Full wwPDB X-ray Structure Validation Report (i)

Jun 10, 2025 – 12:48 PM JST

PDB ID	:	9J3P / pdb_00009j3p
Title	:	Human Pigment Epithelium-Derived Factor with Zinc Ions Crystallized in P2(1)2(1)2(1) Space Group
Authors	:	Belousov, A.S.; Chistyakov, D.V.; Baksheeva, V.E.; Bulgakov, T.K.; Bukhdruker, S.S.; Zamyatnin, A.A.; Zinchenko, D.V.; Tsvetkov, P.O.; Permyakov, S.E.; Zernii, E.Y.; Borshchevskiy, V.I.
Deposited on	:	2024-08-08
Resolution	:	2.10 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 (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:

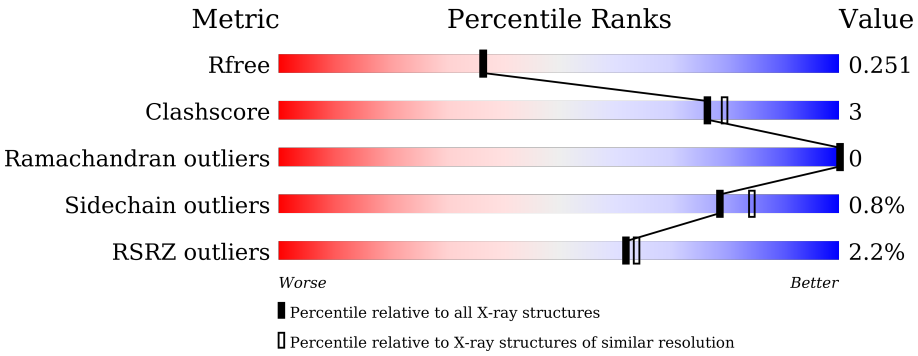
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	A	398	86% 9% 5%
1	B	398	87% 6% 7%
1	C	398	87% 6% 7%
1	D	398	3% 86% 8% 7%
1	E	398	3% 86% 7% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30200 atoms, of which 14830 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.

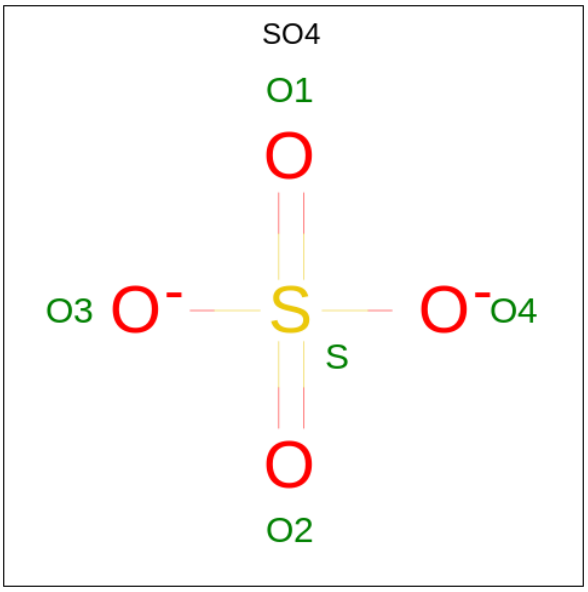
- Molecule 1 is a protein called Pigment epithelium-derived factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	377	Total	C	H	N	O	S	0	5	0
			5992	1911	3014	495	566	6			
1	B	369	Total	C	H	N	O	S	0	6	0
			5856	1873	2946	483	547	7			
1	C	371	Total	C	H	N	O	S	0	4	0
			5841	1874	2932	483	546	6			
1	D	371	Total	C	H	N	O	S	0	8	0
			5960	1903	3009	489	553	6			
1	E	368	Total	C	H	N	O	S	0	3	0
			5725	1840	2860	477	541	7			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

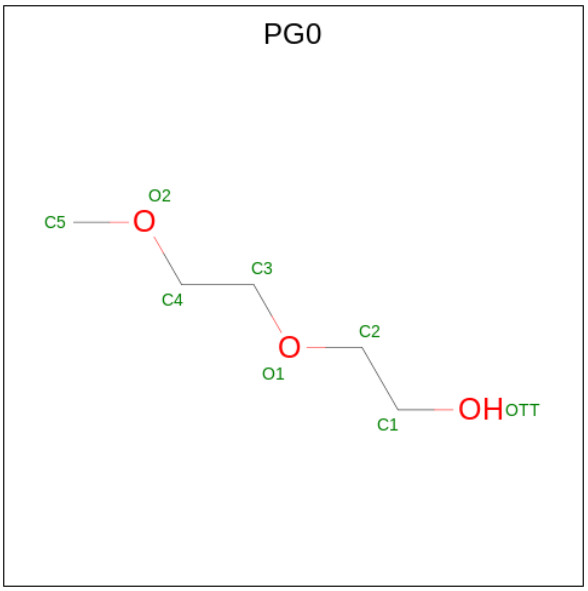
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	C	2	Total	Zn	0	0
			2	2		
2	D	1	Total	Zn	0	0
			1	1		
2	E	3	Total	Zn	0	0
			3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 20 5 12 3	0	0
4	A	1	Total C H O 20 5 12 3	0	0
4	B	1	Total C H O 20 5 12 3	0	0
4	B	1	Total C H O 12 3 7 2	0	0
4	B	1	Total C H O 20 5 12 3	0	0
4	D	1	Total C H O 12 3 7 2	0	0
4	E	1	Total C H O 12 3 7 2	0	0

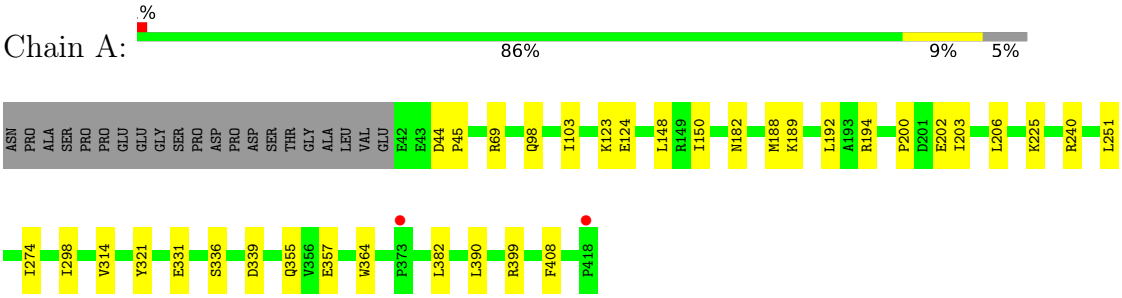
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	194	Total O 194 194	0	0
5	B	168	Total O 168 168	0	0
5	C	89	Total O 89 89	0	0
5	D	143	Total O 143 143	0	0
5	E	64	Total O 64 64	0	0

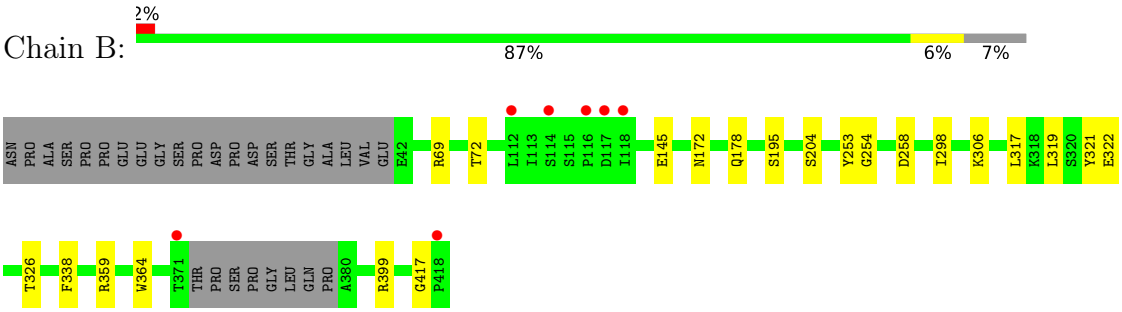
3 Residue-property plots (i)

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.

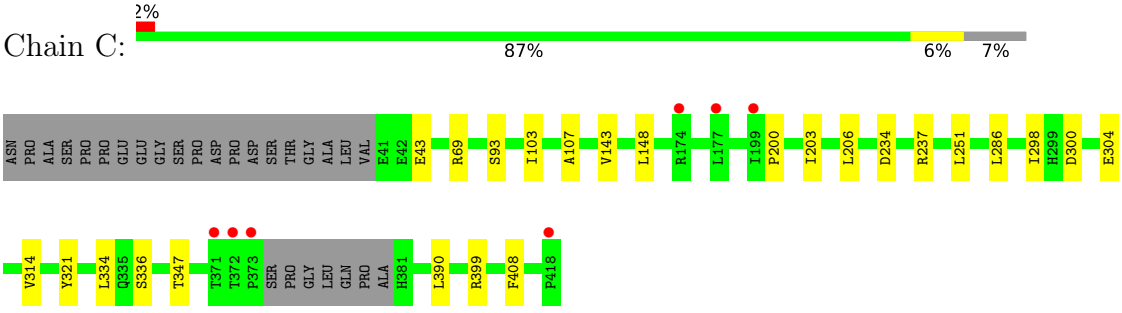
• Molecule 1: Pigment epithelium-derived factor



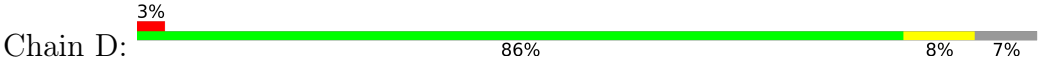
• Molecule 1: Pigment epithelium-derived factor

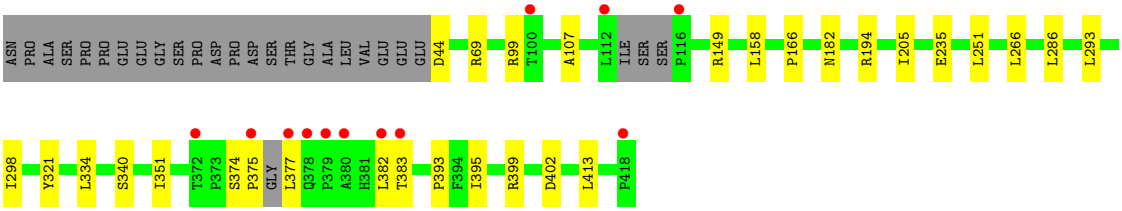


• Molecule 1: Pigment epithelium-derived factor

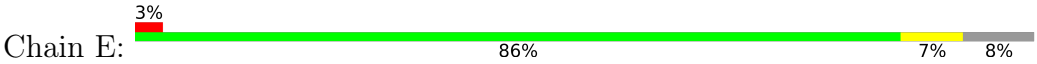


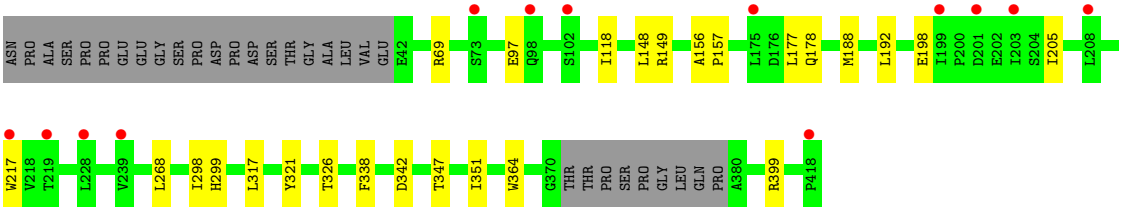
• Molecule 1: Pigment epithelium-derived factor





• Molecule 1: Pigment epithelium-derived factor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.23Å 131.57Å 227.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.10 19.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.95-2.10) 97.5 (19.95-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.217 , 0.251 0.217 , 0.251	Depositor DCC
R_{free} test set	6649 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	30200	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: PG0, SO4, 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	0.16	0/3054	0.35	0/4143
1	B	0.16	0/2986	0.36	0/4049
1	C	0.18	0/2981	0.37	0/4046
1	D	0.16	0/3037	0.35	0/4119
1	E	0.19	0/2932	0.39	1/3980 (0.0%)
All	All	0.17	0/14990	0.36	1/20337 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	299	HIS	N-CA-CB	5.03	117.51	110.12

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	2978	3014	3014	21	1
1	B	2910	2946	2946	15	1
1	C	2909	2932	2932	15	0
1	D	2951	3009	3009	18	0
1	E	2865	2860	2860	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	1
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	3	0	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	1	0
3	D	10	0	0	0	1
3	E	5	0	0	0	0
4	A	16	24	24	3	0
4	B	21	31	31	2	0
4	D	5	7	7	1	0
4	E	5	7	7	0	0
5	A	194	0	0	4	2
5	B	168	0	0	4	0
5	C	89	0	0	3	0
5	D	143	0	0	1	0
5	E	64	0	0	1	0
All	All	15370	14830	14830	84	3

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 (84) 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:C:300:ASP:OD2	5:C:601:HOH:O	2.04	0.75
1:B:172:ASN:OD1	5:B:601:HOH:O	2.04	0.74
1:D:44:ASP:N	5:D:601:HOH:O	2.22	0.71
1:A:44:ASP:OD2	5:A:601:HOH:O	2.08	0.71
1:C:43:GLU:OE2	5:C:602:HOH:O	2.10	0.70
1:C:304:GLU:OE2	5:C:601:HOH:O	2.08	0.69
1:B:417:GLY:O	5:B:602:HOH:O	2.10	0.68
1:D:69:ARG:NH2	1:D:321:TYR:OH	2.28	0.66
1:E:69:ARG:NH2	1:E:321:TYR:OH	2.30	0.64
1:D:149:ARG:HG3	4:D:504:PG0:H52	1.82	0.62
1:D:158:LEU:HD23	1:D:166:PRO:HD3	1.80	0.62
1:C:103[A]:ILE:HD13	1:C:336:SER:OG	2.00	0.62
1:E:298:ILE:HG21	1:E:399:ARG:HD2	1.81	0.61
1:A:355[B]:GLN:NE2	1:A:357:GLU:OE2	2.36	0.57
1:A:189:LYS:NZ	5:A:609:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:NH2	1:B:321:TYR:OH	2.38	0.56
1:D:382[B]:LEU:HD12	1:D:383:THR:N	2.20	0.56
1:E:326:THR:HG23	1:E:338:PHE:CE2	2.41	0.56
1:C:69:ARG:NH2	1:C:321:TYR:OH	2.39	0.56
1:E:205:ILE:HD11	1:E:351:ILE:HD12	1.89	0.55
1:A:148:LEU:HD23	1:A:150:ILE:HD11	1.89	0.54
1:B:319:LEU:HD22	4:B:504:PG0:H42	1.88	0.54
1:D:182:ASN:OD1	1:D:194:ARG:NH2	2.35	0.53
1:D:286:LEU:HD22	1:D:395:ILE:HG13	1.90	0.53
1:A:225:LYS:NZ	5:A:614:HOH:O	2.43	0.52
1:C:234:ASP:OD2	1:C:237:ARG:NE	2.41	0.51
1:B:326:THR:HG23	1:B:338:PHE:CE2	2.45	0.50
1:A:298:ILE:HG21	1:A:399:ARG:HD2	1.93	0.50
1:B:195:SER:OG	1:B:322:GLU:OE2	2.21	0.49
1:C:206:LEU:C	1:C:206:LEU:HD23	2.37	0.49
1:A:274:ILE:HD13	1:A:364:TRP:CZ3	2.47	0.49
1:E:317:LEU:HD12	1:E:364:TRP:CZ2	2.48	0.48
1:E:178:GLN:NE2	5:E:606:HOH:O	2.47	0.47
1:E:148:LEU:HD11	1:E:347:THR:HG21	1.96	0.47
1:B:298:ILE:HG21	1:B:399:ARG:CD	2.45	0.47
1:E:156:ALA:HB3	1:E:157:PRO:HD3	1.96	0.47
1:B:317:LEU:HD12	1:B:364:TRP:CZ2	2.50	0.47
1:C:107:ALA:HB2	1:C:334:LEU:HD21	1.97	0.47
1:C:298:ILE:HG21	1:C:399:ARG:CD	2.45	0.47
1:E:156:ALA:HB3	1:E:157:PRO:CD	2.46	0.46
1:B:298:ILE:HG21	1:B:399:ARG:HD2	1.98	0.46
1:A:200:PRO:HD2	1:A:203:ILE:HD11	1.96	0.46
1:A:103:ILE:HD13	1:A:336:SER:OG	2.16	0.46
1:A:182:ASN:OD1	1:A:194:ARG:NH2	2.47	0.45
1:A:206:LEU:HD13	1:A:355[B]:GLN:HB3	1.98	0.45
1:C:314:VAL:HG22	1:C:390:LEU:HD12	1.99	0.45
1:E:298:ILE:HG21	1:E:399:ARG:CD	2.46	0.45
1:A:188:MET:HG3	1:A:192:LEU:HD12	1.98	0.45
1:D:251:LEU:HD12	1:D:251:LEU:C	2.42	0.45
1:B:178:GLN:OE1	5:B:603:HOH:O	2.21	0.45
1:C:286:LEU:HD12	1:C:286:LEU:N	2.32	0.44
1:D:375:PRO:O	1:D:377:LEU:N	2.51	0.44
1:D:393:PRO:HB3	1:D:413:LEU:HD23	1.98	0.44
1:B:145:GLU:CG	1:B:204:SER:HA	2.48	0.44
1:E:97:GLU:HG3	1:E:342:ASP:OD2	2.18	0.44
1:A:251:LEU:C	1:A:251:LEU:HD12	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLU:HG2	4:A:503:PG0:H51	1.99	0.44
1:C:298:ILE:HG21	1:C:399:ARG:HD2	2.00	0.43
1:C:148:LEU:HD11	1:C:347:THR:HG21	1.99	0.43
1:B:319:LEU:HD22	4:B:504:PG0:C4	2.47	0.43
1:D:298:ILE:HG21	1:D:399:ARG:HD2	1.99	0.43
1:D:293:LEU:HD22	1:D:298:ILE:HD11	2.00	0.43
1:D:235:GLU:OE1	1:D:235:GLU:N	2.45	0.43
1:A:45:PRO:O	5:A:602:HOH:O	2.21	0.42
1:B:359:ARG:NH1	5:B:606:HOH:O	2.34	0.42
1:E:217:TRP:HA	1:E:268:LEU:HD23	2.00	0.42
1:E:177:LEU:HD12	1:E:198:GLU:HA	2.01	0.42
1:C:200:PRO:HD2	1:C:203:ILE:HD11	2.01	0.42
1:C:251:LEU:C	1:C:251:LEU:HD12	2.44	0.42
1:A:298:ILE:HG21	1:A:399:ARG:CD	2.50	0.42
1:A:69:ARG:NH2	1:A:321:TYR:OH	2.52	0.41
1:D:107:ALA:CB	1:D:334:LEU:HD21	2.49	0.41
1:D:205:ILE:HD11	1:D:351:ILE:HD12	2.02	0.41
1:A:123:LYS:HD3	4:A:504:PG0:H52	2.02	0.41
1:A:124:GLU:CG	4:A:504:PG0:H53	2.51	0.41
1:D:99:ARG:NH2	1:D:340:SER:O	2.51	0.41
1:B:253:TYR:CG	1:B:254:GLY:N	2.88	0.41
3:C:503:SO4:O1	1:E:149:ARG:NH1	2.51	0.41
1:A:274:ILE:HD13	1:A:364:TRP:HZ3	1.84	0.41
1:B:72:THR:O	1:B:72:THR:HG22	2.20	0.41
1:E:188:MET:HG3	1:E:192:LEU:HD12	2.02	0.40
1:A:314:VAL:HG22	1:A:390:LEU:HD12	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASP:OD1	2:A:501:ZN:ZN[1_655]	1.70	0.50
1:B:258:ASP:OD2	5:A:680:HOH:O[1_655]	2.16	0.04
3:D:503:SO4:O1	5:A:767:HOH:O[4_555]	2.18	0.02

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	380/398 (96%)	369 (97%)	11 (3%)	0	100	100
1	B	371/398 (93%)	361 (97%)	10 (3%)	0	100	100
1	C	371/398 (93%)	355 (96%)	16 (4%)	0	100	100
1	D	373/398 (94%)	360 (96%)	13 (4%)	0	100	100
1	E	367/398 (92%)	351 (96%)	16 (4%)	0	100	100
All	All	1862/1990 (94%)	1796 (96%)	66 (4%)	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	334/354 (94%)	329 (98%)	5 (2%)	60	67
1	B	322/354 (91%)	321 (100%)	1 (0%)	91	94
1	C	321/354 (91%)	318 (99%)	3 (1%)	75	82
1	D	332/354 (94%)	330 (99%)	2 (1%)	84	89
1	E	313/354 (88%)	312 (100%)	1 (0%)	91	94
All	All	1622/1770 (92%)	1610 (99%)	12 (1%)	79	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	202	GLU
1	A	240	ARG
1	A	382	LEU
1	A	408	PHE
1	B	306	LYS
1	C	93	SER
1	C	143	VAL
1	C	408	PHE
1	D	266	LEU
1	D	374	SER
1	E	118	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	HIS
1	A	309	GLN
1	B	178	GLN
1	B	392	GLN
1	C	98	GLN
1	C	330	GLN
1	C	335	GLN
1	C	392	GLN
1	D	285	ASN
1	D	299	HIS
1	D	392	GLN
1	E	335	GLN

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 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.06	0
4	PG0	B	504	-	4,4,7	0.20	0	3,3,6	0.32	0
4	PG0	D	504	-	4,4,7	0.21	0	3,3,6	0.25	0
3	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.06	0
4	PG0	B	503	-	7,7,7	0.25	0	6,6,6	0.24	0
4	PG0	A	503	-	7,7,7	0.24	0	6,6,6	0.23	0
3	SO4	A	502	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.08	0
4	PG0	B	505	-	7,7,7	0.25	0	6,6,6	0.20	0
4	PG0	E	505	-	4,4,7	0.21	0	3,3,6	0.24	0
3	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	C	503	-	4,4,4	0.13	0	6,6,6	0.06	0
4	PG0	A	504	-	7,7,7	0.26	0	6,6,6	0.11	0
3	SO4	E	504	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG0	B	504	-	-	0/2/2/5	-
4	PG0	D	504	-	-	2/2/2/5	-
4	PG0	B	503	-	-	4/5/5/5	-
4	PG0	A	503	-	-	4/5/5/5	-
4	PG0	E	505	-	-	2/2/2/5	-
4	PG0	B	505	-	-	2/5/5/5	-
4	PG0	A	504	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	PG0	O1-C3-C4-O2
4	A	503	PG0	OTT-C1-C2-O1
4	A	504	PG0	O1-C3-C4-O2
4	D	504	PG0	O1-C3-C4-O2
4	B	503	PG0	OTT-C1-C2-O1
4	B	505	PG0	O1-C3-C4-O2
4	A	504	PG0	OTT-C1-C2-O1
4	A	503	PG0	C4-C3-O1-C2
4	A	504	PG0	C3-C4-O2-C5
4	B	503	PG0	C4-C3-O1-C2
4	E	505	PG0	O1-C3-C4-O2
4	B	505	PG0	OTT-C1-C2-O1
4	E	505	PG0	C3-C4-O2-C5
4	A	503	PG0	C3-C4-O2-C5
4	B	503	PG0	C1-C2-O1-C3
4	D	504	PG0	C3-C4-O2-C5
4	B	503	PG0	O1-C3-C4-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	PG0	2	0
4	D	504	PG0	1	0
4	A	503	PG0	1	0
3	C	503	SO4	1	0
4	A	504	PG0	2	0
3	D	503	SO4	0	1

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	A	377/398 (94%)	-0.03	2 (0%)	87	88	31, 57, 85, 134	5 (1%)
1	B	369/398 (92%)	0.04	7 (1%)	66	67	33, 60, 89, 123	6 (1%)
1	C	371/398 (93%)	0.16	7 (1%)	66	67	36, 67, 96, 120	4 (1%)
1	D	371/398 (93%)	0.17	12 (3%)	50	52	31, 63, 99, 127	8 (2%)
1	E	368/398 (92%)	0.55	13 (3%)	47	49	38, 77, 107, 126	3 (0%)
All	All	1856/1990 (93%)	0.18	41 (2%)	62	64	31, 64, 99, 134	26 (1%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	372	THR	5.2
1	D	372	THR	5.0
1	E	418	PRO	4.9
1	B	114	SER	4.1
1	B	116	PRO	3.8
1	D	418	PRO	3.8
1	D	375	PRO	3.7
1	D	377	LEU	3.5
1	D	379	PRO	3.5
1	B	371	THR	3.4
1	C	371	THR	3.2
1	B	418	PRO	3.1
1	D	382[A]	LEU	3.1
1	E	201	ASP	3.1
1	B	118	ILE	2.9
1	C	177	LEU	2.9
1	C	373	PRO	2.8
1	E	199	ILE	2.8
1	B	112	LEU	2.8
1	E	175	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	378	GLN	2.7
1	A	418	PRO	2.6
1	D	116	PRO	2.6
1	D	383	THR	2.6
1	D	380	ALA	2.5
1	E	228	LEU	2.4
1	D	100	THR	2.4
1	D	112	LEU	2.3
1	E	219	THR	2.3
1	E	208	LEU	2.3
1	A	373	PRO	2.3
1	C	418	PRO	2.2
1	E	98	GLN	2.2
1	B	117	ASP	2.2
1	E	217	TRP	2.2
1	E	73	SER	2.2
1	E	203	ILE	2.1
1	C	174	ARG	2.1
1	C	199	ILE	2.1
1	E	102	SER	2.1
1	E	239	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	SO4	C	504	5/5	0.35	0.09	128,130,135,164	0
4	PG0	B	505	8/8	0.52	0.16	72,88,99,100	0

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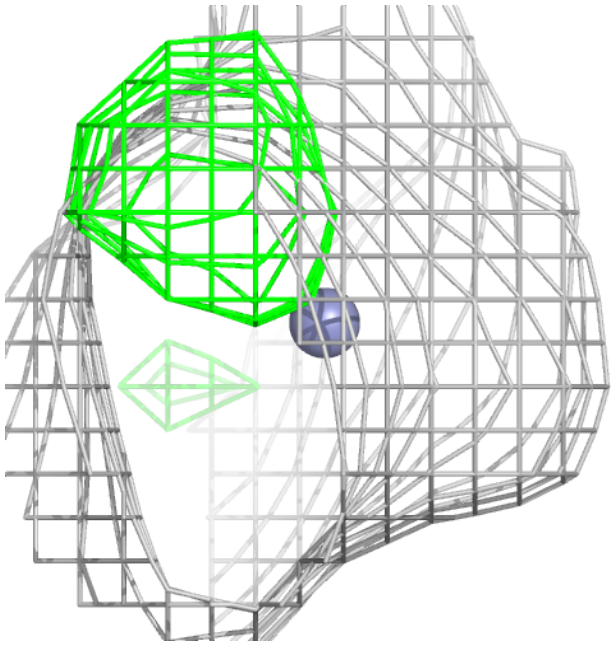
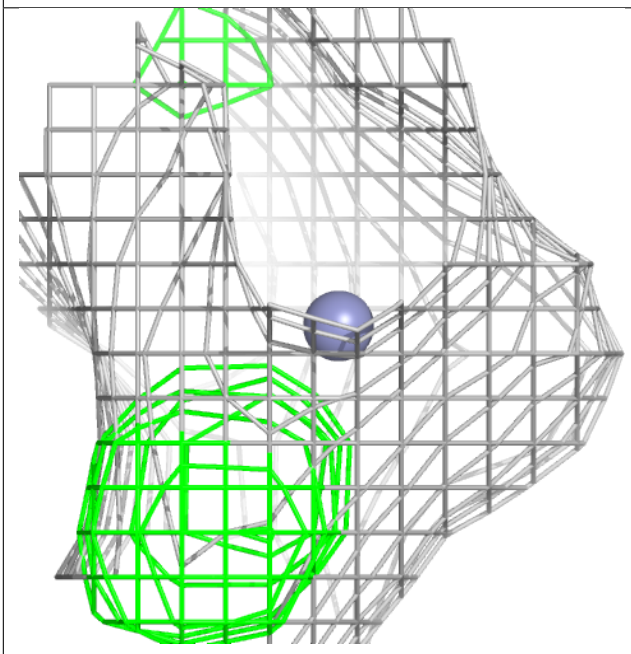
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PG0	A	504	8/8	0.58	0.16	83,89,102,106	0
3	SO4	E	504	5/5	0.58	0.12	104,109,122,142	0
4	PG0	D	504	5/8	0.58	0.24	92,98,99,100	0
3	SO4	C	505	5/5	0.64	0.08	121,121,140,171	0
3	SO4	B	502	5/5	0.66	0.16	113,121,150,170	0
4	PG0	B	503	8/8	0.68	0.17	61,82,84,84	0
4	PG0	A	503	8/8	0.70	0.18	74,87,92,95	0
4	PG0	B	504	5/8	0.74	0.13	75,90,97,101	0
4	PG0	E	505	5/8	0.76	0.12	96,100,110,110	0
3	SO4	A	502	5/5	0.77	0.08	88,89,93,121	0
3	SO4	D	503	5/5	0.84	0.08	68,76,79,106	0
3	SO4	D	502	5/5	0.85	0.08	80,81,92,112	0
3	SO4	B	501	5/5	0.88	0.07	68,75,84,92	0
2	ZN	E	502	1/1	0.91	0.11	85,85,85,85	1
2	ZN	D	501	1/1	0.91	0.07	71,71,71,71	0
3	SO4	C	503	5/5	0.93	0.06	84,85,91,91	0
2	ZN	C	501	1/1	0.94	0.09	75,75,75,75	0
2	ZN	E	503	1/1	0.94	0.12	82,82,82,82	1
2	ZN	C	502	1/1	0.97	0.05	73,73,73,73	1
2	ZN	A	501	1/1	0.97	0.05	59,59,59,59	0
2	ZN	E	501	1/1	0.97	0.05	74,74,74,74	0

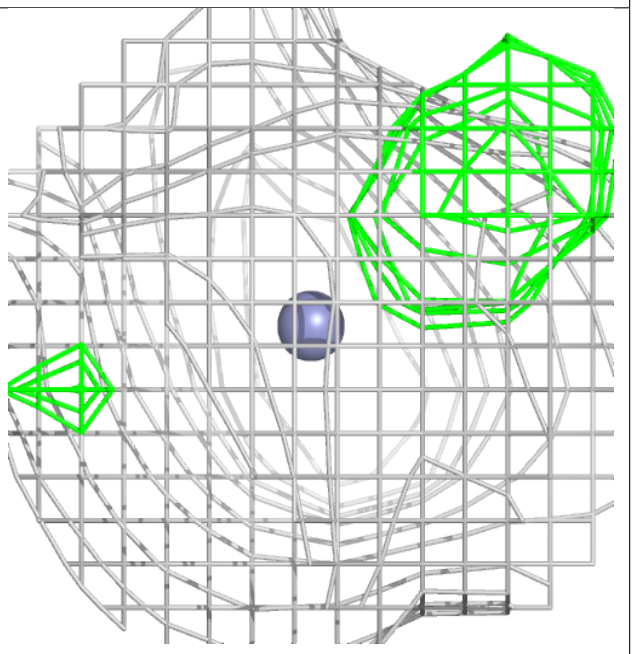
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN E 502:

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

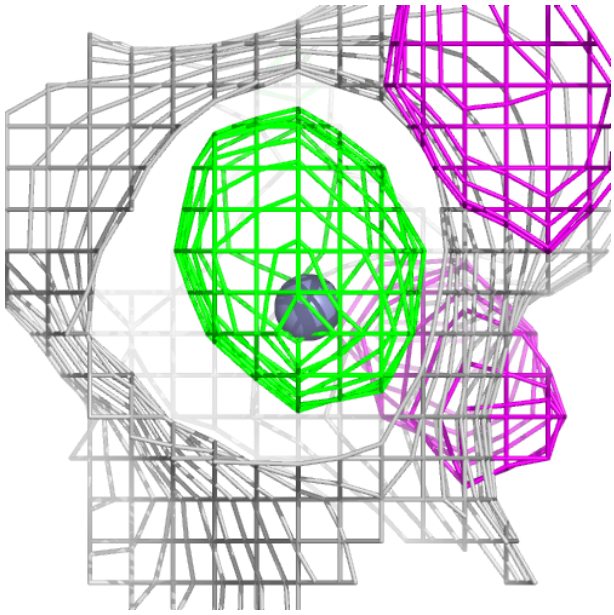


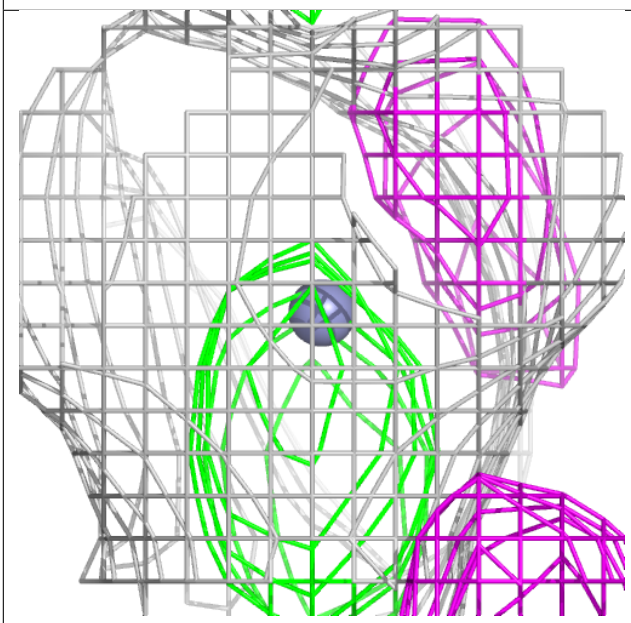


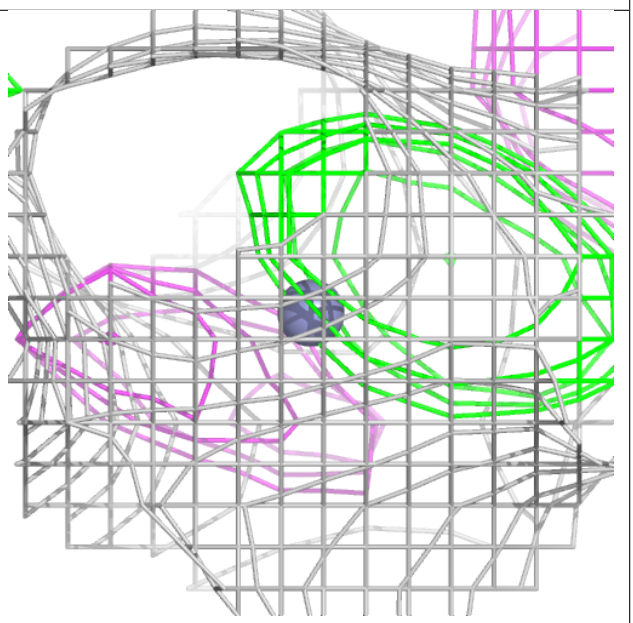


Electron density around ZN D 501:

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

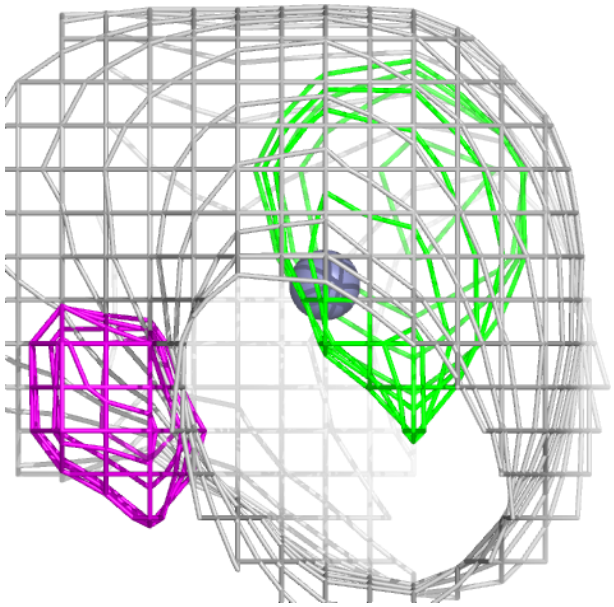


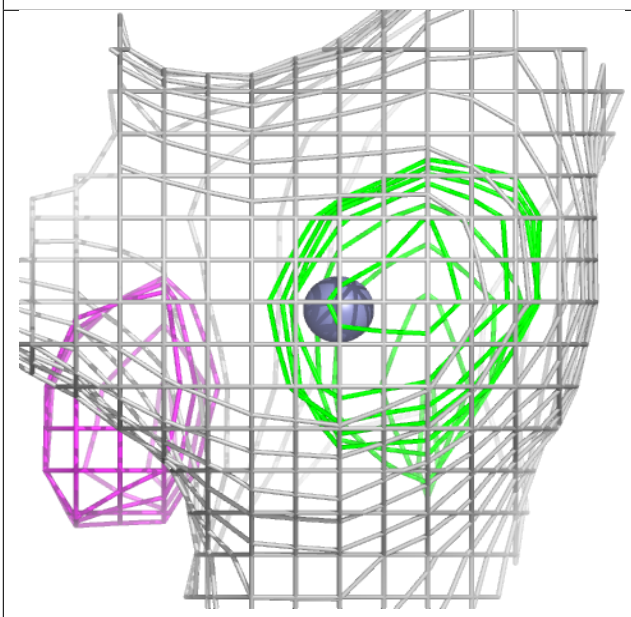


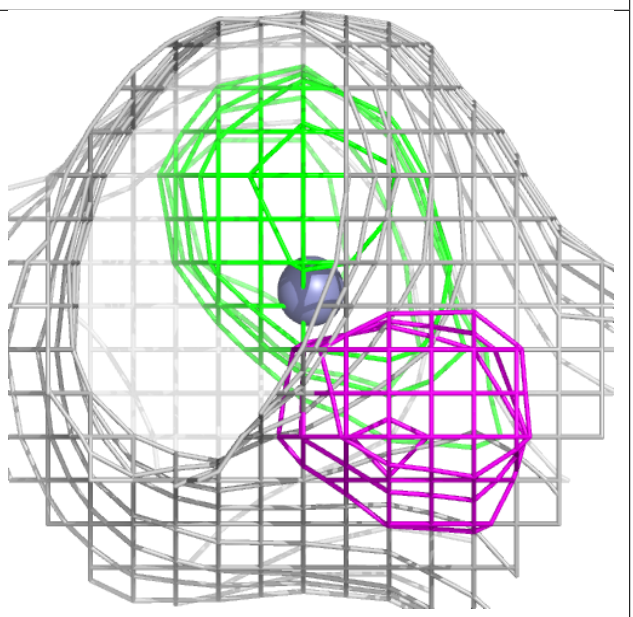


Electron density around ZN C 501:

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

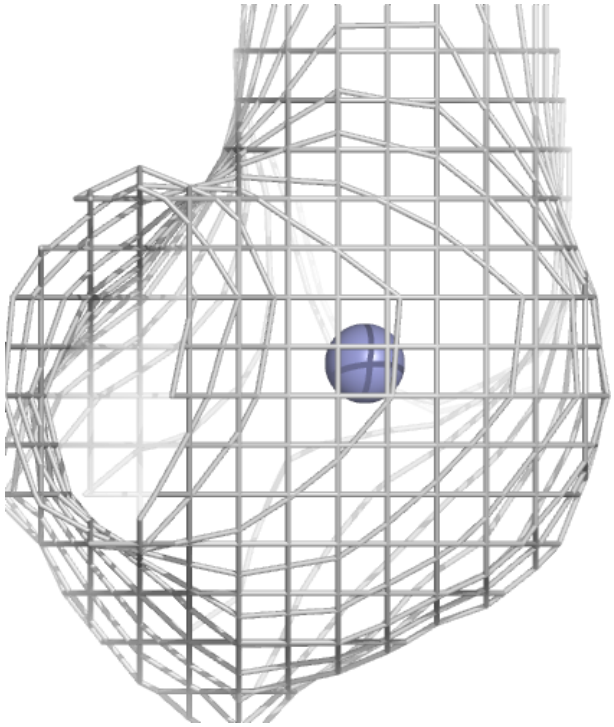


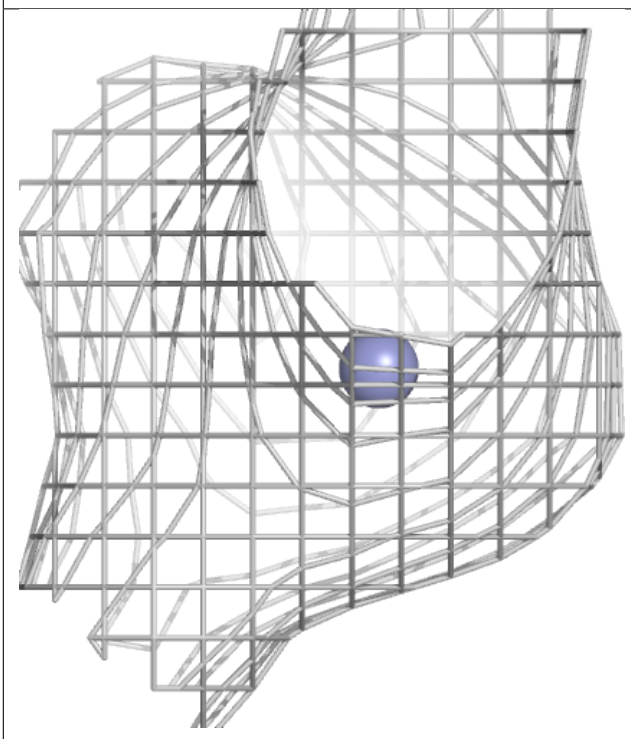


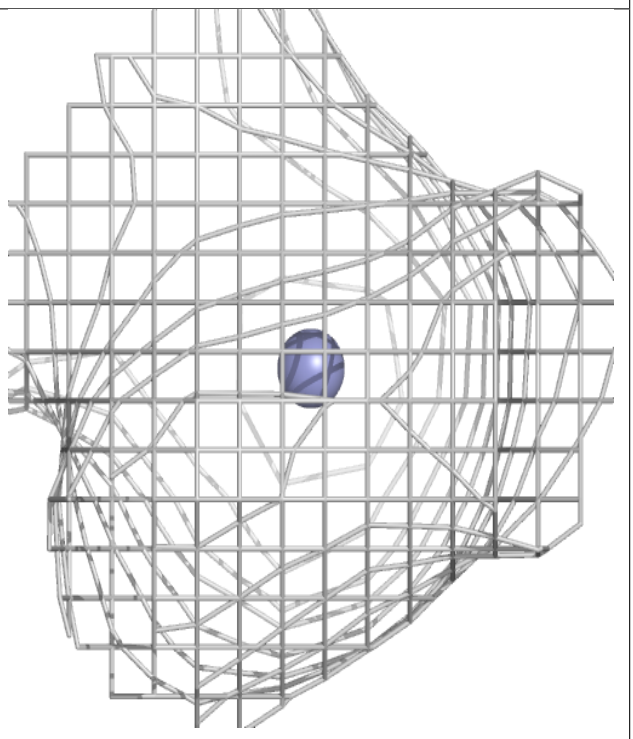


Electron density around ZN E 503:

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

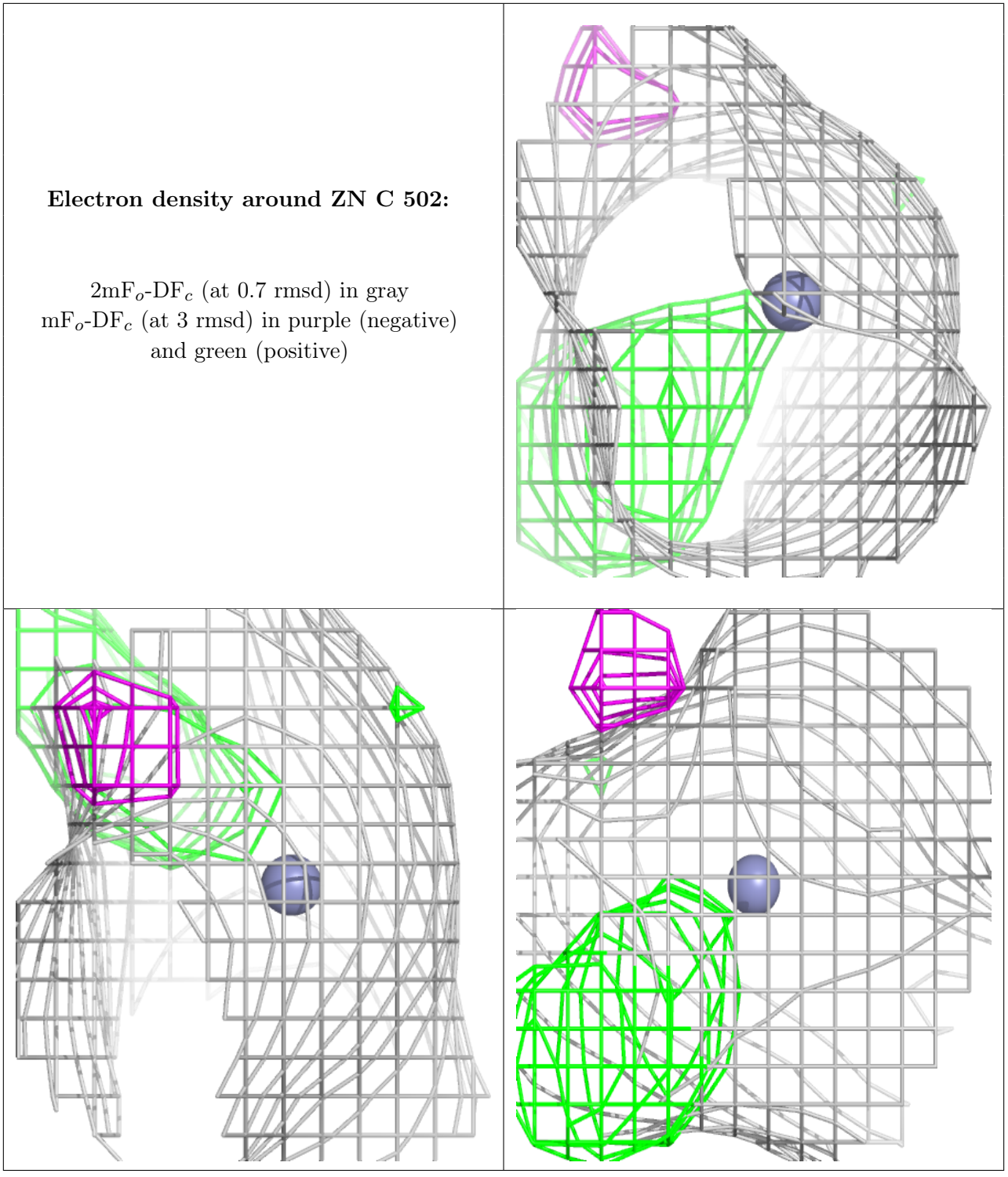






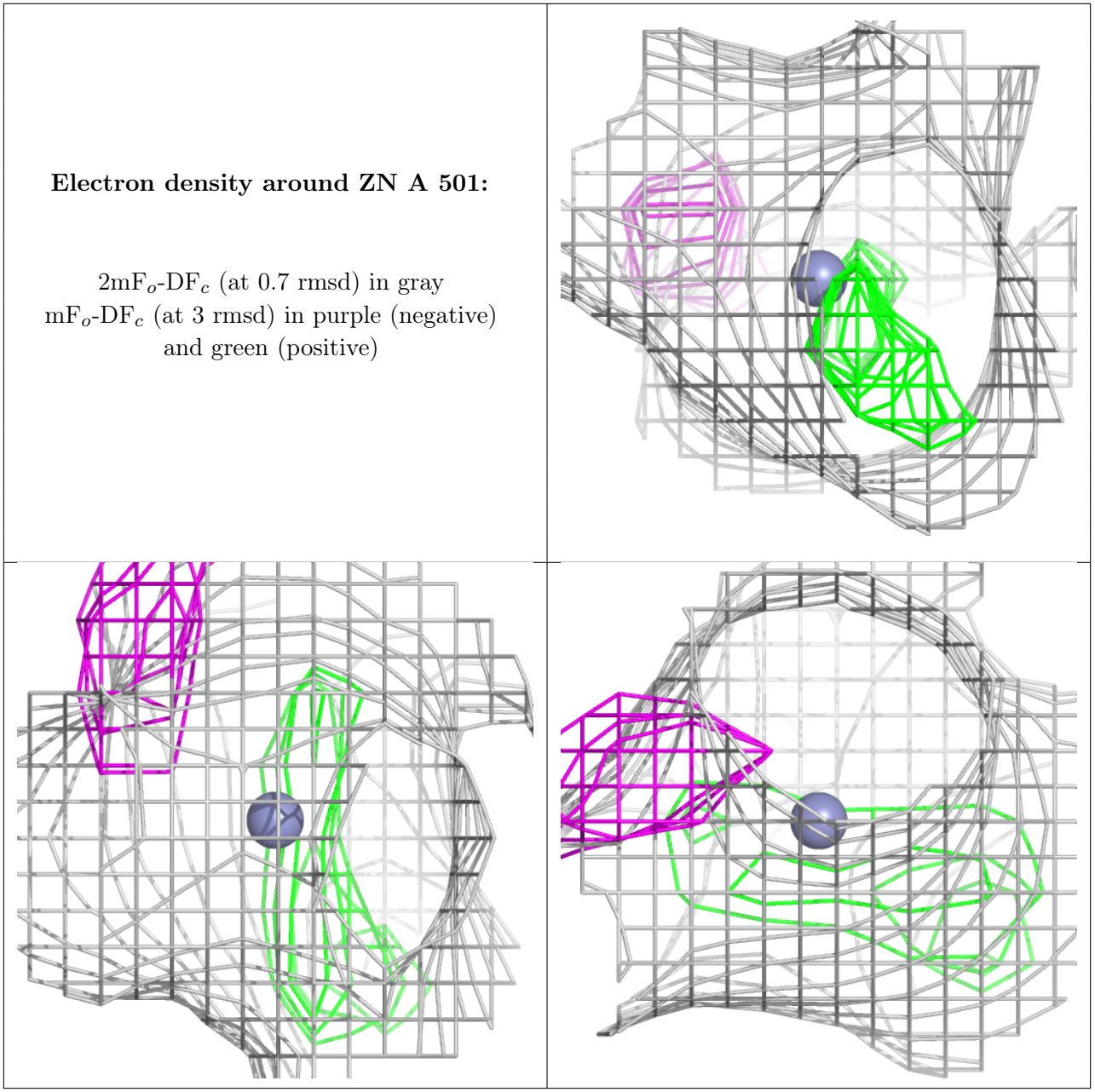
Electron density around ZN C 502:

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



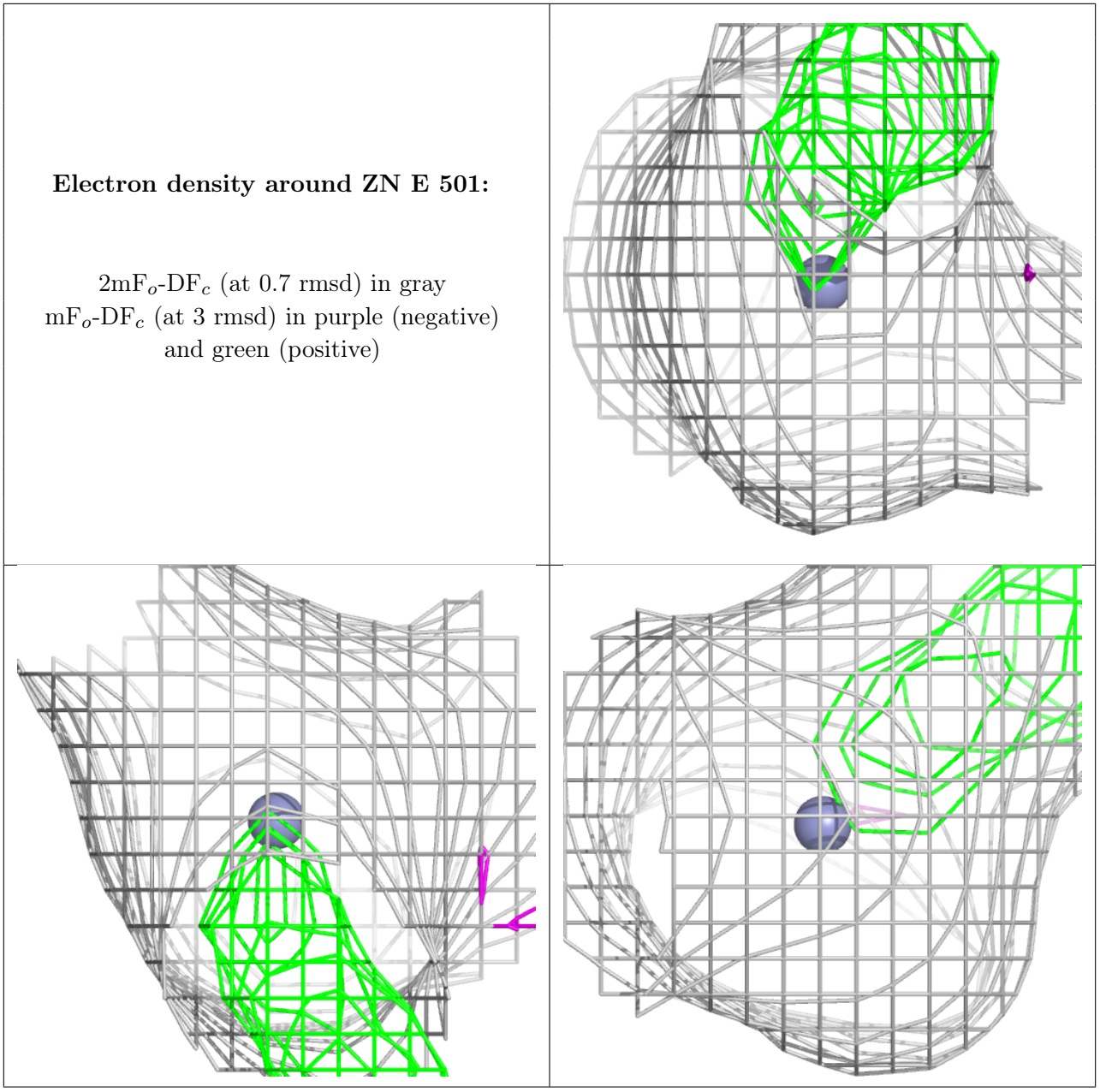
Electron density around ZN A 501:

$2mF_o$-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 E 501:

$2mF_o$-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.