wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 06:14 am GMT

PDB ID	:	6YI1
Title	:	Crystal structure of human glutaminyl cyclase in complex with Glu(gamma-hydrazide)-Phe-Ala
Authors	:	Kupski, O.; Sautner, V.; Tittmann, K.
Deposited on	:	2020-03-31
Resolution	:	1.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

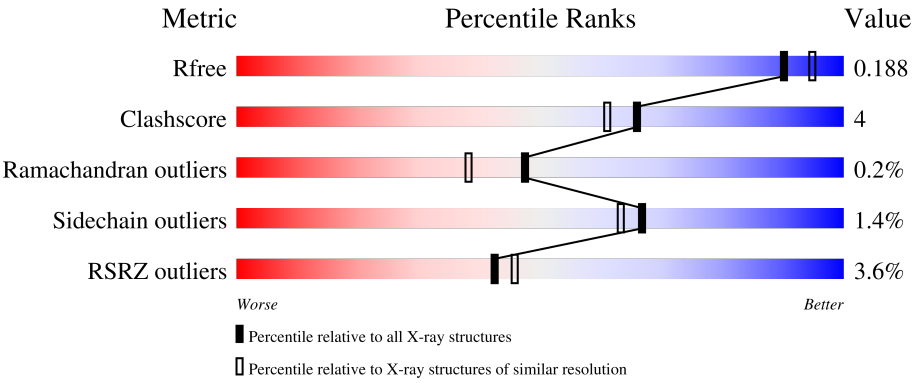
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.92 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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 <=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	329	3% 93% 7%
1	B	329	4% 91% 8%
2	C	4	75% 25%
2	D	4	50% 50%
2	E	4	75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	PEG	A	417	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 6178 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	6	0
			2699	1724	465	501	9			
1	B	329	Total	C	N	O	S	0	14	0
			2745	1752	479	505	9			

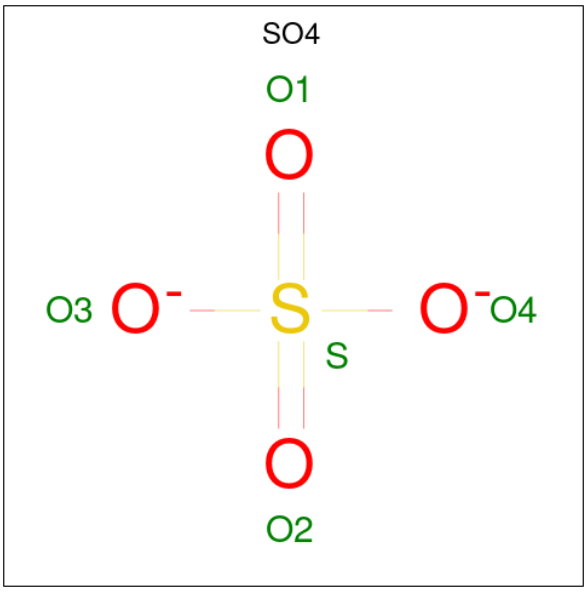
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	expression tag	UNP Q16769
A	34	PRO	-	expression tag	UNP Q16769
B	33	GLY	-	expression tag	UNP Q16769
B	34	PRO	-	expression tag	UNP Q16769

- Molecule 2 is a protein called Glu(gamma-hydrazide)-Phe-Ala.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	1
			27	17	6	4			
2	D	4	Total	C	N	O	0	0	1
			27	17	6	4			
2	E	4	Total	C	N	O	0	2	1
			33	20	8	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

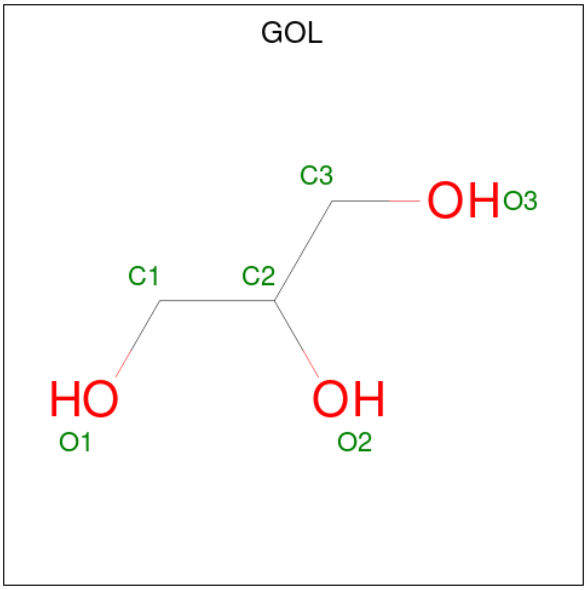


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0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

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

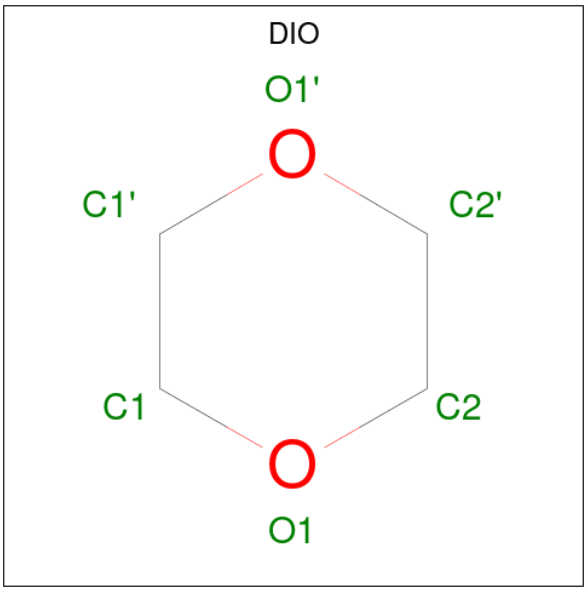
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Zn 5 5	0	0
4	B	5	Total Zn 5 5	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



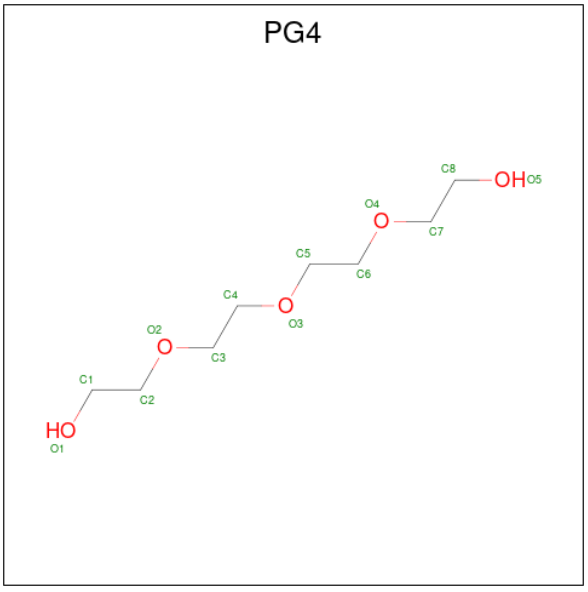
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	1
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



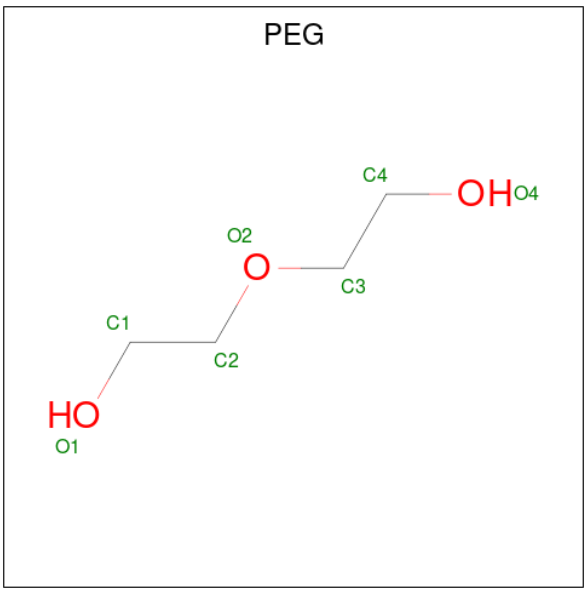
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 4 2	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



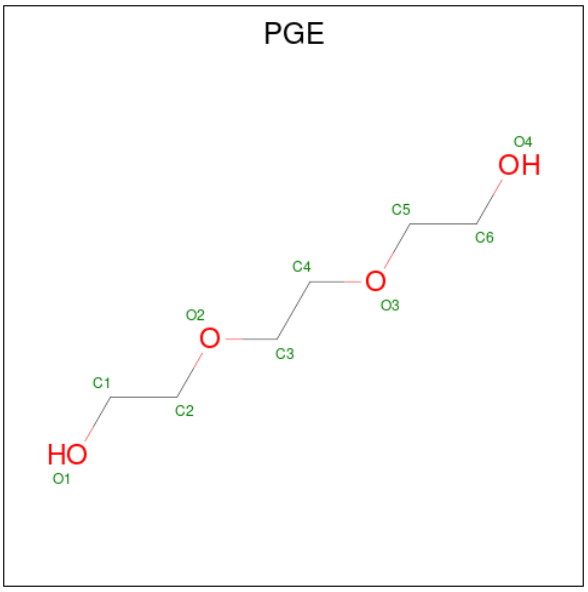
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



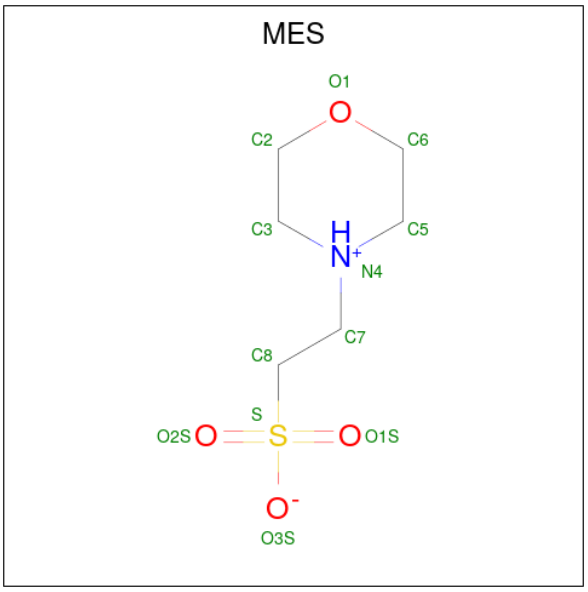
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 10 6 4	0	0
9	B	1	Total C O 10 6 4	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N O S 12 6 1 4 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is water.

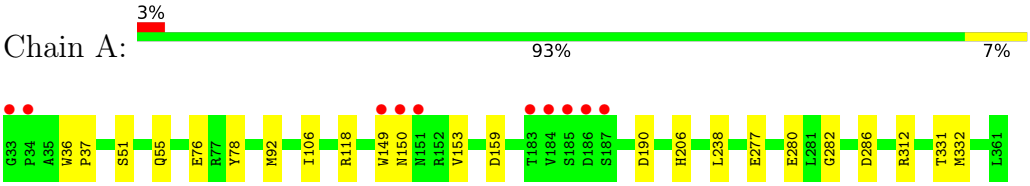
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	231	Total	O	0	3
			234	234		
11	B	192	Total	O	0	5
			194	194		

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.

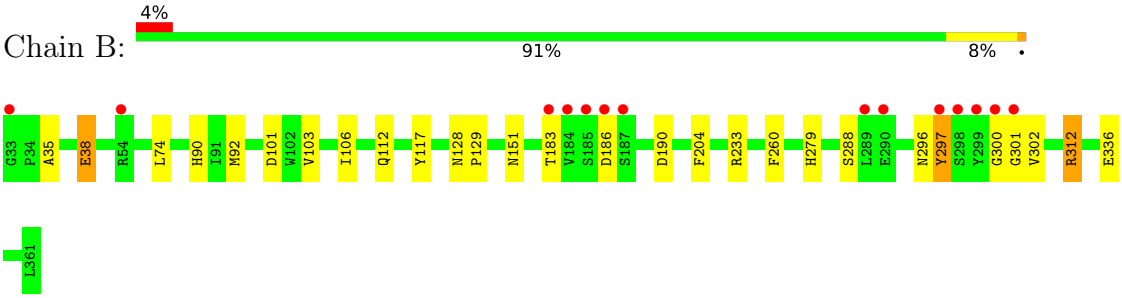
• Molecule 1: Glutaminyl-peptide cyclotransferase

Chain A:



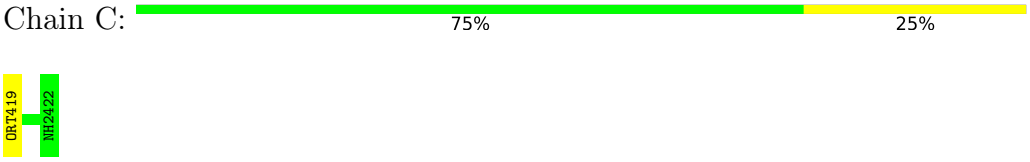
• Molecule 1: Glutaminyl-peptide cyclotransferase

Chain B:



• Molecule 2: Glu(gamma-hydrazide)-Phe-Ala

Chain C:



• Molecule 2: Glu(gamma-hydrazide)-Phe-Ala

Chain D:

• Molecule 2: Glu(gamma-hydrazide)-Phe-Ala

Chain E:


ORT422
NH2425

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	120.38Å 120.38Å 331.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	88.28 – 1.92 88.28 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.4 (88.28-1.92) 94.2 (88.28-1.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.92Å)	Xtriage
Refinement program	PHENIX dev_2940	Depositor
R, R_{free}	0.159 , 0.186 0.161 , 0.188	Depositor DCC
R_{free} test set	3497 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.6	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	0.97	EDS
Total number of atoms	6178	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: PEG, PGE, GOL, PG4, ORT, SO4, ZN, NH2, DIO, MES

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	0.49	0/2778	0.59	0/3782
1	B	2.40	2/2831 (0.1%)	1.31	6/3854 (0.2%)
2	C	0.48	0/16	0.51	0/20
2	D	0.40	0/16	0.43	0/20
2	E	0.65	0/20	0.45	0/24
All	All	1.73	2/5661 (0.0%)	1.02	6/7700 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297[A]	TYR	CB-CG	88.68	2.84	1.51
1	B	297[B]	TYR	CB-CG	88.68	2.84	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	297[A]	TYR	CA-CB-CG	-38.32	40.59	113.40
1	B	297[B]	TYR	CA-CB-CG	-38.32	40.59	113.40
1	B	297[A]	TYR	CB-CG-CD1	-25.41	105.75	121.00
1	B	297[B]	TYR	CB-CG-CD1	-25.41	105.75	121.00
1	B	297[A]	TYR	CB-CG-CD2	24.57	135.74	121.00

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	2699	0	2605	19	0
1	B	2745	0	2651	20	0
2	C	27	0	14	1	0
2	D	27	0	14	2	0
2	E	33	0	19	1	0
3	A	20	0	0	0	0
3	B	35	0	0	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	12	0	16	0	0
5	B	18	0	24	0	0
6	A	6	0	8	0	0
7	A	39	0	54	5	0
8	A	21	0	30	7	0
8	B	14	0	20	3	0
9	B	20	0	28	1	0
10	B	24	0	24	7	0
11	A	234	0	0	3	0
11	B	194	0	0	4	0
All	All	6178	0	5507	45	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 4.

The worst 5 of 45 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)
11:A:502:HOH:O	2:D:425:NH2:N	2.20	0.74
1:A:118:ARG:HH12	8:A:418:PEG:H22	1.61	0.65
1:B:183:THR:HG22	11:B:638:HOH:O	1.99	0.63
1:A:312:ARG:HA	7:A:415:PG4:H41	1.81	0.63
1:A:277:GLU:HA	7:A:413:PG4:H52	1.82	0.62

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	333/329 (101%)	324 (97%)	9 (3%)	0	100 100
1	B	341/329 (104%)	325 (95%)	14 (4%)	2 (1%)	25 14
2	C	2/4 (50%)	2 (100%)	0	0	100 100
2	D	2/4 (50%)	2 (100%)	0	0	100 100
2	E	3/4 (75%)	3 (100%)	0	0	100 100
All	All	681/670 (102%)	656 (96%)	23 (3%)	2 (0%)	47 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	302[A]	VAL
1	B	302[B]	VAL

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	296/290 (102%)	293 (99%)	3 (1%)	76 75
1	B	298/290 (103%)	292 (98%)	6 (2%)	55 49
2	C	1/1 (100%)	1 (100%)	0	100 100
2	D	1/1 (100%)	1 (100%)	0	100 100
2	E	1/1 (100%)	1 (100%)	0	100 100
All	All	597/583 (102%)	588 (98%)	9 (2%)	67 61

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	297[B]	TYR
1	B	312	ARG
1	B	38	GLU
1	B	186	ASP
1	B	204	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 10 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
8	PEG	A	417	-	6,6,6	0.40	0	5,5,5	0.92	0
3	SO4	B	407	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	A	401	-	4,4,4	0.15	0	6,6,6	0.11	0
6	DIO	A	412	-	6,6,6	0.58	0	6,6,6	0.27	0
3	SO4	A	407	-	4,4,4	0.15	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	B	421[A]	-	4,4,4	0.15	0	6,6,6	0.22	0
5	GOL	B	412[A]	-	5,5,5	0.97	0	5,5,5	1.35	0
3	SO4	B	409	4	4,4,4	0.27	0	6,6,6	0.19	0
5	GOL	A	411	-	5,5,5	1.25	1 (20%)	5,5,5	1.02	0
3	SO4	B	410	-	4,4,4	0.16	0	6,6,6	0.12	0
5	GOL	B	413	-	5,5,5	0.80	0	5,5,5	0.88	0
10	MES	B	420	-	12,12,12	2.24	1 (8%)	14,16,16	2.14	4 (28%)
3	SO4	A	409	-	4,4,4	0.24	0	6,6,6	0.30	0
3	SO4	B	418	-	4,4,4	0.11	0	6,6,6	0.26	0
7	PG4	A	414	-	12,12,12	0.64	0	11,11,11	0.42	0
3	SO4	A	408	-	4,4,4	0.12	0	6,6,6	0.13	0
7	PG4	A	415	-	12,12,12	0.48	0	11,11,11	0.53	0
8	PEG	B	417	-	6,6,6	0.56	0	5,5,5	0.48	0
8	PEG	A	418	-	6,6,6	0.51	0	5,5,5	0.67	0
9	PGE	B	414	-	9,9,9	0.39	0	8,8,8	0.60	0
3	SO4	B	401	-	4,4,4	0.16	0	6,6,6	0.37	0
3	SO4	B	408	-	4,4,4	0.14	0	6,6,6	0.15	0
8	PEG	B	416	-	6,6,6	0.64	0	5,5,5	0.73	0
7	PG4	A	413	-	12,12,12	0.58	0	11,11,11	0.83	0
5	GOL	B	411	-	5,5,5	0.71	0	5,5,5	1.30	0
8	PEG	A	416	-	6,6,6	0.65	0	5,5,5	0.94	0
10	MES	B	419	-	12,12,12	2.27	1 (8%)	14,16,16	2.07	3 (21%)
5	GOL	A	410	-	5,5,5	1.02	0	5,5,5	0.74	0
9	PGE	B	415	-	9,9,9	0.48	0	8,8,8	0.58	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
7	PG4	A	415	-	-	0/10/10/10	-
8	PEG	A	417	-	-	0/4/4/4	-
5	GOL	A	411	-	-	0/4/4/4	-
5	GOL	B	413	-	-	0/4/4/4	-
5	GOL	B	411	-	-	2/4/4/4	-
7	PG4	A	413	-	-	2/10/10/10	-
8	PEG	B	417	-	-	0/4/4/4	-
7	PG4	A	414	-	-	1/10/10/10	-
8	PEG	A	416	-	-	0/4/4/4	-
10	MES	B	420	-	-	4/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DIO	A	412	-	-	-	0/1/1/1
10	MES	B	419	-	-	4/6/14/14	0/1/1/1
8	PEG	A	418	-	-	0/4/4/4	-
9	PGE	B	414	-	-	0/7/7/7	-
5	GOL	A	410	-	-	0/4/4/4	-
9	PGE	B	415	-	-	0/7/7/7	-
8	PEG	B	416	-	-	1/4/4/4	-
5	GOL	B	412[A]	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	419	MES	C8-S	-7.60	1.66	1.77
10	B	420	MES	C8-S	-7.55	1.66	1.77
5	A	411	GOL	C1-C2	2.03	1.60	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	420	MES	C5-N4-C3	5.95	122.22	108.83
10	B	419	MES	C5-N4-C3	4.51	118.98	108.83
10	B	419	MES	O1S-S-C8	4.18	111.94	106.92
10	B	420	MES	C7-N4-C3	2.59	117.85	111.23
10	B	420	MES	O3S-S-C8	2.41	109.67	105.77

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	411	GOL	C1-C2-C3-O3
5	B	411	GOL	O2-C2-C3-O3
5	B	412[A]	GOL	C1-C2-C3-O3
5	B	412[A]	GOL	O2-C2-C3-O3
10	B	419	MES	N4-C7-C8-S

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	417	PEG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	421[A]	SO4	1	0
10	B	420	MES	4	0
3	B	418	SO4	1	0
7	A	414	PG4	1	0
7	A	415	PG4	1	0
8	B	417	PEG	2	0
8	A	418	PEG	3	0
8	B	416	PEG	1	0
7	A	413	PG4	3	0
10	B	419	MES	3	0
9	B	415	PGE	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	329/329 (100%)	-0.30	10 (3%) 50 53	16, 23, 47, 102	0
1	B	329/329 (100%)	-0.22	14 (4%) 35 38	17, 27, 56, 95	1 (0%)
2	C	2/4 (50%)	0.12	0 100 100	20, 20, 20, 22	0
2	D	2/4 (50%)	1.40	0 100 100	55, 55, 55, 59	0
2	E	2/4 (50%)	0.29	0 100 100	26, 26, 26, 28	0
All	All	664/670 (99%)	-0.25	24 (3%) 42 46	16, 25, 55, 102	1 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299[A]	TYR	8.6
1	B	186	ASP	6.5
1	A	184	VAL	6.1
1	A	186	ASP	5.9
1	A	149	TRP	5.7

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 monosaccharides 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, 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.

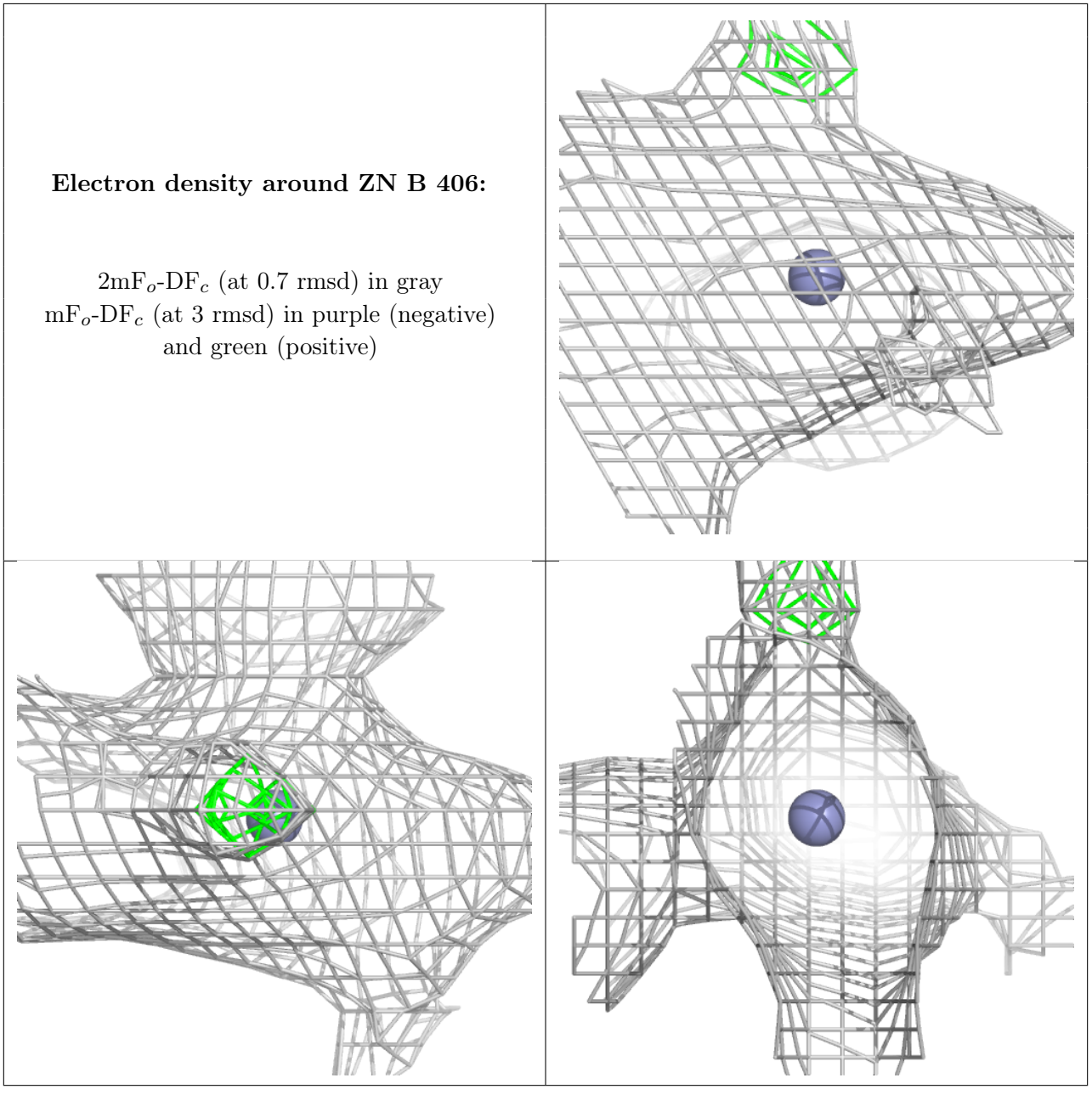
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	413	6/6	0.76	0.17	52,55,57,59	0
8	PEG	A	418	7/7	0.77	0.21	51,59,64,67	0
8	PEG	A	417	7/7	0.79	0.18	59,59,62,62	0
3	SO4	B	418	5/5	0.79	0.20	80,82,82,85	0
8	PEG	B	416	7/7	0.79	0.30	54,57,58,58	0
9	PGE	B	415	10/10	0.79	0.28	46,58,61,63	0
8	PEG	B	417	7/7	0.80	0.26	58,58,60,60	0
10	MES	B	419	12/12	0.81	0.22	52,58,73,74	0
3	SO4	B	421[A]	5/5	0.82	0.19	36,41,43,46	5
5	GOL	B	412[A]	6/6	0.83	0.27	24,25,27,28	6
3	SO4	A	409	5/5	0.87	0.16	61,61,70,70	0
5	GOL	A	411	6/6	0.87	0.13	24,38,39,40	0
7	PG4	A	413	13/13	0.88	0.12	43,49,53,53	0
9	PGE	B	414	10/10	0.88	0.18	41,43,50,55	0
7	PG4	A	414	13/13	0.89	0.17	41,46,55,60	0
7	PG4	A	415	13/13	0.90	0.22	47,50,59,60	0
3	SO4	B	410	5/5	0.90	0.17	79,80,81,82	5
8	PEG	A	416	7/7	0.91	0.14	43,46,49,50	0
10	MES	B	420	12/12	0.91	0.30	68,81,89,90	0
3	SO4	A	408	5/5	0.92	0.20	76,76,79,79	0
3	SO4	B	407	5/5	0.92	0.17	93,94,95,95	0
6	DIO	A	412	6/6	0.93	0.15	44,45,45,45	0
5	GOL	B	411	6/6	0.94	0.10	25,34,36,36	0
4	ZN	B	406	1/1	0.94	0.11	48,48,48,48	1
3	SO4	B	408	5/5	0.95	0.10	68,70,72,72	0
5	GOL	A	410	6/6	0.97	0.10	40,42,42,43	0
3	SO4	A	401	5/5	0.97	0.11	65,65,66,66	5
4	ZN	A	406	1/1	0.98	0.05	26,26,26,26	1
3	SO4	B	401	5/5	0.98	0.07	32,32,33,33	5
3	SO4	A	407	5/5	0.98	0.13	40,42,49,50	5
4	ZN	A	405	1/1	0.98	0.04	32,32,32,32	0
4	ZN	A	404	1/1	0.99	0.03	26,26,26,26	1
4	ZN	B	404	1/1	0.99	0.09	24,24,24,24	1
3	SO4	B	409	5/5	0.99	0.09	28,28,29,30	0
4	ZN	B	405	1/1	1.00	0.09	21,21,21,21	1
4	ZN	A	402	1/1	1.00	0.08	18,18,18,18	0
4	ZN	B	402	1/1	1.00	0.09	20,20,20,20	0
4	ZN	B	403	1/1	1.00	0.06	21,21,21,21	0
4	ZN	A	403	1/1	1.00	0.07	20,20,20,20	1

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.

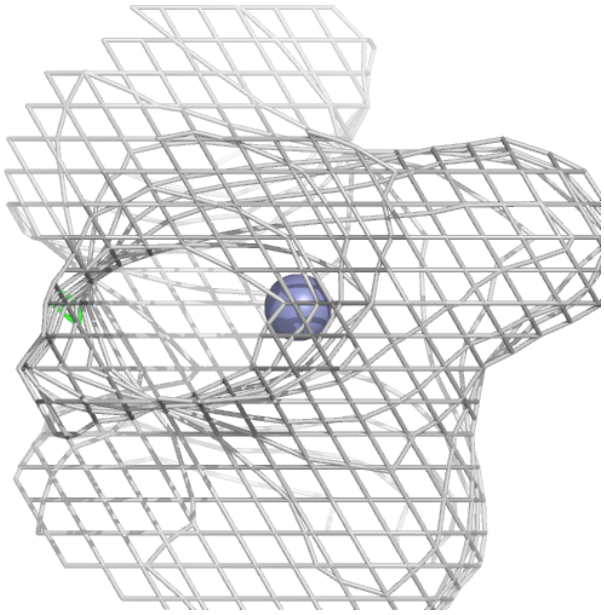
Electron density around ZN B 406:

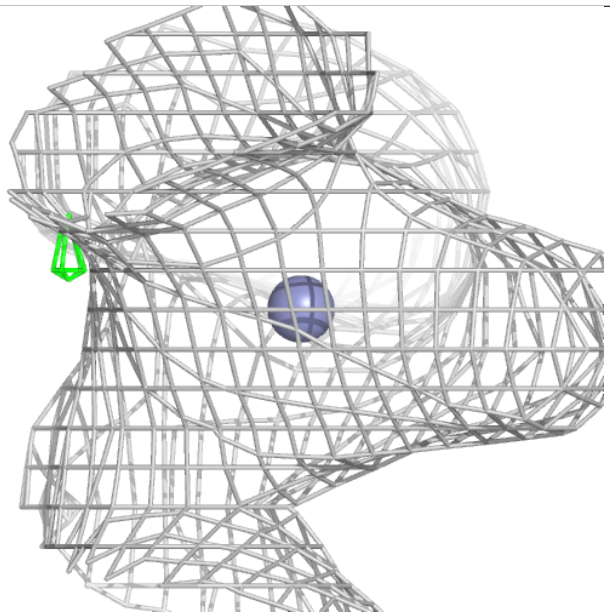
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

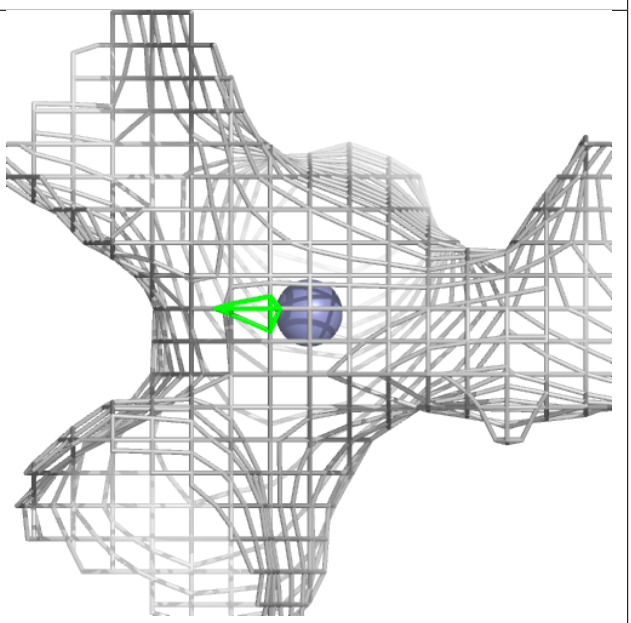


Electron density around ZN A 406:

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

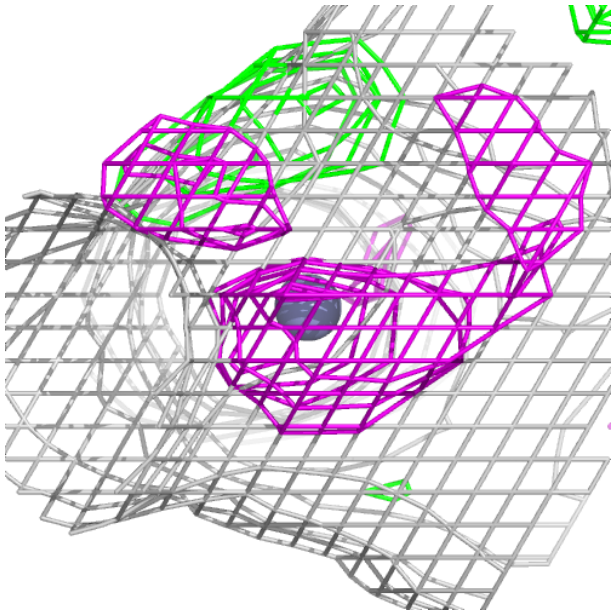


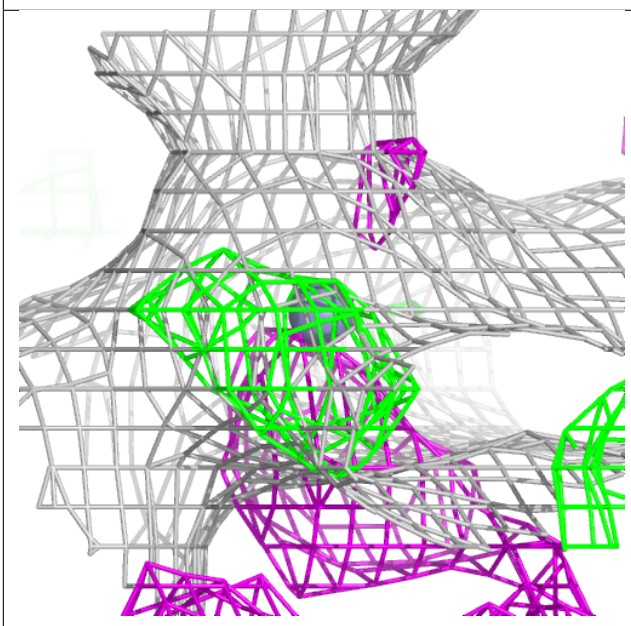


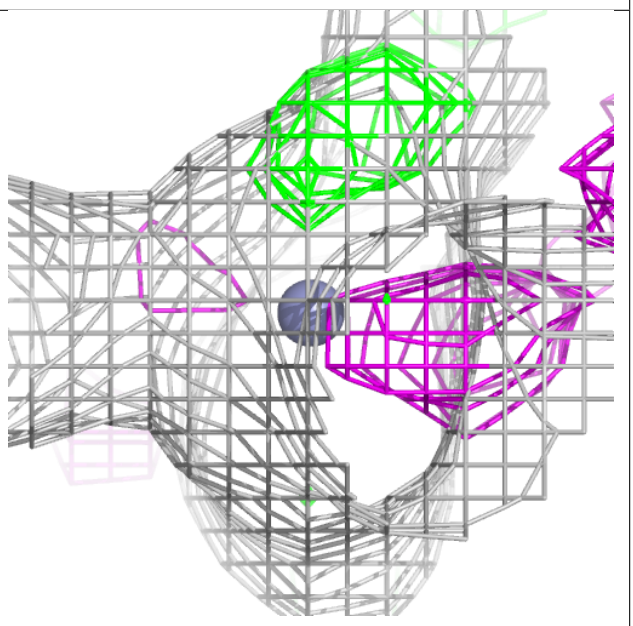


Electron density around ZN A 405:

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

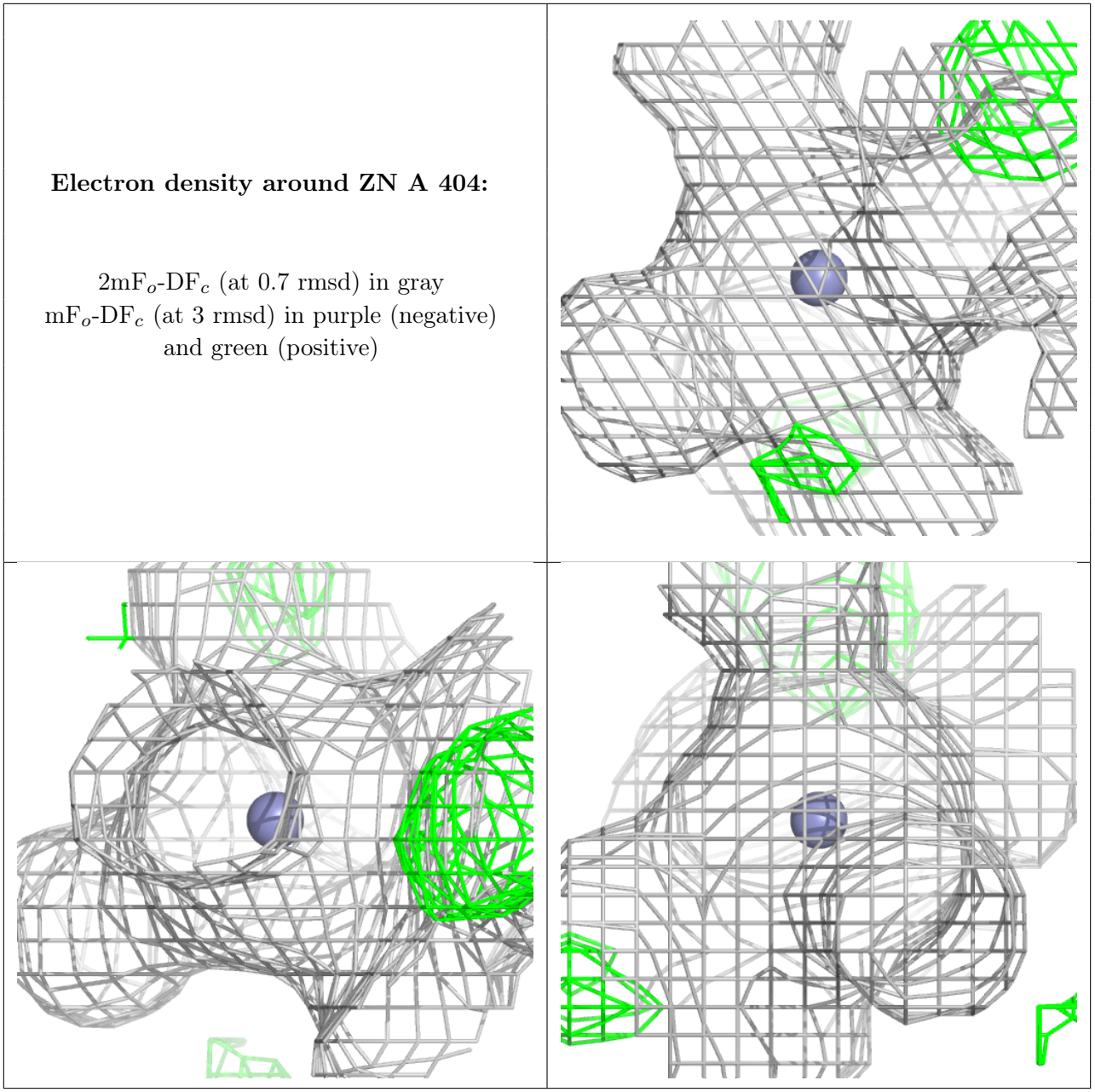






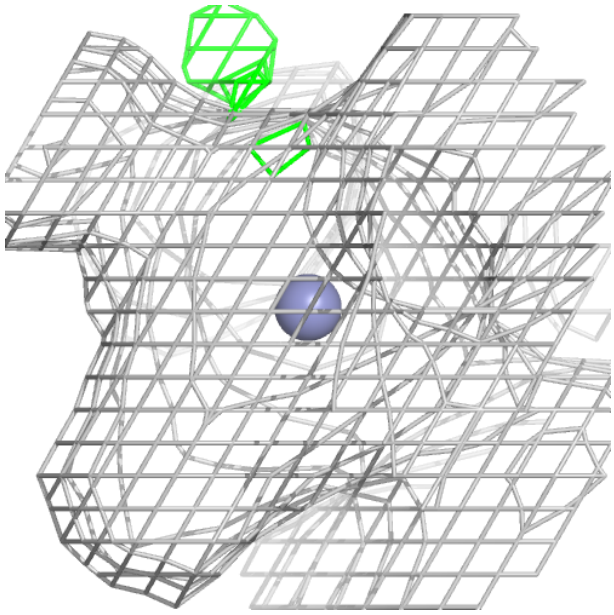
Electron density around ZN A 404:

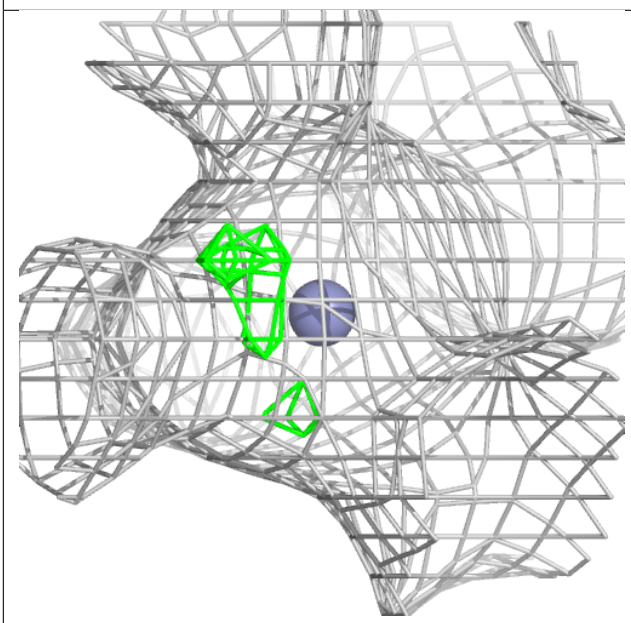
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

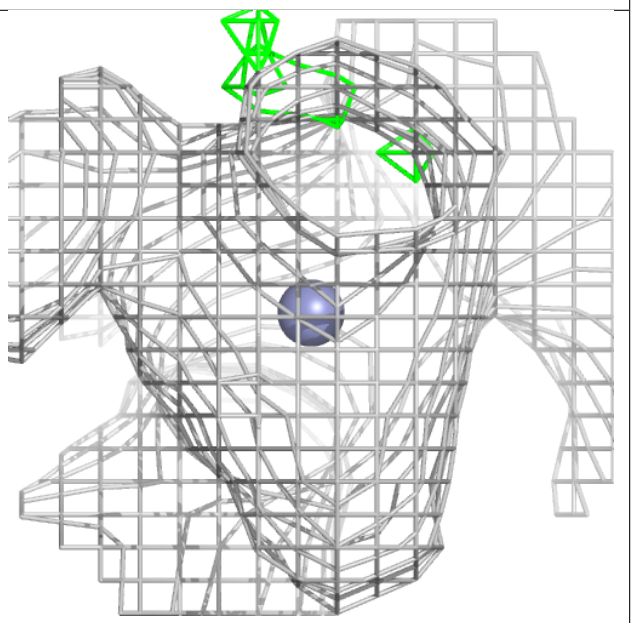


Electron density around ZN B 404:

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

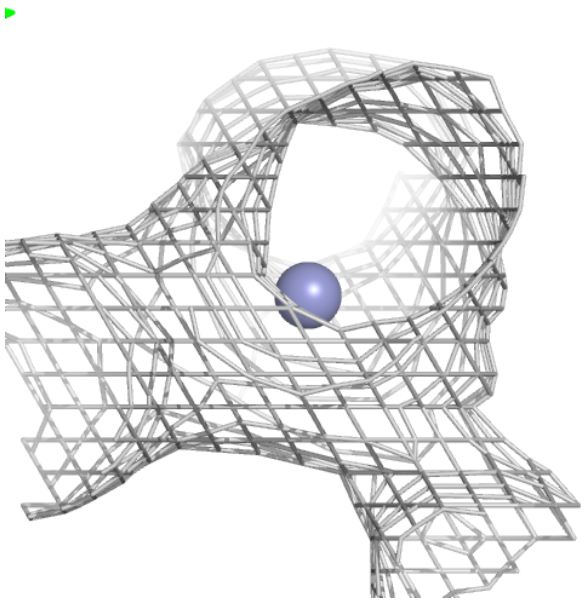


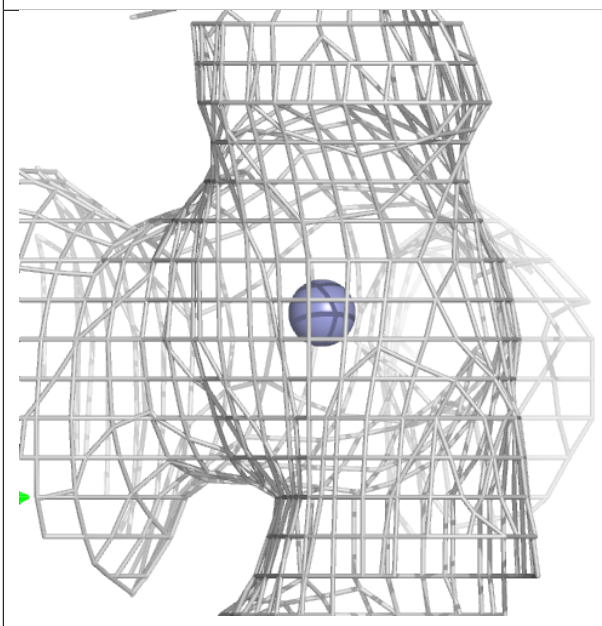


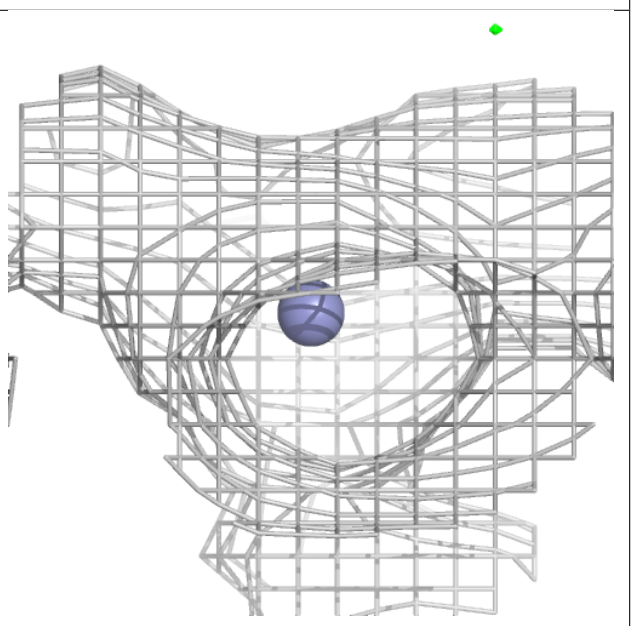


Electron density around ZN B 405:

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

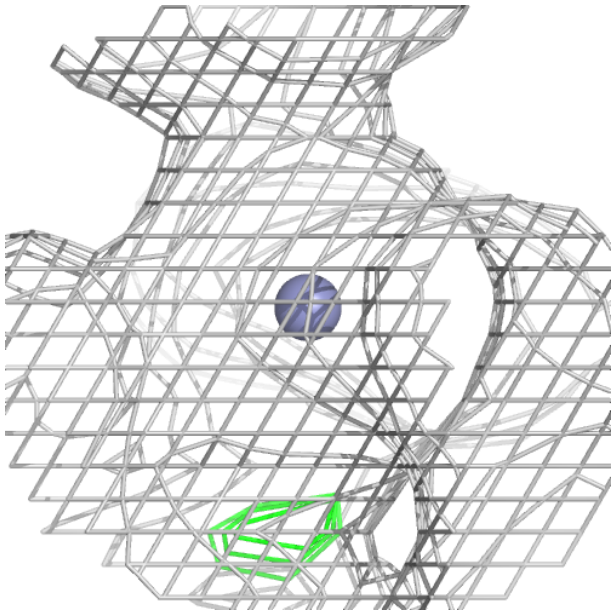


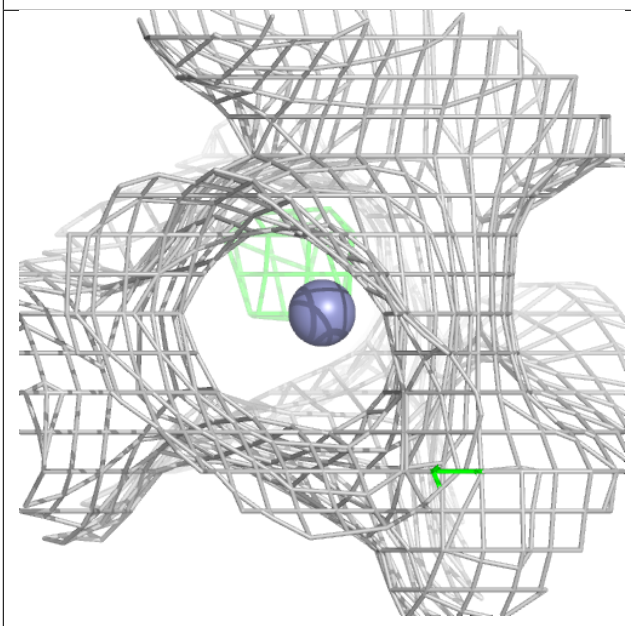


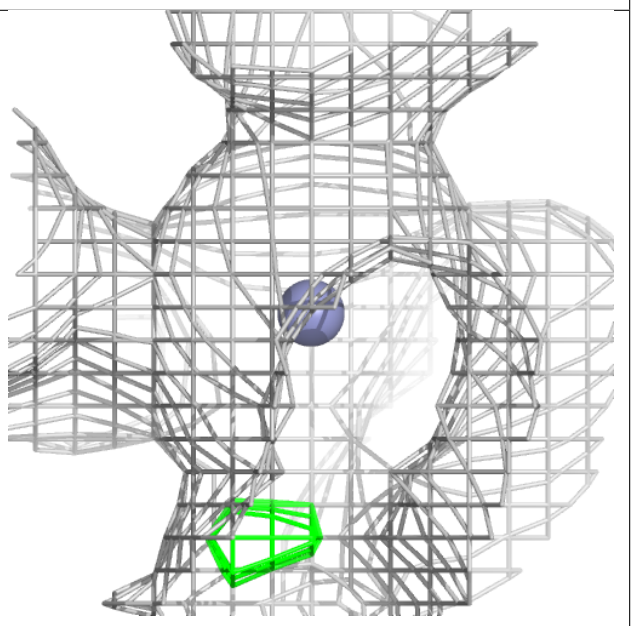


Electron density around ZN A 402:

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

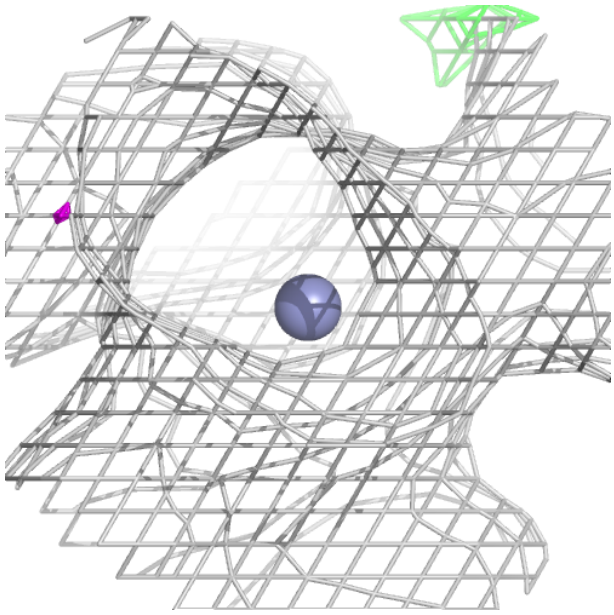


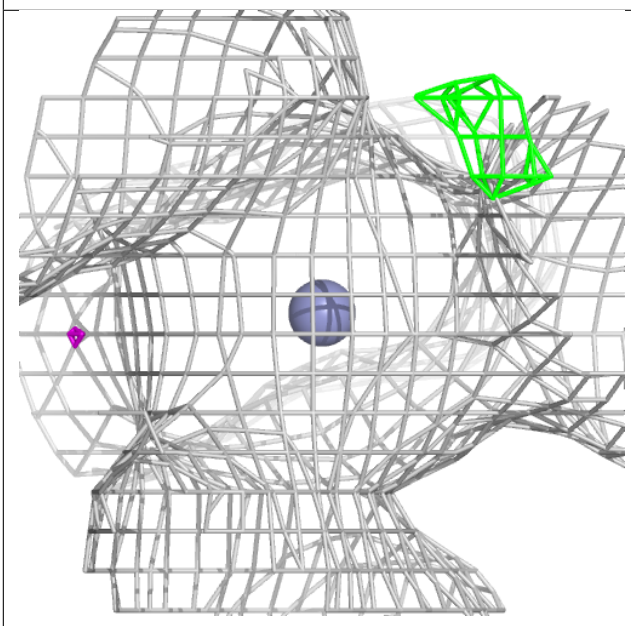


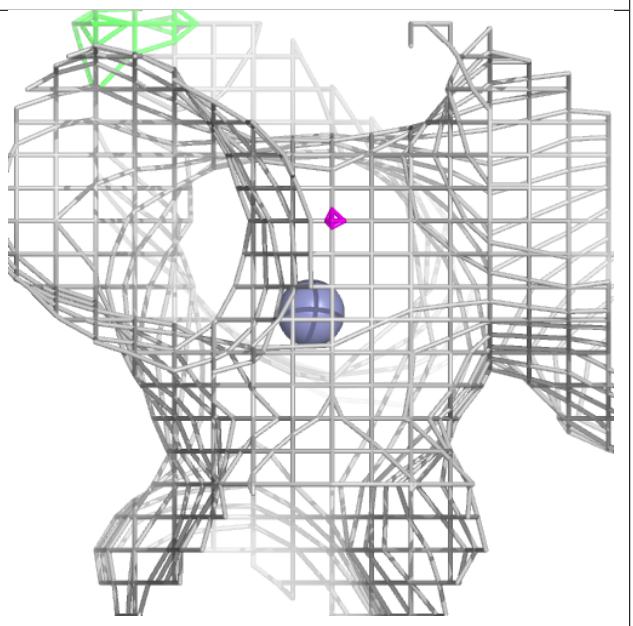


Electron density around ZN B 402:

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

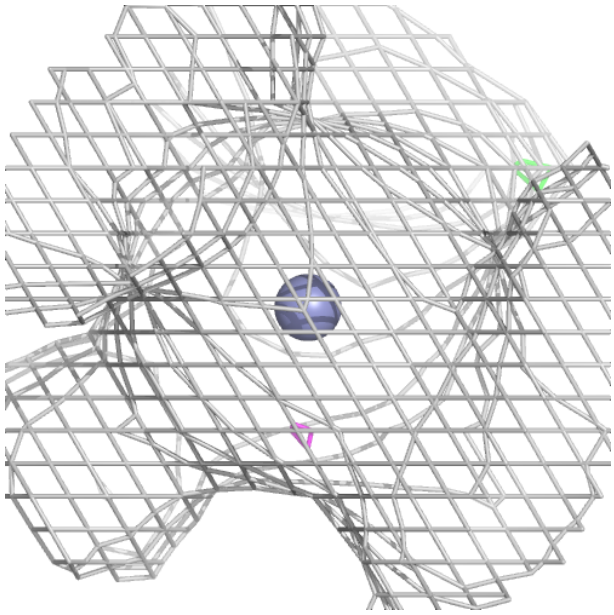


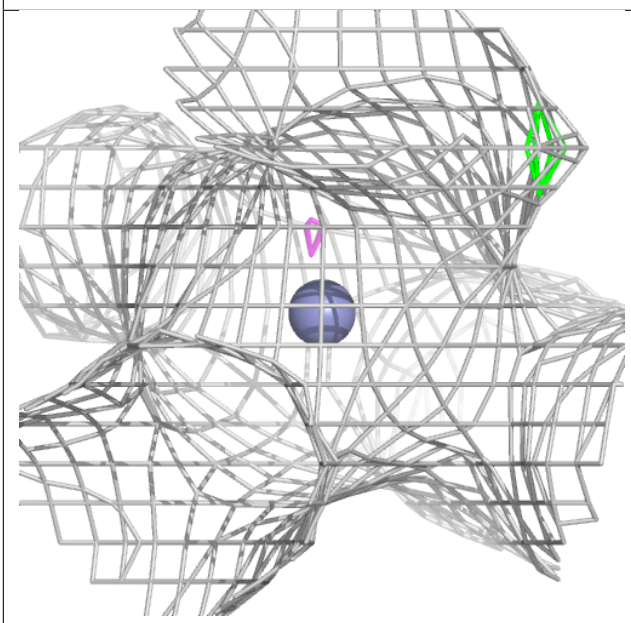


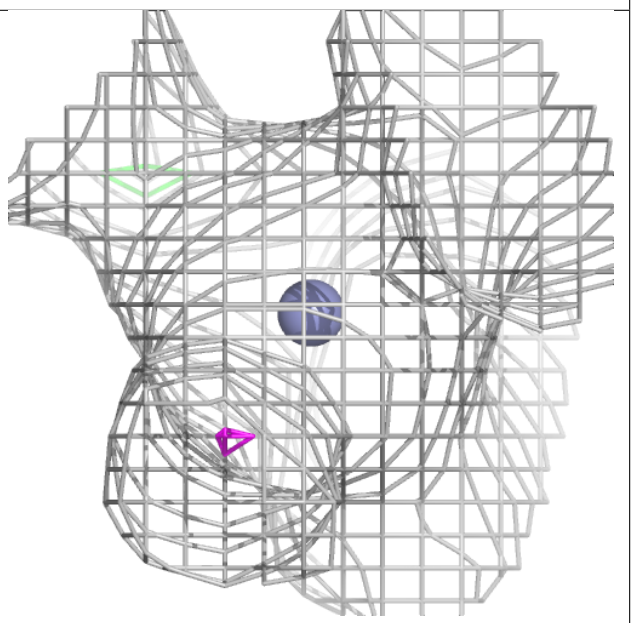


Electron density around ZN B 403:

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

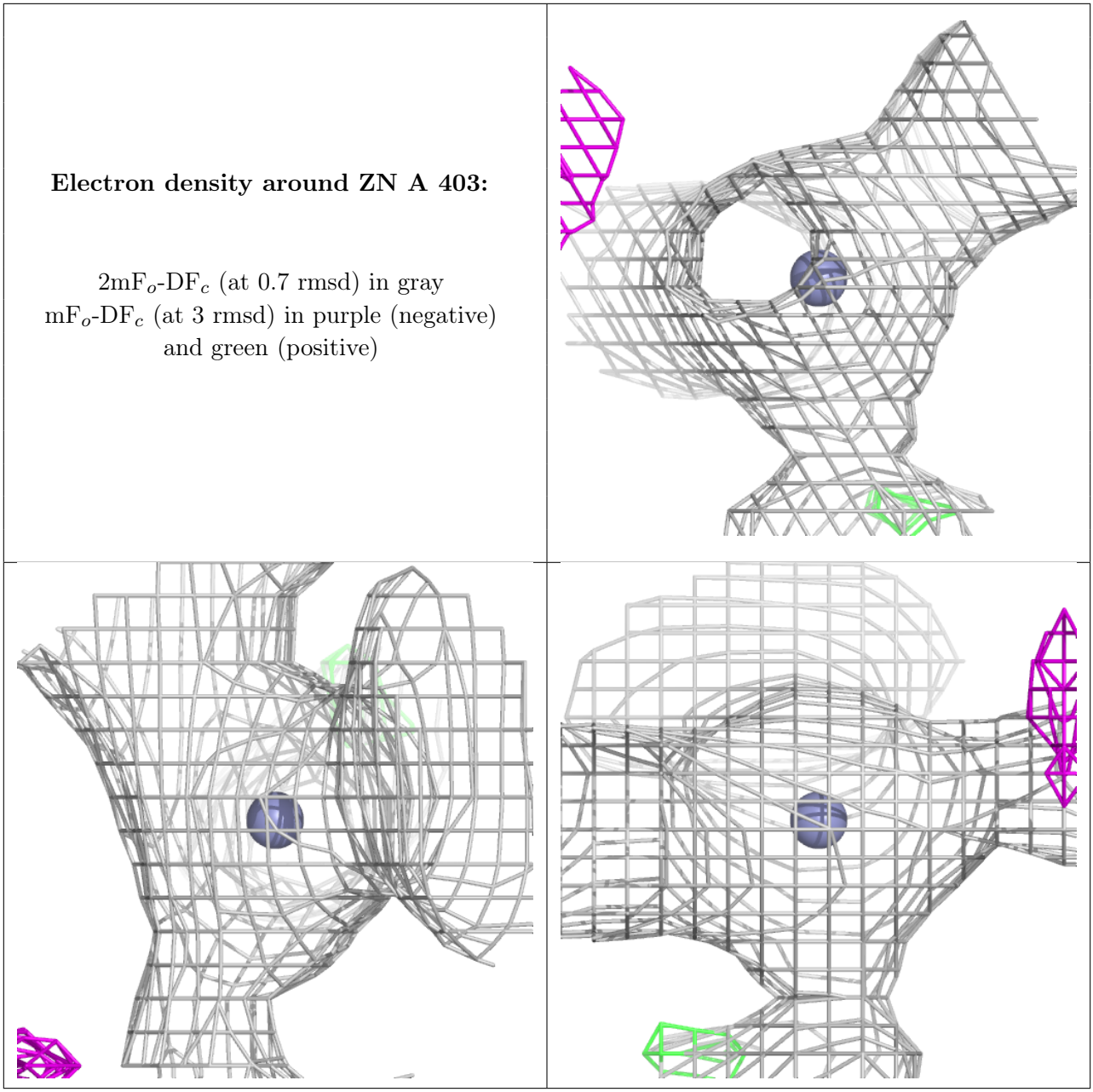






Electron density around ZN A 403:

$2mF_o$-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.