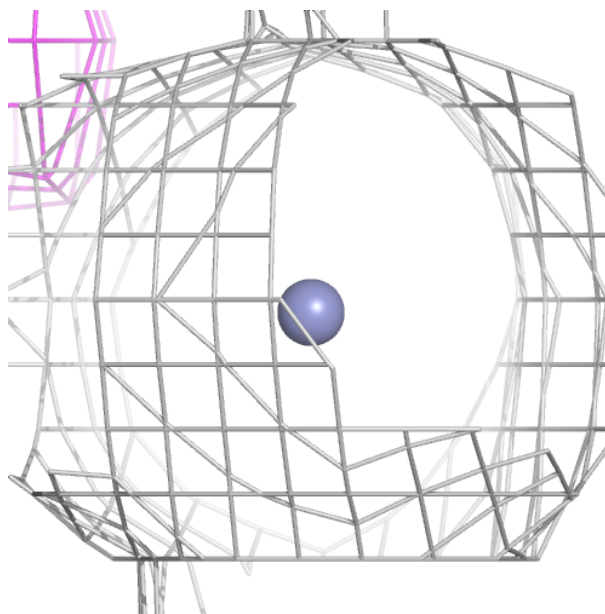
Electron density around ZN G 301:

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



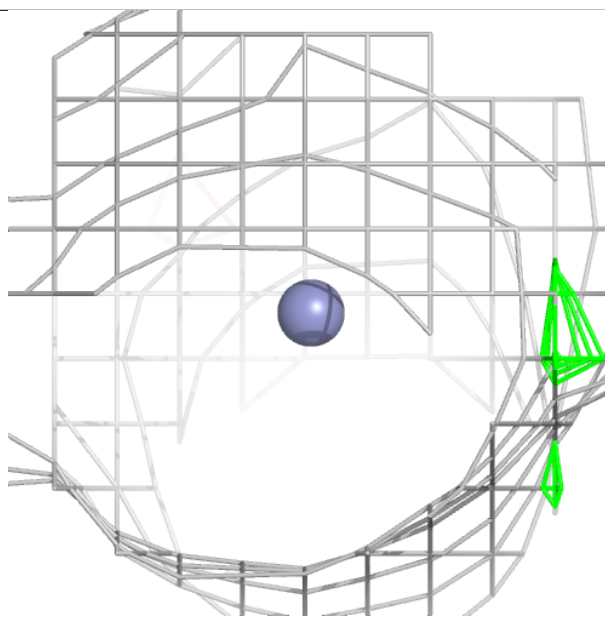
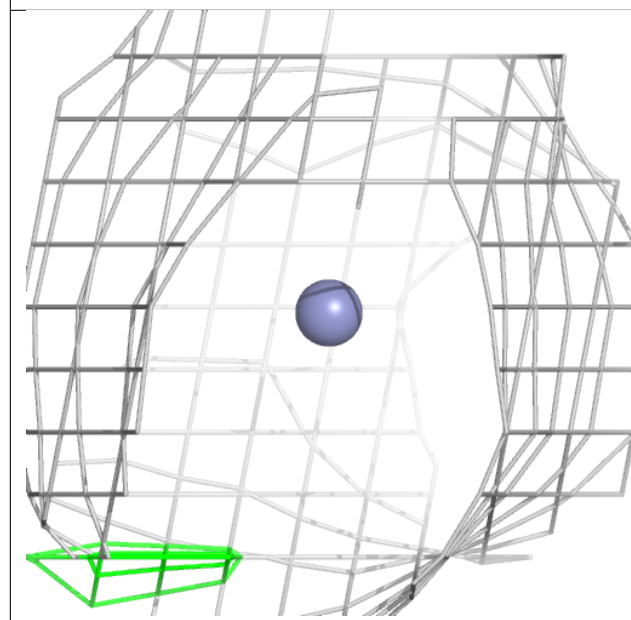
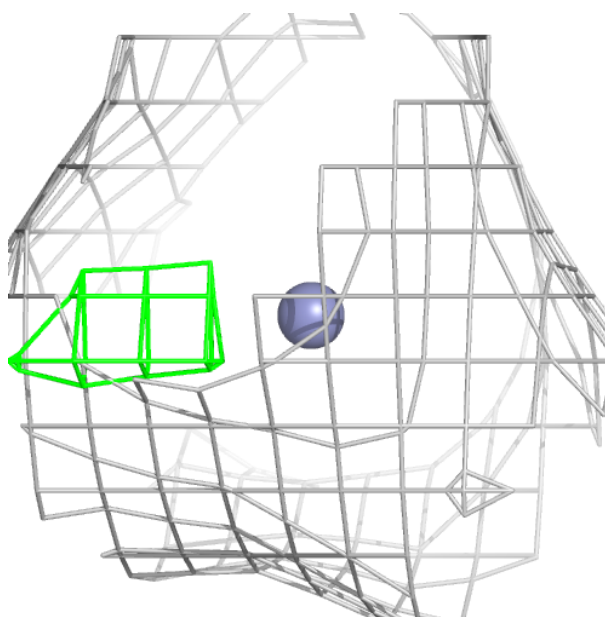
Electron density around ZN G 302:

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



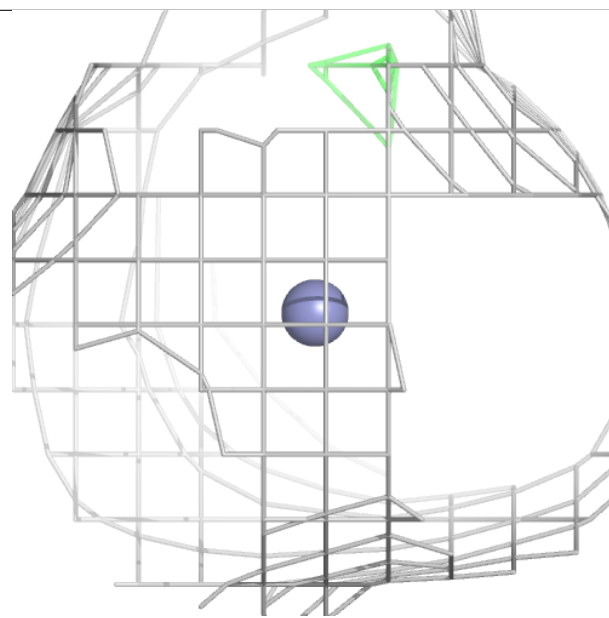
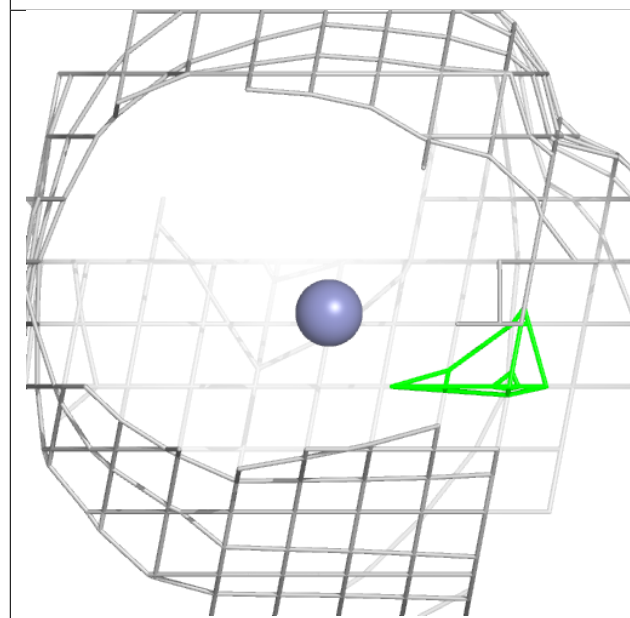
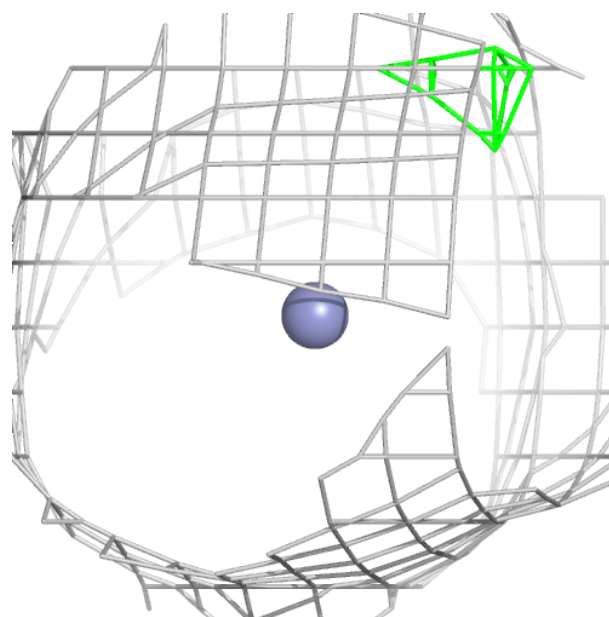
Electron density around ZN A 301:

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



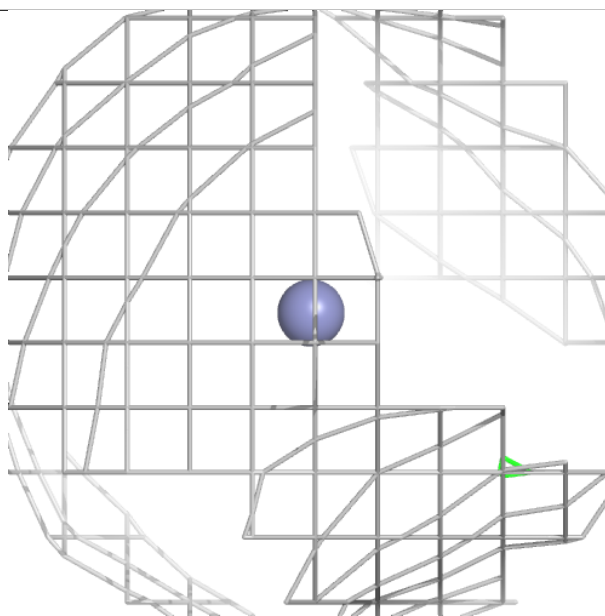
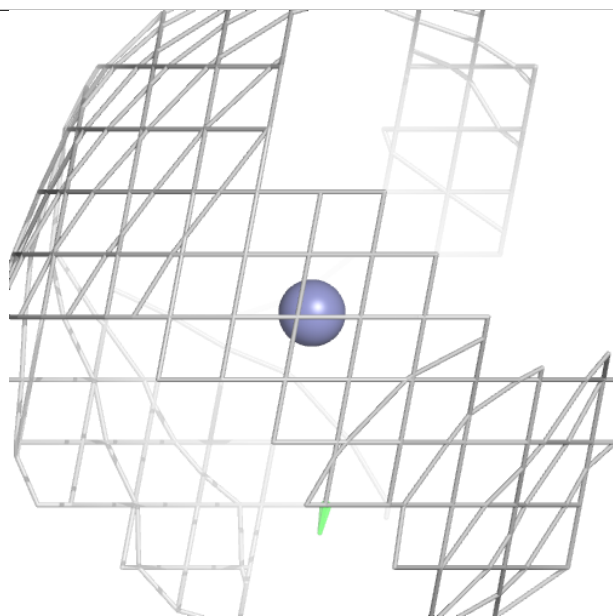
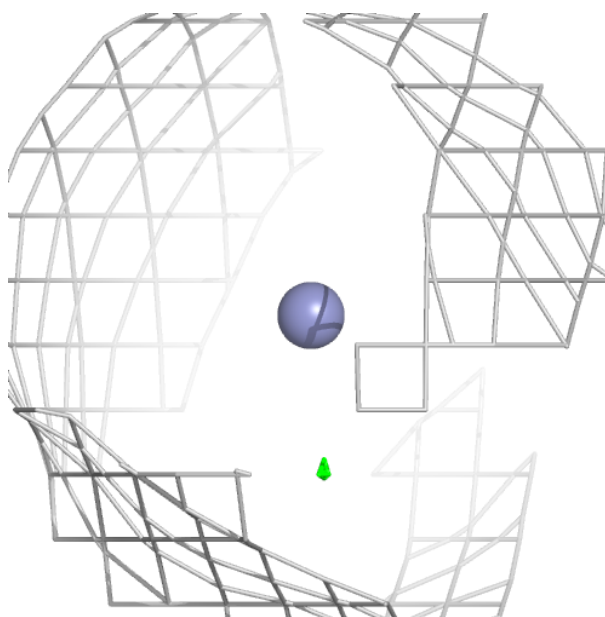
Electron density around ZN J 302:

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



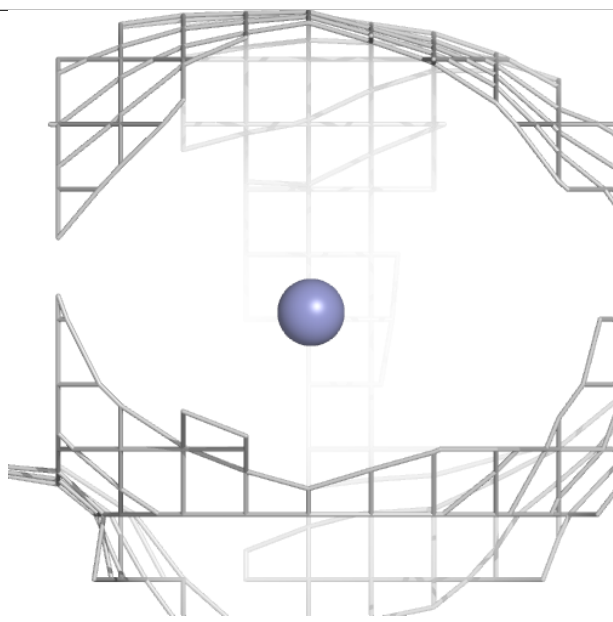
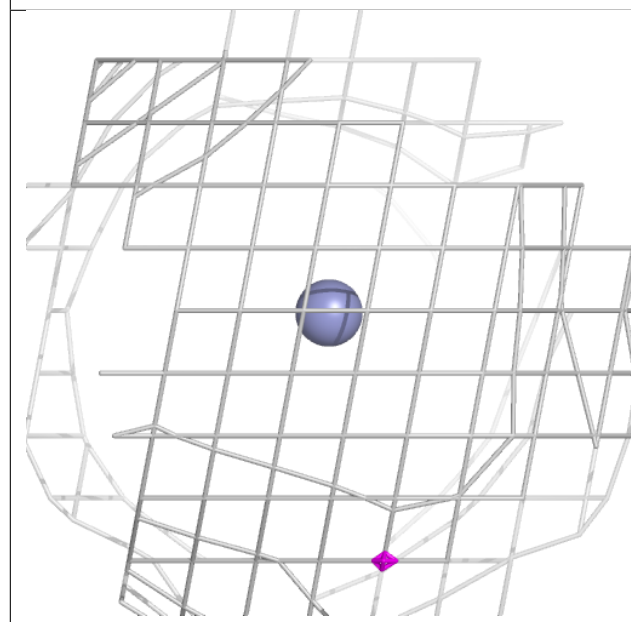
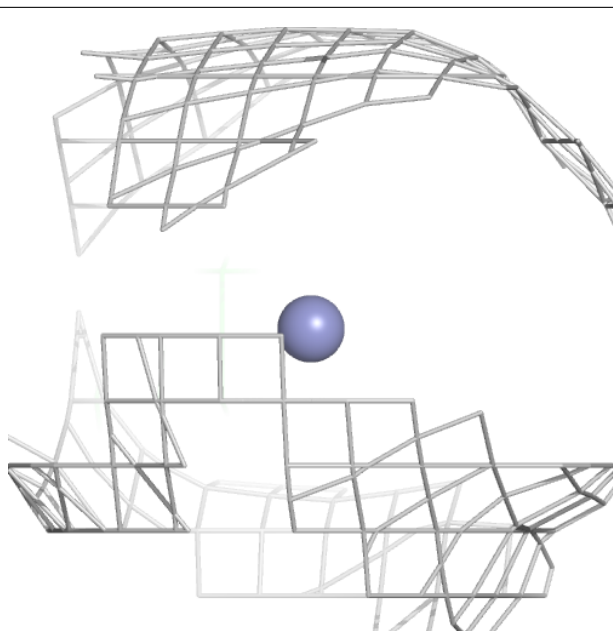
Electron density around ZN M 301:

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and green (positive)



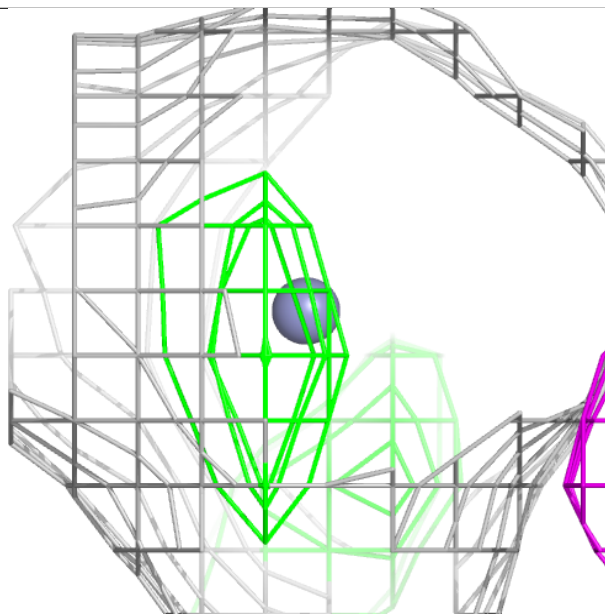
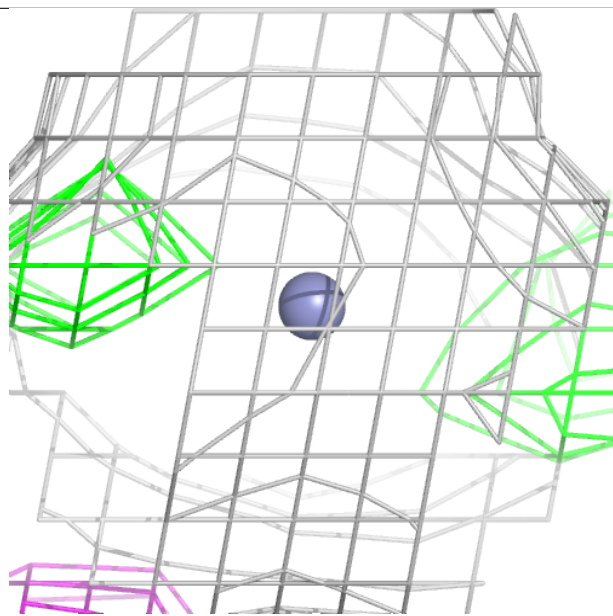
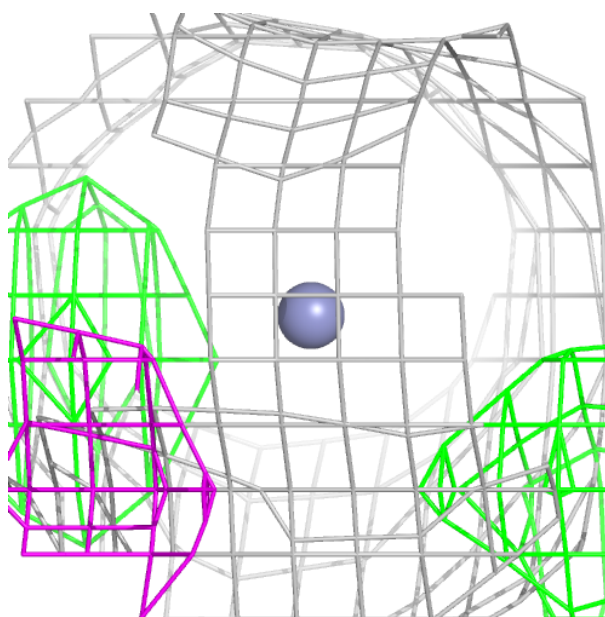
Electron density around ZN M 302:

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



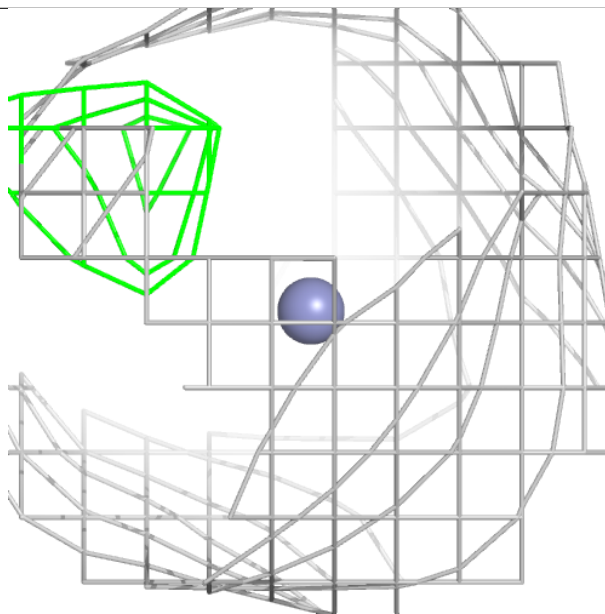
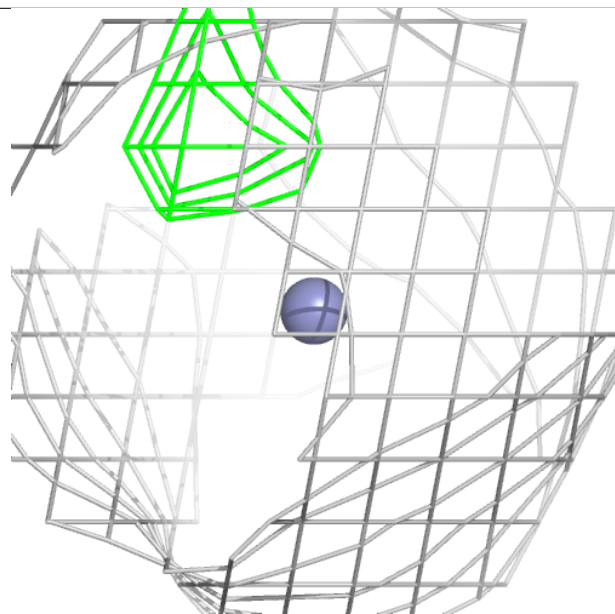
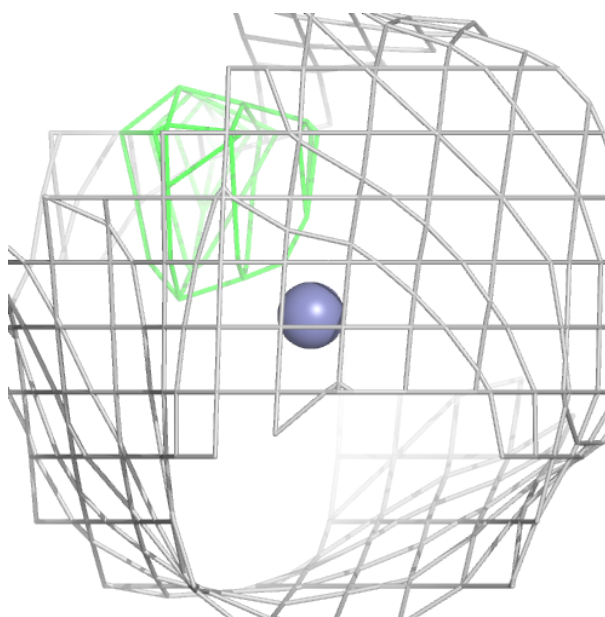
Electron density around ZN P 302:

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



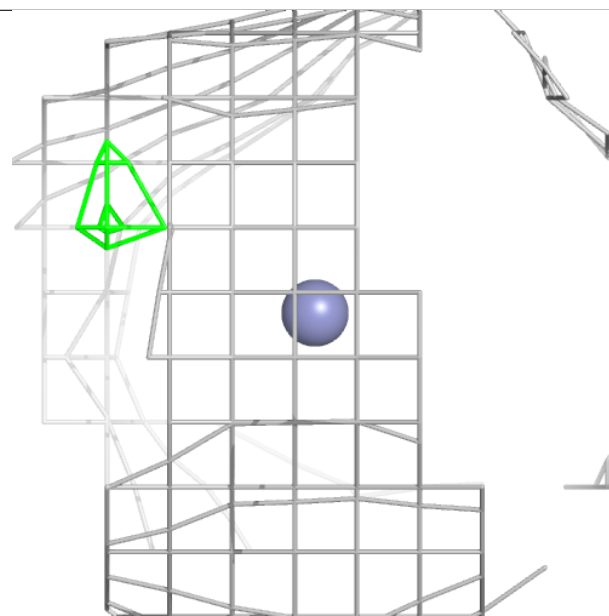
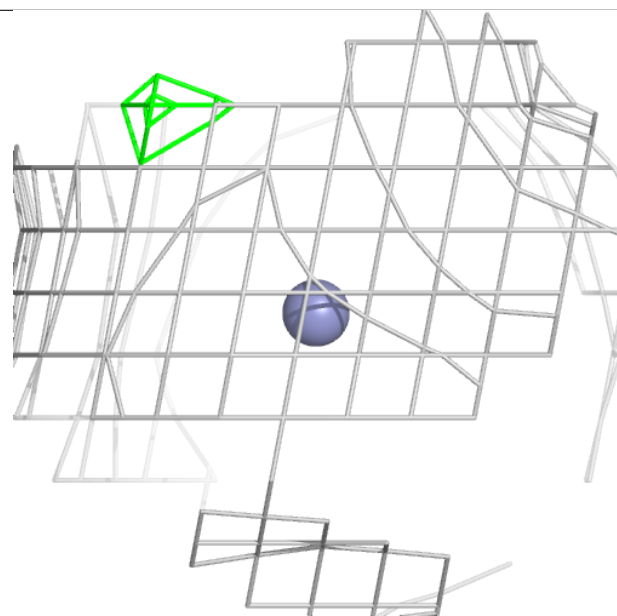
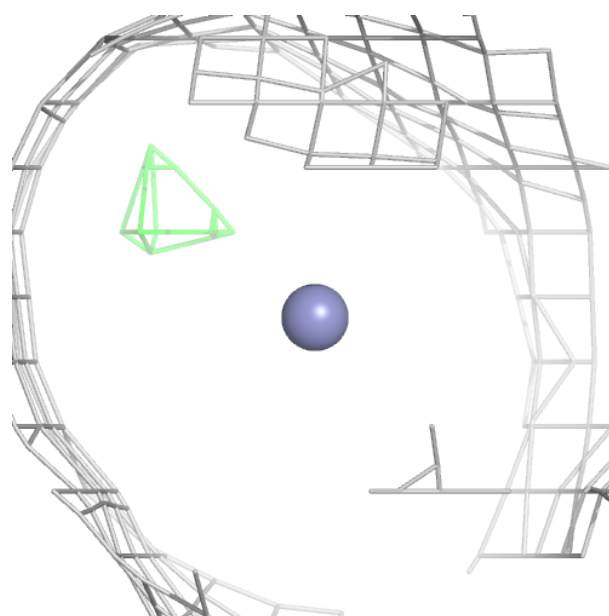
Electron density around ZN S 301:

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and green (positive)



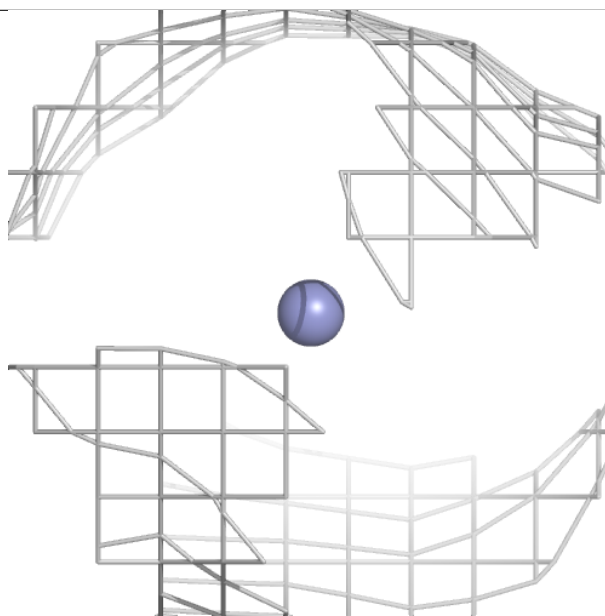
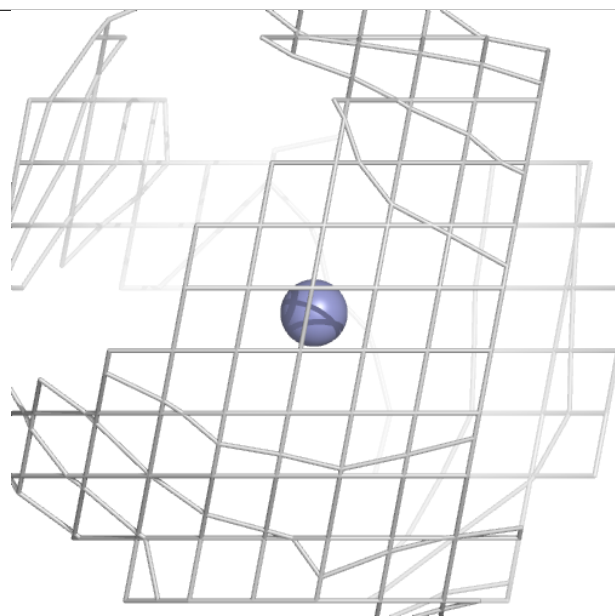
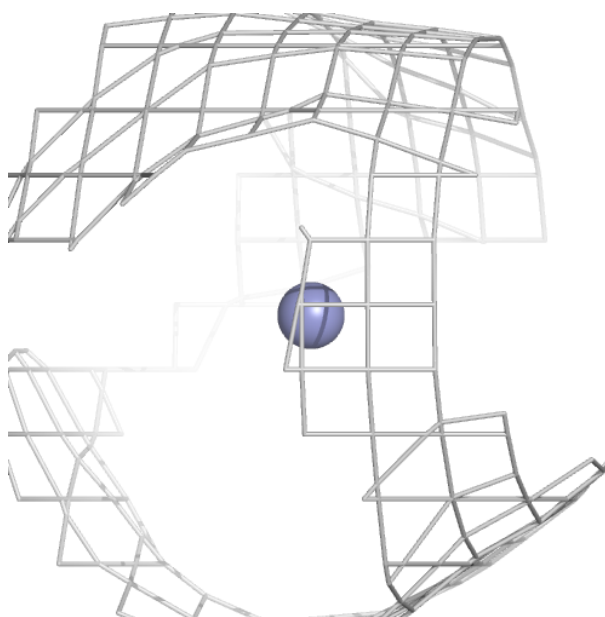
Electron density around ZN S 302:

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



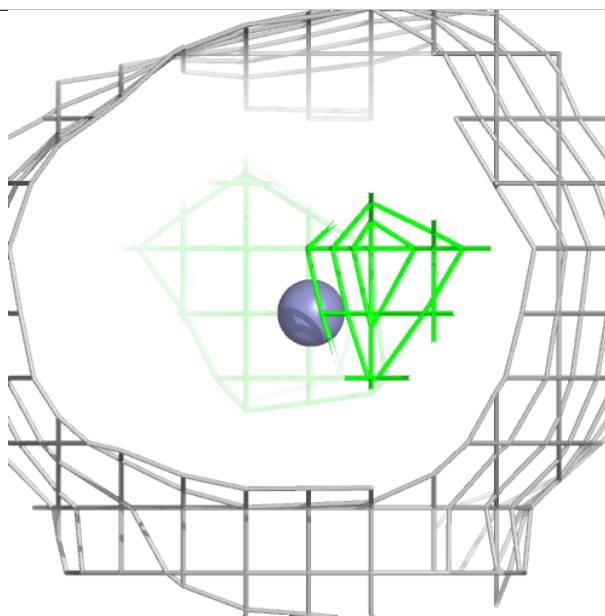
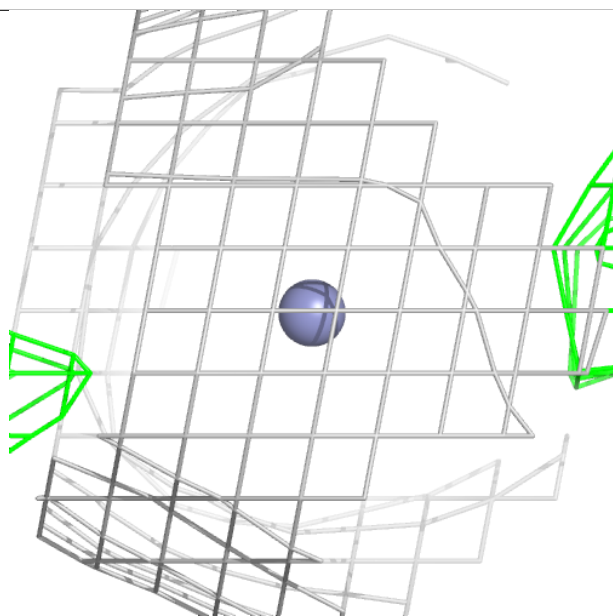
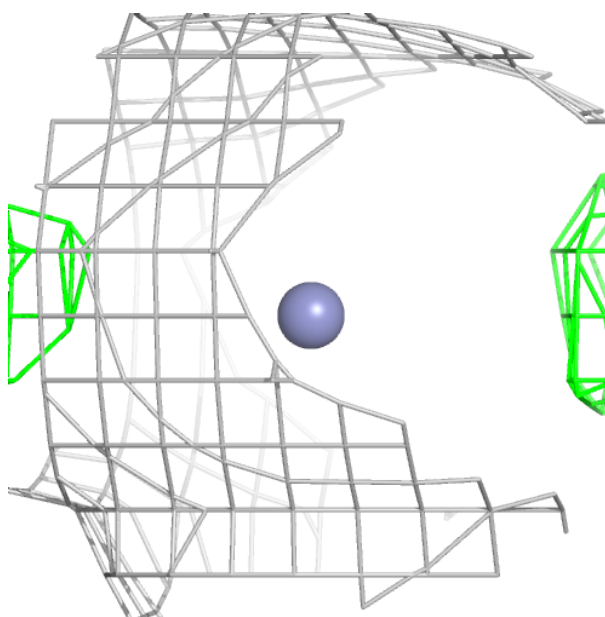
Electron density around ZN V 301:

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



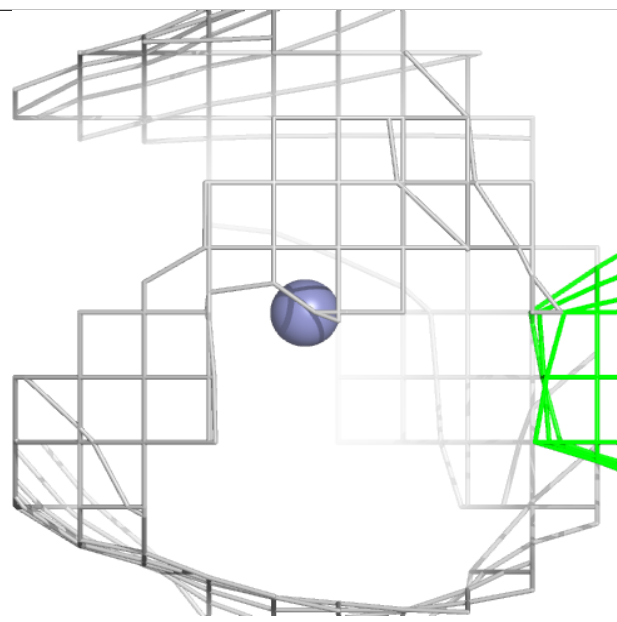
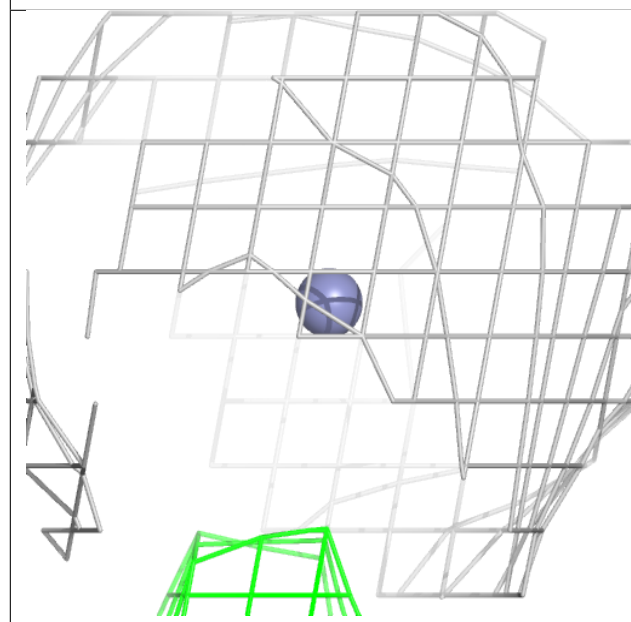
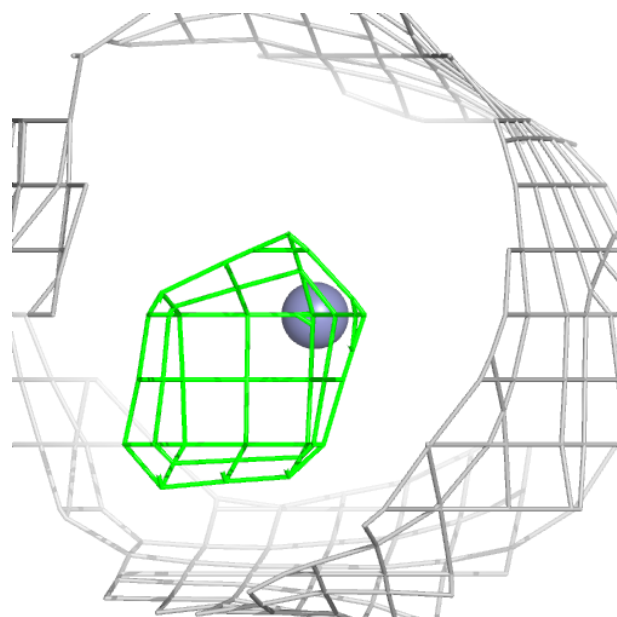
Electron density around ZN V 302:

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



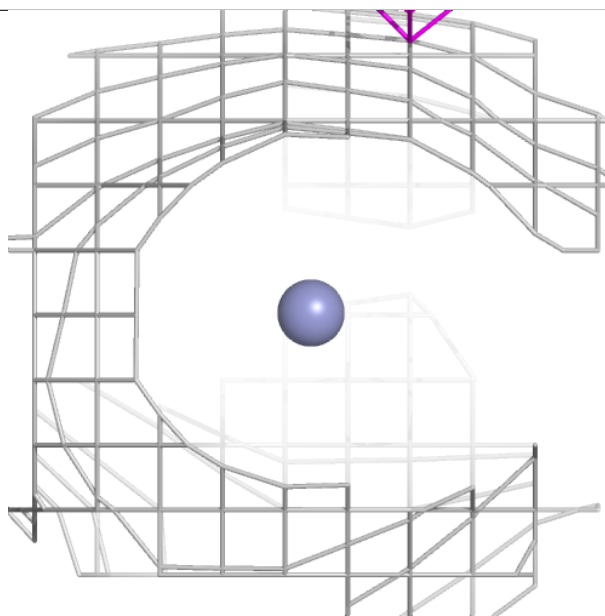
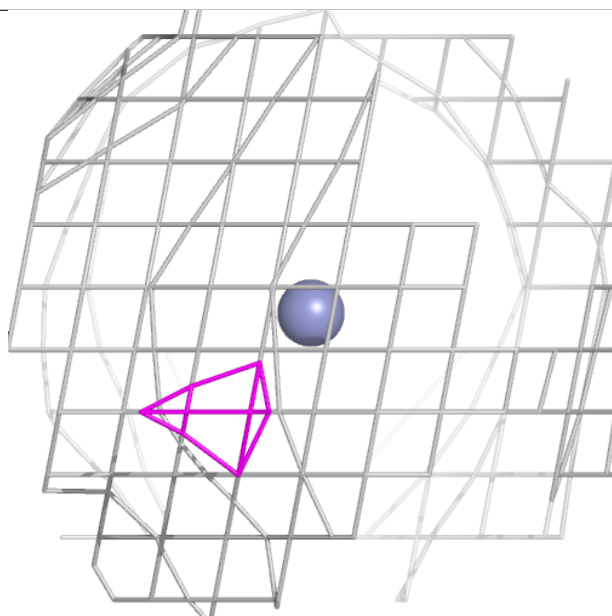
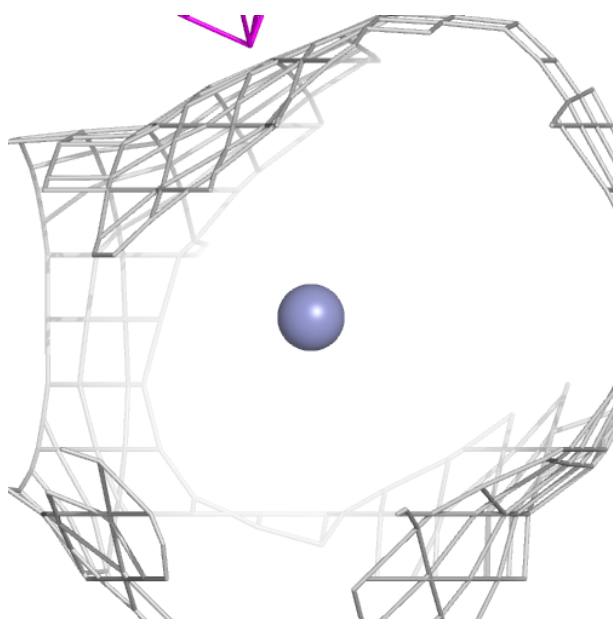
Electron density around ZN Y 301:

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and green (positive)



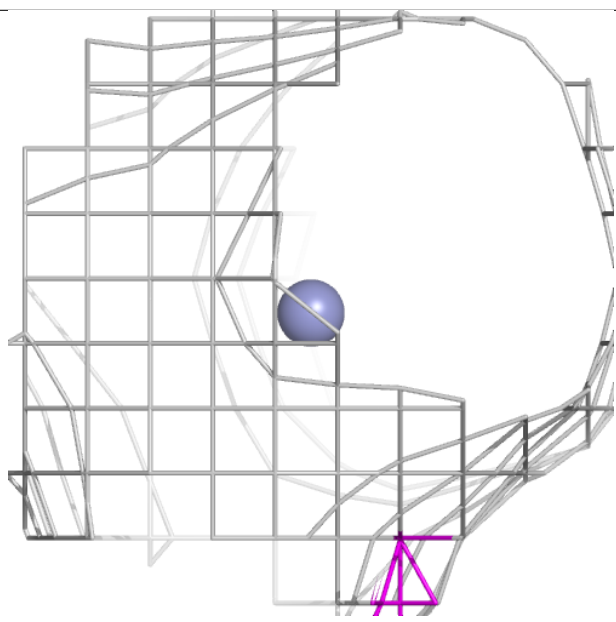
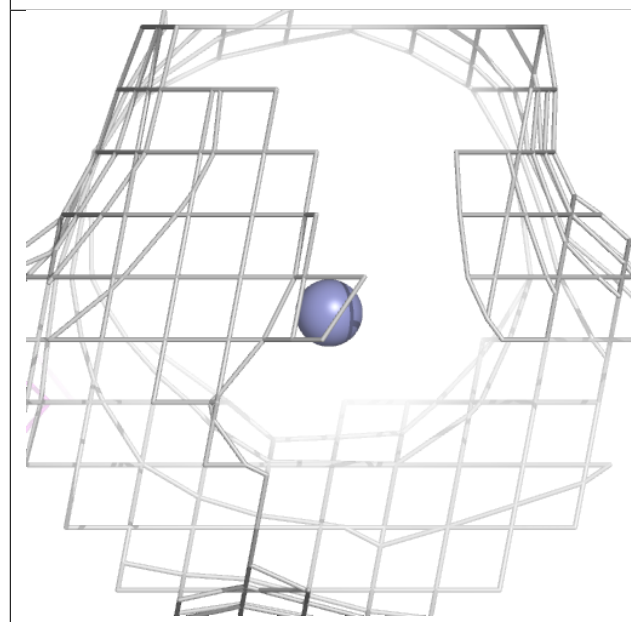
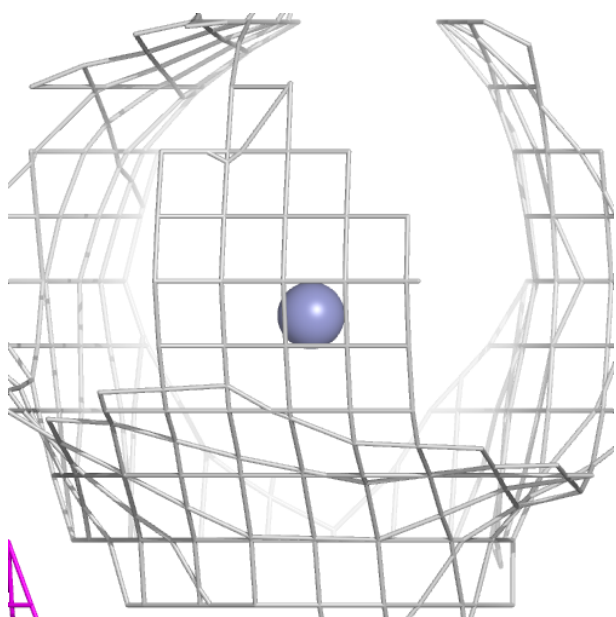
Electron density around ZN Y 302:

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



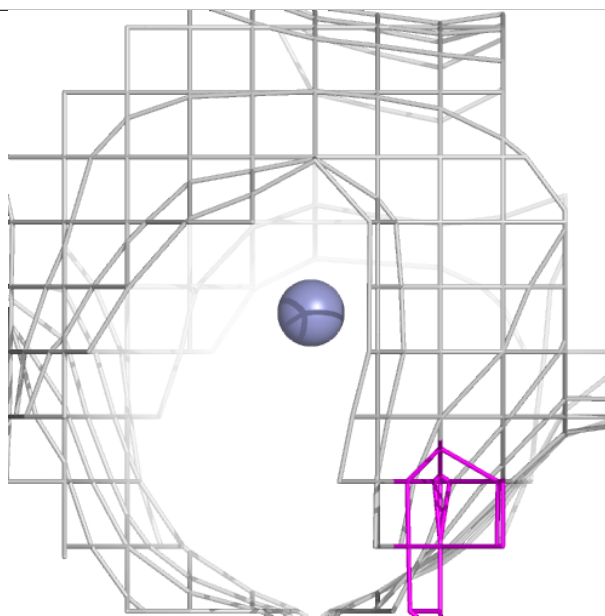
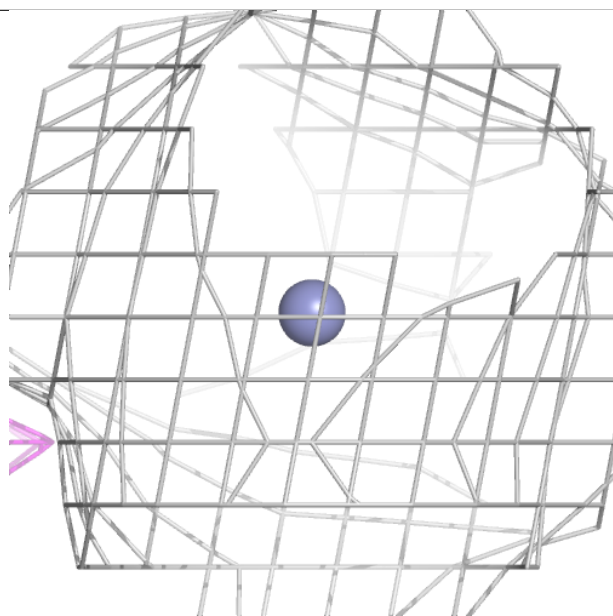
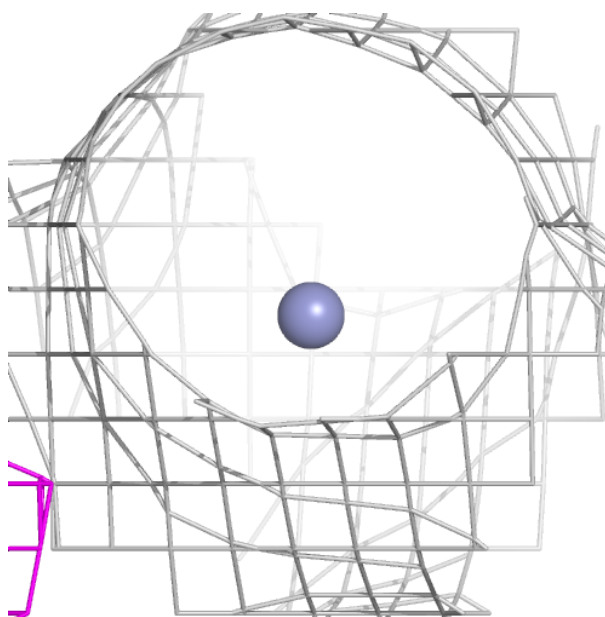
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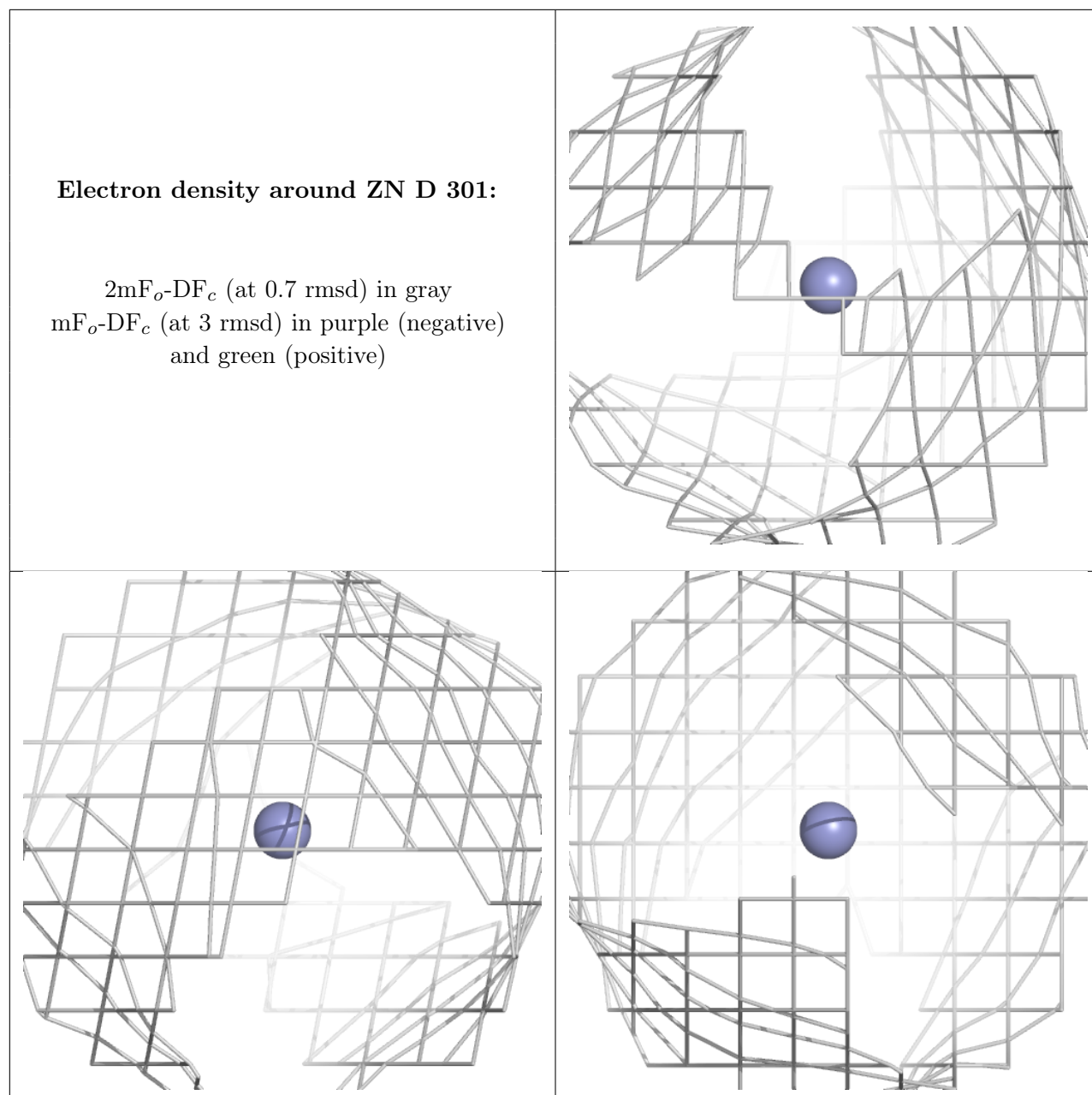
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and green (positive)



Electron density around ZN P 301:

$2mF_o-DF_c$ (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.