



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:13 PM UTC

PDB ID : 7XZ2 / pdb_00007xz2
Title : TRIM E3 ubiquitin ligase
Authors : Park, S.H.; Song, H.K.
Deposited on : 2022-06-02
Resolution : 3.50 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

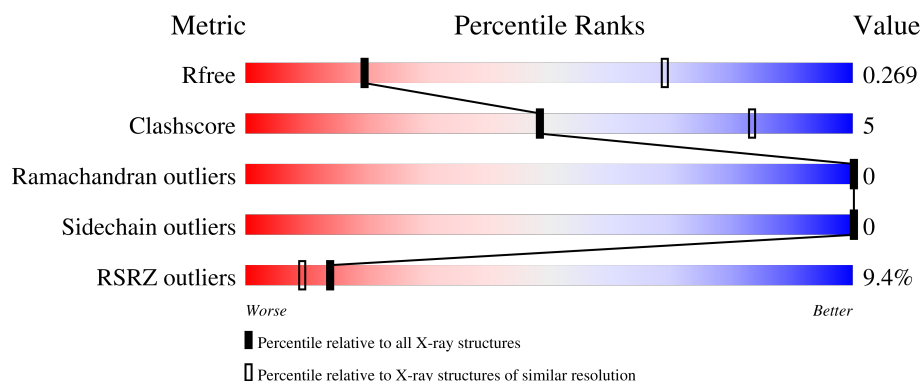
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	466	7% 70%12%18%
1	B	466	7% 72%11%17%
1	C	466	10% 71%11%18%
1	D	466	7% 72%11%17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12162 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 Tripartite motif-containing protein 72.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3022	1907	544	556	15			
1	B	386	Total	C	N	O	S	0	0	0
			3054	1926	551	562	15			
1	C	382	Total	C	N	O	S	0	0	0
			3022	1907	544	556	15			
1	D	386	Total	C	N	O	S	0	0	0
			3054	1926	551	562	15			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	expression tag	UNP Q1XH17
A	6	SER	-	expression tag	UNP Q1XH17
A	55	SER	CYS	engineered mutation	UNP Q1XH17
A	144	SER	CYS	engineered mutation	UNP Q1XH17
A	242	SER	CYS	engineered mutation	UNP Q1XH17
A	279	HIS	LYS	engineered mutation	UNP Q1XH17
A	283	HIS	ALA	engineered mutation	UNP Q1XH17
B	5	GLY	-	expression tag	UNP Q1XH17
B	6	SER	-	expression tag	UNP Q1XH17
B	55	SER	CYS	engineered mutation	UNP Q1XH17
B	144	SER	CYS	engineered mutation	UNP Q1XH17
B	242	SER	CYS	engineered mutation	UNP Q1XH17
B	279	HIS	LYS	engineered mutation	UNP Q1XH17
B	283	HIS	ALA	engineered mutation	UNP Q1XH17
C	5	GLY	-	expression tag	UNP Q1XH17
C	6	SER	-	expression tag	UNP Q1XH17
C	55	SER	CYS	engineered mutation	UNP Q1XH17
C	144	SER	CYS	engineered mutation	UNP Q1XH17
C	242	SER	CYS	engineered mutation	UNP Q1XH17
C	279	HIS	LYS	engineered mutation	UNP Q1XH17
C	283	HIS	ALA	engineered mutation	UNP Q1XH17

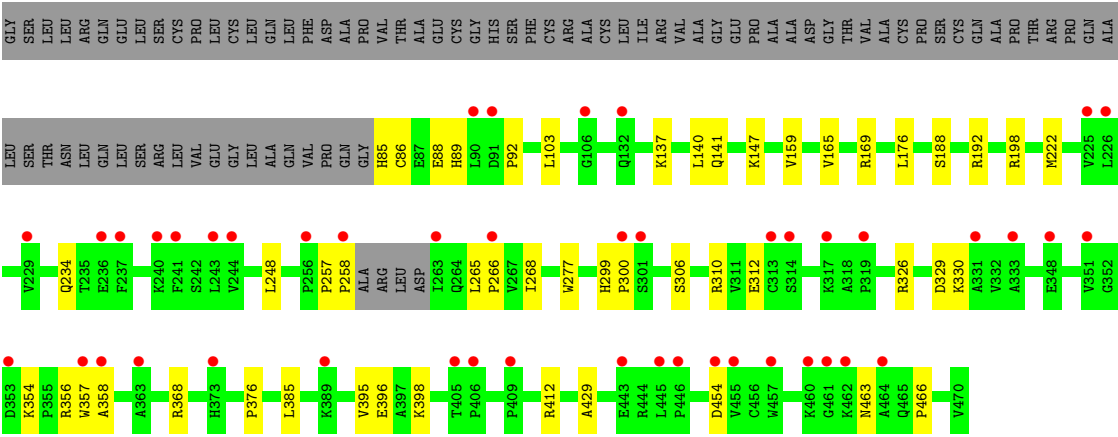
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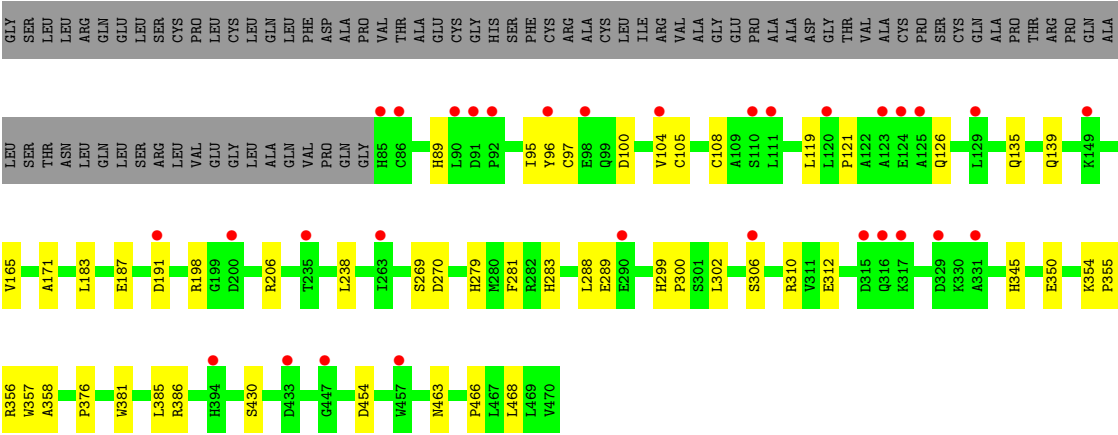
Chain	Residue	Modelled	Actual	Comment	Reference
D	5	GLY	-	expression tag	UNP Q1XH17
D	6	SER	-	expression tag	UNP Q1XH17
D	55	SER	CYS	engineered mutation	UNP Q1XH17
D	144	SER	CYS	engineered mutation	UNP Q1XH17
D	242	SER	CYS	engineered mutation	UNP Q1XH17
D	279	HIS	LYS	engineered mutation	UNP Q1XH17
D	283	HIS	ALA	engineered mutation	UNP Q1XH17

- 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	2	Total Zn 2 2	0	0
2	B	3	Total Zn 3 3	0	0
2	C	2	Total Zn 2 2	0	0
2	D	3	Total Zn 3 3	0	0



● Molecule 1: Tripartite motif-containing protein 72



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.00Å 326.95Å 120.95Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	38.23 – 3.50 38.23 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.23-3.50) 88.2 (38.23-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.249 , 0.269 0.249 , 0.269	Depositor DCC
R_{free} test set	2011 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 107.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12162	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.50% 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	0.10	0/3088	0.26	0/4177
1	B	0.10	0/3121	0.29	0/4223
1	C	0.10	0/3088	0.24	0/4177
1	D	0.10	0/3121	0.27	0/4223
All	All	0.10	0/12418	0.27	0/16800

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 [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	3022	0	3021	40	0
1	B	3054	0	3055	38	0
1	C	3022	0	3021	34	0
1	D	3054	0	3055	41	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
All	All	12162	0	12152	133	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 5.

All (133) 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:D:89:HIS:ND1	1:D:105:CYS:SG	2.26	1.09
1:D:89:HIS:CE1	1:D:108:CYS:SG	2.55	0.99
1:C:354:LYS:HD3	1:C:357:TRP:HB3	1.64	0.79
1:B:354:LYS:HD3	1:B:357:TRP:HB3	1.66	0.78
1:B:222:MET:HE2	1:B:248:LEU:HB2	1.71	0.73
1:C:356:ARG:HA	1:C:385:LEU:O	1.89	0.73
1:D:354:LYS:HD3	1:D:357:TRP:HB3	1.69	0.72
1:C:165:VAL:HG21	1:D:198:ARG:HB2	1.71	0.72
1:D:97:CYS:HB3	1:D:100:ASP:HB2	1.72	0.71
1:D:312:GLU:HB3	1:D:466:PRO:HB3	1.74	0.70
1:D:89:HIS:HE1	1:D:108:CYS:SG	2.12	0.69
1:C:358:ALA:HB3	1:C:454:ASP:HB3	1.74	0.69
1:A:188:SER:OG	1:A:192:ARG:NH1	2.26	0.68
1:A:222:MET:HE2	1:A:248:LEU:HB2	1.75	0.68
1:A:358:ALA:HB3	1:A:454:ASP:HB3	1.77	0.67
1:D:95:ILE:HA	1:D:121:PRO:HG3	1.75	0.67
1:A:165:VAL:HG21	1:B:198:ARG:HB2	1.77	0.67
1:D:358:ALA:HB3	1:D:454:ASP:HB3	1.78	0.66
1:B:356:ARG:HA	1:B:385:LEU:O	1.97	0.65
1:B:135:GLN:HE21	1:B:139:GLN:HE21	1.44	0.65
1:D:135:GLN:HE21	1:D:139:GLN:HE21	1.43	0.65
1:C:234:GLN:NE2	1:D:126:GLN:OE1	2.28	0.65
1:B:358:ALA:HB3	1:B:454:ASP:HB3	1.78	0.65
1:C:354:LYS:NZ	1:C:463:ASN:OD1	2.31	0.64
1:D:356:ARG:HA	1:D:385:LEU:O	1.96	0.64
1:A:198:ARG:HB2	1:B:165:VAL:HG21	1.78	0.64
1:A:354:LYS:HD3	1:A:357:TRP:HB3	1.79	0.63
1:A:356:ARG:HA	1:A:385:LEU:O	1.97	0.63
1:C:188:SER:OG	1:C:192:ARG:NH1	2.31	0.63
1:C:198:ARG:HB2	1:D:165:VAL:HG21	1.80	0.63
1:B:322:GLY:O	1:B:369:ARG:NH1	2.31	0.63
1:D:89:HIS:CE1	1:D:105:CYS:SG	2.92	0.62
1:A:354:LYS:NZ	1:A:463:ASN:OD1	2.33	0.61
1:C:86:CYS:HB3	1:C:89:HIS:H	1.67	0.59
1:B:206:ARG:NH2	1:D:430:SER:O	2.36	0.59
1:B:86:CYS:HB3	1:B:89:HIS:H	1.67	0.59
1:A:265:LEU:HD12	1:A:266:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD23	1:B:164:THR:HG22	1.83	0.58
1:A:86:CYS:HB3	1:A:89:HIS:H	1.68	0.58
1:B:306:SER:HB3	1:B:310:ARG:HB3	1.87	0.57
1:C:137:LYS:O	1:C:141:GLN:NE2	2.38	0.56
1:A:234:GLN:NE2	1:B:126:GLN:OE1	2.36	0.56
1:D:299:HIS:HB3	1:D:302:LEU:HG	1.89	0.55
1:C:326:ARG:HA	1:C:368:ARG:HD2	1.89	0.55
1:A:137:LYS:O	1:A:141:GLN:NE2	2.39	0.53
1:C:268:ILE:HD11	1:D:171:ALA:HB1	1.90	0.53
1:B:430:SER:O	1:D:206:ARG:NH2	2.43	0.52
1:D:97:CYS:HA	1:D:119:LEU:HA	1.92	0.51
1:A:356:ARG:HG3	1:A:386:ARG:HA	1.93	0.51
1:D:89:HIS:ND1	1:D:108:CYS:SG	2.82	0.51
1:C:265:LEU:HD12	1:C:266:PRO:HD2	1.91	0.51
1:D:279:HIS:NE2	1:D:283:HIS:CD2	2.78	0.51
1:D:355:PRO:HG2	1:D:463:ASN:HD22	1.77	0.50
1:A:326:ARG:HA	1:A:368:ARG:HD2	1.93	0.50
1:B:354:LYS:NZ	1:B:463:ASN:OD1	2.42	0.50
1:C:176:LEU:HD12	1:D:187:GLU:HB2	1.92	0.50
1:D:356:ARG:HG3	1:D:386:ARG:HA	1.93	0.49
1:A:147:LYS:HD2	1:B:212:LEU:HD22	1.94	0.49
1:D:306:SER:HB3	1:D:310:ARG:HB3	1.95	0.49
1:B:355:PRO:HG2	1:B:463:ASN:HD22	1.78	0.48
1:B:86:CYS:C	1:B:88:GLU:H	2.22	0.48
1:B:290:GLU:OE2	1:B:309:ARG:NH1	2.47	0.48
1:A:354:LYS:HE3	1:A:455:VAL:HG23	1.96	0.48
1:B:468:LEU:HD23	1:C:159:VAL:HG23	1.96	0.47
1:A:268:ILE:HD11	1:B:171:ALA:HB1	1.96	0.47
1:C:86:CYS:C	1:C:88:GLU:H	2.22	0.47
1:B:354:LYS:HE3	1:B:455:VAL:HG23	1.96	0.47
1:A:221:GLN:O	1:A:224:LYS:HG3	2.14	0.47
1:B:299:HIS:CG	1:B:332:VAL:HG12	2.50	0.47
1:B:329:ASP:CG	1:B:370:GLY:H	2.22	0.46
1:A:86:CYS:C	1:A:88:GLU:H	2.22	0.46
1:D:289:GLU:OE1	1:D:345:HIS:ND1	2.48	0.46
1:A:300:PRO:HG3	1:A:321:ALA:HB2	1.99	0.45
1:C:222:MET:HE2	1:C:248:LEU:HB2	1.98	0.45
1:C:169:ARG:NE	1:D:191:ASP:OD1	2.41	0.45
1:A:145:MET:HE2	1:A:145:MET:HB2	1.85	0.45
1:B:222:MET:HE1	1:B:244:VAL:HG13	1.99	0.45
1:A:376:PRO:HD2	1:A:396:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:SER:OG	1:D:270:ASP:N	2.50	0.45
1:C:176:LEU:HD22	1:D:183:LEU:HD22	1.99	0.45
1:D:89:HIS:CG	1:D:105:CYS:SG	3.08	0.45
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.87	0.44
1:A:299:HIS:CG	1:A:300:PRO:HD2	2.53	0.44
1:C:103:LEU:HD21	1:D:238:LEU:HD13	2.00	0.44
1:D:95:ILE:HB	1:D:104:VAL:HG23	2.00	0.44
1:A:228:GLU:O	1:A:232:LYS:NZ	2.45	0.43
1:B:250:LYS:NZ	1:B:254:GLU:OE1	2.41	0.43
1:A:459:ASP:O	1:A:462:LYS:HG2	2.19	0.43
1:D:97:CYS:SG	1:D:119:LEU:HG	2.58	0.43
1:B:299:HIS:HB3	1:B:302:LEU:HG	2.01	0.43
1:A:457:TRP:CD1	1:A:457:TRP:N	2.87	0.43
1:C:376:PRO:HD2	1:C:396:GLU:HB2	2.01	0.43
1:C:398:LYS:H	1:C:398:LYS:HG2	1.62	0.43
1:D:96:TYR:H	1:D:121:PRO:HB3	1.83	0.43
1:A:120:LEU:HD12	1:A:121:PRO:HD2	1.99	0.43
1:B:356:ARG:HG3	1:B:386:ARG:HA	2.01	0.43
1:B:393:ALA:HB2	1:B:403:LEU:HD11	2.00	0.43
1:A:225:VAL:HG11	1:A:247:ARG:HH21	1.84	0.42
1:A:304:VAL:HG12	1:A:308:GLY:HA2	2.01	0.42
1:B:329:ASP:OD1	1:B:330:LYS:N	2.52	0.42
1:B:329:ASP:OD1	1:B:370:GLY:N	2.43	0.42
1:D:376:PRO:HB3	1:D:381:TRP:NE1	2.34	0.42
1:A:85:HIS:HB3	1:A:92:PRO:HA	2.01	0.42
1:D:350:GLU:HB3	1:D:468:LEU:HB2	2.01	0.42
1:A:147:LYS:HA	1:A:147:LYS:HD3	1.80	0.42
1:A:281:PHE:HB2	1:B:277:TRP:CZ2	2.55	0.42
1:C:265:LEU:HD22	1:D:165:VAL:HG22	2.02	0.42
1:A:289:GLU:OE1	1:A:345:HIS:ND1	2.52	0.42
1:C:329:ASP:OD1	1:C:330:LYS:N	2.53	0.42
1:D:96:TYR:N	1:D:121:PRO:HB3	2.35	0.42
1:D:299:HIS:CG	1:D:300:PRO:HD2	2.55	0.42
1:B:323:GLU:HA	1:B:369:ARG:NH1	2.35	0.41
1:C:299:HIS:CG	1:C:300:PRO:HD2	2.55	0.41
1:C:257:PRO:HG2	1:C:258:PRO:HD3	2.01	0.41
1:C:312:GLU:HB3	1:C:466:PRO:HB3	2.02	0.41
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.88	0.41
1:B:299:HIS:CG	1:B:300:PRO:HD2	2.55	0.41
1:B:362:MET:HE1	1:B:368:ARG:HA	2.02	0.41
1:A:257:PRO:HG2	1:A:258:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LYS:HD3	1:B:147:LYS:HA	1.77	0.41
1:C:85:HIS:HB3	1:C:92:PRO:HA	2.03	0.41
1:C:277:TRP:CZ2	1:D:281:PHE:HB2	2.56	0.41
1:D:288:LEU:HD23	1:D:288:LEU:HA	1.93	0.41
1:A:188:SER:HG	1:A:192:ARG:HH12	1.64	0.41
1:A:427:TYR:CD1	1:A:437:PRO:HA	2.56	0.40
1:B:398:LYS:H	1:B:398:LYS:HG2	1.66	0.40
1:A:273:LYS:HE2	1:A:273:LYS:HB2	1.91	0.40
1:B:395:VAL:HG12	1:B:396:GLU:N	2.36	0.40
1:C:147:LYS:HA	1:C:147:LYS:HD3	1.77	0.40
1:A:222:MET:HE1	1:A:244:VAL:HG13	2.03	0.40
1:C:395:VAL:HG12	1:C:396:GLU:N	2.36	0.40
1:C:306:SER:HB3	1:C:310:ARG:HB3	2.02	0.40
1:C:412:ARG:HG2	1:C:429:ALA:HB3	2.03	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	378/466 (81%)	361 (96%)	17 (4%)	0	100	100
1	B	384/466 (82%)	366 (95%)	18 (5%)	0	100	100
1	C	378/466 (81%)	360 (95%)	18 (5%)	0	100	100
1	D	384/466 (82%)	362 (94%)	22 (6%)	0	100	100
All	All	1524/1864 (82%)	1449 (95%)	75 (5%)	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	327/394 (83%)	327 (100%)	0	100	100
1	B	330/394 (84%)	330 (100%)	0	100	100
1	C	327/394 (83%)	327 (100%)	0	100	100
1	D	330/394 (84%)	330 (100%)	0	100	100
All	All	1314/1576 (83%)	1314 (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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	458	HIS
1	B	114	HIS
1	B	135	GLN
1	B	337	GLN
1	B	345	HIS
1	C	114	HIS
1	D	135	GLN
1	D	156	HIS
1	D	442	HIS

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 10 ligands modelled in this entry, 10 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	382/466 (81%)	0.82	34 (8%)	15 10	52, 166, 263, 384	0
1	B	386/466 (82%)	0.70	33 (8%)	16 11	39, 101, 264, 335	0
1	C	382/466 (81%)	0.87	46 (12%)	9 6	52, 179, 261, 372	0
1	D	386/466 (82%)	0.64	31 (8%)	18 12	45, 101, 263, 362	0
All	All	1536/1864 (82%)	0.76	144 (9%)	14 9	39, 143, 264, 384	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	VAL	8.1
1	D	315	ASP	6.5
1	A	229	VAL	5.6
1	C	457	TRP	5.5
1	B	457	TRP	5.5
1	B	322	GLY	5.4
1	C	461	GLY	5.1
1	A	263	ILE	4.9
1	A	457	TRP	4.5
1	C	258	PRO	4.5
1	C	389	LYS	4.4
1	A	90	LEU	4.2
1	C	462	LYS	4.2
1	A	258	PRO	4.2
1	C	237	PHE	4.1
1	D	85	HIS	4.0
1	B	315	ASP	4.0
1	D	92	PRO	4.0
1	C	460	LYS	3.9
1	B	321	ALA	3.7
1	C	455	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	125	ALA	3.6
1	D	457	TRP	3.6
1	A	407	GLU	3.6
1	C	454	ASP	3.6
1	C	240	LYS	3.5
1	C	263	ILE	3.5
1	A	106	GLY	3.5
1	A	266	PRO	3.5
1	B	103	LEU	3.4
1	A	313	CYS	3.4
1	D	104	VAL	3.4
1	C	358	ALA	3.4
1	B	433	ASP	3.3
1	A	256	PRO	3.3
1	D	306	SER	3.3
1	B	160	GLU	3.3
1	D	263	ILE	3.2
1	C	226	LEU	3.2
1	C	353	ASP	3.1
1	C	266	PRO	3.1
1	A	373	HIS	3.1
1	D	447	GLY	3.0
1	A	103	LEU	3.0
1	B	106	GLY	3.0
1	B	454	ASP	3.0
1	C	90	LEU	3.0
1	D	86	CYS	3.0
1	D	124	GLU	3.0
1	B	111	LEU	3.0
1	C	409	PRO	2.9
1	C	443	GLU	2.9
1	A	443	GLU	2.9
1	A	239	MET	2.9
1	C	331	ALA	2.9
1	C	244	VAL	2.8
1	A	243	LEU	2.8
1	D	129	LEU	2.8
1	A	92	PRO	2.8
1	B	306	SER	2.8
1	B	407	GLU	2.8
1	C	317	LYS	2.8
1	C	406	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	102	THR	2.7
1	D	317	LYS	2.7
1	B	125	ALA	2.7
1	A	460	LYS	2.7
1	B	94	SER	2.7
1	D	90	LEU	2.7
1	B	123	ALA	2.7
1	D	235	THR	2.7
1	C	464	ALA	2.7
1	D	98	GLU	2.7
1	D	91	ASP	2.6
1	D	191	ASP	2.6
1	D	200	ASP	2.6
1	D	331	ALA	2.6
1	D	329	ASP	2.6
1	C	314	SER	2.6
1	B	406	PRO	2.6
1	C	333	ALA	2.6
1	B	104	VAL	2.5
1	B	267	VAL	2.5
1	C	241	PHE	2.5
1	A	226	LEU	2.5
1	D	120	LEU	2.5
1	A	241	PHE	2.5
1	C	301	SER	2.5
1	C	225	VAL	2.5
1	B	470	VAL	2.5
1	D	290	GLU	2.4
1	A	111	LEU	2.4
1	A	230	ALA	2.4
1	B	387	ASP	2.4
1	B	129	LEU	2.4
1	C	243	LEU	2.4
1	C	256	PRO	2.3
1	B	307	SER	2.3
1	C	106	GLY	2.3
1	D	111	LEU	2.3
1	C	351	VAL	2.3
1	A	358	ALA	2.3
1	B	259	ALA	2.3
1	B	133	LEU	2.3
1	C	405	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	461	GLY	2.3
1	D	149	LYS	2.3
1	C	357	TRP	2.3
1	C	319	PRO	2.3
1	D	110	SER	2.2
1	D	123	ALA	2.2
1	A	235	THR	2.2
1	D	394	HIS	2.2
1	C	132	GLN	2.2
1	A	382	LEU	2.2
1	A	387	ASP	2.2
1	B	305	SER	2.2
1	C	445	LEU	2.2
1	B	331	ALA	2.1
1	A	458	HIS	2.1
1	B	101	ARG	2.1
1	C	313	CYS	2.1
1	A	448	PRO	2.1
1	A	240	LYS	2.1
1	B	96	TYR	2.1
1	B	444	ARG	2.1
1	C	300	PRO	2.1
1	C	373	HIS	2.1
1	A	91	ASP	2.1
1	A	406	PRO	2.1
1	C	236	GLU	2.1
1	B	309	ARG	2.1
1	C	363	ALA	2.1
1	D	316	GLN	2.1
1	D	96	TYR	2.0
1	A	409	PRO	2.0
1	C	446	PRO	2.0
1	C	91	ASP	2.0
1	A	389	LYS	2.0
1	D	433	ASP	2.0
1	B	139	GLN	2.0
1	B	263	ILE	2.0
1	C	348	GLU	2.0
1	B	159	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

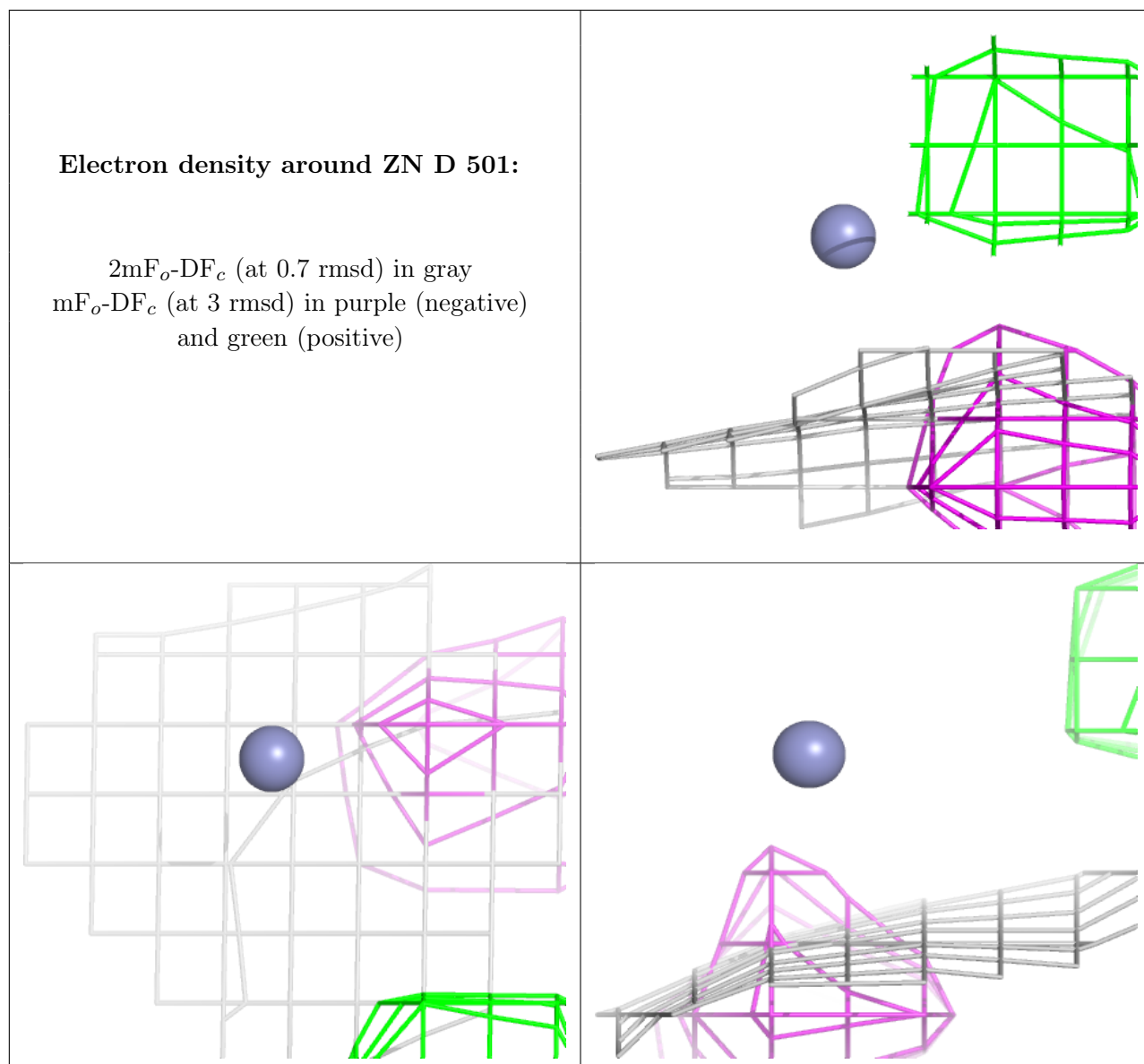
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D	501	1/1	0.80	0.10	399,399,399,399	0
2	ZN	D	502	1/1	0.84	0.12	421,421,421,421	0
2	ZN	B	501	1/1	0.89	0.07	391,391,391,391	0
2	ZN	B	502	1/1	0.89	0.10	402,402,402,402	0
2	ZN	A	502	1/1	0.93	0.07	342,342,342,342	0
2	ZN	B	503	1/1	0.95	0.13	98,98,98,98	0
2	ZN	A	501	1/1	0.96	0.05	303,303,303,303	0
2	ZN	C	501	1/1	0.97	0.05	343,343,343,343	0
2	ZN	C	502	1/1	0.97	0.05	321,321,321,321	0
2	ZN	D	503	1/1	0.98	0.06	61,61,61,61	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.

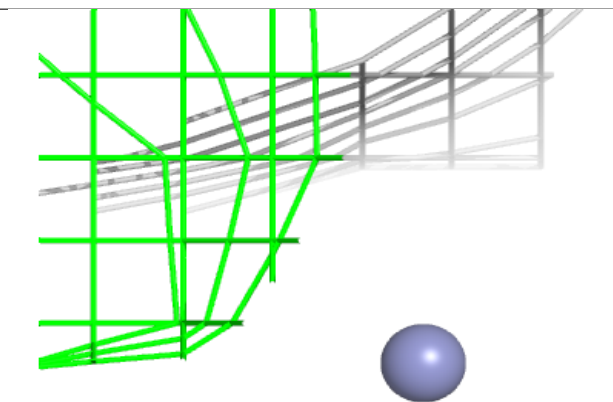
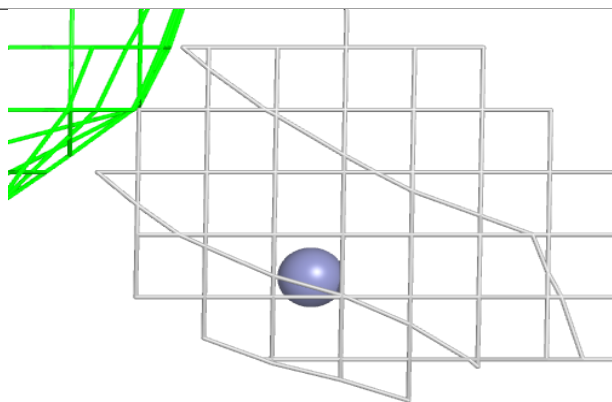
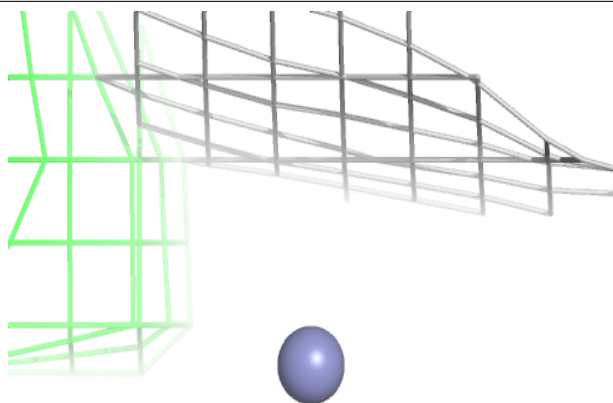
Electron density around ZN D 501:

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

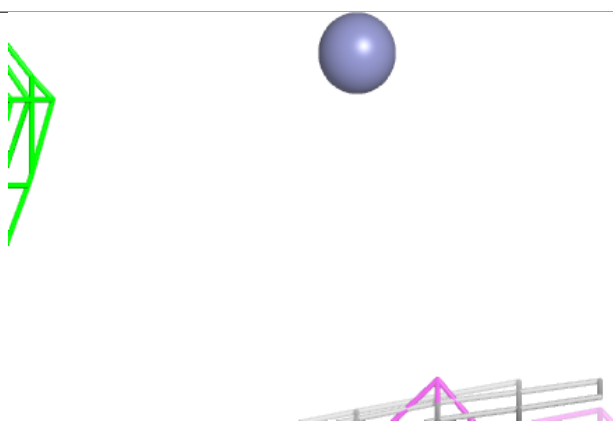
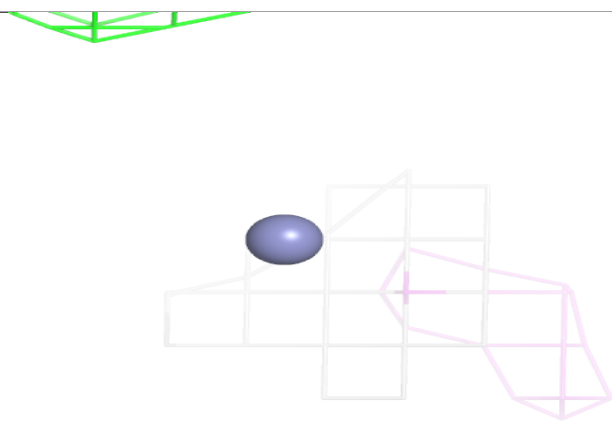
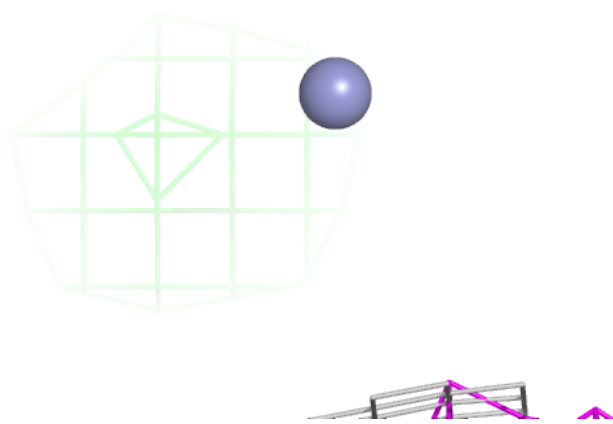


Electron density around ZN D 502:

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

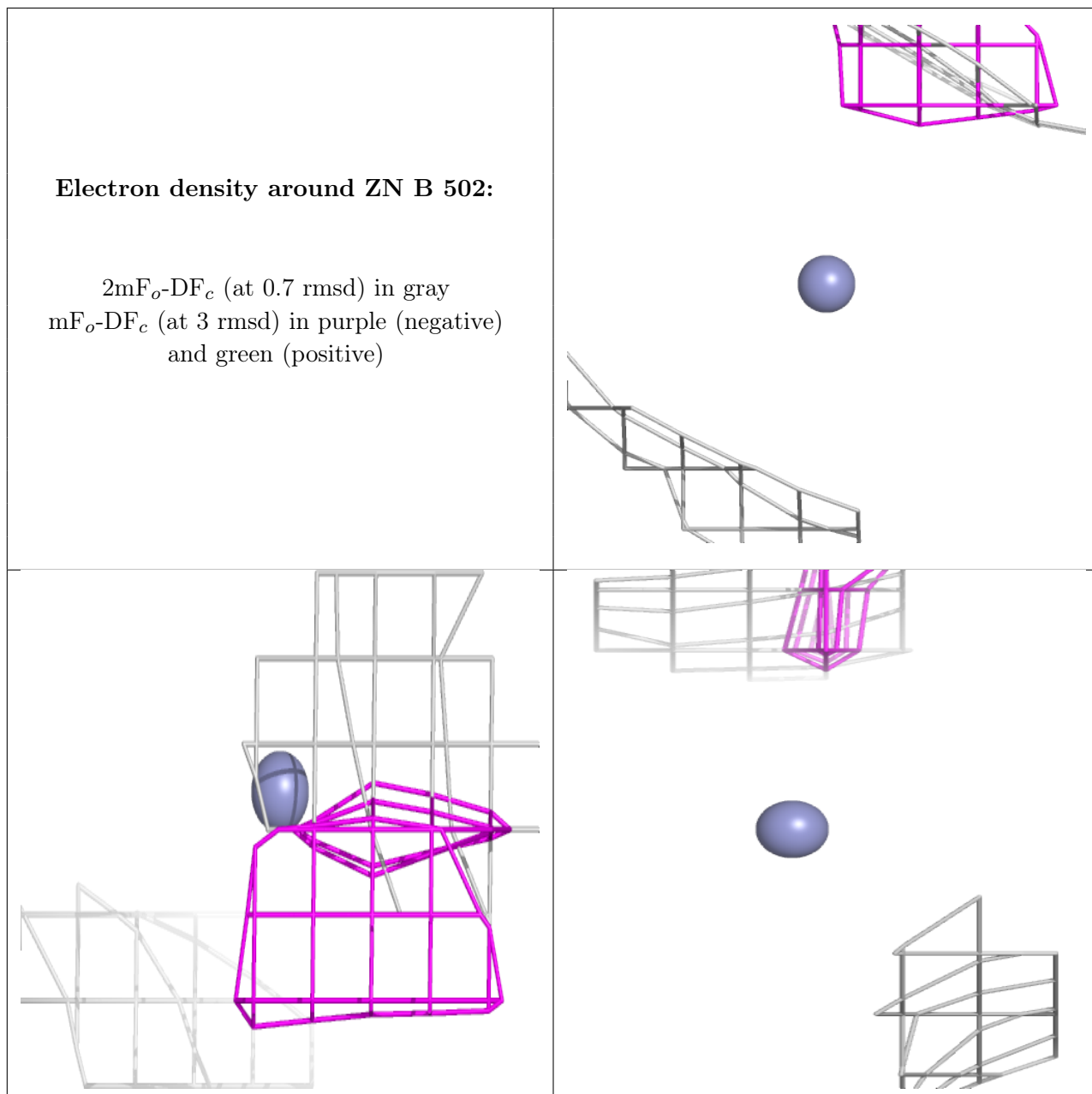
**Electron density around ZN B 501:**

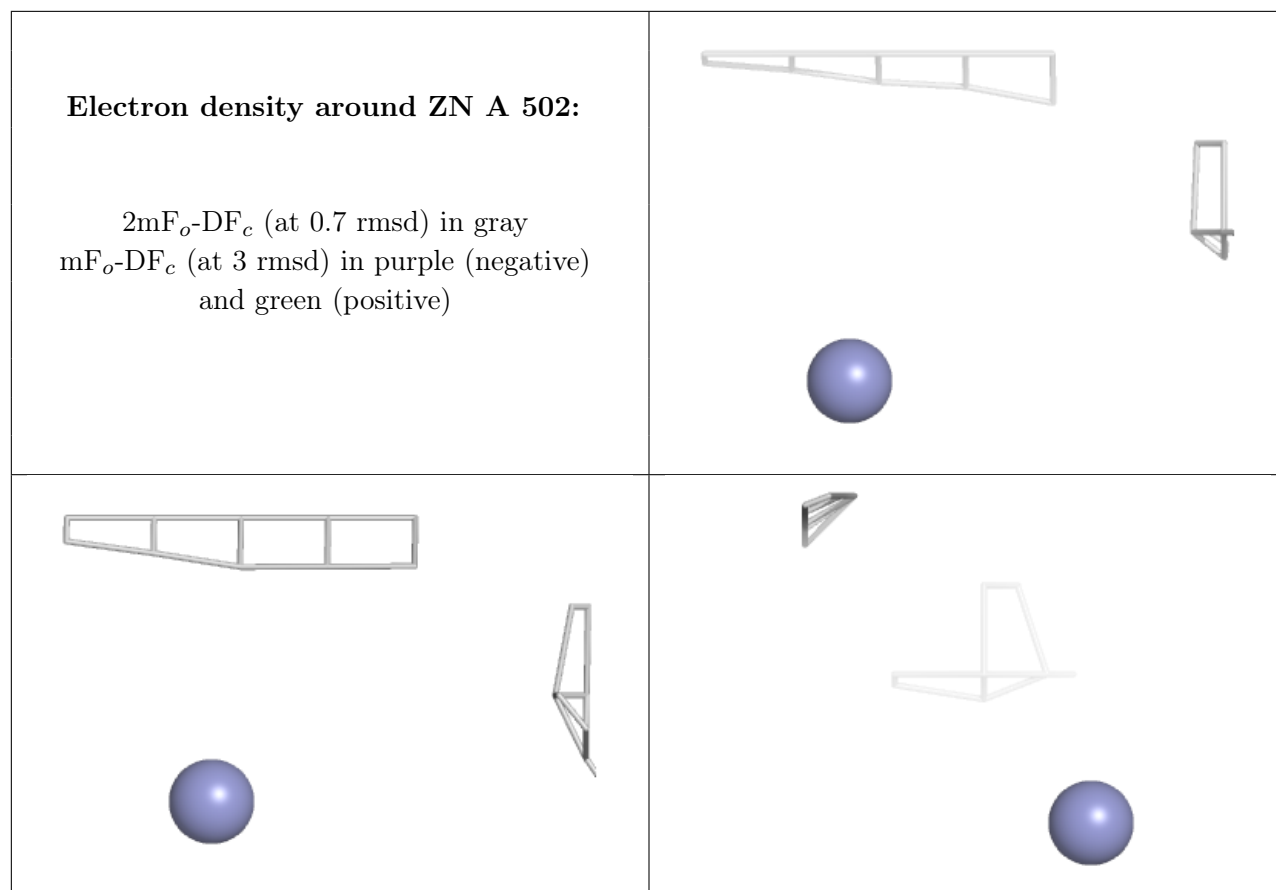
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 502:

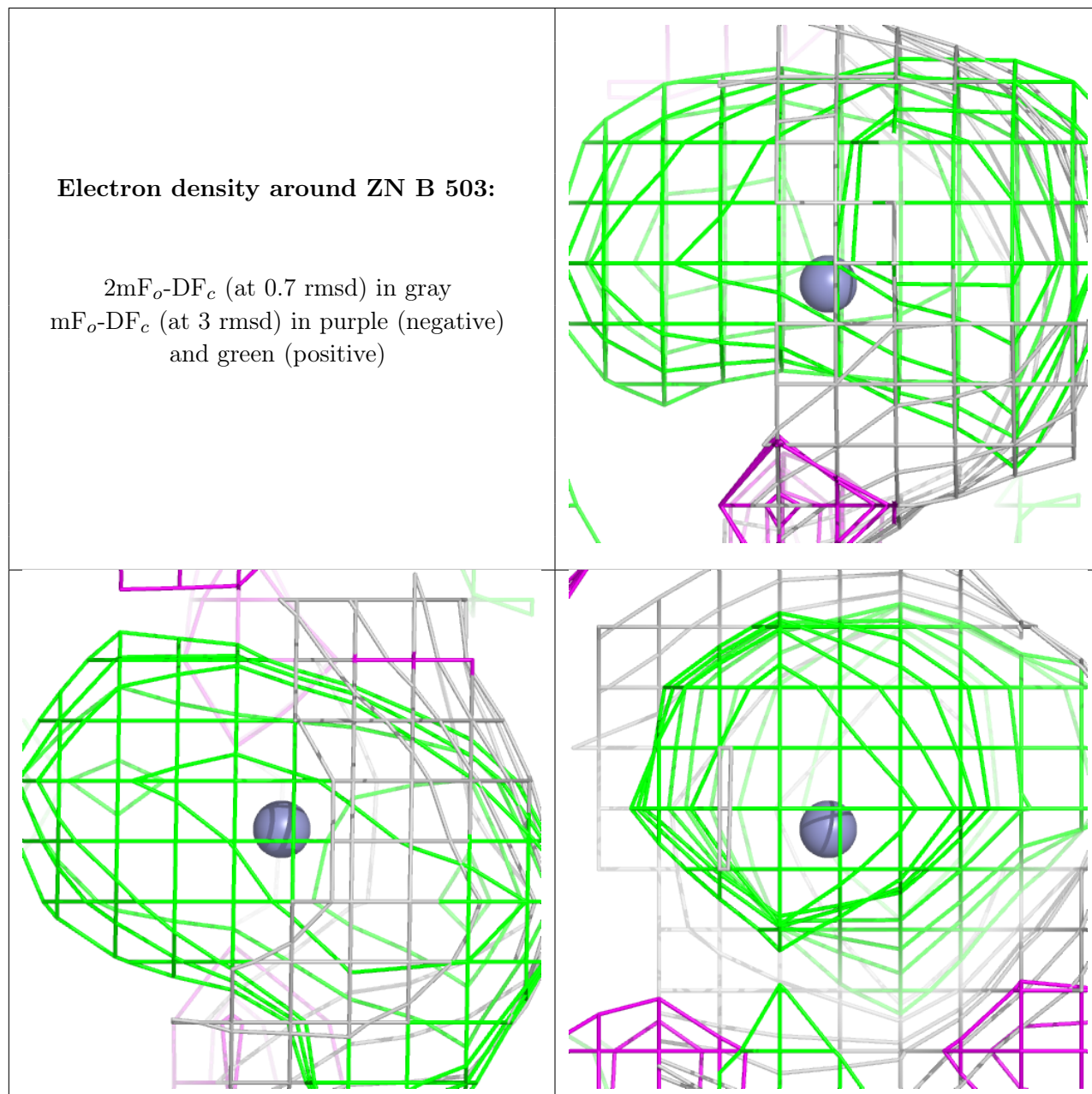
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





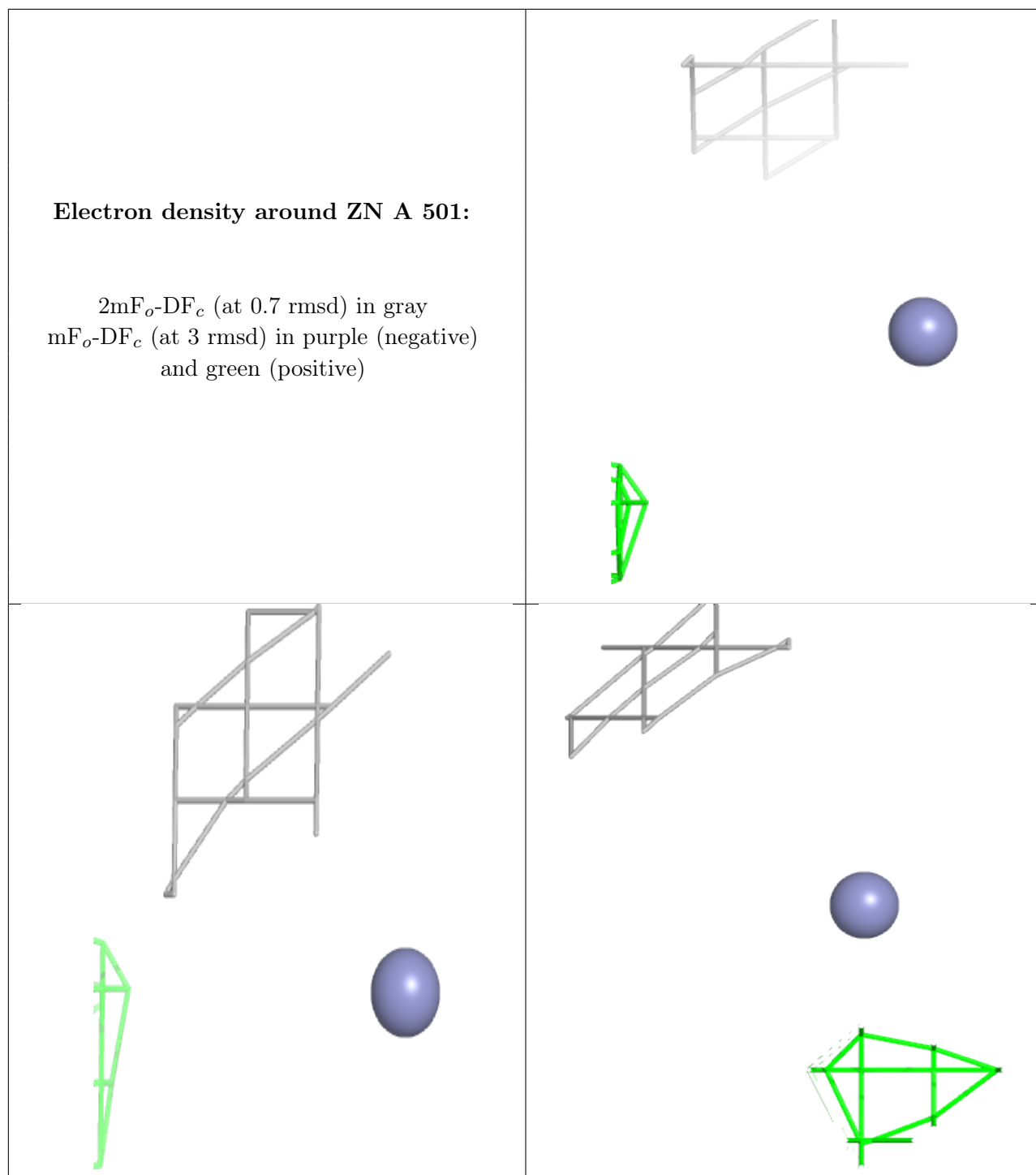
Electron density around ZN B 503:

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



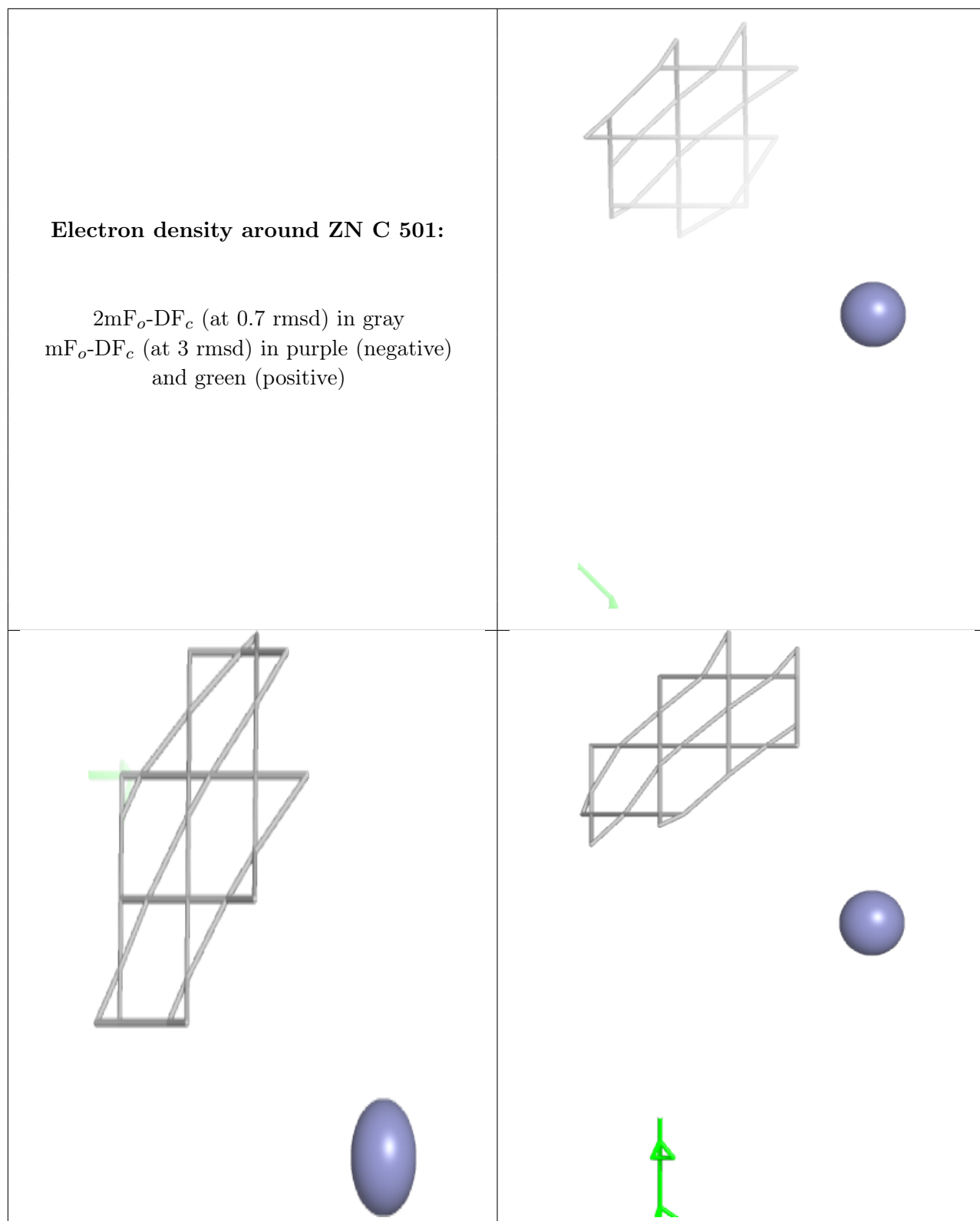
Electron density around ZN A 501:

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



Electron density around ZN C 501:

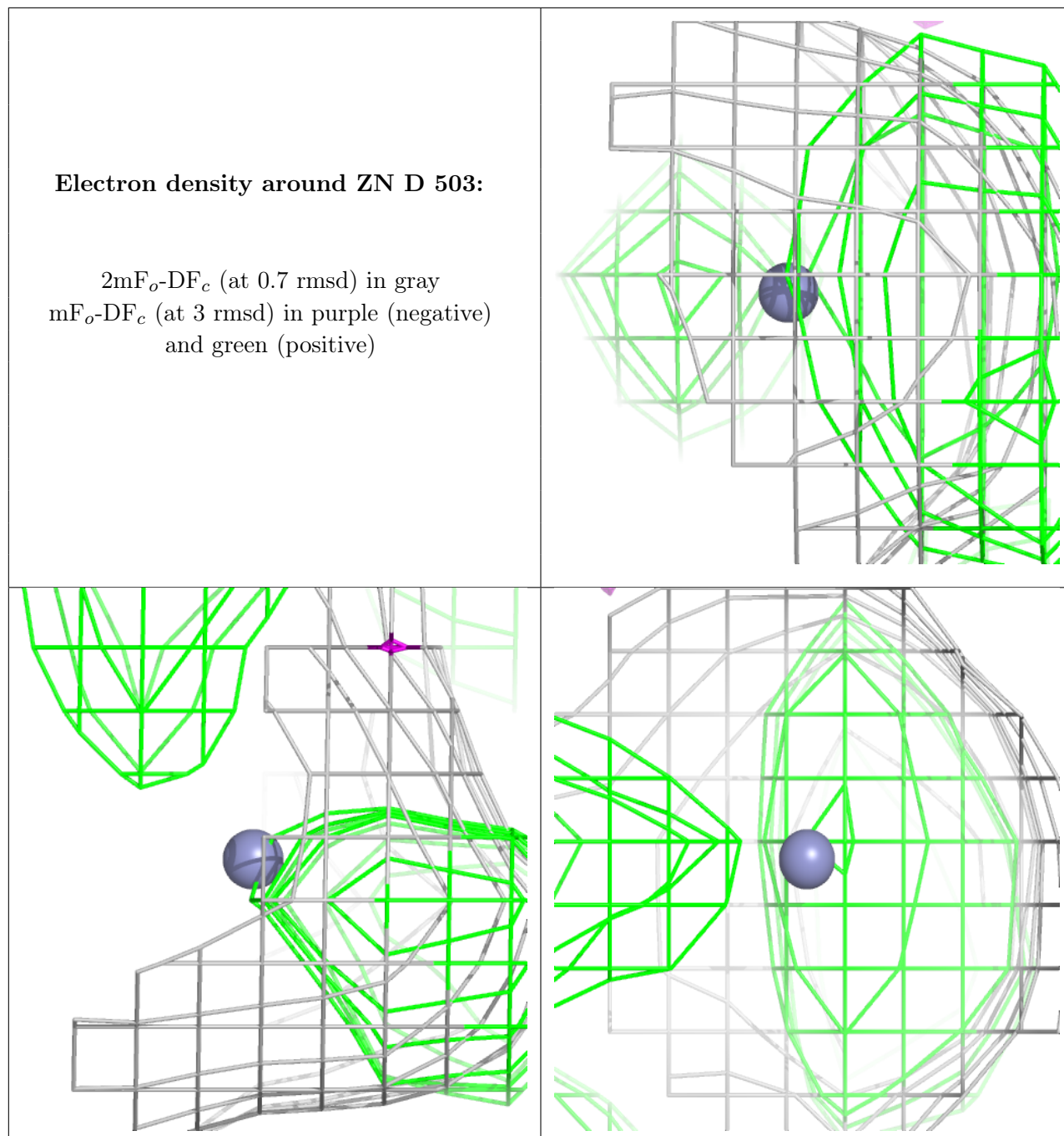
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN C 502: $2mF_o - DF_c$ (at 0.7 rmsd) in gray $mF_o - DF_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around ZN D 503:

$2mF_o-DF_c$ (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.