



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 12:55 pm GMT

PDB ID : 8C0H
Title : Crystal structure of guanidinase from Nitrospira inopinata
Authors : Puehringer, D.
Deposited on : 2022-12-16
Resolution : 1.58 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 : 4.02b-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

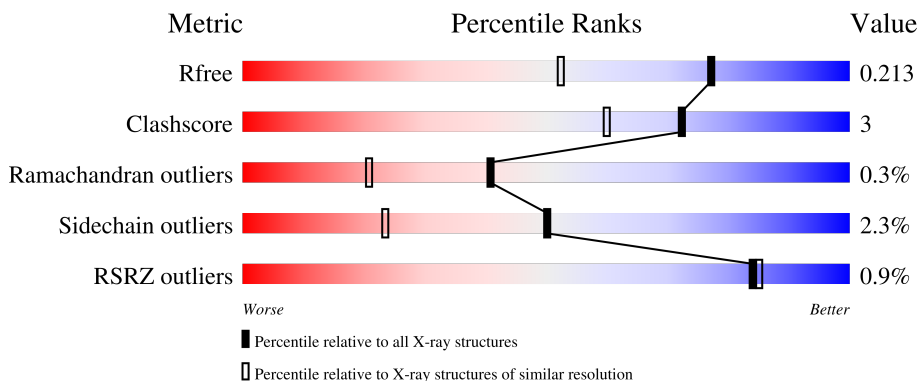
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	384	90% 7% ..
1	B	384	87% 10% ..
1	C	384	90% 7% ..
1	D	384	91% 5% ..
1	E	384	90% 7% ..

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Mol	Chain	Length	Quality of chain	
1	F	384		90% 7% ..
1	G	384		89% 8% ..
1	H	384		88% 9% ..
1	I	384		89% 8% ..
1	J	384		89% 8% ..
1	K	384		89% 8% ..
1	L	384		89% 7% ..

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
2	NI	B	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 71341 atoms, of which 33940 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 Putative agmatinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	374	5703	1826	2831	495	539	12	0	4	0
1	B	374	5701	1826	2829	495	539	12	0	4	0
1	C	374	5717	1829	2839	498	539	12	0	5	0
1	D	373	5664	1815	2810	492	535	12	0	2	0
1	E	374	5700	1826	2828	495	539	12	0	4	0
1	F	374	5701	1826	2829	495	539	12	0	3	0
1	G	377	5720	1830	2844	496	537	13	0	0	0
1	H	374	5702	1826	2830	495	539	12	0	4	0
1	I	375	5736	1835	2849	498	542	12	0	5	0
1	J	374	5669	1816	2815	492	534	12	0	0	0
1	K	373	5646	1810	2801	490	533	12	0	0	0
1	L	374	5713	1829	2835	496	541	12	0	5	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0S4KUT0
A	0	PRO	-	expression tag	UNP A0A0S4KUT0
B	-1	GLY	-	expression tag	UNP A0A0S4KUT0
B	0	PRO	-	expression tag	UNP A0A0S4KUT0
C	-1	GLY	-	expression tag	UNP A0A0S4KUT0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	PRO	-	expression tag	UNP A0A0S4KUT0
D	-1	GLY	-	expression tag	UNP A0A0S4KUT0
D	0	PRO	-	expression tag	UNP A0A0S4KUT0
E	-1	GLY	-	expression tag	UNP A0A0S4KUT0
E	0	PRO	-	expression tag	UNP A0A0S4KUT0
F	-1	GLY	-	expression tag	UNP A0A0S4KUT0
F	0	PRO	-	expression tag	UNP A0A0S4KUT0
G	-1	GLY	-	expression tag	UNP A0A0S4KUT0
G	0	PRO	-	expression tag	UNP A0A0S4KUT0
H	-1	GLY	-	expression tag	UNP A0A0S4KUT0
H	0	PRO	-	expression tag	UNP A0A0S4KUT0
I	-1	GLY	-	expression tag	UNP A0A0S4KUT0
I	0	PRO	-	expression tag	UNP A0A0S4KUT0
J	-1	GLY	-	expression tag	UNP A0A0S4KUT0
J	0	PRO	-	expression tag	UNP A0A0S4KUT0
K	-1	GLY	-	expression tag	UNP A0A0S4KUT0
K	0	PRO	-	expression tag	UNP A0A0S4KUT0
L	-1	GLY	-	expression tag	UNP A0A0S4KUT0
L	0	PRO	-	expression tag	UNP A0A0S4KUT0

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

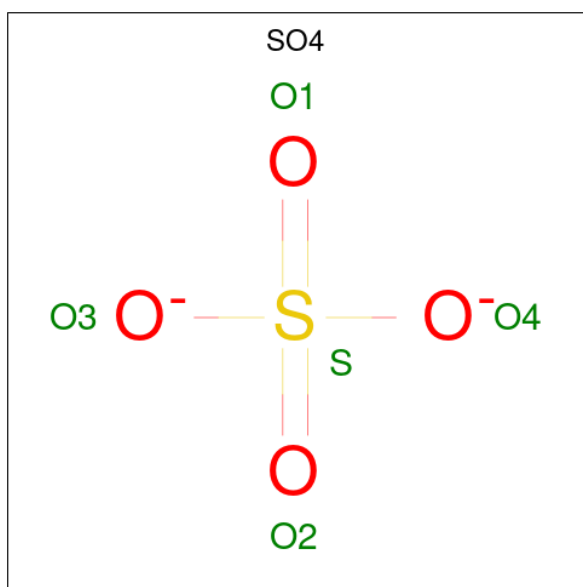
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ni 2 2	0	0
2	B	2	Total Ni 2 2	0	0
2	C	2	Total Ni 2 2	0	0
2	D	2	Total Ni 2 2	0	0
2	E	2	Total Ni 2 2	0	0
2	F	2	Total Ni 2 2	0	0
2	G	2	Total Ni 2 2	0	0
2	H	2	Total Ni 2 2	0	0
2	I	2	Total Ni 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	2	Total 2	Ni 2	0	0
2	K	2	Total 2	Ni 2	0	0
2	L	2	Total 2	Ni 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	231	Total O 231 231	0	0
4	B	243	Total O 243 243	0	0
4	C	240	Total O 240 240	0	0

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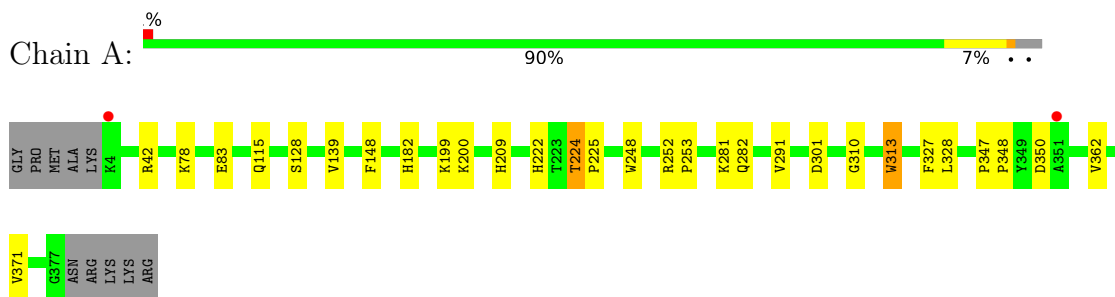
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	241	Total 241	O 241	0	0
4	E	236	Total 236	O 236	0	0
4	F	211	Total 211	O 211	0	0
4	G	256	Total 256	O 256	0	0
4	H	222	Total 222	O 222	0	0
4	I	246	Total 246	O 246	0	0
4	J	243	Total 243	O 243	0	0
4	K	237	Total 237	O 237	0	0
4	L	219	Total 219	O 219	0	0

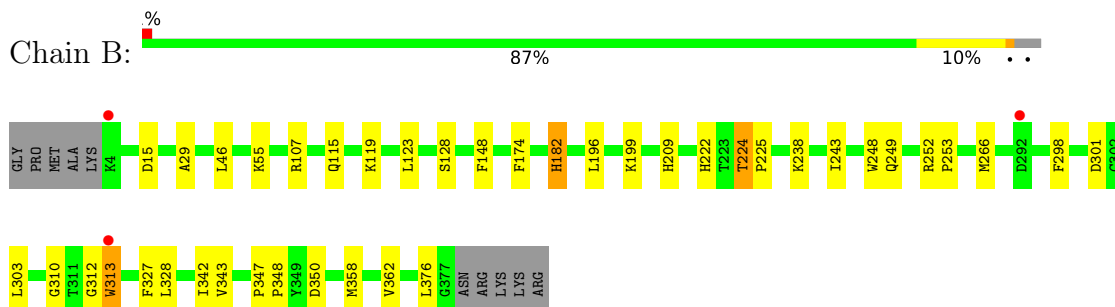
3 Residue-property plots [i](#)

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.

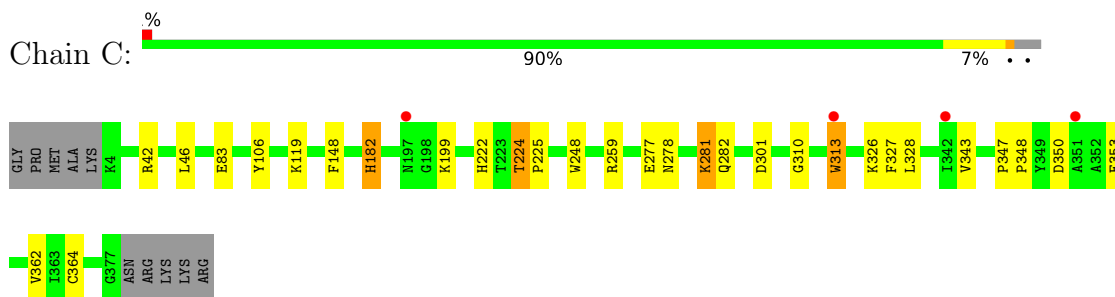
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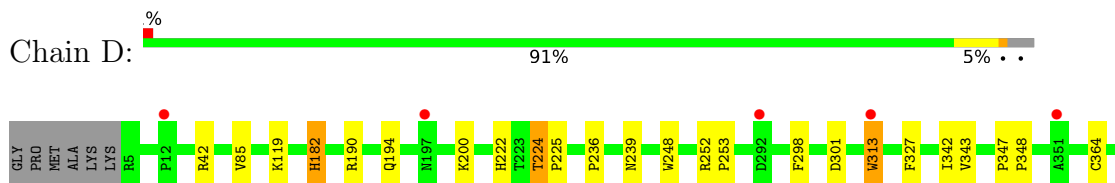
- Molecule 1: Putative agmatinase 2

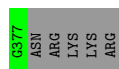


- Molecule 1: Putative agmatinase 2

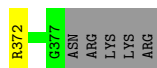
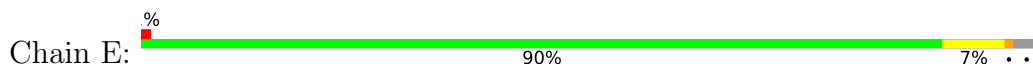


- Molecule 1: Putative agmatinase 2

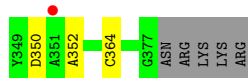
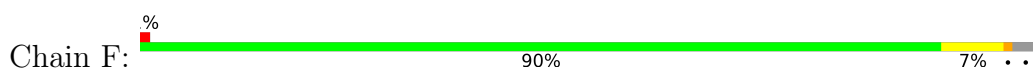




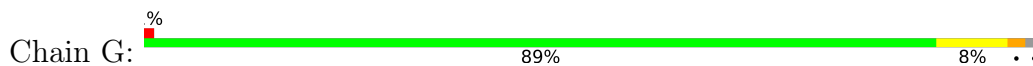
- Molecule 1: Putative agmatinase 2



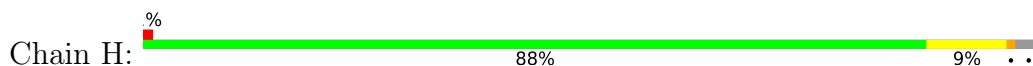
- Molecule 1: Putative agmatinase 2



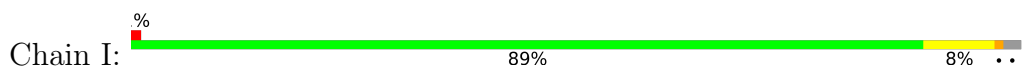
- Molecule 1: Putative agmatinase 2

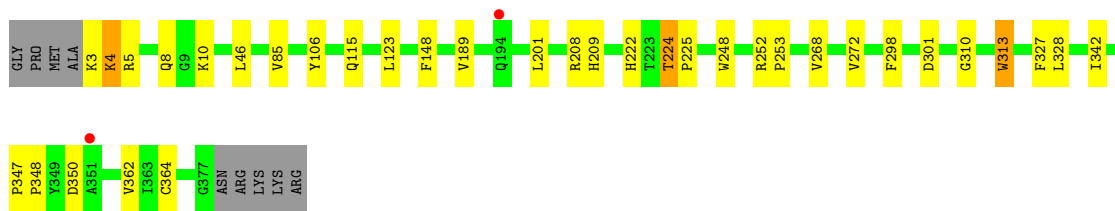


- Molecule 1: Putative agmatinase 2

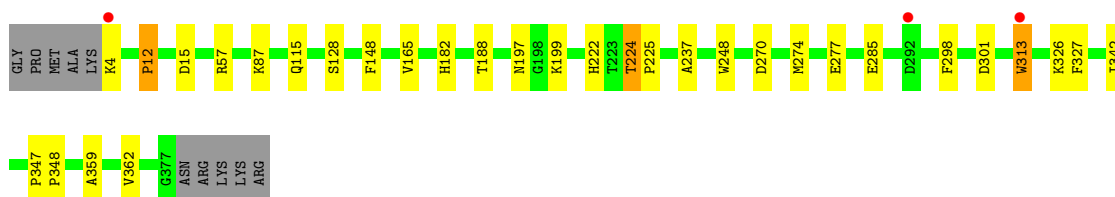
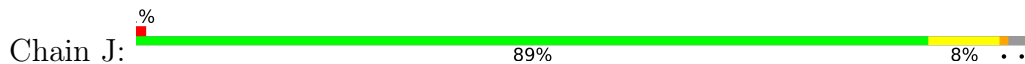


- Molecule 1: Putative agmatinase 2

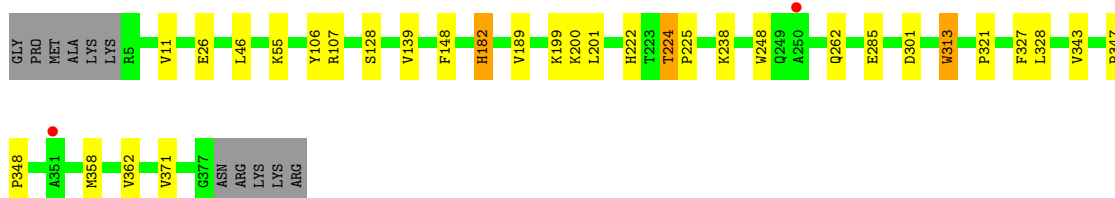
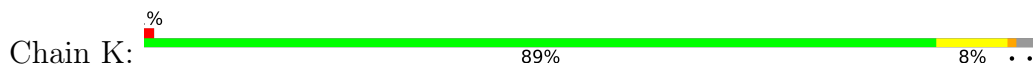




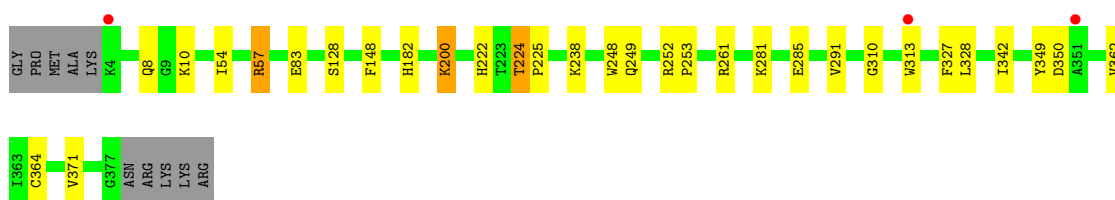
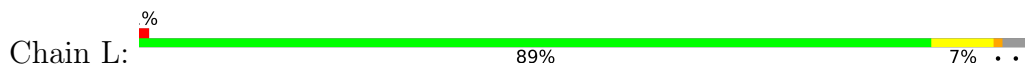
● Molecule 1: Putative agmatinase 2



● Molecule 1: Putative agmatinase 2



● Molecule 1: Putative agmatinase 2



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.97Å 164.79Å 143.97Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	45.01 – 1.58 45.01 – 1.58	Depositor EDS
% Data completeness (in resolution range)	92.9 (45.01-1.58) 82.2 (45.01-1.58)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 1.58Å)	Xtrriage
Refinement program	PHENIX 1.20.1-4478	Depositor
R, R_{free}	0.200 , 0.214 0.200 , 0.213	Depositor DCC
R_{free} test set	2001 reflections (0.34%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtrriage
Anisotropy	0.352	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.159 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	71341	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5951e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, NI

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	0.44	0/2949	0.63	0/4008
1	B	0.47	0/2949	0.66	0/4008
1	C	0.43	0/2960	0.64	0/4022
1	D	0.47	0/2931	0.65	0/3984
1	E	0.44	0/2949	0.63	0/4008
1	F	0.44	1/2940 (0.0%)	0.62	0/3996
1	G	0.57	1/2944 (0.0%)	0.65	0/3999
1	H	0.49	0/2949	0.64	0/4008
1	I	0.44	0/2962	0.63	0/4025
1	J	0.50	1/2922 (0.0%)	0.66	1/3971 (0.0%)
1	K	0.45	0/2913	0.64	0/3960
1	L	0.47	0/2953	0.66	0/4014
All	All	0.47	3/35321 (0.0%)	0.64	1/48003 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3
1	F	0	2
1	G	0	1
1	H	0	1
1	I	0	2
1	L	0	2
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	12	PRO	N-CD	-15.97	1.25	1.47
1	F	12	PRO	N-CD	-5.46	1.40	1.47
1	J	237	ALA	C-N	-5.12	1.22	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	12	PRO	CA-N-CD	-8.30	99.88	111.50

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	352[A]	ALA	Mainchain
1	E	352[B]	ALA	Mainchain
1	E	372	ARG	Sidechain
1	F	352[B]	ALA	Mainchain
1	F	42	ARG	Sidechain
1	G	5	ARG	Sidechain
1	H	361	ARG	Sidechain
1	I	208	ARG	Sidechain
1	I	5	ARG	Sidechain
1	L	261	ARG	Sidechain
1	L	349	TYR	Mainchain

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	2872	2831	2822	18	0
1	B	2872	2829	2822	26	0
1	C	2878	2839	2825	23	0
1	D	2854	2810	2802	16	0
1	E	2872	2828	2822	24	0
1	F	2872	2829	2827	24	0
1	G	2876	2844	2844	23	0
1	H	2872	2830	2822	29	0
1	I	2887	2849	2836	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2854	2815	2813	19	0
1	K	2845	2801	2801	16	0
1	L	2878	2835	2823	24	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	G	10	0	0	0	0
3	H	10	0	0	0	0
3	I	10	0	0	0	0
3	J	10	0	0	0	0
3	K	10	0	0	0	0
3	L	10	0	0	0	0
4	A	231	0	0	2	0
4	B	243	0	0	0	0
4	C	240	0	0	1	0
4	D	241	0	0	0	0
4	E	236	0	0	1	0
4	F	211	0	0	2	0
4	G	256	0	0	0	0
4	H	222	0	0	0	0
4	I	246	0	0	0	0
4	J	243	0	0	1	0
4	K	237	0	0	0	0
4	L	219	0	0	0	0
All	All	37401	33940	33859	232	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 (232) 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:G:281:LYS:O	1:G:285:GLU:HG3	1.73	0.87
1:G:83:GLU:HG2	1:I:46:LEU:HD13	1.58	0.84
1:J:298:PHE:HB3	1:J:342:ILE:HD13	1.61	0.82
1:L:238:LYS:HD3	1:L:238:LYS:N	2.03	0.73
1:C:301:ASP:OD2	1:C:313:TRP:NE1	2.24	0.70
1:L:8:GLN:CB	1:L:10:LYS:HE3	2.22	0.69
1:B:249:GLN:OE1	1:F:123:LEU:HD11	1.92	0.68
1:D:200:LYS:HD3	1:D:236:PRO:HD3	1.75	0.66
1:A:83:GLU:HG2	1:C:46:LEU:HD13	1.78	0.65
1:E:55:LYS:HD2	1:F:156:LYS:HZ1	1.62	0.65
1:G:83:GLU:CG	1:I:46:LEU:HD13	2.27	0.64
1:L:238:LYS:HD3	1:L:238:LYS:H	1.60	0.64
1:E:301:ASP:OD2	1:E:313:TRP:NE1	2.30	0.64
1:A:301:ASP:OD2	1:A:313:TRP:NE1	2.31	0.63
1:I:301:ASP:OD2	1:I:313:TRP:NE1	2.32	0.63
1:J:12:PRO:HD2	1:J:12:PRO:O	1.98	0.63
1:K:46:LEU:HD13	1:L:83:GLU:HG2	1.80	0.63
1:F:123:LEU:HD12	1:F:123:LEU:O	1.99	0.62
1:H:10:LYS:HE3	1:H:30:LEU:HD11	1.80	0.62
1:F:238:LYS:H	1:F:238:LYS:HD2	1.63	0.62
1:G:301:ASP:OD2	1:G:313:TRP:NE1	2.33	0.62
1:C:42:ARG:NH1	1:C:46:LEU:HD21	2.15	0.61
1:E:55:LYS:HD2	1:F:156:LYS:NZ	2.14	0.61
1:E:238:LYS:HD3	1:E:238:LYS:N	2.17	0.59
1:J:87:LYS:NZ	4:J:502:HOH:O	2.36	0.57
1:E:55:LYS:CD	1:F:156:LYS:HZ1	2.15	0.57
1:I:268:VAL:O	1:I:272:VAL:HG13	2.04	0.57
1:B:46:LEU:O	1:D:85:VAL:HG22	2.06	0.56
1:J:224:THR:N	1:J:225:PRO:CD	2.69	0.55
1:L:238:LYS:H	1:L:238:LYS:CD	2.18	0.55
1:H:303:LEU:HD13	1:H:358:MET:HG2	1.89	0.55
1:L:310:GLY:HA3	1:L:350[A]:ASP:HB2	1.89	0.55
1:B:298:PHE:HB3	1:B:342:ILE:HD13	1.88	0.54
1:E:209:HIS:ND1	1:E:313:TRP:CD2	2.75	0.54
1:L:8:GLN:HB2	1:L:10:LYS:HE3	1.90	0.54
1:A:139:VAL:HG11	1:A:371:VAL:CG2	2.38	0.54
1:F:310:GLY:HA3	1:F:350[B]:ASP:HB2	1.90	0.54
1:H:301:ASP:OD2	1:H:313:TRP:NE1	2.40	0.53
1:J:197:ASN:O	1:J:199:LYS:HE3	2.08	0.53
1:F:238:LYS:HE3	4:F:548:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:ARG:NH2	1:I:85:VAL:HG22	2.23	0.53
1:D:224:THR:N	1:D:225:PRO:CD	2.72	0.53
1:I:224:THR:N	1:I:225:PRO:CD	2.72	0.53
1:C:42:ARG:CZ	1:C:46:LEU:HD21	2.39	0.53
1:L:224:THR:N	1:L:225:PRO:CD	2.72	0.53
1:H:10:LYS:HE3	1:H:30:LEU:CD1	2.38	0.52
1:I:4:LYS:HD2	1:I:4:LYS:N	2.24	0.52
1:J:12:PRO:O	1:J:12:PRO:CD	2.57	0.52
1:C:199:LYS:HD2	4:C:608:HOH:O	2.08	0.52
1:I:310:GLY:HA3	1:I:350[B]:ASP:HB2	1.92	0.52
1:I:298:PHE:CD1	1:I:342:ILE:HD12	2.45	0.52
1:I:364:CYS:HB3	1:L:248:TRP:CZ2	2.44	0.52
1:B:224:THR:N	1:B:225:PRO:CD	2.73	0.52
1:G:199:LYS:HE3	1:G:199:LYS:HA	1.92	0.51
1:G:224:THR:N	1:G:225:PRO:CD	2.73	0.51
1:E:209:HIS:ND1	1:E:313:TRP:CE3	2.79	0.51
1:A:139:VAL:HG11	1:A:371:VAL:HG22	1.92	0.51
1:D:298:PHE:CD2	1:D:342:ILE:HD12	2.46	0.51
1:H:224:THR:N	1:H:225:PRO:CD	2.74	0.51
1:F:224:THR:N	1:F:225:PRO:CD	2.74	0.50
1:I:8:GLN:HB2	1:I:10:LYS:HE2	1.93	0.50
1:K:285:GLU:C	1:K:285:GLU:OE1	2.50	0.50
1:E:238:LYS:CD	1:E:238:LYS:H	2.24	0.50
1:F:238:LYS:H	1:F:238:LYS:CD	2.24	0.50
1:I:8:GLN:CB	1:I:10:LYS:HE2	2.41	0.50
1:E:224:THR:N	1:E:225:PRO:CD	2.75	0.50
1:E:238:LYS:HD3	1:E:238:LYS:H	1.77	0.50
1:K:224:THR:N	1:K:225:PRO:CD	2.75	0.50
1:D:342:ILE:HG23	1:D:342:ILE:O	2.11	0.50
1:C:350[B]:ASP:OD2	1:C:353:GLU:HA	2.11	0.50
1:B:303:LEU:HD13	1:B:358:MET:HG2	1.95	0.49
1:K:301:ASP:OD2	1:K:313:TRP:NE1	2.45	0.49
1:J:342:ILE:HG21	1:J:359:ALA:HB1	1.94	0.49
1:L:281:LYS:O	1:L:285:GLU:HG3	2.12	0.49
1:F:238:LYS:CE	4:F:548:HOH:O	2.61	0.49
1:B:174:PHE:HB2	1:B:376:LEU:HD21	1.95	0.49
1:L:54:ILE:O	1:L:57:ARG:NH1	2.45	0.49
1:E:209:HIS:CE1	1:E:313:TRP:CD2	3.01	0.49
1:E:238:LYS:N	1:E:238:LYS:CD	2.76	0.48
1:E:33:THR:O	1:E:37:GLU:HG2	2.14	0.48
1:H:6:THR:HG22	1:H:7:TYR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:128:SER:HB2	1:K:248:TRP:CE2	2.48	0.48
1:J:224:THR:N	1:J:225:PRO:HD2	2.27	0.48
1:G:200:LYS:HD2	1:G:200:LYS:N	2.27	0.48
1:H:139:VAL:HG11	1:H:371:VAL:CG2	2.43	0.48
1:A:224:THR:N	1:A:225:PRO:CD	2.77	0.48
1:J:347:PRO:N	1:J:348:PRO:CD	2.77	0.48
1:B:243:ILE:HG12	1:B:266:MET:HE2	1.96	0.48
1:K:139:VAL:HG11	1:K:371:VAL:HG22	1.96	0.48
1:A:78:LYS:HE2	4:A:540:HOH:O	2.13	0.47
1:I:224:THR:N	1:I:225:PRO:HD2	2.29	0.47
1:C:281:LYS:HD2	1:C:282:GLN:N	2.28	0.47
1:K:199:LYS:HE3	1:K:200:LYS:H	1.79	0.47
1:L:238:LYS:N	1:L:238:LYS:CD	2.72	0.47
1:G:328:LEU:HD13	1:G:362:VAL:HG13	1.95	0.47
1:J:301:ASP:OD2	1:J:313:TRP:NE1	2.48	0.47
1:B:310:GLY:HA3	1:B:350[A]:ASP:HB2	1.95	0.47
1:D:224:THR:N	1:D:225:PRO:HD2	2.29	0.47
1:K:182:HIS:ND1	1:K:343:VAL:HG21	2.29	0.47
1:G:347:PRO:N	1:G:348:PRO:CD	2.78	0.47
1:C:224:THR:N	1:C:225:PRO:CD	2.78	0.47
1:D:236:PRO:HG2	1:D:239:ASN:HB2	1.97	0.47
1:B:347:PRO:N	1:B:348:PRO:CD	2.78	0.46
1:D:301:ASP:OD2	1:D:313:TRP:NE1	2.48	0.46
1:H:269:THR:HA	1:H:272:VAL:HG22	1.96	0.46
1:E:115:GLN:NE2	1:F:119:LYS:HE2	2.31	0.46
1:L:224:THR:N	1:L:225:PRO:HD2	2.30	0.46
1:A:248:TRP:CZ2	1:E:364:CYS:HB3	2.51	0.46
1:C:364:CYS:HB3	1:F:248:TRP:CZ2	2.50	0.46
1:F:257:ALA:O	1:F:261:ARG:HG3	2.15	0.46
1:H:107:ARG:HB2	1:H:312:GLY:HA2	1.97	0.46
1:I:298:PHE:HD1	1:I:342:ILE:HD12	1.80	0.46
1:D:182:HIS:ND1	1:D:343:VAL:HG21	2.31	0.46
1:H:139:VAL:CG1	1:H:371:VAL:HG22	2.46	0.46
1:A:328:LEU:HD13	1:A:362:VAL:HG13	1.97	0.46
1:H:139:VAL:HG11	1:H:371:VAL:HG22	1.98	0.46
1:A:310:GLY:HA3	1:A:350[A]:ASP:HB2	1.98	0.45
1:H:328:LEU:HD13	1:H:362:VAL:HG13	1.98	0.45
1:B:107:ARG:HB2	1:B:312:GLY:HA2	1.98	0.45
1:D:347:PRO:N	1:D:348:PRO:CD	2.79	0.45
1:H:128:SER:HB2	1:I:248:TRP:CE2	2.51	0.45
1:B:182:HIS:ND1	1:B:343:VAL:HG21	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:LYS:HD3	1:F:236:PRO:HG3	1.98	0.45
1:F:301:ASP:OD2	1:F:313:TRP:NE1	2.49	0.45
1:K:328:LEU:HD13	1:K:362:VAL:HG13	1.98	0.45
1:C:278:ASN:O	1:C:281:LYS:HE3	2.17	0.45
1:G:205:HIS:CD2	1:G:226:TRP:HE1	2.35	0.45
1:J:199:LYS:HE2	1:J:199:LYS:N	2.32	0.45
1:I:342:ILE:HG23	1:I:342:ILE:O	2.17	0.45
1:E:106:TYR:CD2	1:E:107:ARG:HG3	2.52	0.45
1:G:165:VAL:HG21	1:G:188:THR:HG22	1.99	0.45
1:A:347:PRO:N	1:A:348:PRO:CD	2.80	0.44
1:G:3:LYS:HE3	1:G:5:ARG:NH2	2.33	0.44
1:B:128:SER:HB2	1:C:248:TRP:CE2	2.53	0.44
1:D:190:ARG:O	1:D:194:GLN:HG3	2.17	0.44
1:E:55:LYS:CE	1:F:156:LYS:HZ1	2.30	0.44
1:H:161:VAL:HG21	1:H:184:LEU:HD22	1.99	0.44
1:B:301:ASP:OD2	1:B:313:TRP:NE1	2.51	0.44
1:H:310:GLY:HA3	1:H:350[A]:ASP:HB2	2.00	0.44
1:I:8:GLN:HG3	1:I:10:LYS:HE2	1.99	0.44
1:J:342:ILE:HD11	1:J:362:VAL:HG11	2.00	0.44
1:B:328:LEU:HD13	1:B:362:VAL:HG13	2.00	0.44
1:H:119:LYS:HE2	1:J:115:GLN:OE1	2.18	0.44
1:K:238:LYS:NZ	1:K:262:GLN:OE1	2.51	0.44
1:B:115:GLN:OE1	1:D:119:LYS:HE2	2.18	0.44
1:D:298:PHE:CD2	1:D:342:ILE:CD1	3.00	0.44
1:E:199:LYS:HG3	4:E:554:HOH:O	2.18	0.44
1:G:119:LYS:HE3	1:I:115:GLN:OE1	2.18	0.44
1:H:248:TRP:CZ2	1:L:364:CYS:HB3	2.53	0.44
1:E:238:LYS:H	1:E:238:LYS:CE	2.31	0.43
1:H:123:LEU:HD13	1:I:106:TYR:CD2	2.53	0.43
1:C:310:GLY:HA3	1:C:350[A]:ASP:HB2	1.99	0.43
1:I:189:VAL:HG13	1:I:201:LEU:HD23	2.00	0.43
1:G:128:SER:HB2	1:J:248:TRP:CE2	2.53	0.43
1:I:209:HIS:ND1	1:I:313:TRP:CD2	2.87	0.43
1:A:252:ARG:N	1:A:253:PRO:HD2	2.33	0.43
1:F:209:HIS:CD2	1:F:209:HIS:N	2.86	0.43
1:H:224:THR:N	1:H:225:PRO:HD2	2.33	0.43
1:I:301:ASP:OD2	1:I:313:TRP:CD1	2.71	0.43
1:J:277:GLU:HG3	1:J:326:LYS:CE	2.48	0.43
1:C:277:GLU:HG3	1:C:326:LYS:HE2	2.00	0.43
1:I:123:LEU:HD11	1:L:249:GLN:OE1	2.18	0.43
1:J:270:ASP:O	1:J:274:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:PRO:N	1:H:348:PRO:CD	2.82	0.43
1:K:11:VAL:HB	1:K:26:GLU:HG3	1.99	0.43
1:A:200:LYS:O	1:A:291:VAL:HG13	2.18	0.43
1:L:200:LYS:HB2	1:L:291:VAL:HG12	1.99	0.43
1:A:128:SER:HB2	1:D:248:TRP:CE2	2.54	0.43
1:F:347:PRO:N	1:F:348:PRO:CD	2.82	0.43
1:B:209:HIS:ND1	1:B:313:TRP:CE3	2.87	0.43
1:B:248:TRP:CZ2	1:F:364:CYS:HB3	2.54	0.43
1:C:182:HIS:ND1	1:C:343:VAL:HG21	2.33	0.43
1:E:46:LEU:HD13	1:F:83:GLU:HG2	2.00	0.43
1:G:248:TRP:CE2	1:K:128:SER:HB2	2.54	0.43
1:H:209:HIS:HE1	1:H:313:TRP:CG	2.37	0.43
1:I:347:PRO:N	1:I:348:PRO:CD	2.82	0.43
1:L:328:LEU:HD13	1:L:362:VAL:HG13	2.00	0.42
1:B:196:LEU:O	1:B:199:LYS:NZ	2.45	0.42
1:B:248:TRP:CE2	1:F:128:SER:HB2	2.55	0.42
1:J:165:VAL:HG21	1:J:188:THR:HG22	2.02	0.42
1:B:224:THR:N	1:B:225:PRO:HD2	2.33	0.42
1:G:224:THR:N	1:G:225:PRO:HD2	2.34	0.42
1:K:347:PRO:N	1:K:348:PRO:CD	2.82	0.42
1:C:301:ASP:OD1	1:C:301:ASP:C	2.58	0.42
1:H:182:HIS:CE1	1:H:299:ASP:HB2	2.55	0.42
1:K:106:TYR:CD2	1:K:107:ARG:HG3	2.55	0.42
1:K:321:PRO:HB3	1:K:358:MET:HE1	2.00	0.42
1:A:42:ARG:NH2	1:C:83:GLU:OE1	2.52	0.42
1:D:364:CYS:HB3	1:E:248:TRP:CZ2	2.55	0.42
1:I:252:ARG:N	1:I:253:PRO:HD2	2.34	0.42
1:C:347:PRO:N	1:C:348:PRO:CD	2.83	0.42
1:C:301:ASP:OD2	1:C:313:TRP:CD1	2.73	0.42
1:E:347:PRO:N	1:E:348:PRO:CD	2.83	0.42
1:H:226:TRP:HA	1:H:226:TRP:CE3	2.55	0.42
1:I:328:LEU:HD13	1:I:362:VAL:HG13	2.02	0.42
4:A:567:HOH:O	1:E:55:LYS:HD3	2.20	0.42
1:A:209:HIS:CE1	1:A:313:TRP:CG	3.08	0.41
1:B:123:LEU:HD13	1:C:106:TYR:CD2	2.55	0.41
1:F:209:HIS:ND1	1:F:313:TRP:CD2	2.88	0.41
1:H:209:HIS:CE1	1:H:313:TRP:CD2	3.09	0.41
1:H:248:TRP:CE2	1:L:128:SER:HB2	2.55	0.41
1:K:189:VAL:HG13	1:K:201:LEU:HD23	2.02	0.41
1:H:209:HIS:CD2	1:H:209:HIS:N	2.88	0.41
1:H:342:ILE:HG23	1:H:342:ILE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:342:ILE:HG23	1:L:342:ILE:O	2.19	0.41
1:J:199:LYS:N	1:J:199:LYS:CE	2.84	0.41
1:L:57:ARG:HD2	1:L:57:ARG:HA	1.70	0.41
1:B:55:LYS:HD2	1:B:55:LYS:HA	1.79	0.41
1:L:8:GLN:HG3	1:L:10:LYS:HE3	2.03	0.41
1:C:281:LYS:HE3	1:C:281:LYS:HB3	1.95	0.41
1:G:342:ILE:O	1:G:342:ILE:HG23	2.21	0.41
1:E:310:GLY:HA3	1:E:350[A]:ASP:HB2	2.03	0.41
1:A:139:VAL:CG1	1:A:371:VAL:HG22	2.50	0.41
1:C:328:LEU:HD13	1:C:362:VAL:HG13	2.02	0.41
1:D:252:ARG:N	1:D:253:PRO:HD2	2.35	0.41
1:G:8:GLN:HB3	1:G:10:LYS:HZ3	1.86	0.41
1:L:252:ARG:N	1:L:253:PRO:HD2	2.35	0.41
1:G:303:LEU:HD13	1:G:358:MET:HG2	2.03	0.40
1:F:269:THR:HA	1:F:272:VAL:HG22	2.03	0.40
1:G:139:VAL:HG11	1:G:371:VAL:CG2	2.52	0.40
1:G:199:LYS:HA	1:G:199:LYS:CE	2.51	0.40
1:H:139:VAL:CG1	1:H:371:VAL:CG2	2.99	0.40
1:G:226:TRP:CE3	1:G:226:TRP:HA	2.56	0.40
1:A:115:GLN:OE1	1:C:119:LYS:HE2	2.21	0.40
1:B:29:ALA:HB2	1:C:259[A]:ARG:CZ	2.51	0.40
1:B:252:ARG:N	1:B:253:PRO:HD2	2.37	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	376/384 (98%)	367 (98%)	8 (2%)	1 (0%)	41 21
1	B	376/384 (98%)	366 (97%)	9 (2%)	1 (0%)	41 21
1	C	377/384 (98%)	368 (98%)	8 (2%)	1 (0%)	41 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	373/384 (97%)	365 (98%)	7 (2%)	1 (0%)	41	21
1	E	376/384 (98%)	365 (97%)	10 (3%)	1 (0%)	41	21
1	F	375/384 (98%)	364 (97%)	10 (3%)	1 (0%)	41	21
1	G	375/384 (98%)	366 (98%)	8 (2%)	1 (0%)	41	21
1	H	376/384 (98%)	366 (97%)	9 (2%)	1 (0%)	41	21
1	I	378/384 (98%)	367 (97%)	10 (3%)	1 (0%)	41	21
1	J	372/384 (97%)	362 (97%)	9 (2%)	1 (0%)	41	21
1	K	371/384 (97%)	361 (97%)	9 (2%)	1 (0%)	41	21
1	L	377/384 (98%)	366 (97%)	10 (3%)	1 (0%)	41	21
All	All	4502/4608 (98%)	4383 (97%)	107 (2%)	12 (0%)	41	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	THR
1	B	224	THR
1	D	224	THR
1	F	224	THR
1	H	224	THR
1	J	224	THR
1	K	224	THR
1	L	224	THR
1	C	224	THR
1	E	224	THR
1	G	224	THR
1	I	224	THR

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	301/307 (98%)	293 (97%)	8 (3%)	44	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	301/307 (98%)	294 (98%)	7 (2%)	50	23
1	C	302/307 (98%)	296 (98%)	6 (2%)	55	29
1	D	300/307 (98%)	295 (98%)	5 (2%)	60	36
1	E	301/307 (98%)	294 (98%)	7 (2%)	50	23
1	F	300/307 (98%)	294 (98%)	6 (2%)	55	29
1	G	301/307 (98%)	293 (97%)	8 (3%)	44	18
1	H	301/307 (98%)	295 (98%)	6 (2%)	55	29
1	I	303/307 (99%)	297 (98%)	6 (2%)	55	29
1	J	299/307 (97%)	290 (97%)	9 (3%)	41	15
1	K	298/307 (97%)	292 (98%)	6 (2%)	55	29
1	L	302/307 (98%)	295 (98%)	7 (2%)	50	23
All	All	3609/3684 (98%)	3528 (98%)	81 (2%)	50	25

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	PHE
1	A	182	HIS
1	A	199	LYS
1	A	222	HIS
1	A	281	LYS
1	A	282	GLN
1	A	313	TRP
1	A	327	PHE
1	B	15	ASP
1	B	148	PHE
1	B	182	HIS
1	B	222	HIS
1	B	238	LYS
1	B	313	TRP
1	B	327	PHE
1	C	148	PHE
1	C	182	HIS
1	C	222	HIS
1	C	281	LYS
1	C	313	TRP
1	C	327	PHE
1	D	42	ARG

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Mol	Chain	Res	Type
1	D	182	HIS
1	D	222	HIS
1	D	313	TRP
1	D	327	PHE
1	E	4	LYS
1	E	148	PHE
1	E	182	HIS
1	E	194	GLN
1	E	222	HIS
1	E	313	TRP
1	E	327	PHE
1	F	148	PHE
1	F	182	HIS
1	F	222	HIS
1	F	238	LYS
1	F	313	TRP
1	F	327	PHE
1	G	3	LYS
1	G	148	PHE
1	G	182	HIS
1	G	200	LYS
1	G	222	HIS
1	G	303	LEU
1	G	313	TRP
1	G	327	PHE
1	H	148	PHE
1	H	182	HIS
1	H	222	HIS
1	H	303	LEU
1	H	313	TRP
1	H	327	PHE
1	I	3	LYS
1	I	4	LYS
1	I	148	PHE
1	I	222	HIS
1	I	313	TRP
1	I	327	PHE
1	J	4	LYS
1	J	15	ASP
1	J	57	ARG
1	J	148	PHE
1	J	182	HIS

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Mol	Chain	Res	Type
1	J	222	HIS
1	J	285	GLU
1	J	313	TRP
1	J	327	PHE
1	K	55	LYS
1	K	148	PHE
1	K	182	HIS
1	K	222	HIS
1	K	313	TRP
1	K	327	PHE
1	L	57	ARG
1	L	148	PHE
1	L	182	HIS
1	L	200	LYS
1	L	222	HIS
1	L	313	TRP
1	L	327	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	8	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	H	404	-	4,4,4	0.11	0	6,6,6	0.18	0
3	SO4	L	404	-	4,4,4	0.22	0	6,6,6	0.21	0
3	SO4	I	403	-	4,4,4	0.21	0	6,6,6	0.23	0
3	SO4	C	404	-	4,4,4	0.17	0	6,6,6	0.22	0
3	SO4	F	404	-	4,4,4	0.11	0	6,6,6	0.28	0
3	SO4	B	404	-	4,4,4	0.10	0	6,6,6	0.17	0
3	SO4	E	403	-	4,4,4	0.13	0	6,6,6	0.24	0
3	SO4	J	404	-	4,4,4	0.53	0	6,6,6	0.10	0
3	SO4	G	403	-	4,4,4	0.27	0	6,6,6	0.29	0
3	SO4	G	404	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	D	404	-	4,4,4	0.19	0	6,6,6	0.15	0
3	SO4	A	403	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	D	403	-	4,4,4	0.20	0	6,6,6	0.16	0
3	SO4	E	404	-	4,4,4	0.18	0	6,6,6	0.13	0
3	SO4	K	404	-	4,4,4	0.11	0	6,6,6	0.15	0
3	SO4	J	403	-	4,4,4	0.21	0	6,6,6	0.19	0
3	SO4	K	403	-	4,4,4	0.23	0	6,6,6	0.16	0
3	SO4	C	403	-	4,4,4	0.18	0	6,6,6	0.15	0
3	SO4	A	404	-	4,4,4	0.11	0	6,6,6	0.10	0
3	SO4	L	403	-	4,4,4	0.26	0	6,6,6	0.14	0
3	SO4	H	403	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	B	403	-	4,4,4	0.18	0	6,6,6	0.30	0
3	SO4	I	404	-	4,4,4	0.12	0	6,6,6	0.14	0
3	SO4	F	403	-	4,4,4	0.15	0	6,6,6	0.14	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	374/384 (97%)	-0.07	2 (0%) 91 91	16, 23, 37, 68	0
1	B	374/384 (97%)	-0.12	3 (0%) 86 87	16, 23, 35, 58	0
1	C	374/384 (97%)	-0.10	4 (1%) 80 82	15, 22, 35, 55	0
1	D	373/384 (97%)	-0.12	5 (1%) 77 78	15, 22, 35, 55	0
1	E	374/384 (97%)	-0.07	5 (1%) 77 78	15, 23, 37, 68	0
1	F	374/384 (97%)	-0.04	4 (1%) 80 82	16, 24, 38, 68	0
1	G	377/384 (98%)	-0.09	4 (1%) 80 82	15, 23, 36, 52	0
1	H	374/384 (97%)	-0.08	2 (0%) 91 91	16, 23, 38, 68	0
1	I	375/384 (97%)	-0.08	2 (0%) 91 91	16, 24, 38, 58	0
1	J	374/384 (97%)	-0.13	3 (0%) 86 87	16, 23, 36, 72	0
1	K	373/384 (97%)	-0.09	2 (0%) 91 91	15, 24, 37, 52	0
1	L	374/384 (97%)	-0.04	3 (0%) 86 87	15, 23, 36, 75	0
All	All	4490/4608 (97%)	-0.09	39 (0%) 84 85	15, 23, 37, 75	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	313	TRP	4.6
1	C	351[A]	ALA	4.2
1	B	292	ASP	4.0
1	L	4	LYS	4.0
1	D	12	PRO	3.9
1	L	351[A]	ALA	3.8
1	D	292	ASP	3.6
1	D	351	ALA	3.5
1	J	292	ASP	3.4
1	E	351[A]	ALA	3.4
1	G	313	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	4	LYS	3.3
1	E	4	LYS	3.3
1	G	1	MET	3.2
1	A	4	LYS	3.0
1	I	351[A]	ALA	2.9
1	C	313	TRP	2.9
1	D	197	ASN	2.8
1	E	8	GLN	2.8
1	K	351	ALA	2.6
1	L	313	TRP	2.5
1	D	313	TRP	2.5
1	G	351	ALA	2.4
1	E	313	TRP	2.4
1	E	342	ILE	2.4
1	A	351[A]	ALA	2.3
1	F	250	ALA	2.3
1	C	342	ILE	2.3
1	B	313	TRP	2.3
1	F	351[A]	ALA	2.2
1	F	313	TRP	2.2
1	I	194	GLN	2.2
1	H	292	ASP	2.2
1	B	4	LYS	2.2
1	F	4	LYS	2.2
1	K	250	ALA	2.1
1	G	2	ALA	2.1
1	H	351[A]	ALA	2.1
1	C	197	ASN	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, 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.

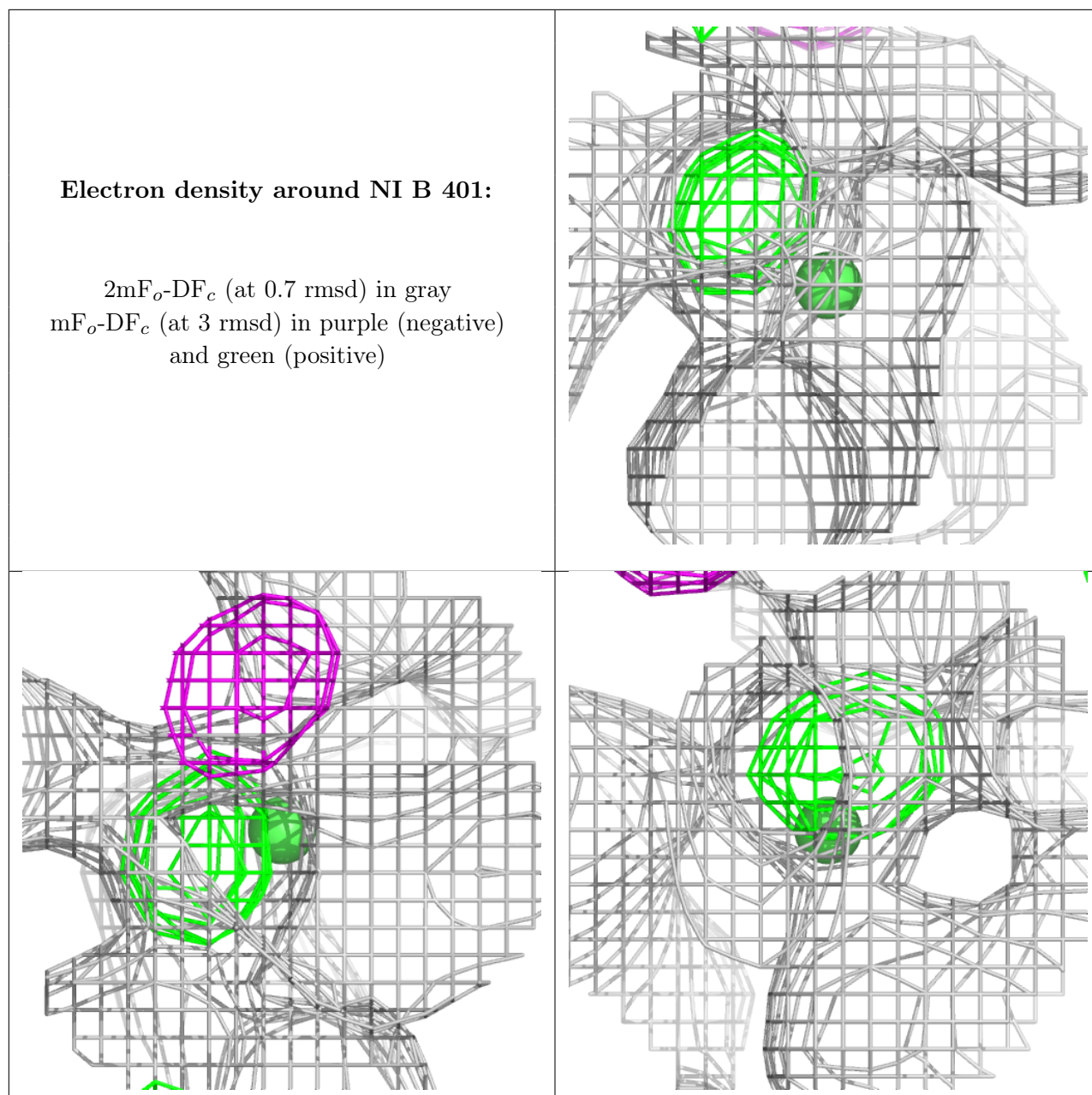
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NI	B	401	1/1	-0.01	0.45	49,49,49,49	1
2	NI	D	402	1/1	0.39	0.17	48,48,48,48	1
2	NI	F	401	1/1	0.69	0.28	42,42,42,42	1
2	NI	K	401	1/1	0.69	0.16	40,40,40,40	1
2	NI	K	402	1/1	0.78	0.17	43,43,43,43	1
2	NI	G	401	1/1	0.79	0.13	45,45,45,45	1
2	NI	E	402	1/1	0.81	0.15	40,40,40,40	1
2	NI	H	402	1/1	0.81	0.23	42,42,42,42	1
2	NI	I	401	1/1	0.82	0.22	43,43,43,43	1
2	NI	J	402	1/1	0.85	0.10	44,44,44,44	1
2	NI	C	401	1/1	0.85	0.10	41,41,41,41	1
2	NI	D	401	1/1	0.85	0.14	41,41,41,41	1
2	NI	B	402	1/1	0.86	0.15	45,45,45,45	1
2	NI	H	401	1/1	0.88	0.13	42,42,42,42	1
2	NI	F	402	1/1	0.88	0.17	41,41,41,41	1
2	NI	G	402	1/1	0.88	0.09	40,40,40,40	1
2	NI	L	401	1/1	0.88	0.17	43,43,43,43	1
2	NI	A	402	1/1	0.89	0.12	42,42,42,42	1
2	NI	J	401	1/1	0.89	0.10	40,40,40,40	1
2	NI	I	402	1/1	0.91	0.10	37,37,37,37	1
2	NI	E	401	1/1	0.93	0.10	38,38,38,38	1
2	NI	C	402	1/1	0.95	0.07	37,37,37,37	1
3	SO4	C	403	5/5	0.95	0.07	27,29,32,34	0
3	SO4	G	404	5/5	0.95	0.08	35,37,57,58	0
3	SO4	I	404	5/5	0.95	0.12	39,43,55,58	0
3	SO4	J	403	5/5	0.95	0.08	29,29,32,39	0
3	SO4	J	404	5/5	0.95	0.07	28,31,43,43	0
3	SO4	H	403	5/5	0.96	0.08	24,28,33,35	0
3	SO4	A	404	5/5	0.96	0.09	35,39,46,46	0
3	SO4	F	404	5/5	0.97	0.07	40,41,42,48	0
3	SO4	G	403	5/5	0.97	0.07	24,25,31,40	0
2	NI	L	402	1/1	0.97	0.19	39,39,39,39	1
3	SO4	A	403	5/5	0.97	0.07	25,27,35,37	0
3	SO4	C	404	5/5	0.97	0.07	32,36,38,44	0
3	SO4	D	403	5/5	0.97	0.07	34,36,46,47	0
3	SO4	D	404	5/5	0.97	0.12	30,30,34,36	0
3	SO4	K	403	5/5	0.97	0.07	25,29,34,42	0
3	SO4	K	404	5/5	0.97	0.06	37,40,46,48	0
3	SO4	H	404	5/5	0.98	0.07	29,39,45,47	0
3	SO4	I	403	5/5	0.98	0.07	25,31,32,42	0
3	SO4	F	403	5/5	0.98	0.06	28,29,34,42	0

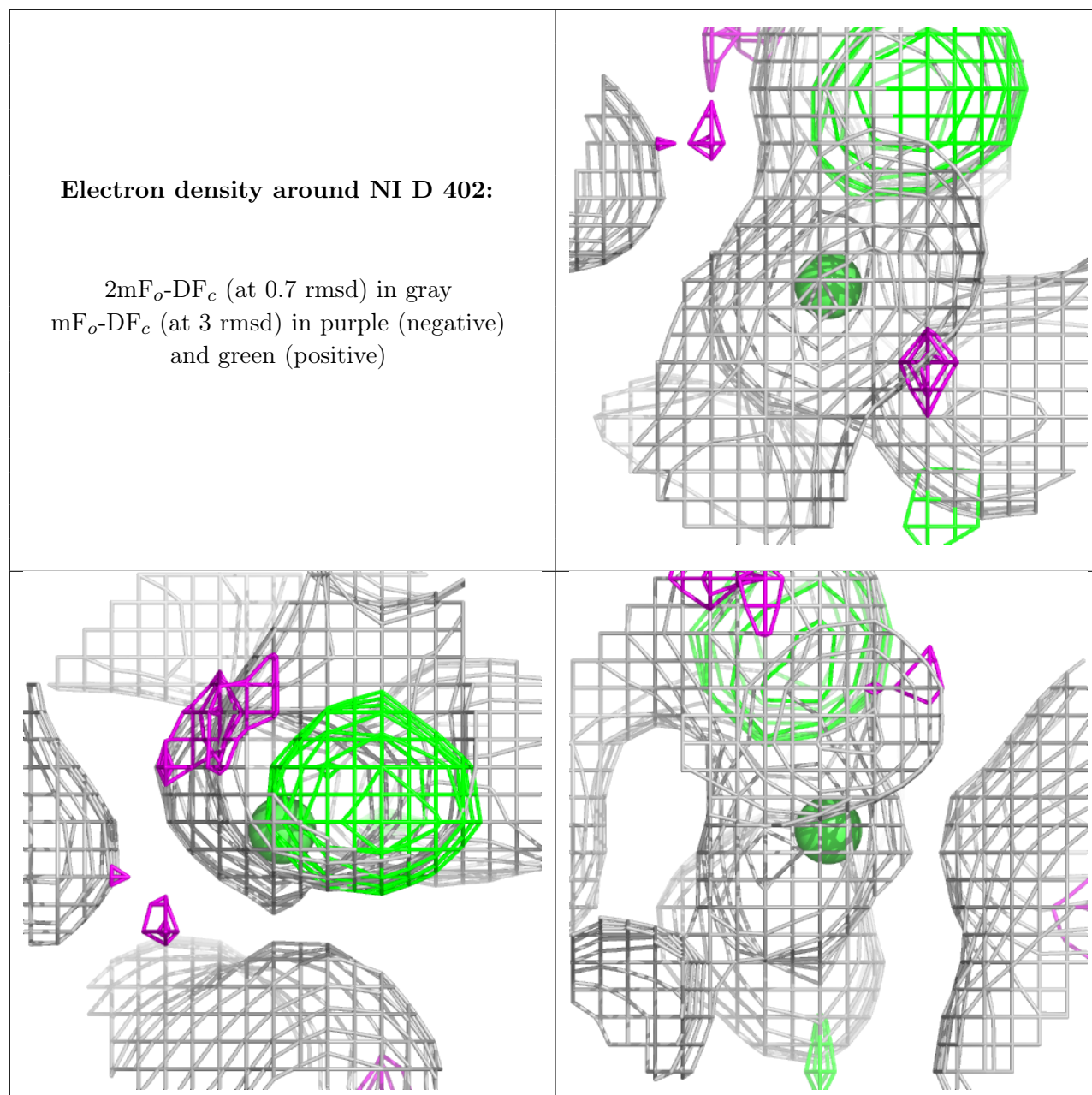
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NI	A	401	1/1	0.98	0.25	41,41,41,41	1
3	SO4	B	403	5/5	0.98	0.06	23,26,31,35	0
3	SO4	E	403	5/5	0.98	0.07	28,29,34,37	0
3	SO4	E	404	5/5	0.98	0.06	33,35,43,49	0
3	SO4	B	404	5/5	0.99	0.07	32,33,43,48	0
3	SO4	L	403	5/5	0.99	0.07	26,27,33,53	0
3	SO4	L	404	5/5	0.99	0.06	29,33,40,45	0

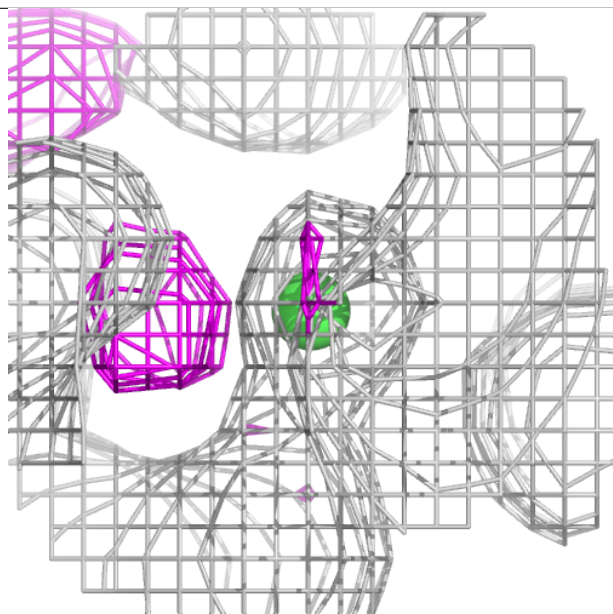
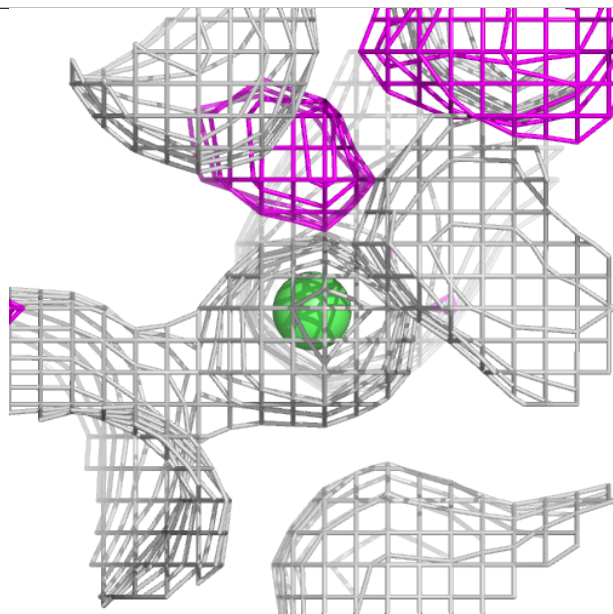
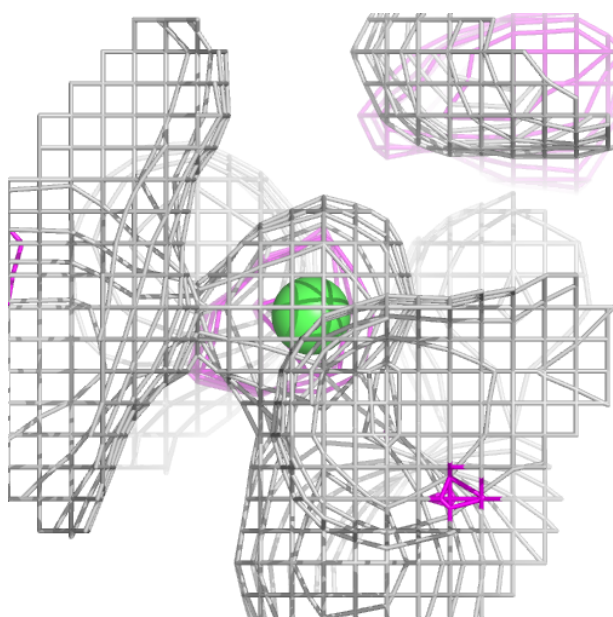
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





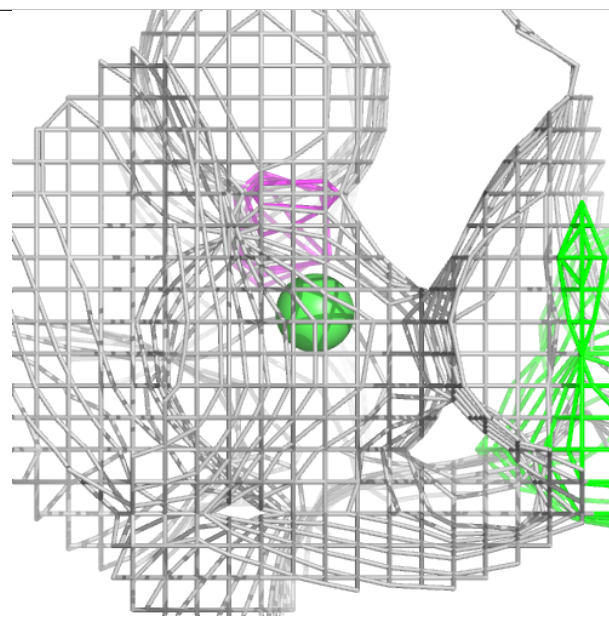
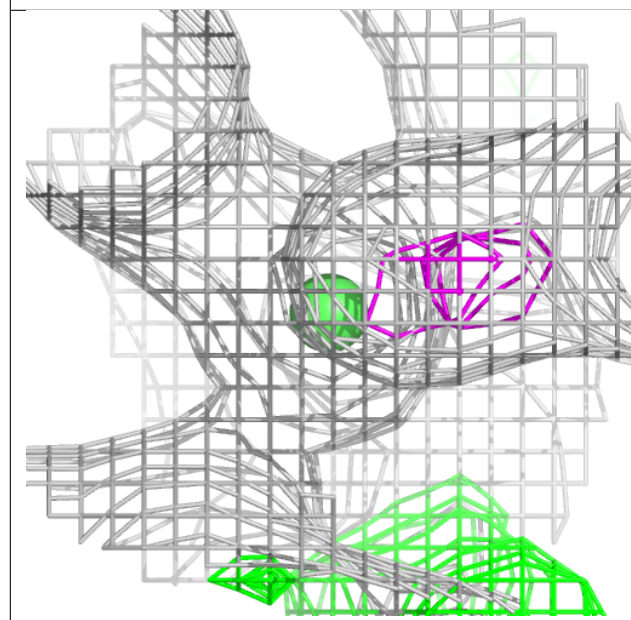
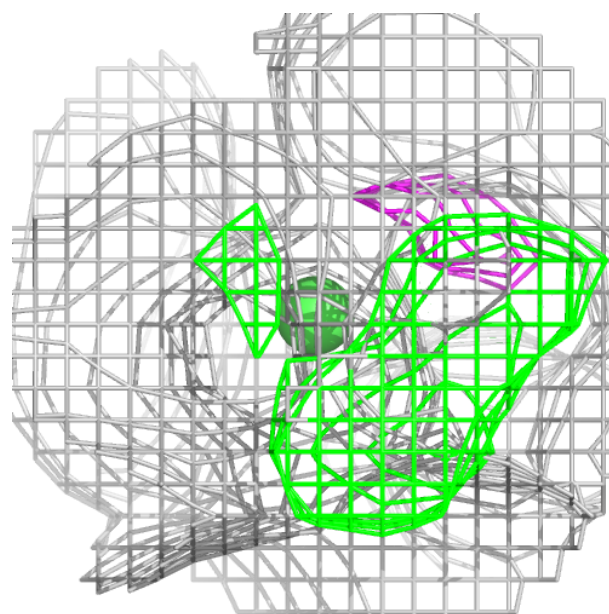
Electron density around NI F 401:

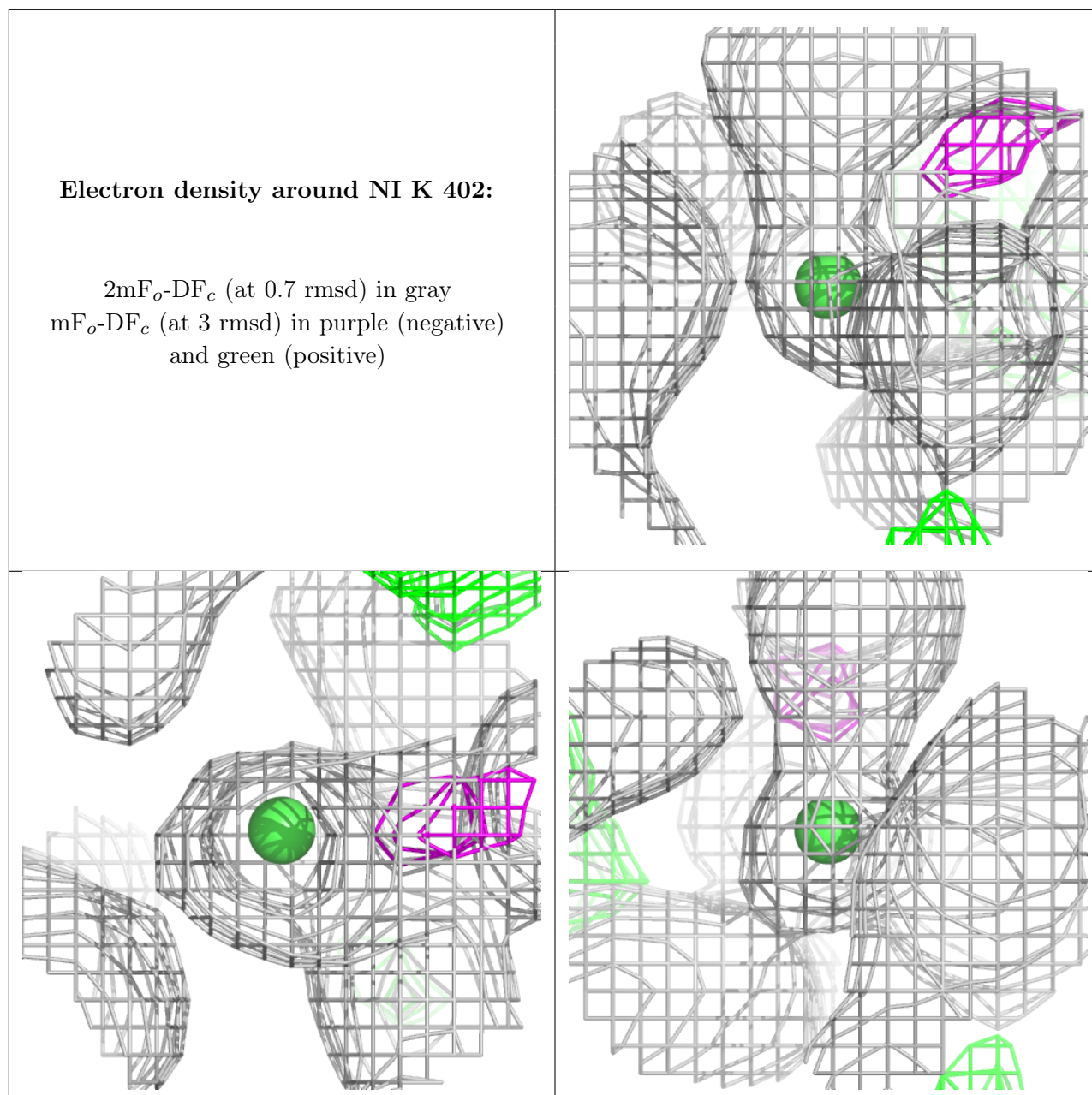
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

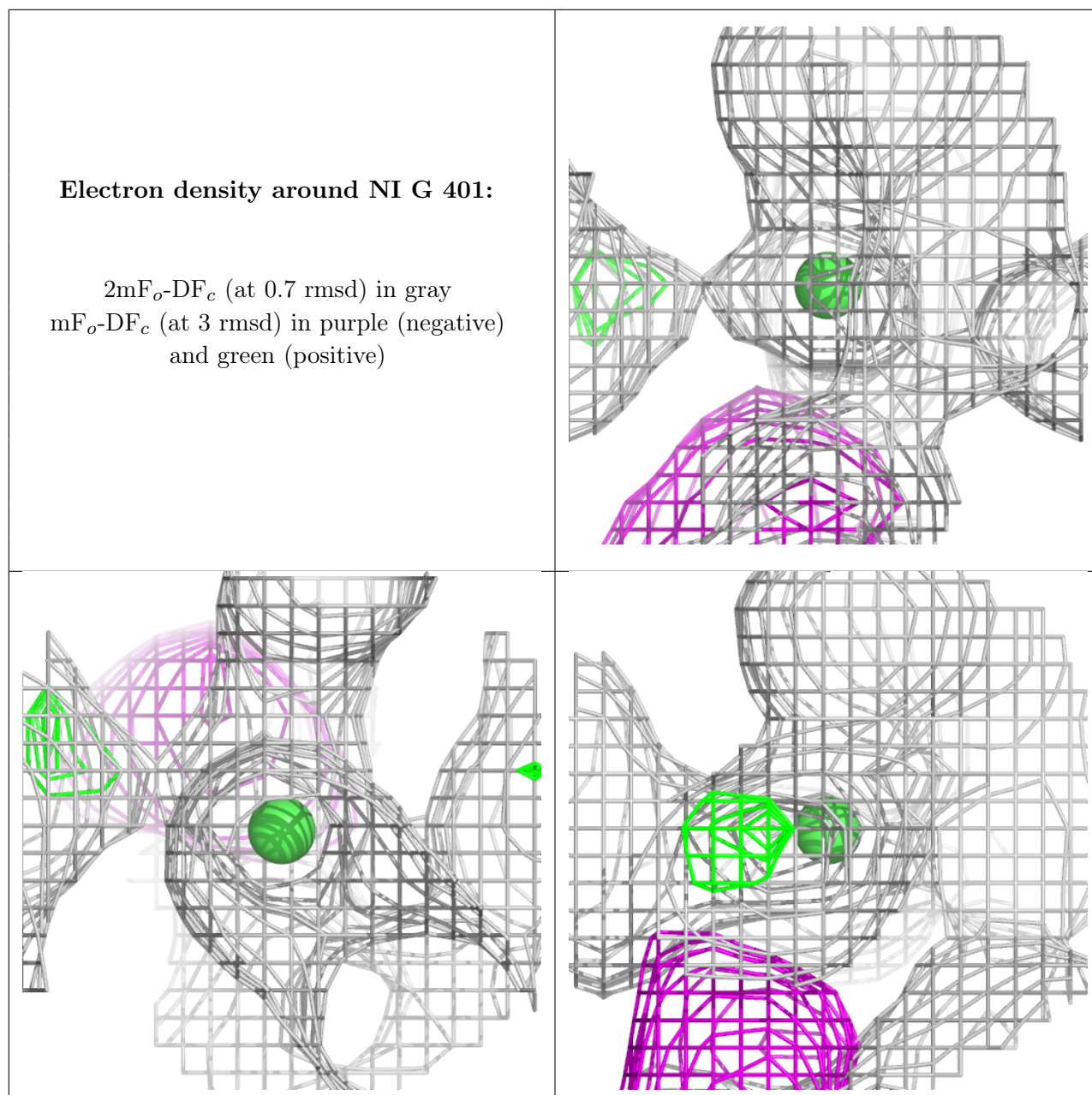


Electron density around NI K 401:

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and green (positive)

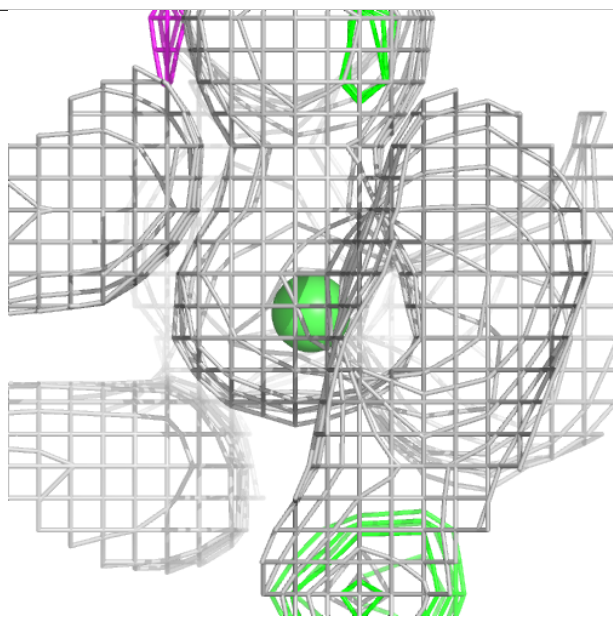
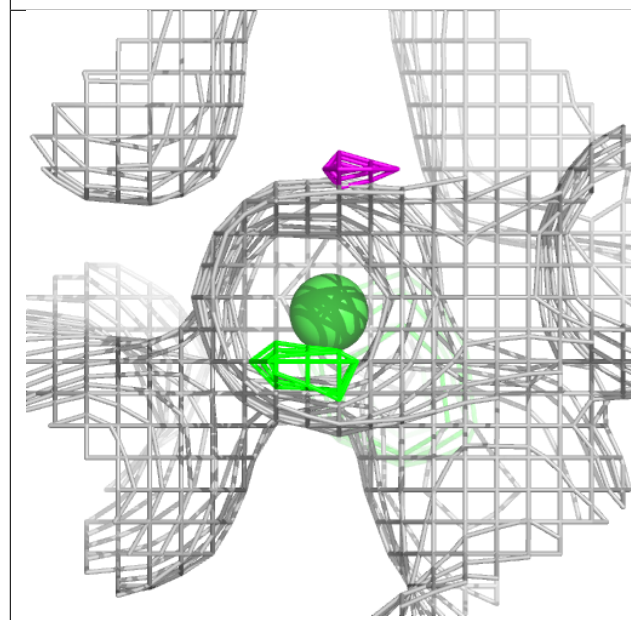
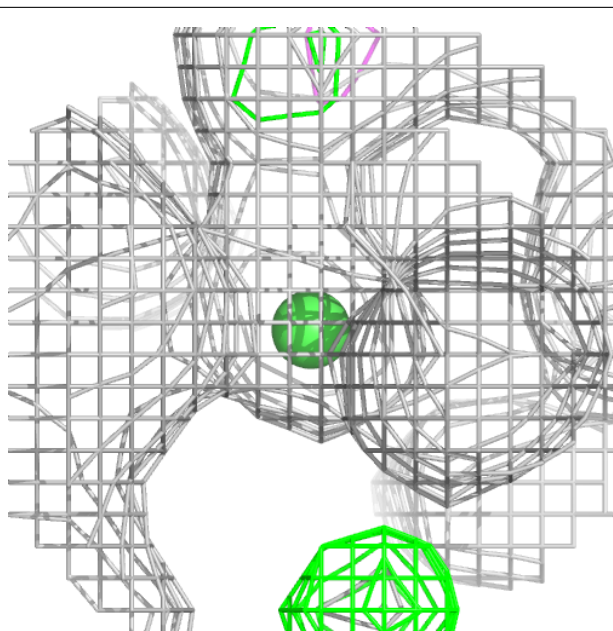






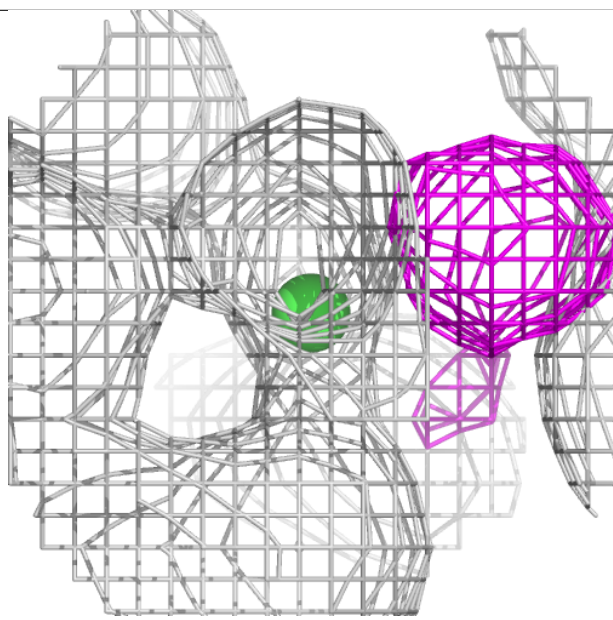
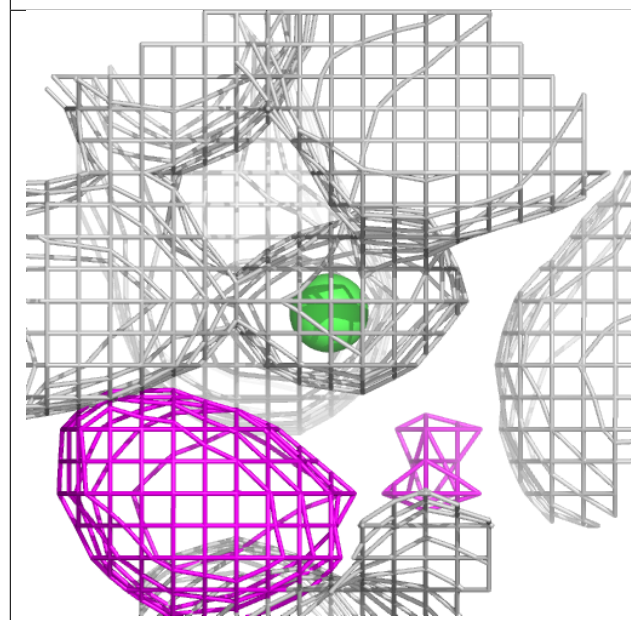
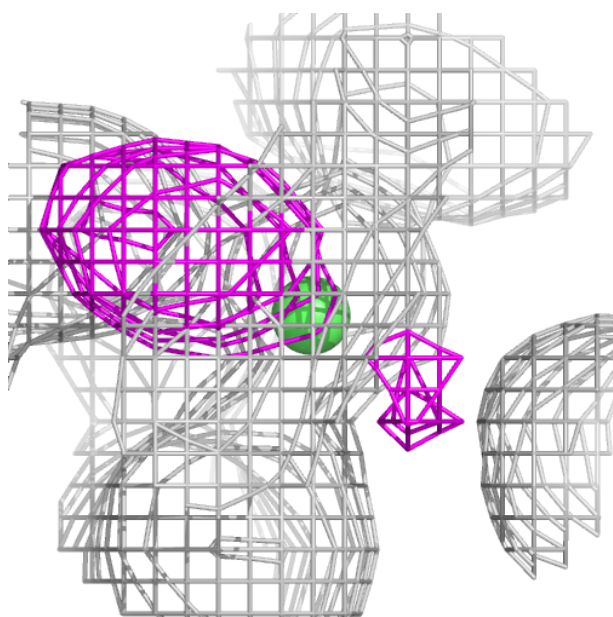
Electron density around NI E 402:

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and green (positive)



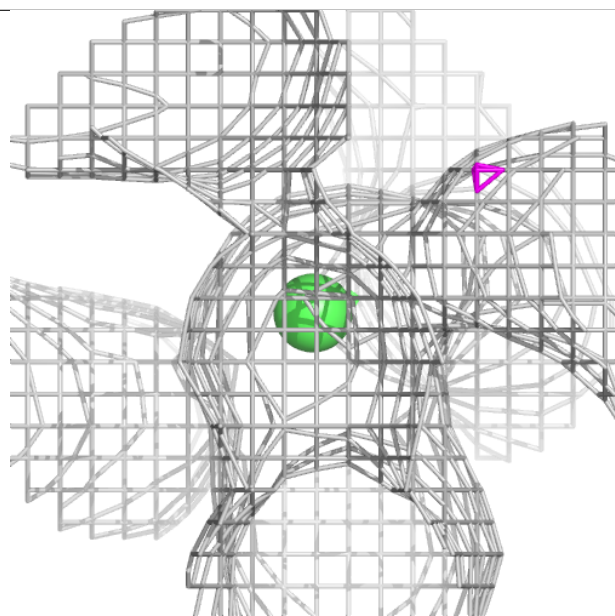
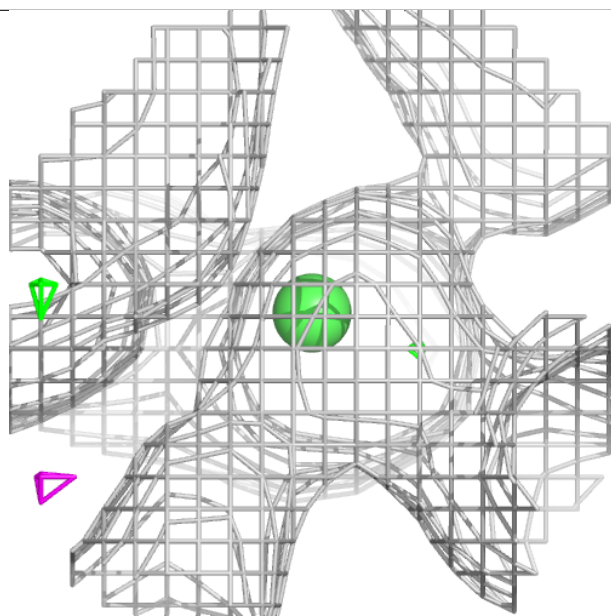
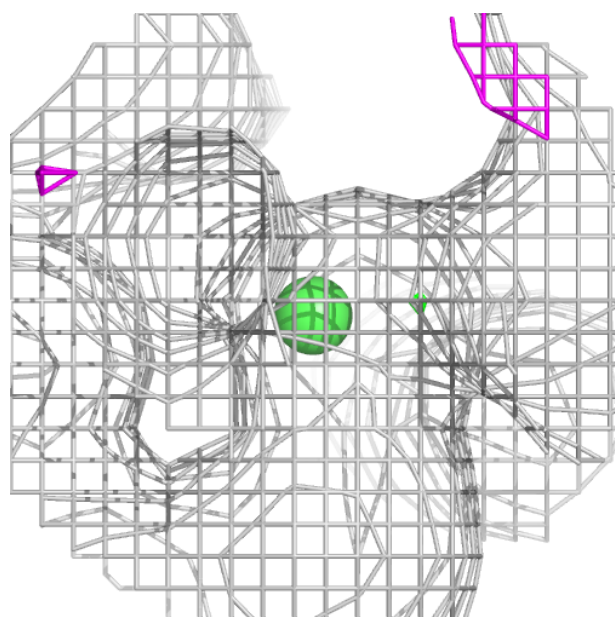
Electron density around NI H 402:

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and green (positive)



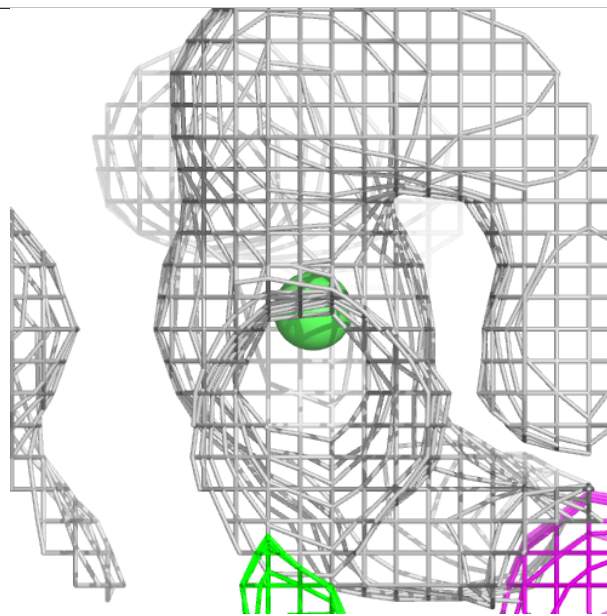
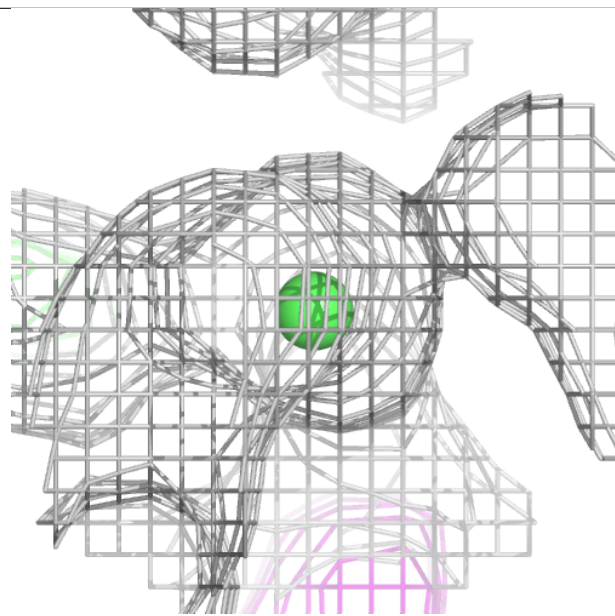
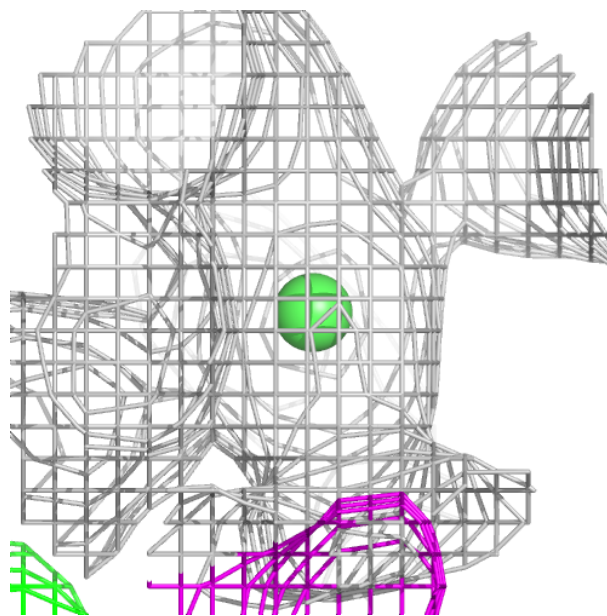
Electron density around NI I 401:

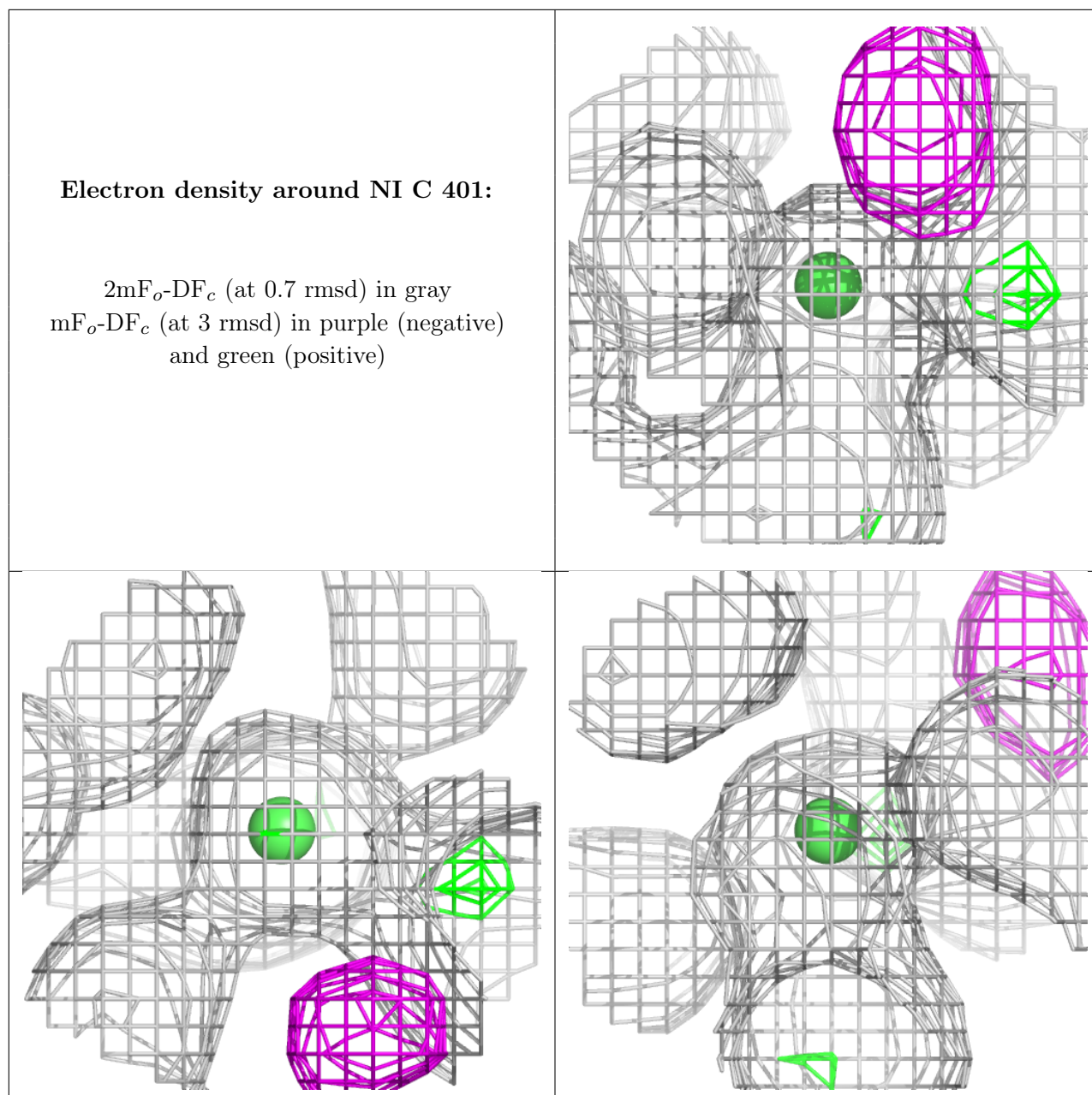
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

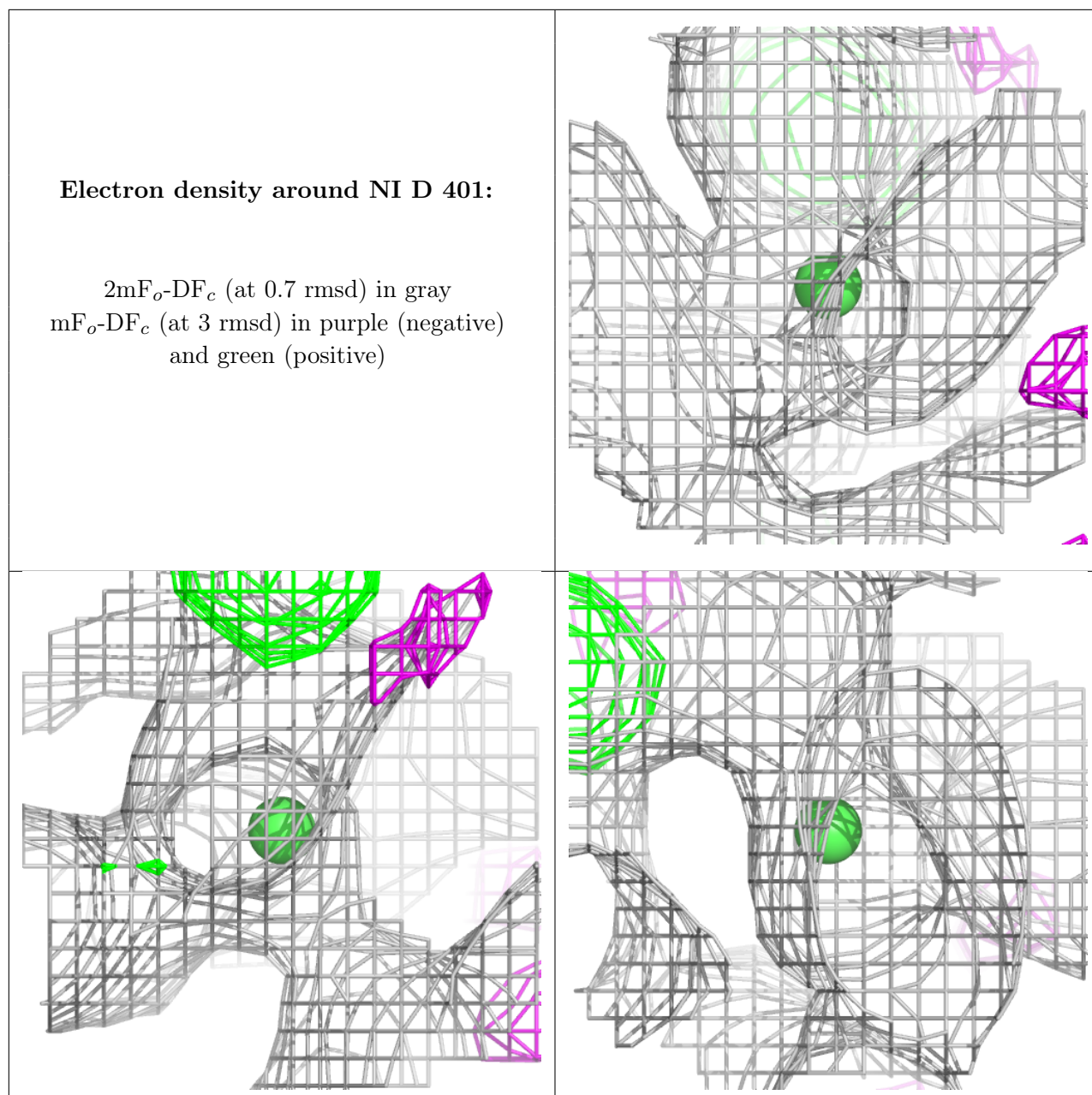


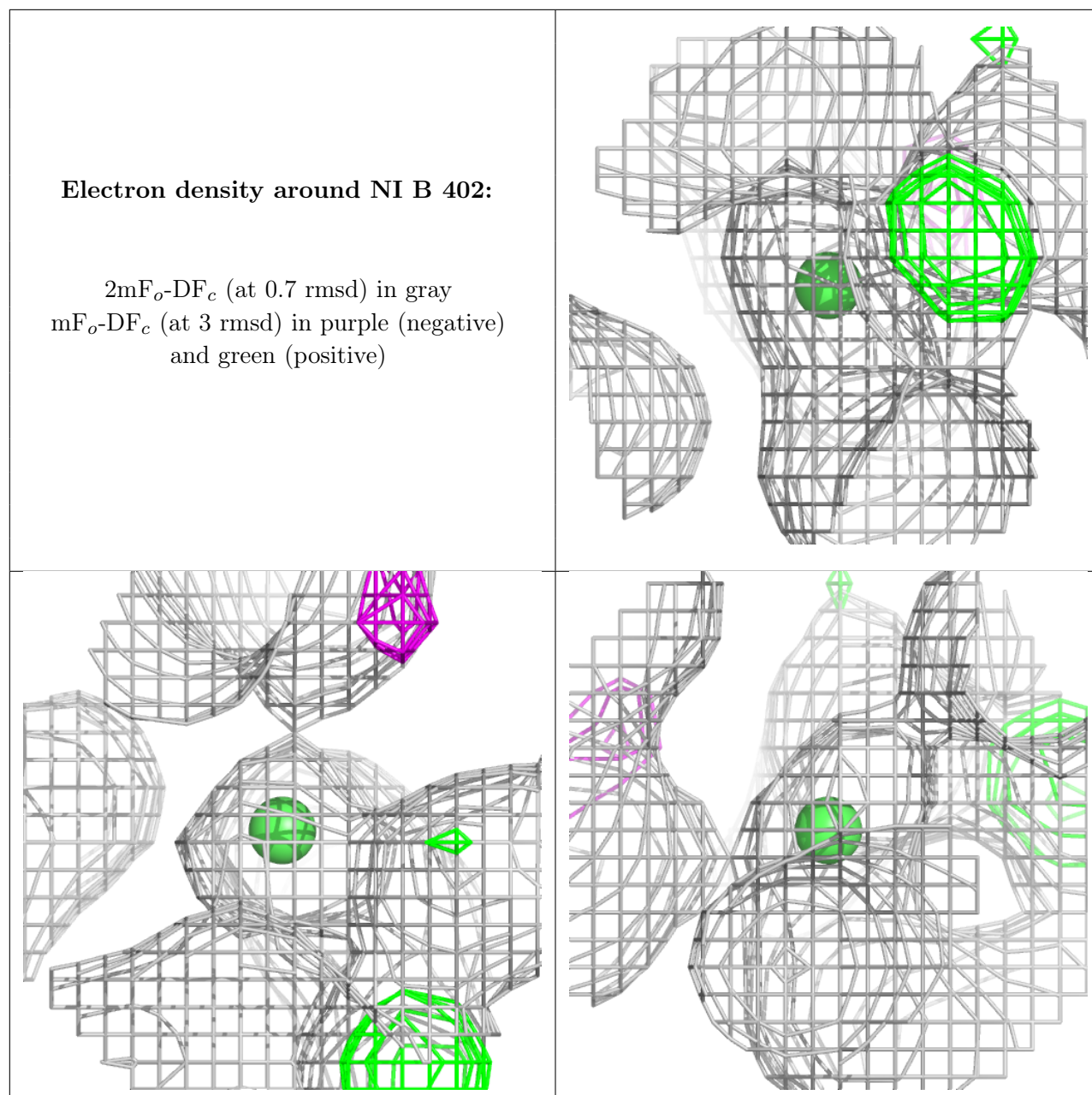
Electron density around NI J 402:

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



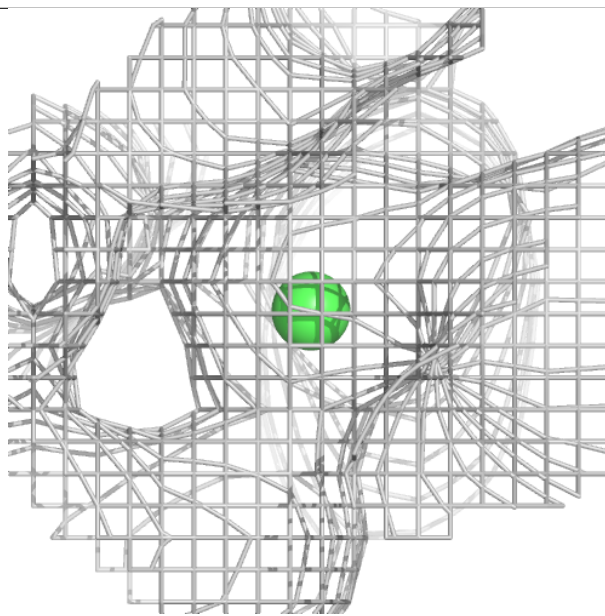
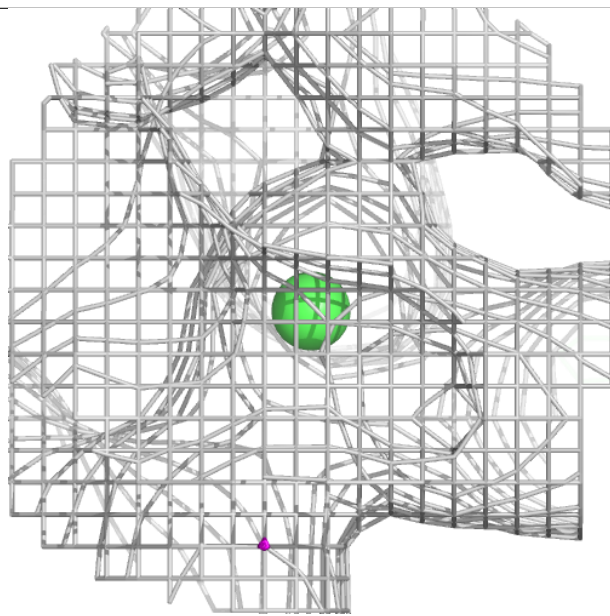
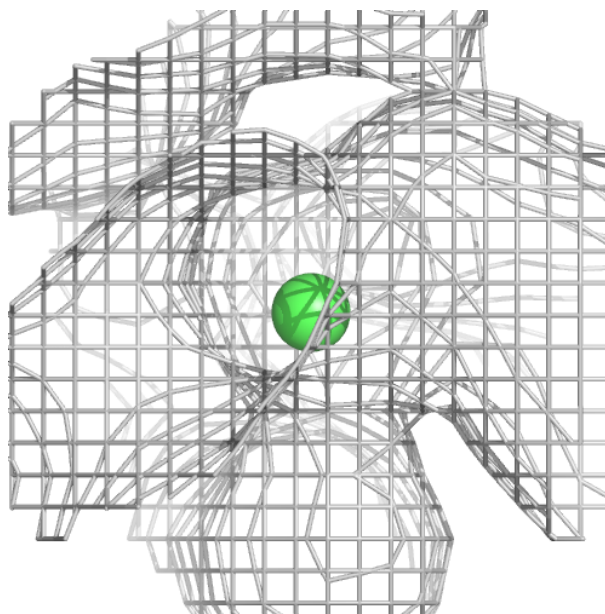






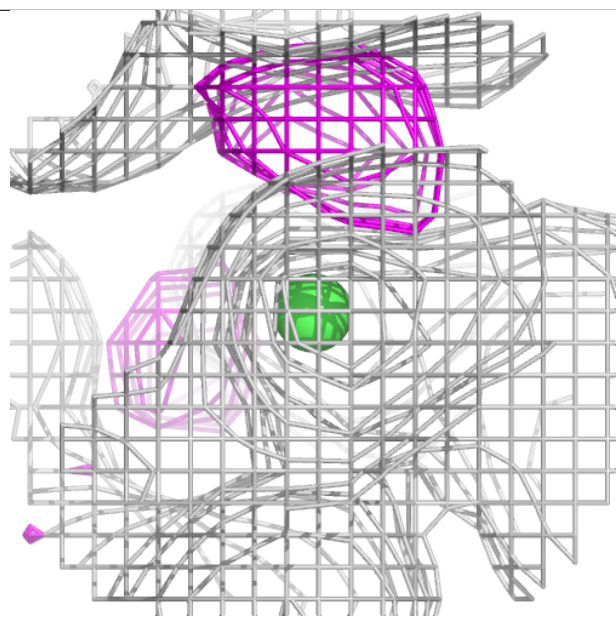
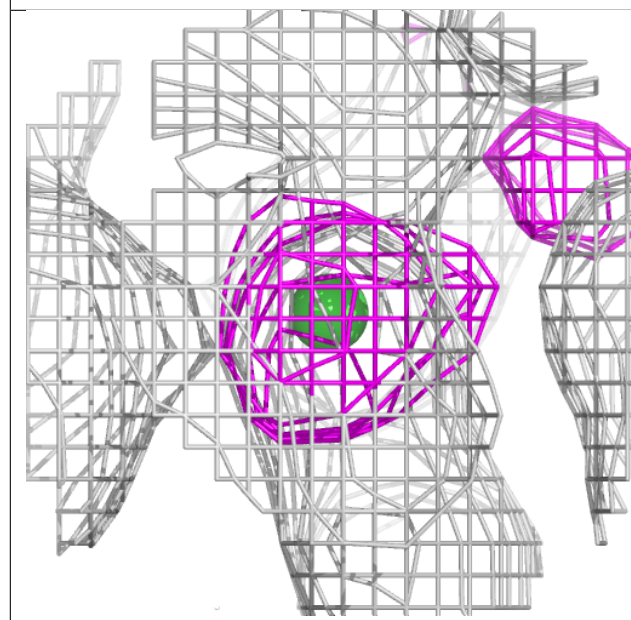
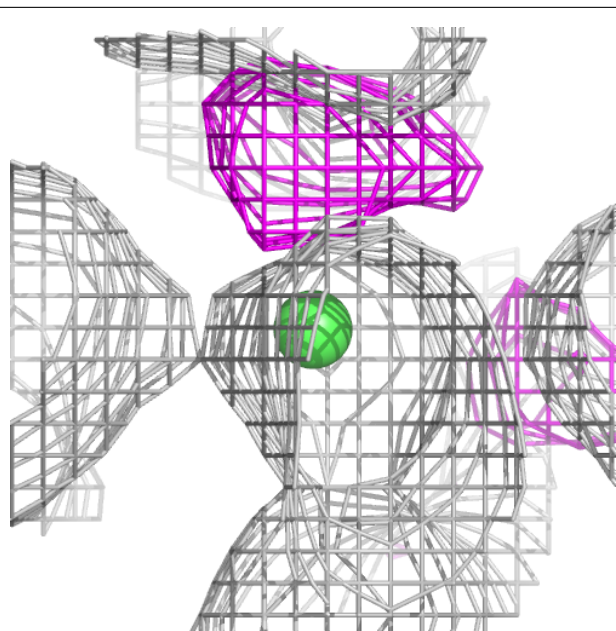
Electron density around NI H 401:

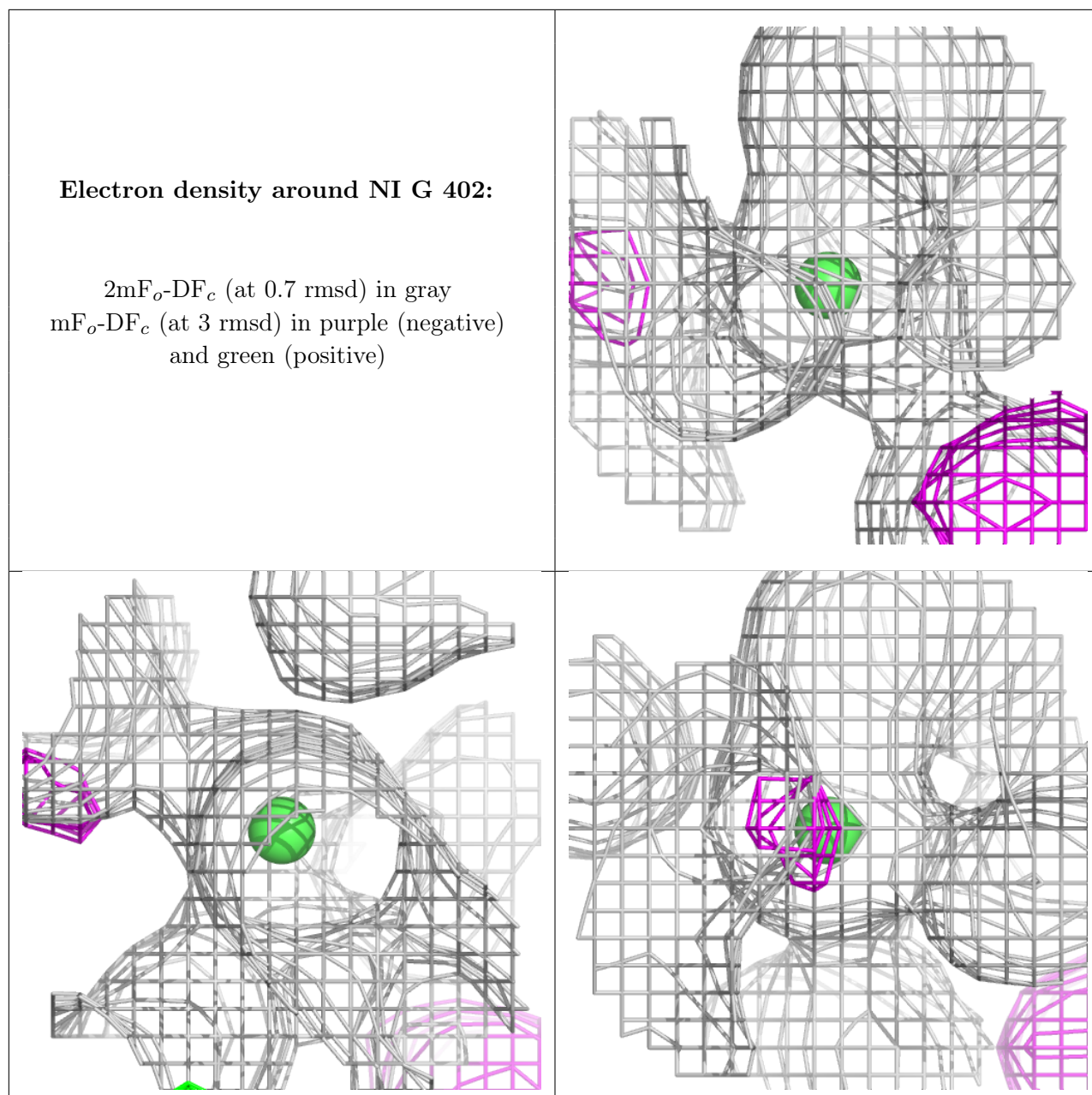
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI F 402:

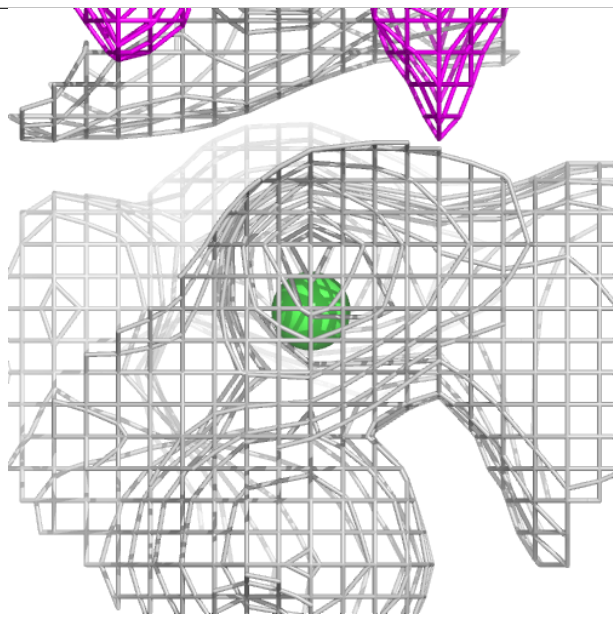
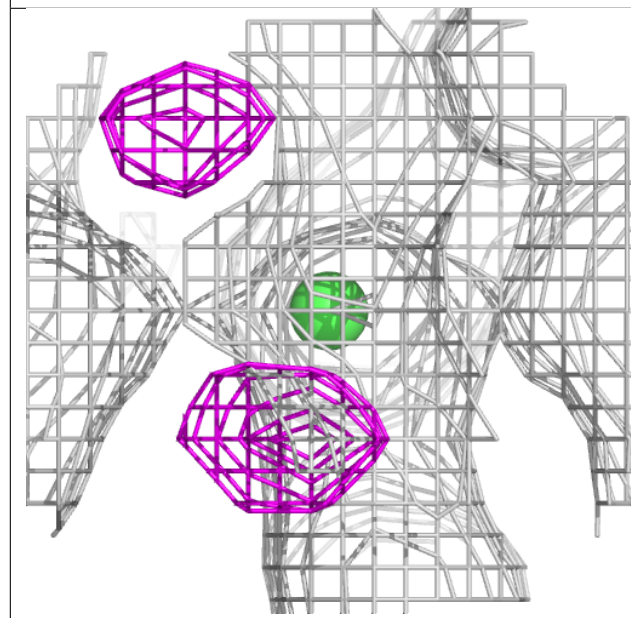
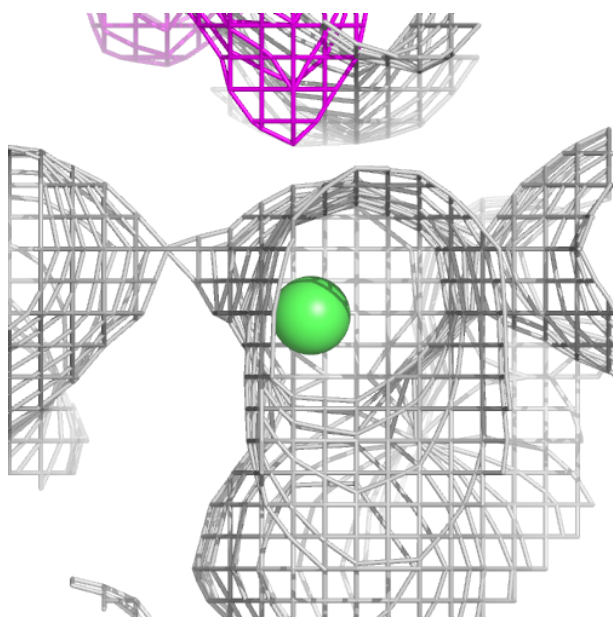
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

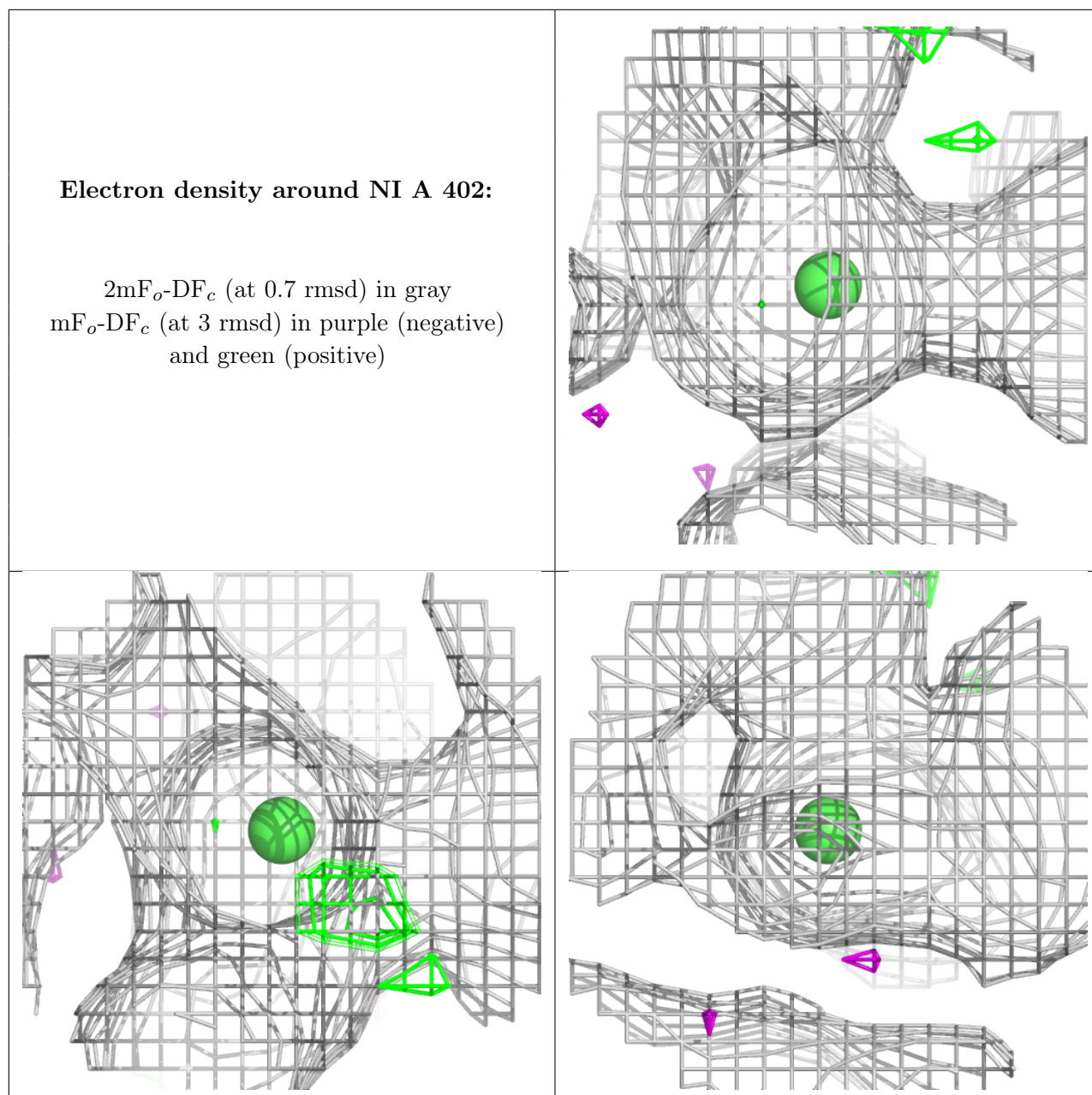




Electron density around NI L 401:

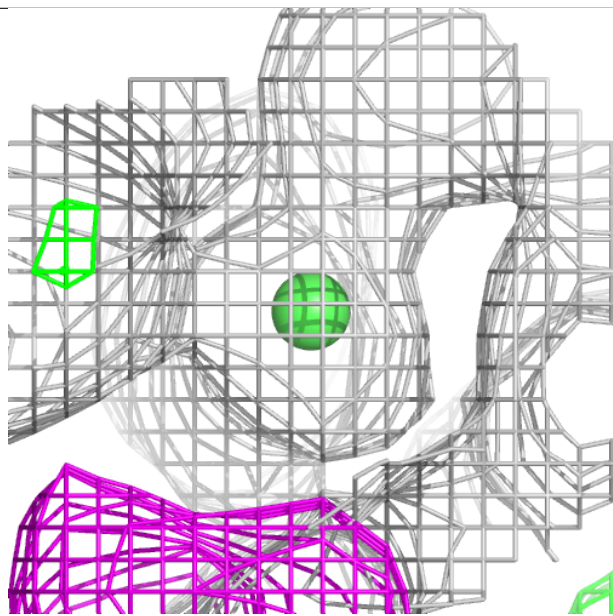
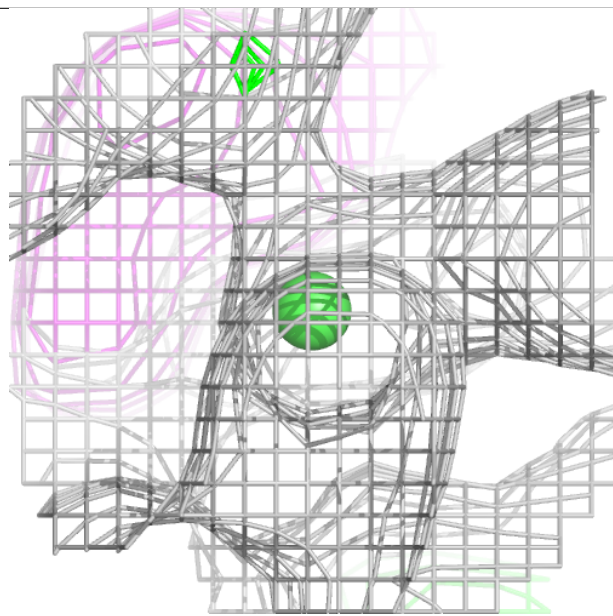
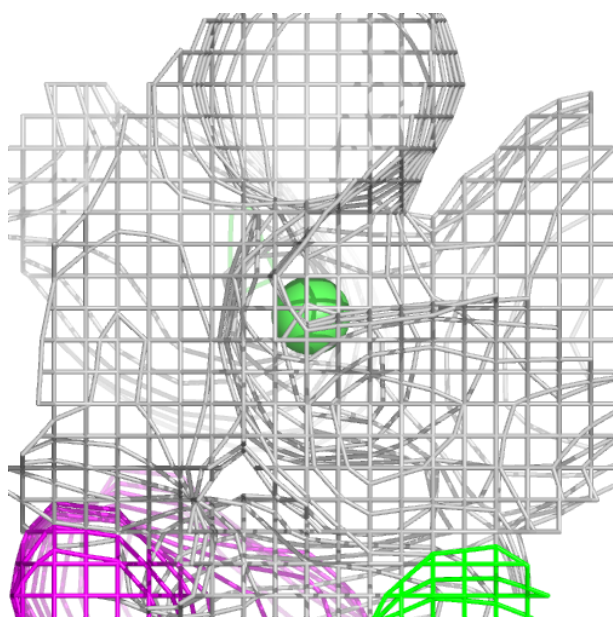
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





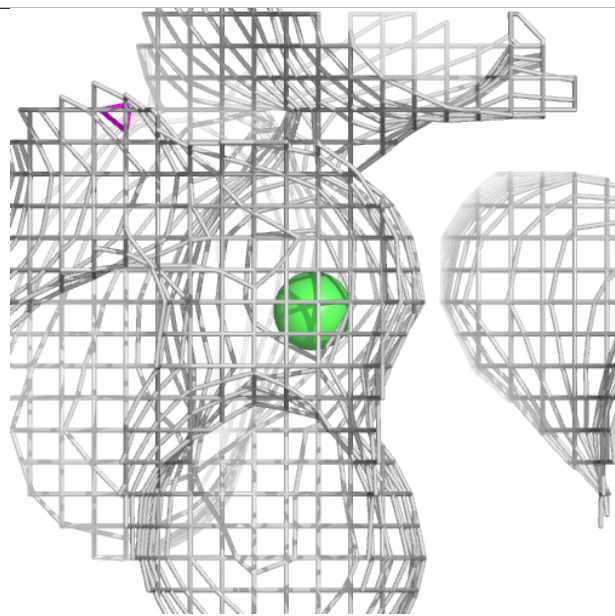
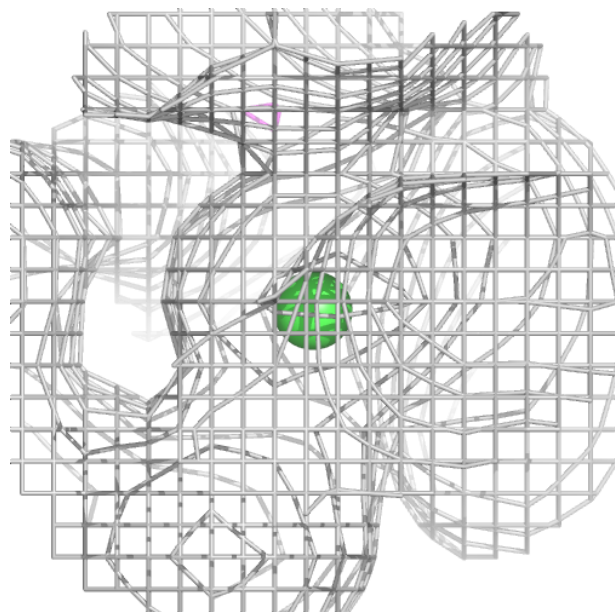
Electron density around NI J 401:

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



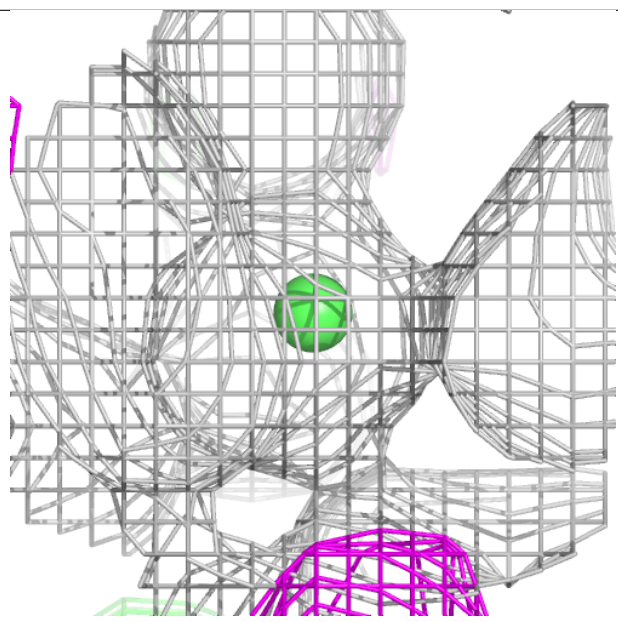
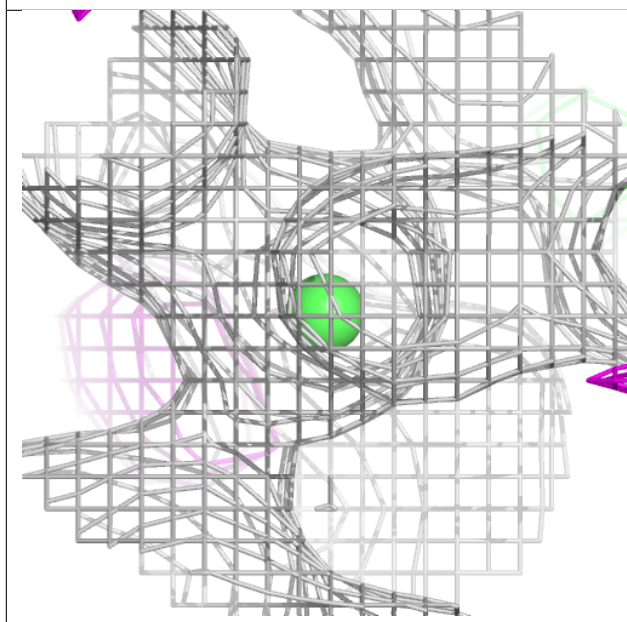
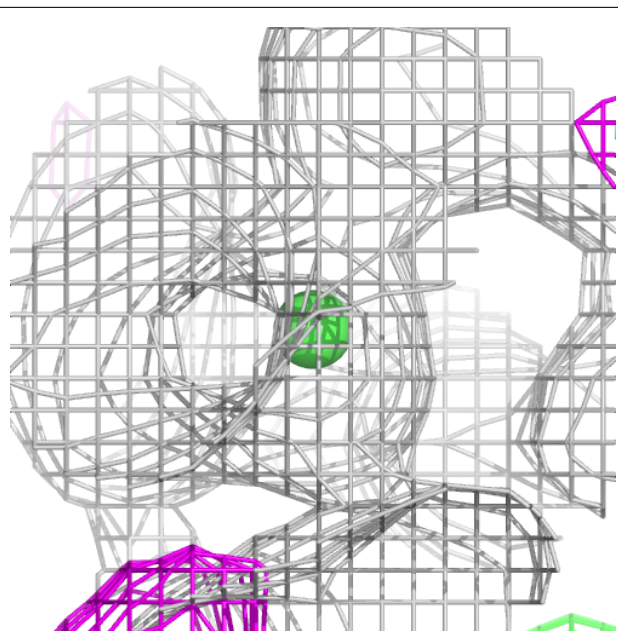
Electron density around NI I 402:

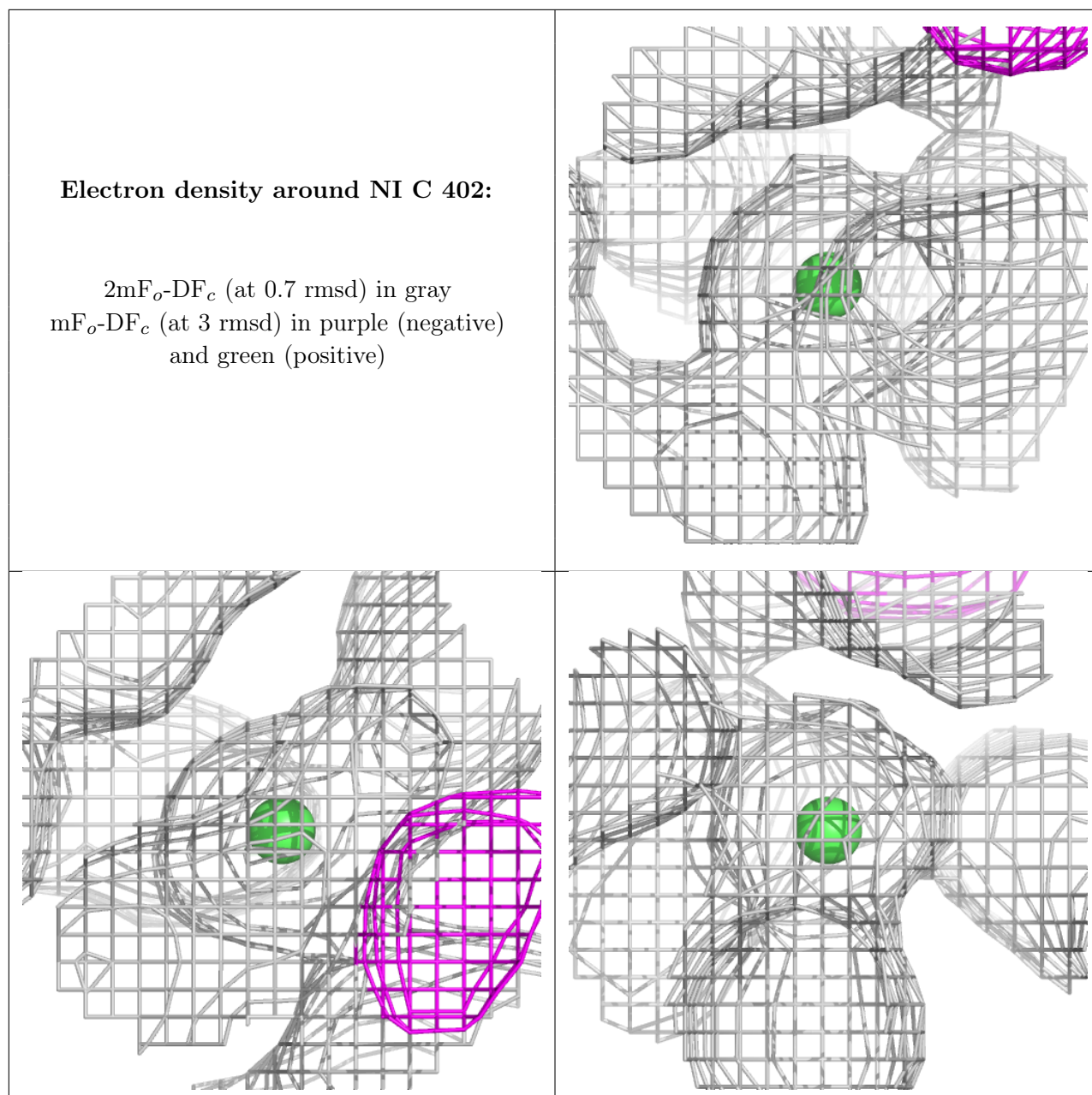
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI E 401:

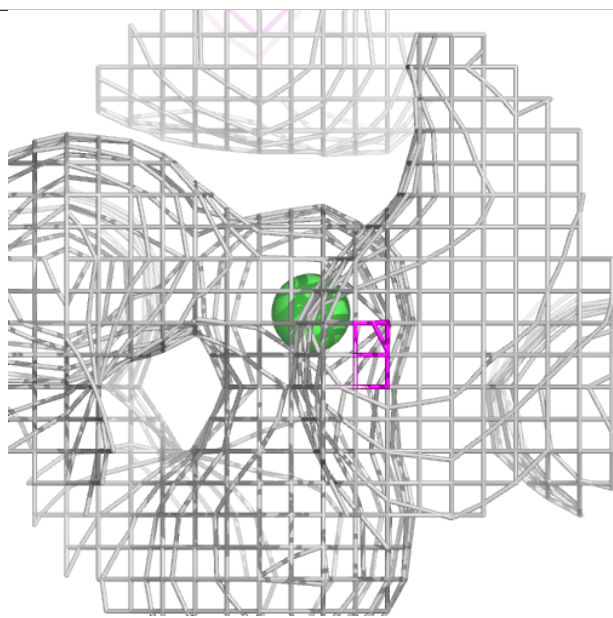
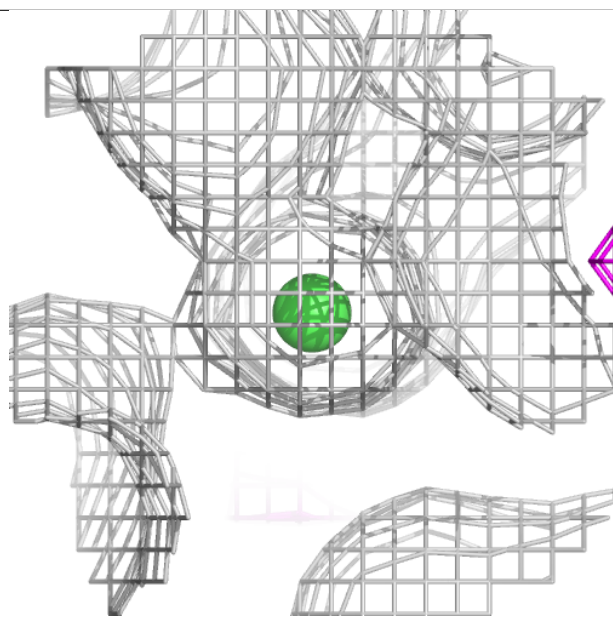
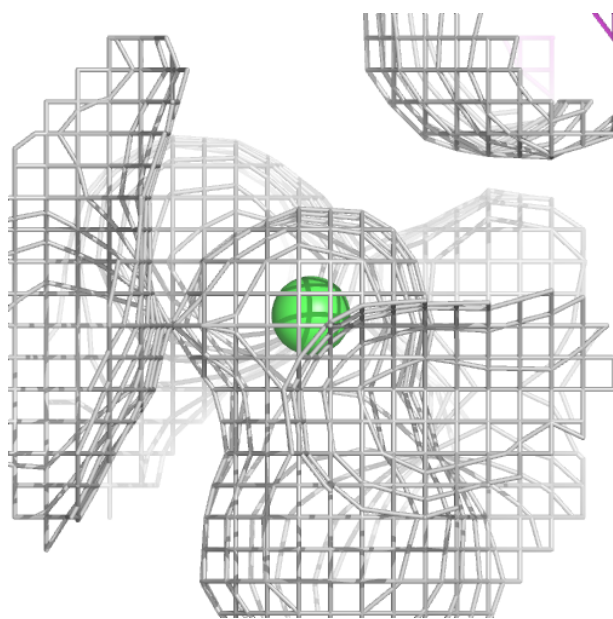
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

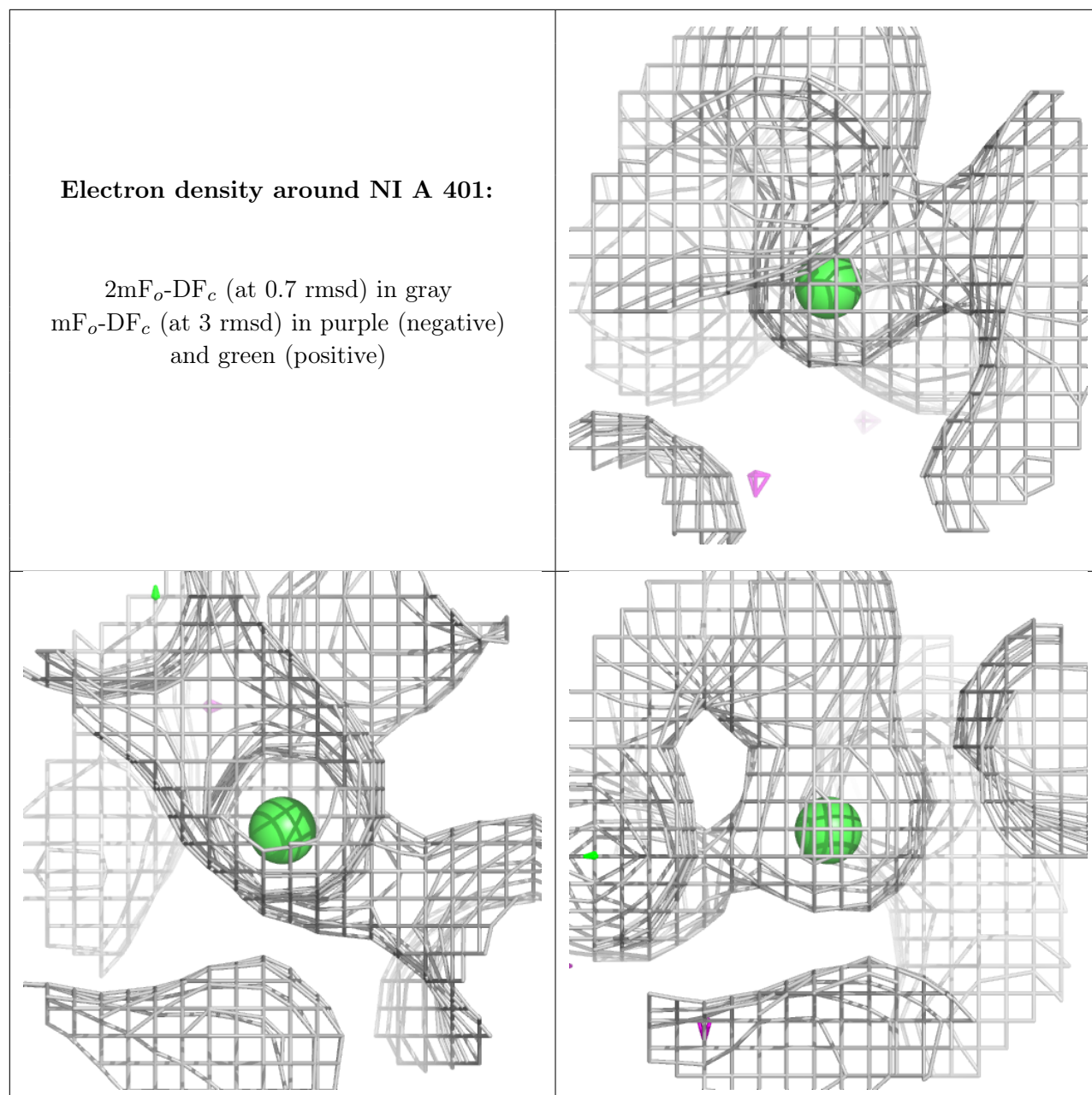




Electron density around NI L 402:

$2mF_o-DF_c$ (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.