



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:10 AM UTC

PDB ID : 9FEK / pdb_00009fek
Title : Crystal structure of guanidinase from Nitrospira inopinata
Authors : Puehringer, D.; Mccarthy, A.
Deposited on : 2024-05-20
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

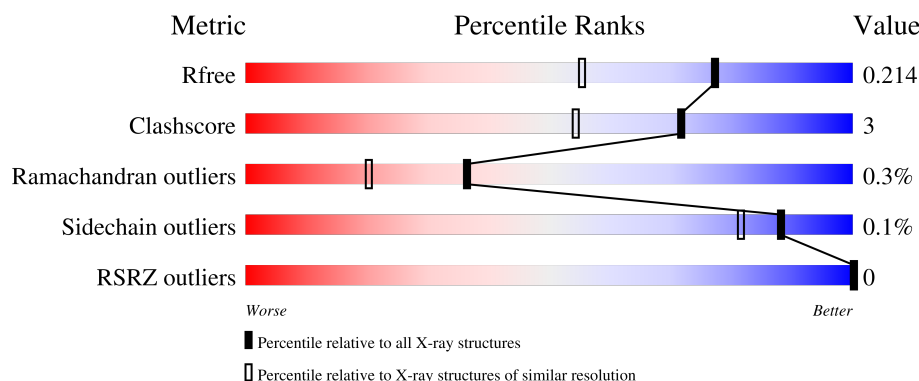
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	89% 8% ..
1	D	384	91% 6% .
1	E	384	92% 5% .

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Mol	Chain	Length	Quality of chain
1	F	384	 90% 8% .
1	G	384	 91% 7% ..
1	H	384	 88% 9% ..
1	I	384	 89% 8% ..
1	J	384	 90% 7% ..
1	K	384	 89% 8% .
1	L	384	 89% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 71343 atoms, of which 33944 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
1	A	374	Total	C	H	N	O	S	0	4	0
			5703	1826	2831	495	539	12			
1	B	374	Total	C	H	N	O	S	0	4	0
			5701	1826	2829	495	539	12			
1	C	374	Total	C	H	N	O	S	0	5	0
			5717	1829	2839	498	539	12			
1	D	373	Total	C	H	N	O	S	0	2	0
			5664	1815	2810	492	535	12			
1	E	374	Total	C	H	N	O	S	0	4	0
			5701	1826	2829	495	539	12			
1	F	374	Total	C	H	N	O	S	0	3	0
			5701	1826	2829	495	539	12			
1	G	377	Total	C	H	N	O	S	0	0	0
			5719	1830	2843	496	537	13			
1	H	374	Total	C	H	N	O	S	0	4	0
			5702	1826	2830	495	539	12			
1	I	375	Total	C	H	N	O	S	0	5	0
			5735	1835	2848	498	542	12			
1	J	374	Total	C	H	N	O	S	0	0	0
			5669	1816	2815	492	534	12			
1	K	373	Total	C	H	N	O	S	0	0	0
			5646	1810	2801	490	533	12			
1	L	375	Total	C	H	N	O	S	0	5	0
			5726	1833	2840	498	543	12			

There are 24 discrepancies between the modelled and reference sequences:

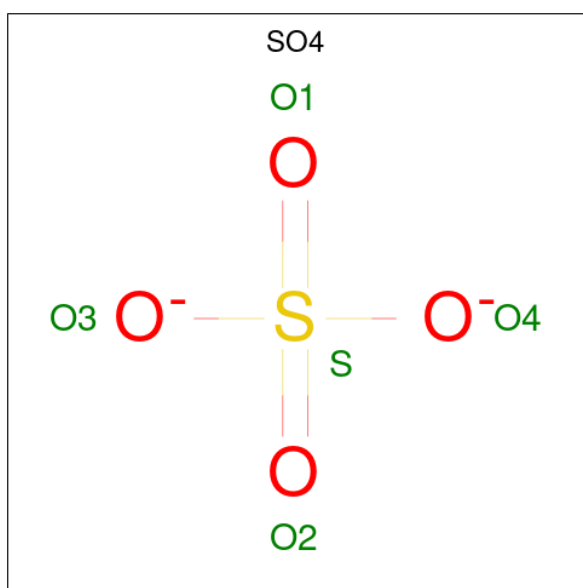
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0S4KUT0
A	0	PRO	-	expression tag	UNP A0A0S4KUT0
B	-1	GLY	-	expression tag	UNP A0A0S4KUT0
B	0	PRO	-	expression tag	UNP A0A0S4KUT0
C	-1	GLY	-	expression tag	UNP A0A0S4KUT0

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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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		
3	G	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		
3	I	1	Total	Mn	0	0
			1	1		
3	J	1	Total	Mn	0	0
			1	1		
3	K	1	Total	Mn	0	0
			1	1		
3	L	1	Total	Mn	0	0
			1	1		

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	B	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	Ni 1	0	0
4	E	1	Total 1	Ni 1	0	0
4	F	1	Total 1	Ni 1	0	0
4	G	1	Total 1	Ni 1	0	0
4	H	1	Total 1	Ni 1	0	0
4	I	1	Total 1	Ni 1	0	0
4	J	1	Total 1	Ni 1	0	0
4	K	1	Total 1	Ni 1	0	0
4	L	1	Total 1	Ni 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	230	Total 230	O 230	0	0
5	B	243	Total 243	O 243	0	0
5	C	238	Total 238	O 238	0	0
5	D	241	Total 241	O 241	0	0
5	E	234	Total 234	O 234	0	0
5	F	210	Total 210	O 210	0	0
5	G	255	Total 255	O 255	0	0
5	H	222	Total 222	O 222	0	0
5	I	245	Total 245	O 245	0	0
5	J	243	Total 243	O 243	0	0

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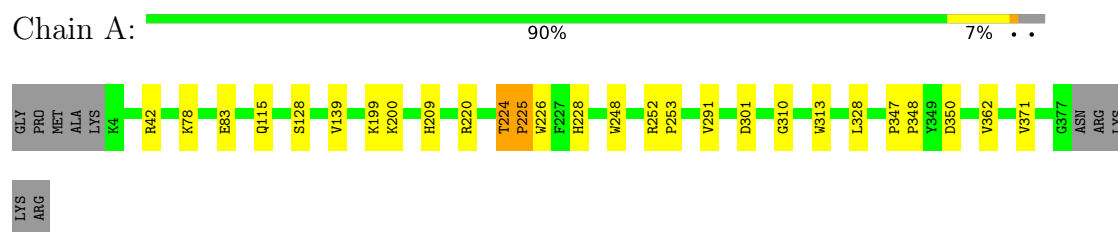
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	236	Total 236	O 236	0	0
5	L	218	Total 218	O 218	0	0

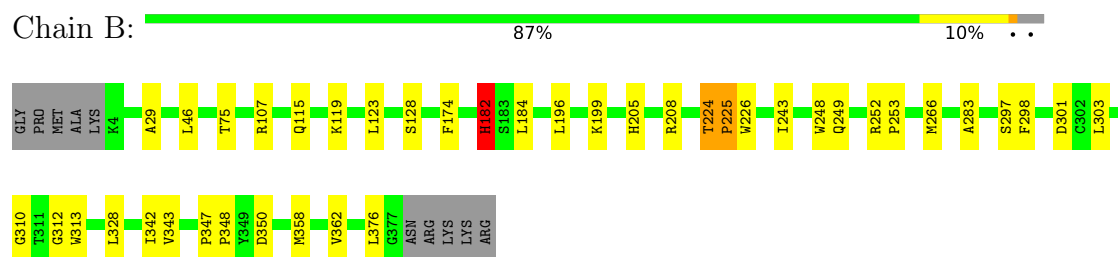
3 Residue-property plots

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.

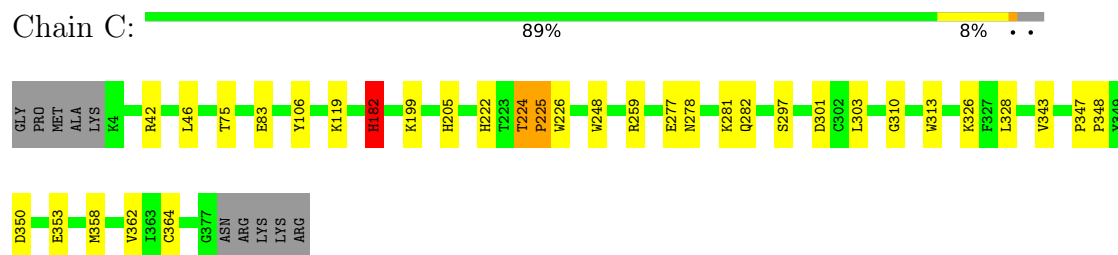
• Molecule 1: Putative agmatinase 2



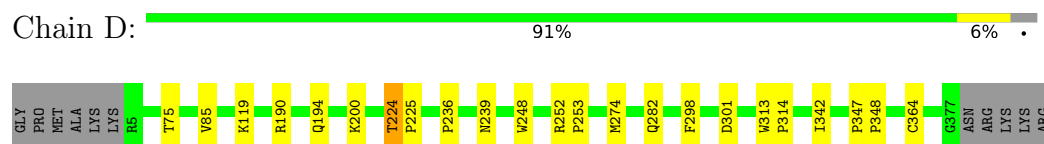
• Molecule 1: Putative agmatinase 2



• Molecule 1: Putative agmatinase 2

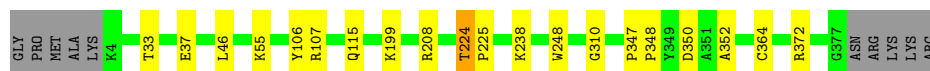


• Molecule 1: Putative agmatinase 2



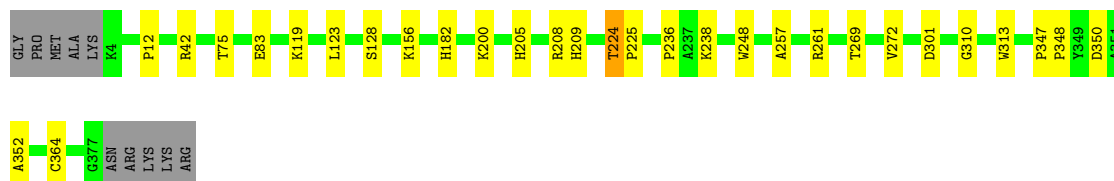
• Molecule 1: Putative agmatinase 2

Chain E:  92% 5% .



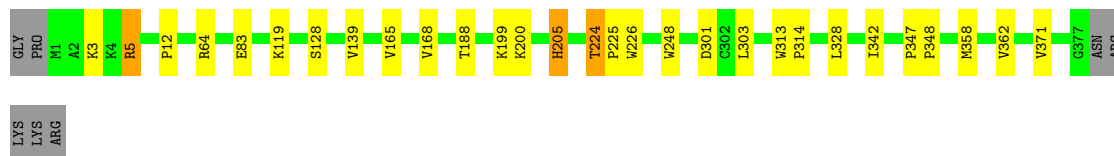
- Molecule 1: Putative agmatinase 2

Chain F:  90% 8% .



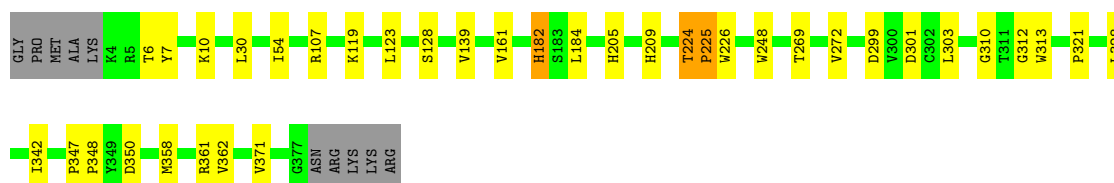
- Molecule 1: Putative agmatinase 2

Chain G:  91% 7% ..



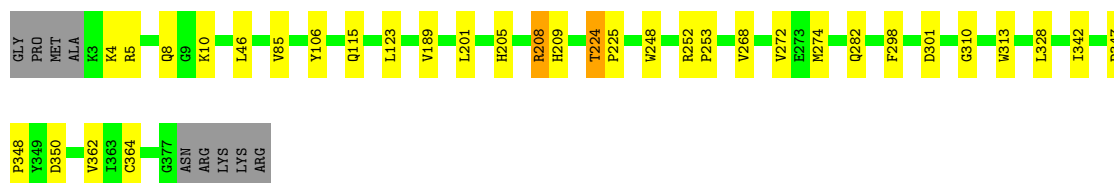
- Molecule 1: Putative agmatinase 2

Chain H:  88% 9% ..



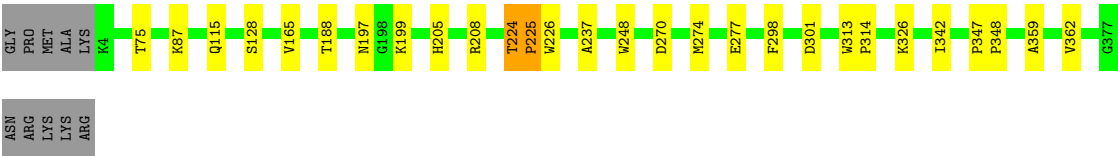
- Molecule 1: Putative agmatinase 2

Chain I:  89% 8% ..

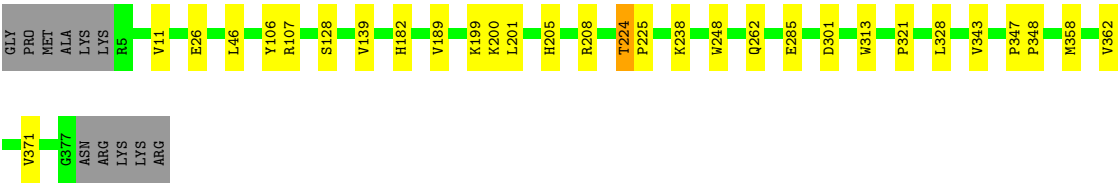
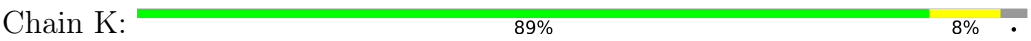


- Molecule 1: Putative agmatinase 2

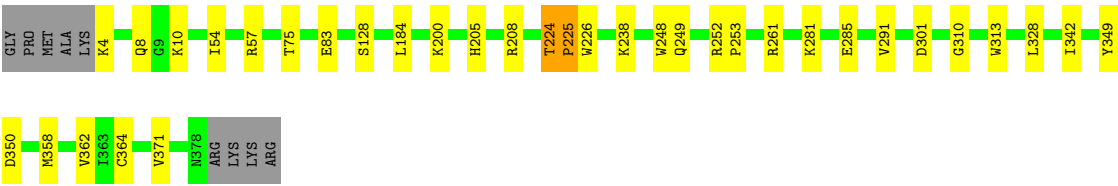
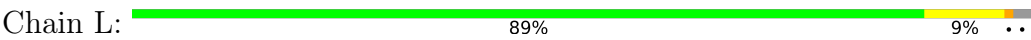
Chain J:  90% 7% ..



● Molecule 1: Putative agmatinase 2



● Molecule 1: Putative agmatinase 2



4 Data and refinement statistics

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) 92.7 (45.01-1.58)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.58Å)	Xtriage
Refinement program	PHENIX (1.21_5184: ???)	Depositor
R, R_{free}	0.200 , 0.214 0.200 , 0.214	Depositor DCC
R_{free} test set	2001 reflections (0.32%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.158 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	71343	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.60 % 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 3.5978e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, NI, SO4

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	0.50	2/2949 (0.1%)	0.65	1/4008 (0.0%)
1	B	0.62	4/2949 (0.1%)	0.76	6/4008 (0.1%)
1	C	0.58	3/2960 (0.1%)	0.72	4/4022 (0.1%)
1	D	0.61	1/2931 (0.0%)	0.73	1/3984 (0.0%)
1	E	0.54	0/2949	0.68	1/4008 (0.0%)
1	F	0.47	2/2940 (0.1%)	0.62	2/3996 (0.1%)
1	G	0.68	4/2944 (0.1%)	0.75	0/3999
1	H	0.58	3/2949 (0.1%)	0.72	1/4008 (0.0%)
1	I	0.52	1/2962 (0.0%)	0.64	2/4025 (0.0%)
1	J	0.64	5/2922 (0.2%)	0.73	2/3971 (0.1%)
1	K	0.53	1/2913 (0.0%)	0.66	2/3960 (0.1%)
1	L	0.62	4/2961 (0.1%)	0.74	2/4025 (0.0%)
All	All	0.57	30/35329 (0.1%)	0.70	24/48014 (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 (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	12	PRO	N-CD	-15.89	1.25	1.47
1	C	205	HIS	C-O	-9.46	1.12	1.24
1	J	237	ALA	C-N	-8.45	1.22	1.33
1	B	226	TRP	C-O	-8.44	1.12	1.24
1	K	205	HIS	C-O	-8.02	1.14	1.24
1	C	226	TRP	C-O	-7.75	1.14	1.24
1	A	226	TRP	C-O	-7.44	1.14	1.24
1	B	205	HIS	C-O	-6.95	1.16	1.24
1	L	225	PRO	C-O	-6.64	1.15	1.24
1	L	226	TRP	C-O	-6.58	1.15	1.24
1	H	54	ILE	C-N	-6.47	1.24	1.33
1	H	225	PRO	C-O	-6.36	1.16	1.24
1	L	184	LEU	C-O	-6.33	1.15	1.24
1	G	168	VAL	C-O	-6.31	1.16	1.24
1	C	225	PRO	C-O	-6.30	1.16	1.24
1	L	205	HIS	C-O	-6.24	1.16	1.24
1	H	321	PRO	C-O	-6.12	1.16	1.24
1	F	205	HIS	C-O	-6.09	1.17	1.24
1	B	225	PRO	C-O	-6.07	1.16	1.24
1	A	225	PRO	C-O	-6.03	1.16	1.24
1	I	205	HIS	C-O	-5.85	1.17	1.24
1	B	184	LEU	C-O	-5.78	1.16	1.24
1	J	205	HIS	C-O	-5.76	1.17	1.24
1	J	225	PRO	C-O	-5.51	1.17	1.24
1	D	314	PRO	C-O	-5.43	1.17	1.23
1	F	12	PRO	N-CD	-5.39	1.40	1.47
1	J	226	TRP	C-O	-5.38	1.17	1.24
1	J	314	PRO	C-O	-5.11	1.18	1.23
1	G	314	PRO	C-O	-5.06	1.18	1.23
1	G	205	HIS	C-O	-5.06	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	HIS	CB-CG-CD2	-12.03	115.56	131.20
1	B	182	HIS	CB-CG-ND1	11.05	139.28	122.70
1	C	182	HIS	CB-CG-ND1	8.55	135.52	122.70
1	C	182	HIS	CB-CG-CD2	-7.83	121.03	131.20
1	K	205	HIS	CA-C-O	-6.33	113.96	120.54
1	B	205	HIS	CA-C-O	-6.19	113.84	120.46
1	K	208	ARG	N-CA-C	-5.63	106.25	113.23
1	L	208	ARG	N-CA-C	-5.61	106.27	113.23
1	D	75	THR	N-CA-C	-5.56	102.52	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	208	ARG	N-CA-C	-5.56	106.33	113.23
1	H	205	HIS	CA-C-O	-5.34	114.74	120.46
1	C	75	THR	N-CA-C	-5.34	102.84	110.59
1	J	75	THR	N-CA-C	-5.34	102.84	110.59
1	F	208	ARG	N-CA-C	-5.32	106.64	113.23
1	F	75	THR	N-CA-C	-5.30	102.67	110.52
1	J	208	ARG	N-CA-C	-5.22	106.91	113.28
1	I	205	HIS	CA-C-O	-5.09	115.01	120.46
1	E	208	ARG	N-CA-C	-5.09	106.92	113.23
1	L	75	THR	N-CA-C	-5.08	103.22	110.59
1	A	226	TRP	CA-C-O	-5.08	113.01	119.31
1	C	205	HIS	CA-C-O	-5.07	115.03	120.46
1	B	208	ARG	N-CA-C	-5.04	106.98	113.23
1	B	75	THR	N-CA-C	-5.03	103.30	110.59
1	B	226	TRP	CA-C-O	-5.01	113.41	119.27

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

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	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2872	2829	2822	26	0
1	C	2878	2839	2825	24	0
1	D	2854	2810	2802	16	0
1	E	2872	2829	2822	18	0
1	F	2872	2829	2827	22	0
1	G	2876	2843	2844	22	0
1	H	2872	2830	2822	29	0
1	I	2887	2848	2836	28	0
1	J	2854	2815	2814	18	0
1	K	2845	2801	2801	16	0
1	L	2886	2840	2829	24	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	0	0
2	K	10	0	0	0	0
2	L	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	230	0	0	2	0
5	B	243	0	0	0	0
5	C	238	0	0	1	0
5	D	241	0	0	0	0
5	E	234	0	0	1	0
5	F	210	0	0	2	0
5	G	255	0	0	0	0
5	H	222	0	0	0	0
5	I	245	0	0	0	0
5	J	243	0	0	1	0
5	K	236	0	0	0	0
5	L	218	0	0	1	0
All	All	37399	33944	33866	228	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 (228) 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:E:55:LYS:HD2	1:F:156:LYS:HZ3	1.26	0.98
1:L:238:LYS:HE2	1:L:238:LYS:H	1.31	0.92
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:E:55:LYS:CD	1:F:156:LYS:HZ3	2.02	0.71
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:G:83:GLU:CG	1:I:46:LEU:HD13	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:274:MET:HE1	1:D:282[B]:GLN:CD	2.27	0.60
1:L:238:LYS:H	1:L:238:LYS:CE	2.09	0.60
1:E:238:LYS:HD3	1:E:238:LYS:N	2.17	0.59
1:J:87:LYS:NZ	5:J:502:HOH:O	2.36	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:K:285:GLU:C	1:K:285:GLU:OE1	2.50	0.55
1:L:4:LYS:NZ	5:L:502:HOH:O	2.39	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:G:358:MET:HE3	1:G:362:VAL:HG23	1.89	0.55
1:B:298:PHE:HB3	1:B:342:ILE:HD13	1.88	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	5:F:547:HOH:O	2.08	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:H:10:LYS:HE3	1:H:30:LEU:CD1	2.38	0.52
1:C:182:HIS:NE2	1:C:297:SER:OG	2.41	0.52
1:C:199:LYS:HD2	5:C:605: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: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:G:64:ARG:NH2	1:I:85:VAL:HG22	2.25	0.51
1:K:321:PRO:HB3	1:K:358:MET:HE1	1.93	0.51
1:A:139:VAL:HG11	1:A:371:VAL:HG22	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:THR:N	1:E:225:PRO:CD	2.75	0.50
1:C:301:ASP:OD2	1:C:313:TRP:CD1	2.64	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:I:274:MET:HE1	1:I:282:GLN:OE1	2.13	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	5:F:547: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: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
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:B:182:HIS:CG	1:B:343:VAL:HG21	2.49	0.48
1:J:347:PRO:N	1:J:348:PRO:CD	2.77	0.48
1:C:224:THR:N	1:C:225:PRO:CD	2.77	0.48
1:K:139:VAL:HG11	1:K:371:VAL:HG22	1.96	0.48
1:A:78:LYS:HE2	5:A:539: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: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:B:243:ILE:HG12	1:B:266:MET:HE2	1.97	0.47
1:G:347:PRO:N	1:G:348:PRO:CD	2.78	0.47
1:L:224:THR:N	1:L: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:ALA:O	1:F:261:ARG:HG3	2.15	0.46
1:I:4:LYS:HD3	1:I:4:LYS:N	2.31	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:B:224:THR:N	1:B:225:PRO:CD	2.79	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:F:200:LYS:HD3	1:F:236:PRO:HG3	1.98	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:K:301:ASP:OD2	1:K:313:TRP:NE1	2.49	0.45
1:I:342:ILE:HG23	1:I:342:ILE:O	2.17	0.45
1:A:224:THR:N	1:A:225:PRO:CD	2.80	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:H:161:VAL:HG21	1:H:184:LEU:HD22	1.99	0.44
1:B:266:MET:HE1	1:B:283:ALA:HB2	1.98	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:301:ASP:OD2	1:B:313:TRP:NE1	2.51	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:E:199:LYS:HG3	5:E:553: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:K:182:HIS:ND1	1:K:343:VAL:HG21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:182:HIS:CG	1:C:343:VAL:HG21	2.54	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
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:248:TRP:CZ2	1:F:364:CYS:HB3	2.54	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:B:303:LEU:HD21	1:B:358:MET:HE2	2.00	0.42
1:J:165:VAL:HG21	1:J:188:THR:HG22	2.02	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:328:LEU:HD13	1:I:362:VAL:HG13	2.02	0.42
5: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:L:342:ILE:HG23	1:L:342:ILE:O	2.19	0.41
1:B:182:HIS:NE2	1:B:297:SER:OG	2.46	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:L:358:MET:HE2	1:L:358:MET:HB2	1.97	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:C:303:LEU:HD11	1:C:358:MET:HE2	2.03	0.41
1:D:301:ASP:OD2	1:D:313:TRP:NE1	2.54	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:222:HIS:CE1	1:C:313:TRP:CE3	3.08	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:D:274:MET:HE1	1:D:282[B]:GLN:NE2	2.36	0.41
1:D:298:PHE:HB3	1:D:342:ILE:HD12	2.02	0.41
1:J:301:ASP:OD1	1:J:301:ASP:C	2.63	0.41
1:L:252:ARG:N	1:L:253:PRO:HD2	2.35	0.41
1:I:301:ASP:C	1:I:301:ASP:OD1	2.64	0.41
1:A:220:ARG:HD2	1:A:228:HIS:CD2	2.56	0.40
1:F:301:ASP:OD1	1:F:301:ASP:C	2.63	0.40
1:G:303:LEU:HD13	1:G:358:MET:HG2	2.03	0.40
1:H:342:ILE:O	1:H:342:ILE:HG23	2.19	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:L:301:ASP:OD2	1:L:313:TRP:NE1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	20
1	B	376/384 (98%)	366 (97%)	9 (2%)	1 (0%)	36	20
1	C	377/384 (98%)	368 (98%)	8 (2%)	1 (0%)	36	20
1	D	373/384 (97%)	365 (98%)	7 (2%)	1 (0%)	36	20
1	E	376/384 (98%)	365 (97%)	10 (3%)	1 (0%)	36	20
1	F	375/384 (98%)	364 (97%)	10 (3%)	1 (0%)	36	20
1	G	375/384 (98%)	366 (98%)	8 (2%)	1 (0%)	36	20
1	H	376/384 (98%)	366 (97%)	9 (2%)	1 (0%)	36	20
1	I	378/384 (98%)	367 (97%)	10 (3%)	1 (0%)	36	20
1	J	372/384 (97%)	362 (97%)	9 (2%)	1 (0%)	36	20
1	K	371/384 (97%)	361 (97%)	9 (2%)	1 (0%)	36	20
1	L	378/384 (98%)	367 (97%)	10 (3%)	1 (0%)	36	20
All	All	4503/4608 (98%)	4384 (97%)	107 (2%)	12 (0%)	36	20

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	THR
1	B	224	THR
1	D	224	THR

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Mol	Chain	Res	Type
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 ⓘ

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%)	300 (100%)	1 (0%)	86	79
1	B	301/307 (98%)	300 (100%)	1 (0%)	86	79
1	C	302/307 (98%)	301 (100%)	1 (0%)	86	79
1	D	300/307 (98%)	300 (100%)	0	100	100
1	E	301/307 (98%)	301 (100%)	0	100	100
1	F	300/307 (98%)	299 (100%)	1 (0%)	86	79
1	G	301/307 (98%)	301 (100%)	0	100	100
1	H	301/307 (98%)	300 (100%)	1 (0%)	86	79
1	I	303/307 (99%)	303 (100%)	0	100	100
1	J	299/307 (97%)	299 (100%)	0	100	100
1	K	298/307 (97%)	298 (100%)	0	100	100
1	L	303/307 (99%)	303 (100%)	0	100	100
All	All	3610/3684 (98%)	3605 (100%)	5 (0%)	88	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	LYS

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Mol	Chain	Res	Type
1	B	182	HIS
1	C	182	HIS
1	F	182	HIS
1	H	182	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	213	GLN
1	A	242	GLN
1	B	74	ASN
1	B	195	HIS
1	C	213	GLN
1	C	242	GLN
1	D	16	ASN
1	D	115	GLN
1	D	197	ASN
1	D	213	GLN
1	E	115	GLN
1	E	195	HIS
1	E	213	GLN
1	E	239	ASN
1	F	195	HIS
1	F	213	GLN
1	G	8	GLN
1	G	16	ASN
1	G	115	GLN
1	G	195	HIS
1	G	242	GLN
1	H	195	HIS
1	H	213	GLN
1	H	242	GLN
1	I	16	ASN
1	I	74	ASN
1	J	16	ASN
1	J	74	ASN
1	K	115	GLN
1	K	194	GLN
1	K	213	GLN
1	L	74	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	SO4	C	401	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	E	402	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	J	401	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	E	401	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	B	401	-	4,4,4	0.29	0	6,6,6	0.27	0
2	SO4	H	402	-	4,4,4	0.19	0	6,6,6	0.14	0
2	SO4	H	401	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	I	401	-	4,4,4	0.31	0	6,6,6	0.22	0
2	SO4	B	402	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	C	402	-	4,4,4	0.25	0	6,6,6	0.24	0
2	SO4	D	402	-	4,4,4	0.30	0	6,6,6	0.14	0
2	SO4	G	401	-	4,4,4	0.30	0	6,6,6	0.24	0
2	SO4	G	402	-	4,4,4	0.35	0	6,6,6	0.07	0
2	SO4	D	401	-	4,4,4	0.30	0	6,6,6	0.12	0
2	SO4	F	402	-	4,4,4	0.20	0	6,6,6	0.27	0
2	SO4	A	402	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	L	401	-	4,4,4	0.34	0	6,6,6	0.18	0
2	SO4	J	402	-	4,4,4	0.46	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	F	401	-	4,4,4	0.21	0	6,6,6	0.17	0
2	SO4	I	402	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	K	402	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	L	402	-	4,4,4	0.32	0	6,6,6	0.25	0
2	SO4	K	401	-	4,4,4	0.33	0	6,6,6	0.18	0
2	SO4	A	401	-	4,4,4	0.37	0	6,6,6	0.18	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	374/384 (97%)	-0.86	0 100 100	10, 26, 41, 75	3 (0%)
1	B	374/384 (97%)	-0.90	0 100 100	11, 25, 39, 66	3 (0%)
1	C	374/384 (97%)	-0.87	0 100 100	10, 24, 39, 59	3 (0%)
1	D	373/384 (97%)	-0.89	0 100 100	15, 24, 38, 56	1 (0%)
1	E	374/384 (97%)	-0.86	0 100 100	11, 25, 41, 75	3 (0%)
1	F	374/384 (97%)	-0.84	0 100 100	11, 26, 42, 78	3 (0%)
1	G	377/384 (98%)	-0.89	0 100 100	16, 25, 41, 59	0
1	H	374/384 (97%)	-0.85	0 100 100	11, 25, 41, 78	3 (0%)
1	I	375/384 (97%)	-0.84	0 100 100	11, 26, 42, 72	4 (1%)
1	J	374/384 (97%)	-0.89	0 100 100	17, 25, 40, 88	0
1	K	373/384 (97%)	-0.84	0 100 100	15, 26, 40, 56	0
1	L	375/384 (97%)	-0.85	0 100 100	11, 26, 40, 81	4 (1%)
All	All	4491/4608 (97%)	-0.87	0 100 100	10, 25, 41, 88	27 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NI	H	404	1/1	0.93	0.16	40,40,40,40	1
4	NI	D	404	1/1	0.96	0.10	46,46,46,46	1
3	MN	C	403	1/1	0.97	0.06	28,28,28,28	1
4	NI	F	404	1/1	0.97	0.17	41,41,41,41	1
3	MN	G	403	1/1	0.97	0.06	38,38,38,38	1
3	MN	F	403	1/1	0.98	0.09	31,31,31,31	1
2	SO4	E	402	5/5	0.98	0.04	34,35,43,49	0
4	NI	A	404	1/1	0.98	0.15	40,40,40,40	1
4	NI	B	404	1/1	0.98	0.05	44,44,44,44	1
4	NI	C	404	1/1	0.98	0.04	40,40,40,40	1
2	SO4	I	402	5/5	0.98	0.04	39,43,56,58	0
2	SO4	K	401	5/5	0.98	0.05	25,29,34,42	0
4	NI	G	404	1/1	0.98	0.05	39,39,39,39	1
2	SO4	C	401	5/5	0.98	0.04	27,29,31,34	0
4	NI	K	404	1/1	0.98	0.09	42,42,42,42	1
4	NI	L	404	1/1	0.98	0.13	37,37,37,37	1
2	SO4	I	401	5/5	0.99	0.04	26,31,32,42	0
2	SO4	B	401	5/5	0.99	0.03	23,25,31,35	0
2	SO4	J	401	5/5	0.99	0.04	29,29,32,39	0
2	SO4	J	402	5/5	0.99	0.03	28,31,43,43	0
2	SO4	B	402	5/5	0.99	0.03	32,33,43,49	0
2	SO4	K	402	5/5	0.99	0.03	37,40,46,48	0
2	SO4	L	401	5/5	0.99	0.04	25,27,33,53	0
2	SO4	L	402	5/5	0.99	0.04	29,33,41,45	0
3	MN	A	403	1/1	0.99	0.03	35,35,35,35	1
3	MN	B	403	1/1	0.99	0.06	41,41,41,41	1
2	SO4	A	401	5/5	0.99	0.04	25,27,34,38	0
3	MN	D	403	1/1	0.99	0.03	33,33,33,33	1
2	SO4	C	402	5/5	0.99	0.03	32,36,38,44	0
2	SO4	D	401	5/5	0.99	0.03	34,36,46,47	0
3	MN	H	403	1/1	0.99	0.03	34,34,34,34	1
3	MN	I	403	1/1	0.99	0.03	25,25,25,25	1
3	MN	J	403	1/1	0.99	0.05	29,29,29,29	1
3	MN	K	403	1/1	0.99	0.04	33,33,33,33	1
3	MN	L	403	1/1	0.99	0.04	35,35,35,35	1
2	SO4	D	402	5/5	0.99	0.04	30,30,34,36	0
2	SO4	E	401	5/5	0.99	0.04	28,29,35,37	0

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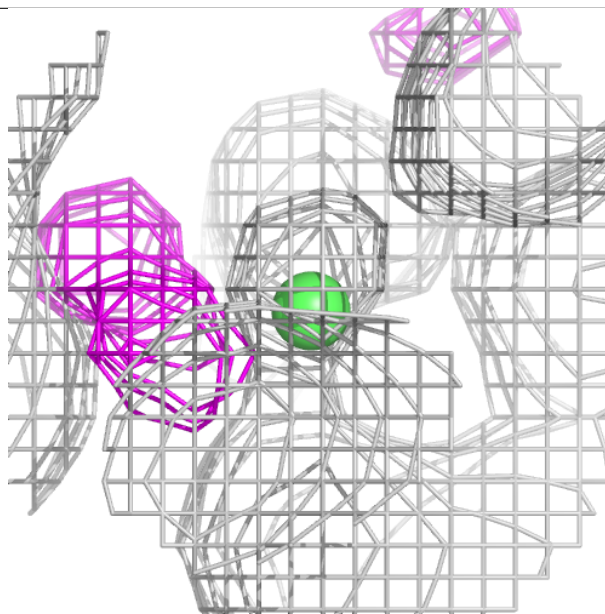
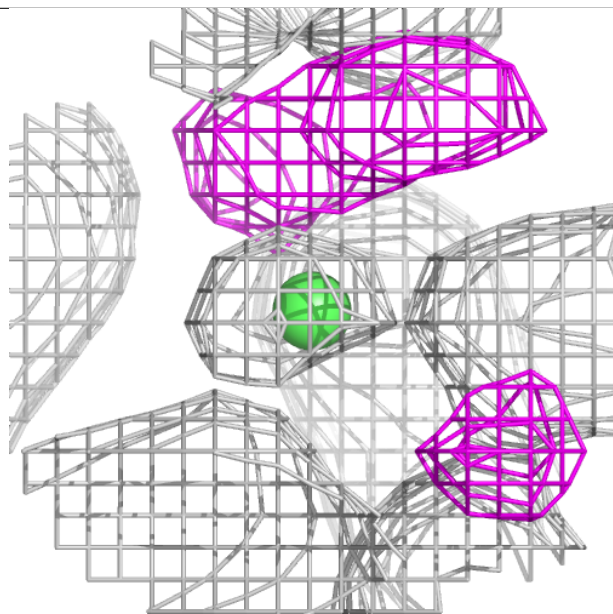
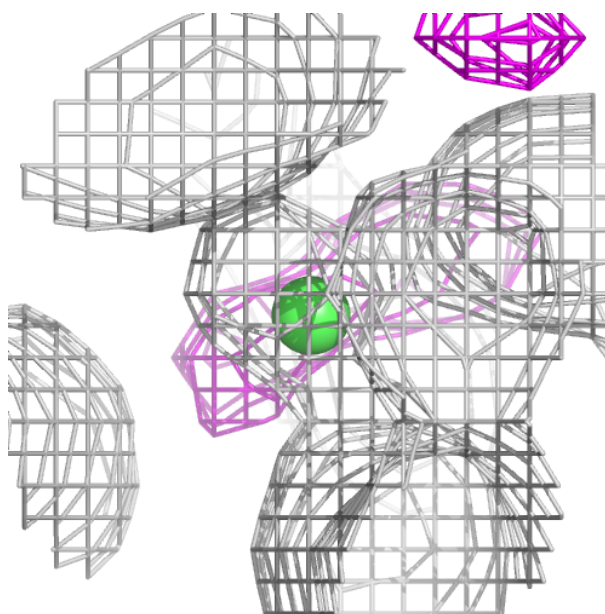
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	402	5/5	0.99	0.04	35,40,46,46	0
2	SO4	F	401	5/5	0.99	0.03	28,29,34,42	0
4	NI	E	404	1/1	0.99	0.07	38,38,38,38	1
2	SO4	F	402	5/5	0.99	0.04	40,42,42,48	0
2	SO4	G	401	5/5	0.99	0.07	24,25,31,40	0
2	SO4	G	402	5/5	0.99	0.04	35,37,57,58	0
4	NI	I	404	1/1	0.99	0.04	42,42,42,42	1
4	NI	J	404	1/1	0.99	0.04	43,43,43,43	1
2	SO4	H	401	5/5	0.99	0.04	24,28,33,35	0
2	SO4	H	402	5/5	0.99	0.04	29,39,45,47	0
3	MN	E	403	1/1	1.00	0.04	27,27,27,27	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.

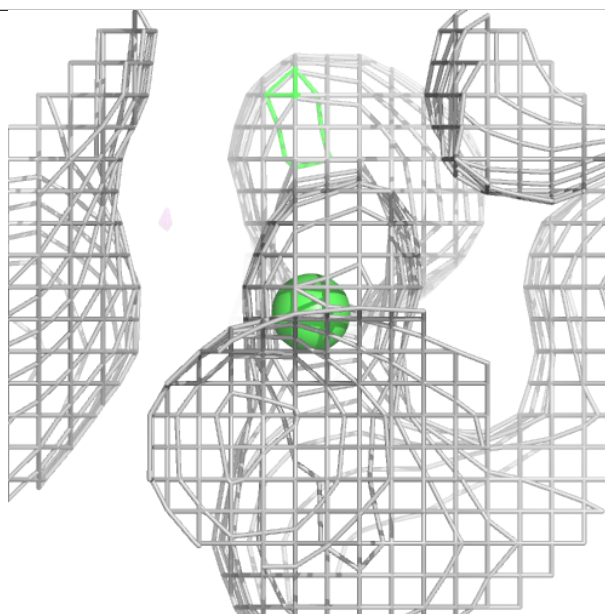
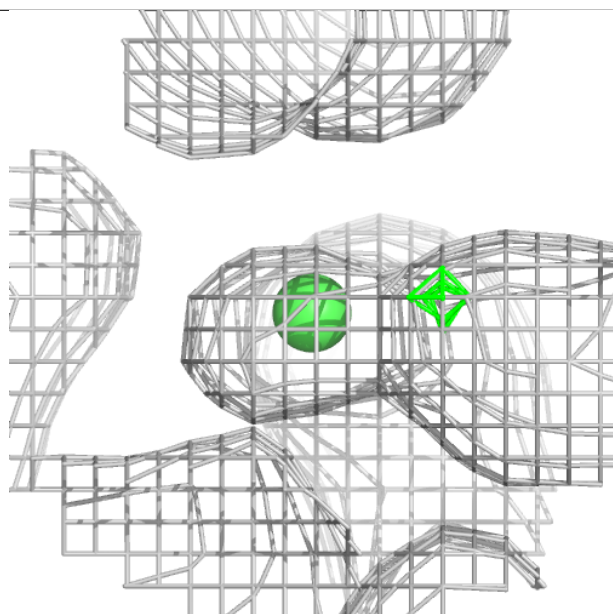
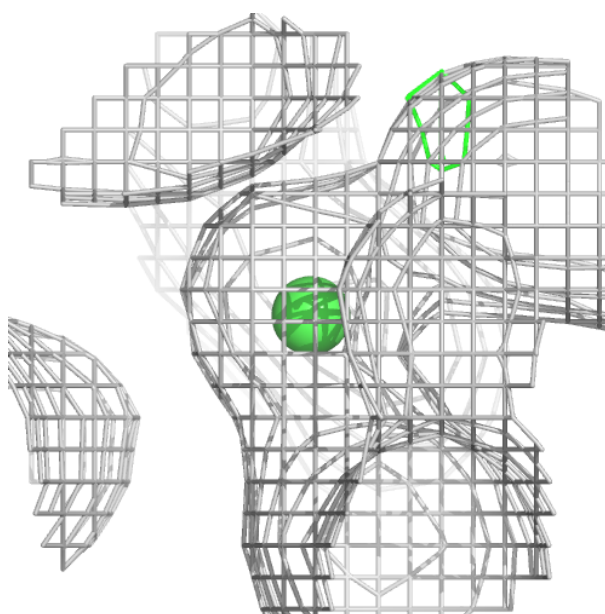
Electron density around NI H 404:

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



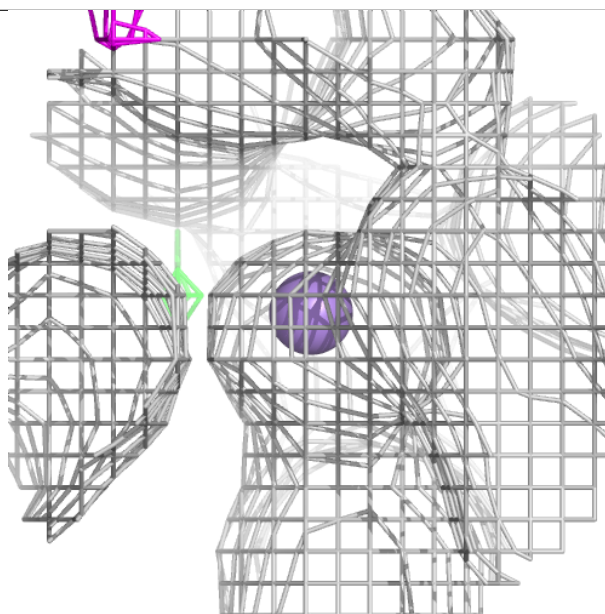
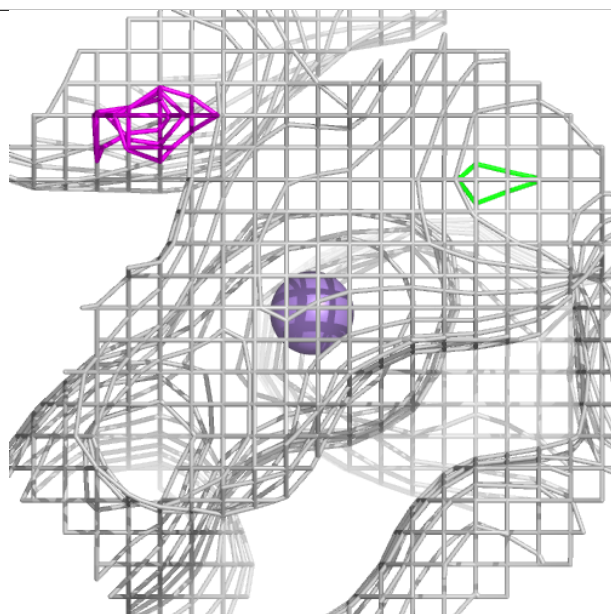
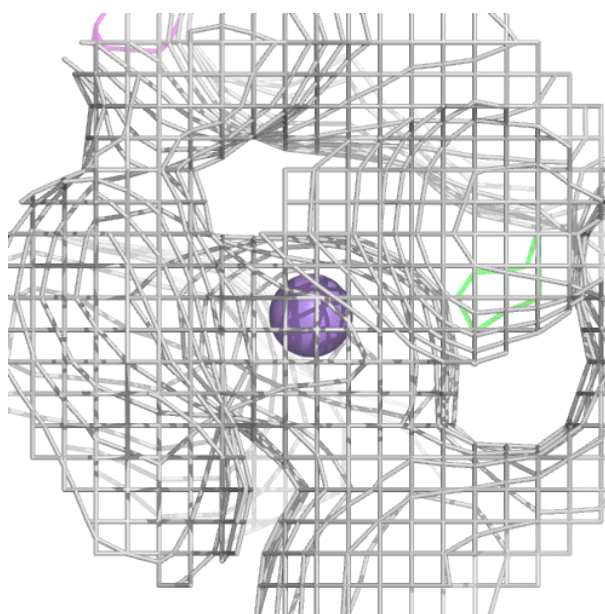
Electron density around NI D 404:

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



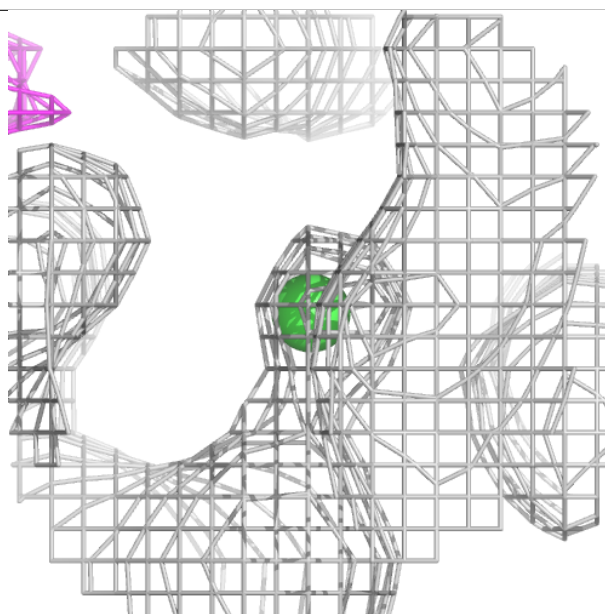
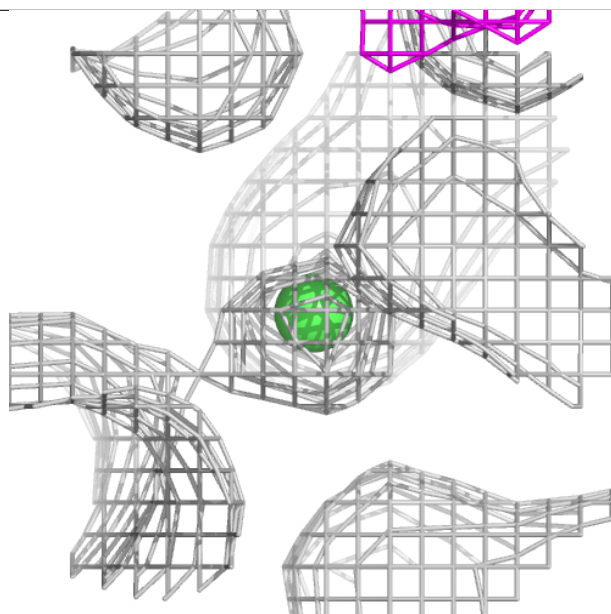
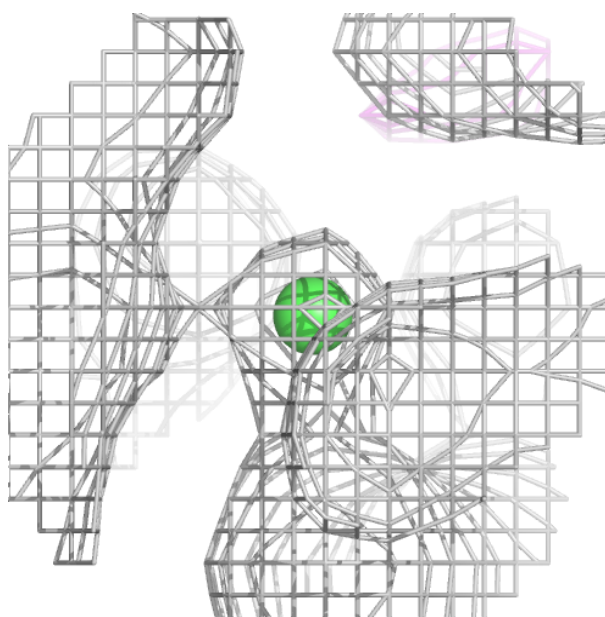
Electron density around MN C 403:

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



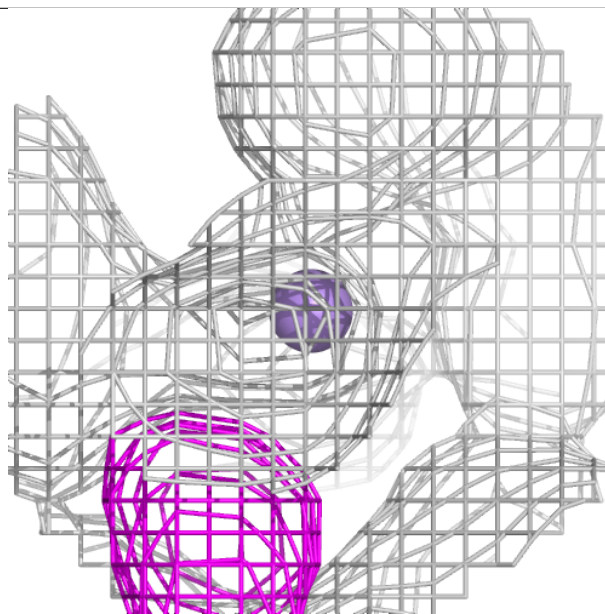
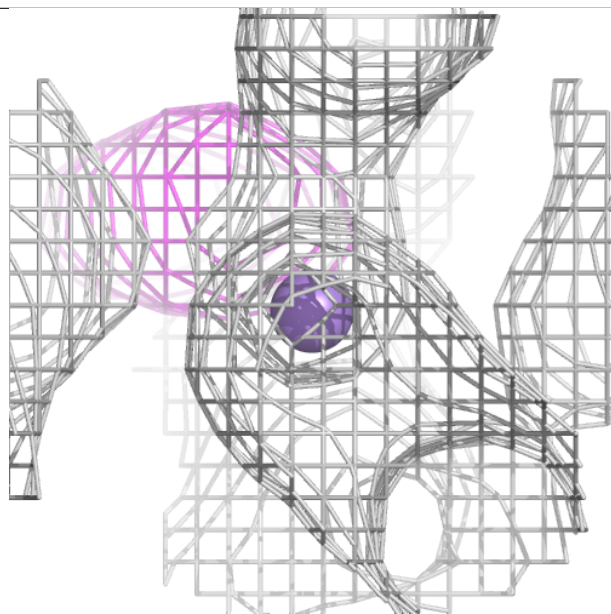
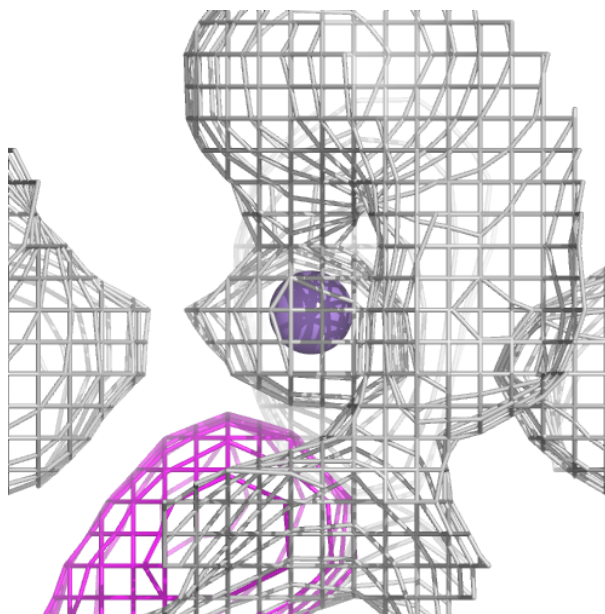
Electron density around NI F 404:

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



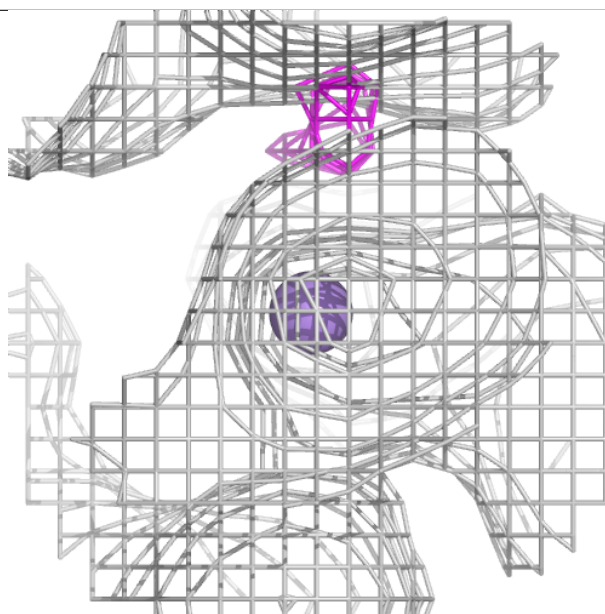
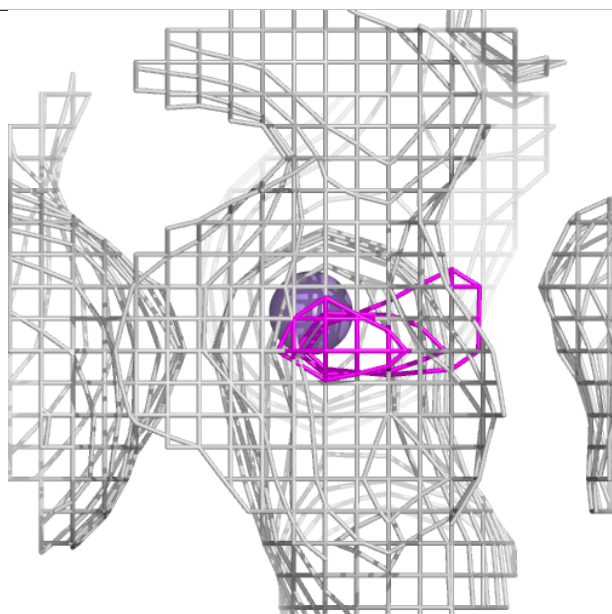
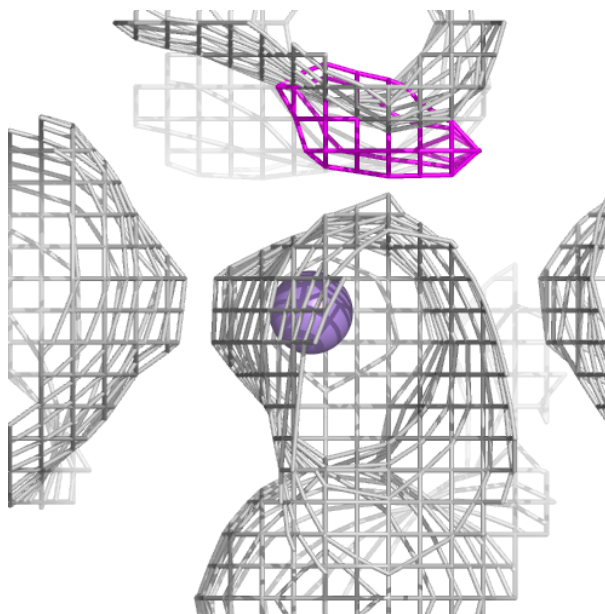
Electron density around MN G 403:

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



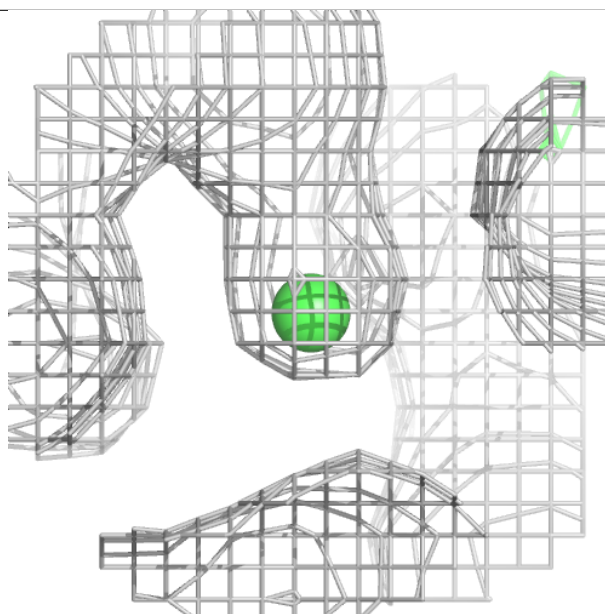
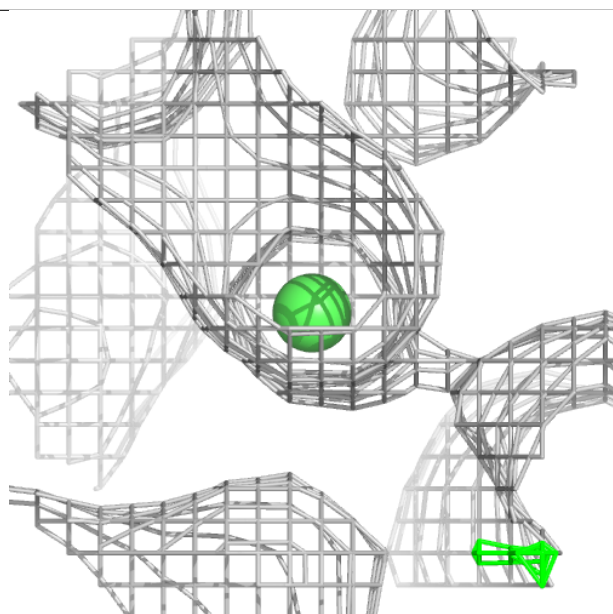
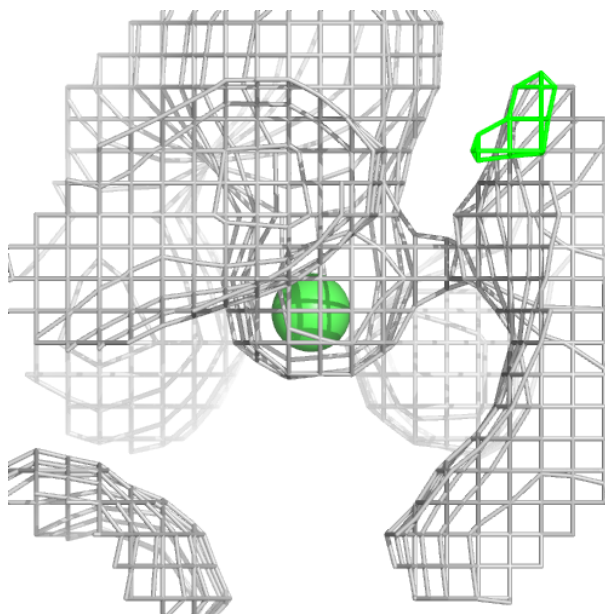
Electron density around MN F 403:

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



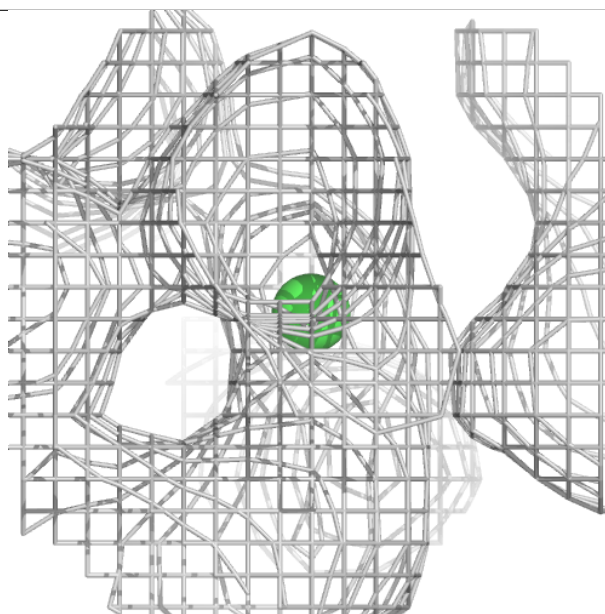
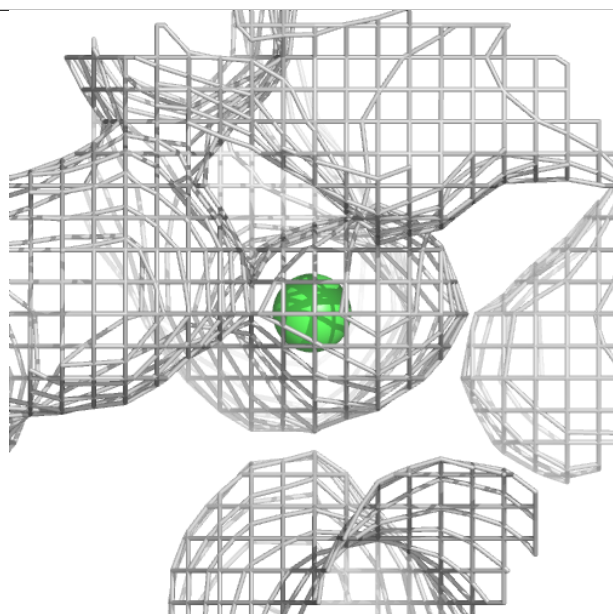
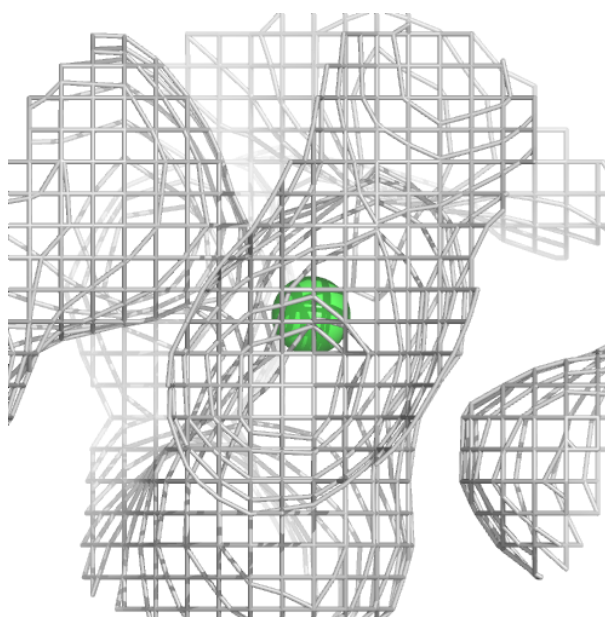
Electron density around NI A 404:

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



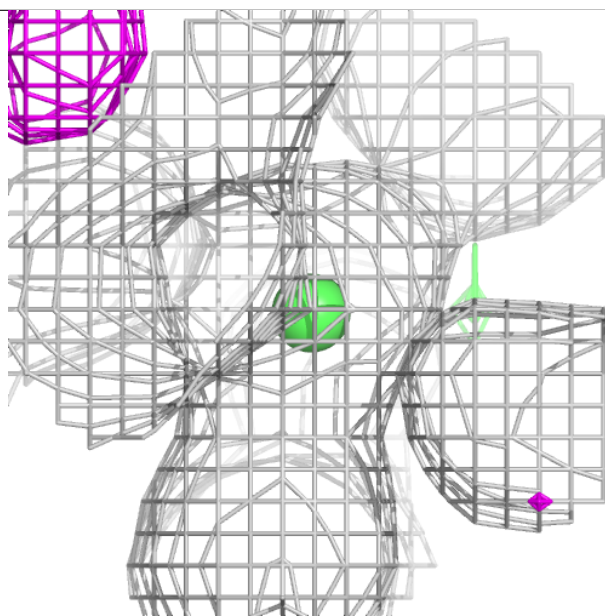
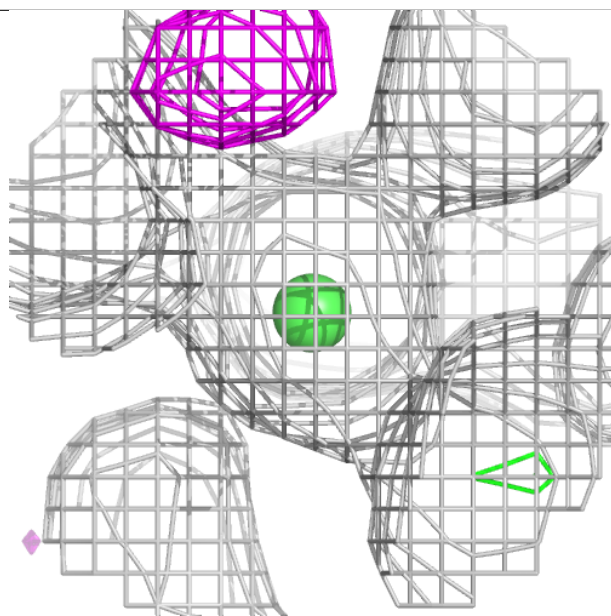
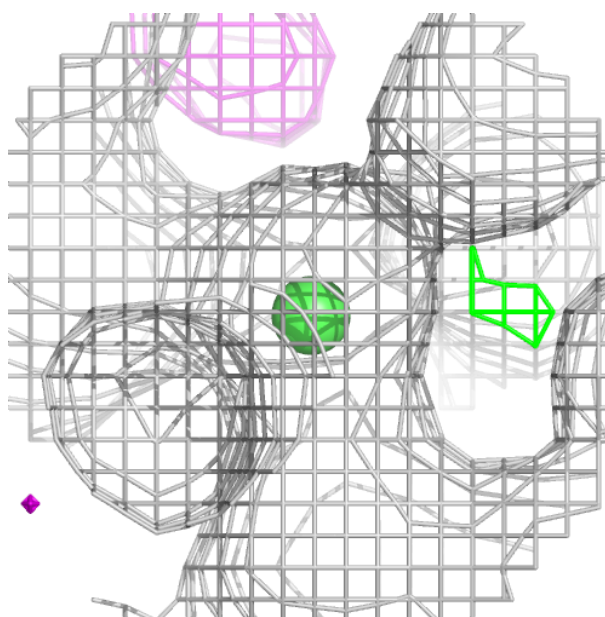
Electron density around NI B 404:

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



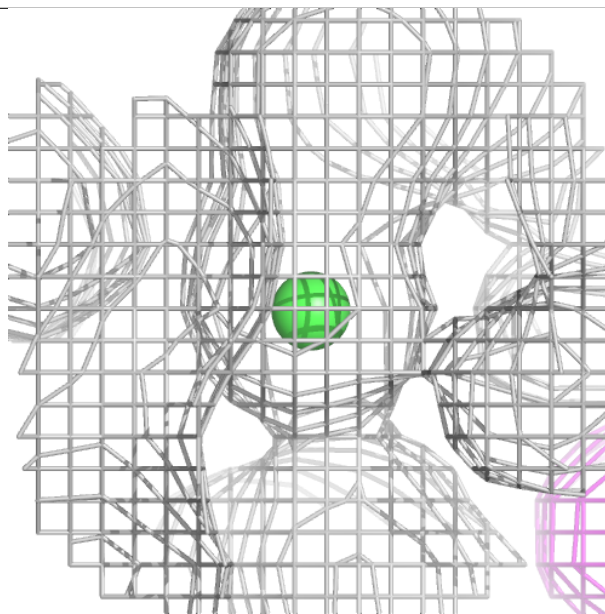
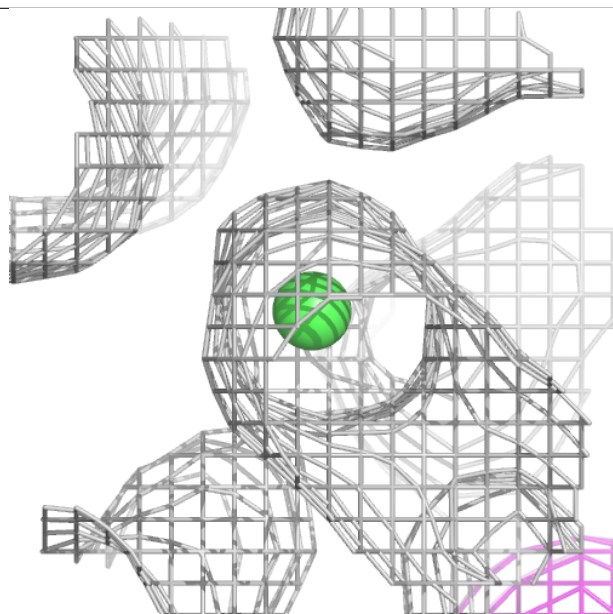
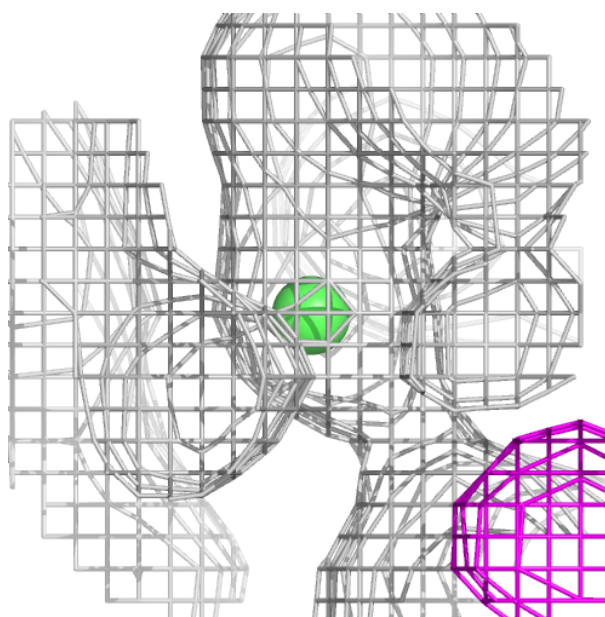
Electron density around NI C 404:

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



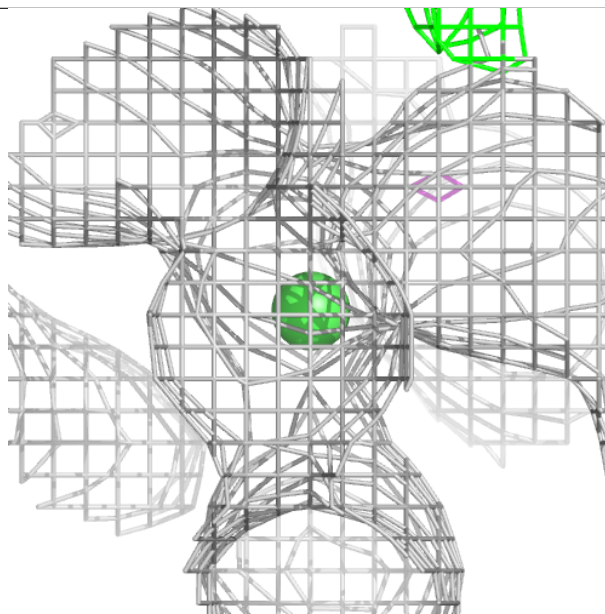
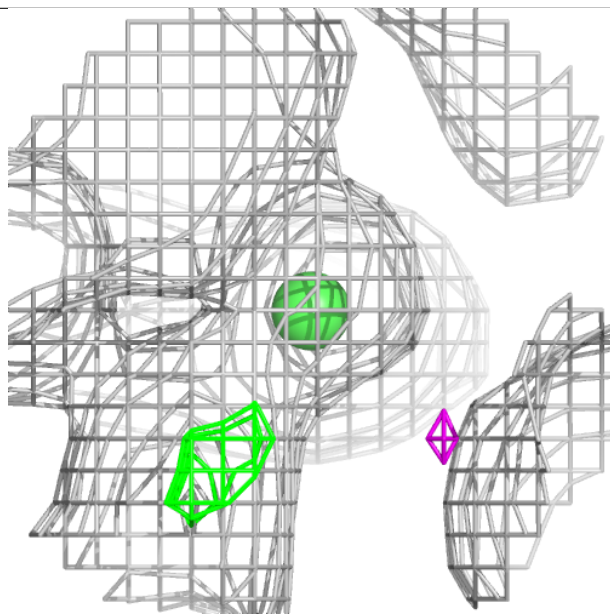
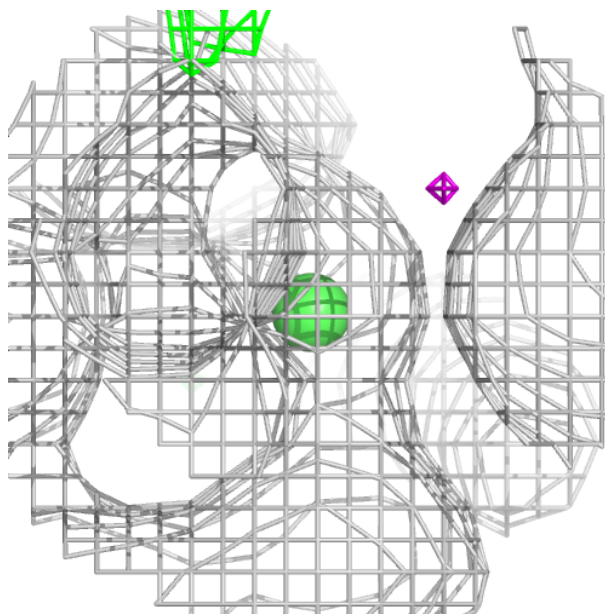
Electron density around NI G 404:

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



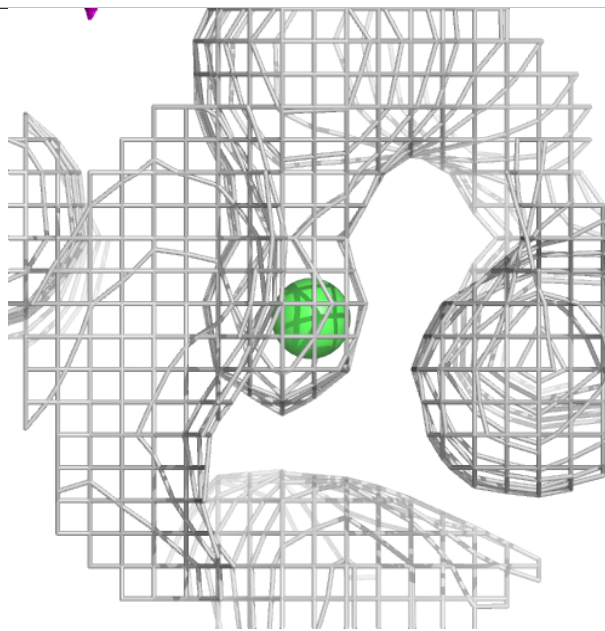
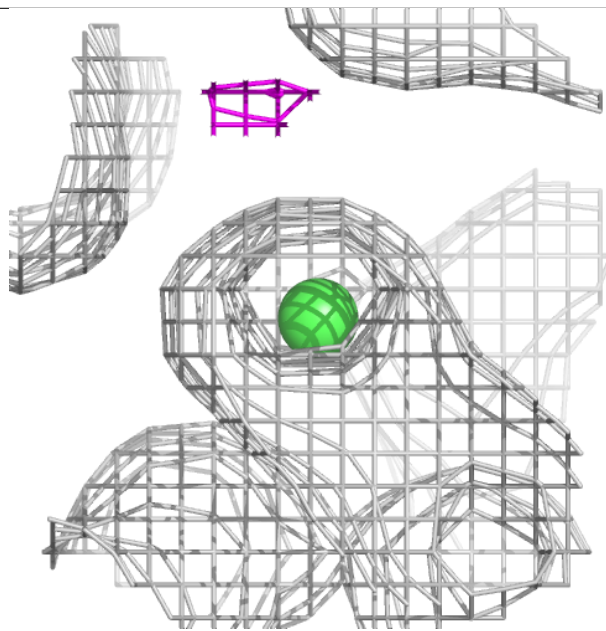
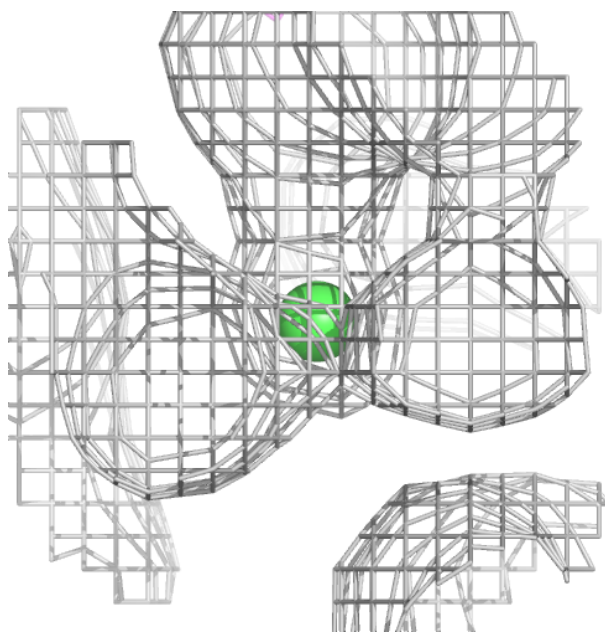
Electron density around NI K 404:

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



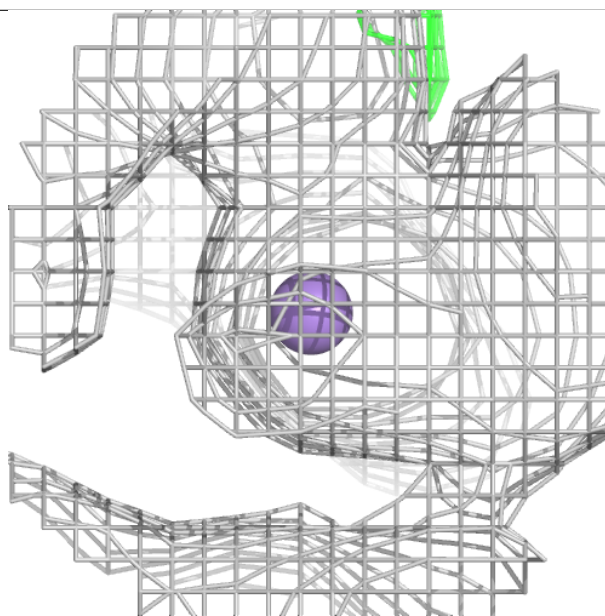
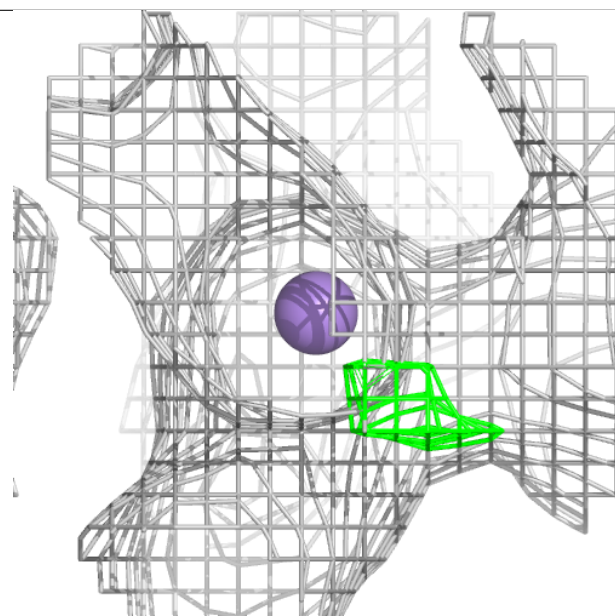
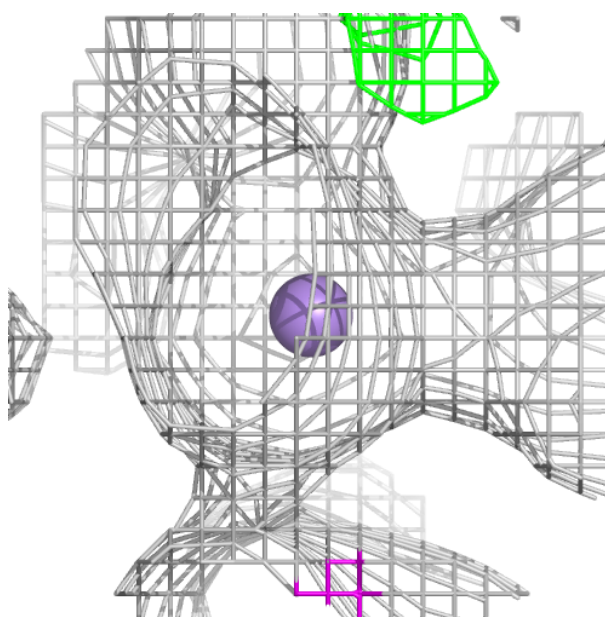
Electron density around NI L 404:

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



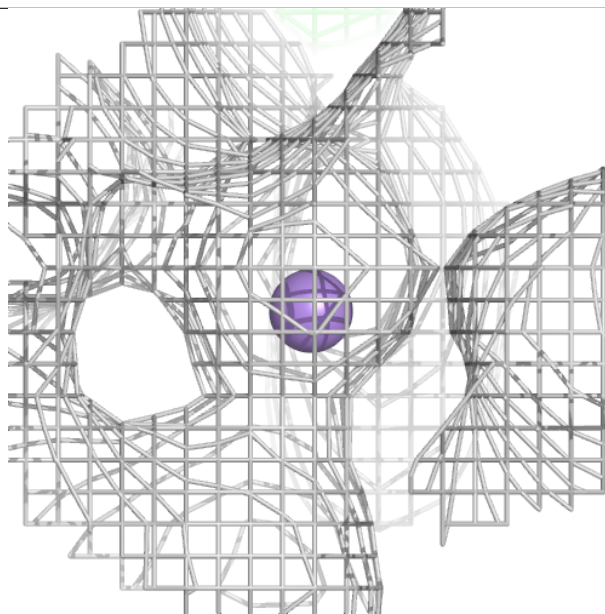
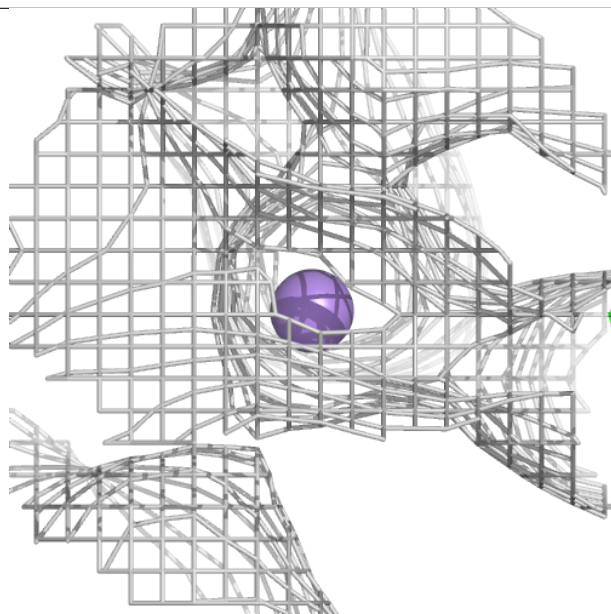
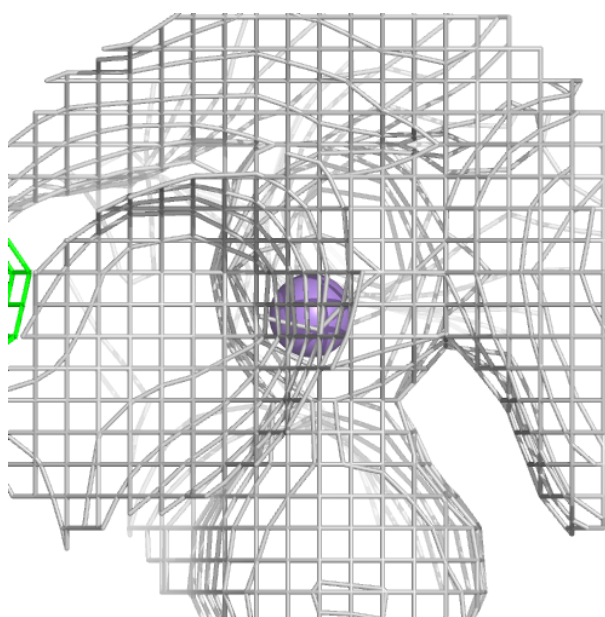
Electron density around MN A 403:

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



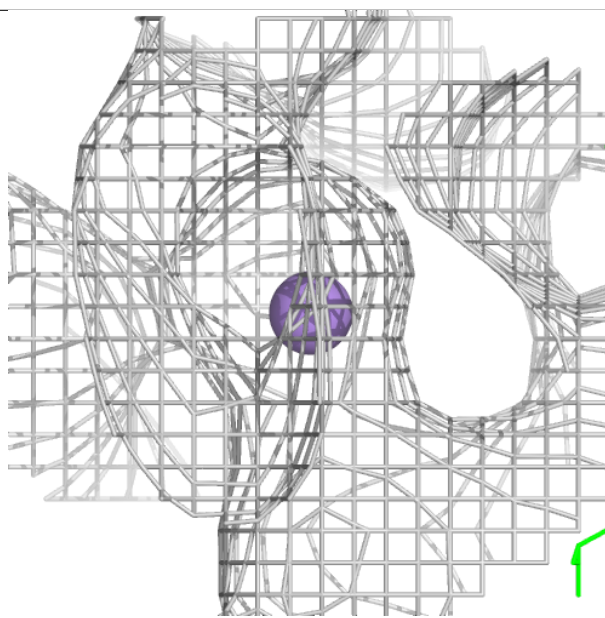
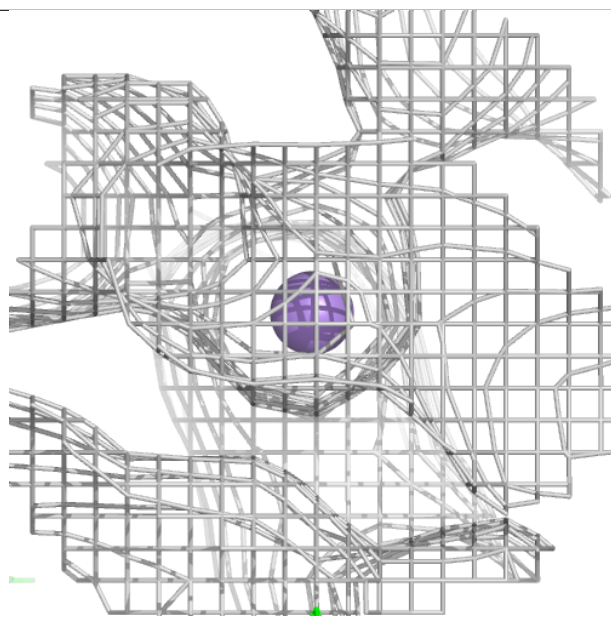
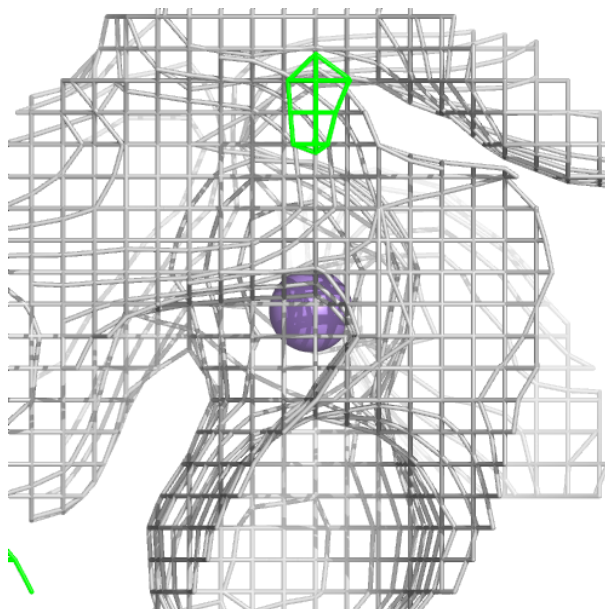
Electron density around MN B 403:

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



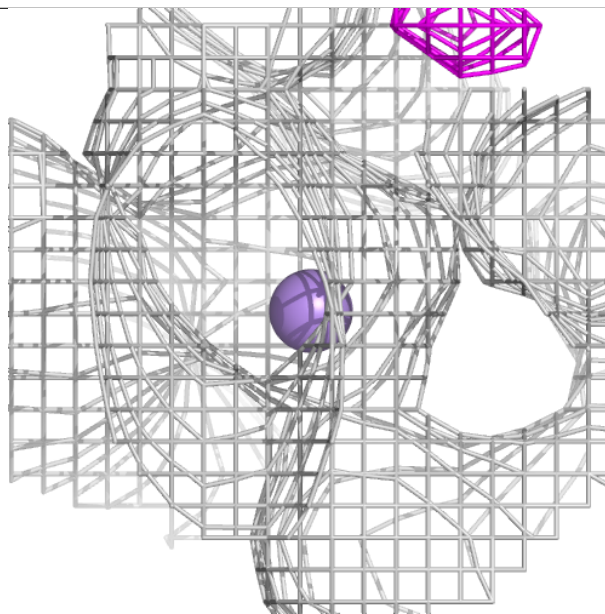
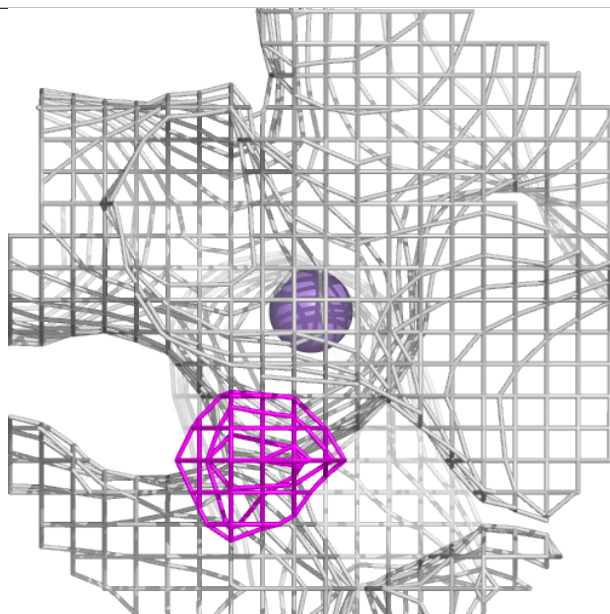
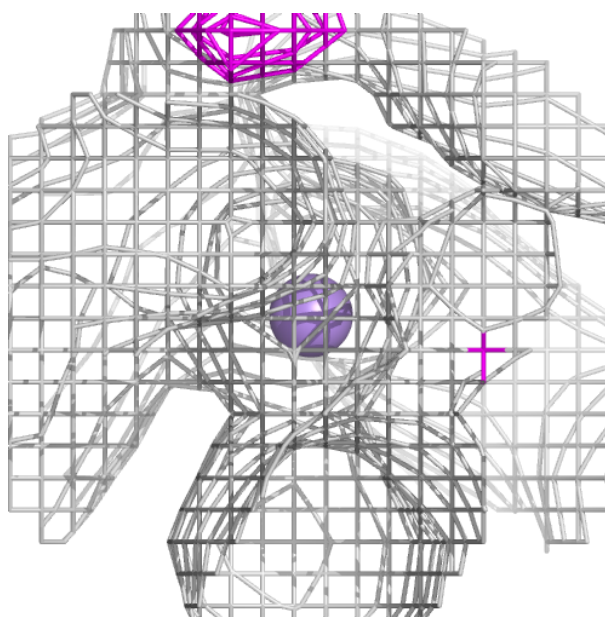
Electron density around MN D 403:

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



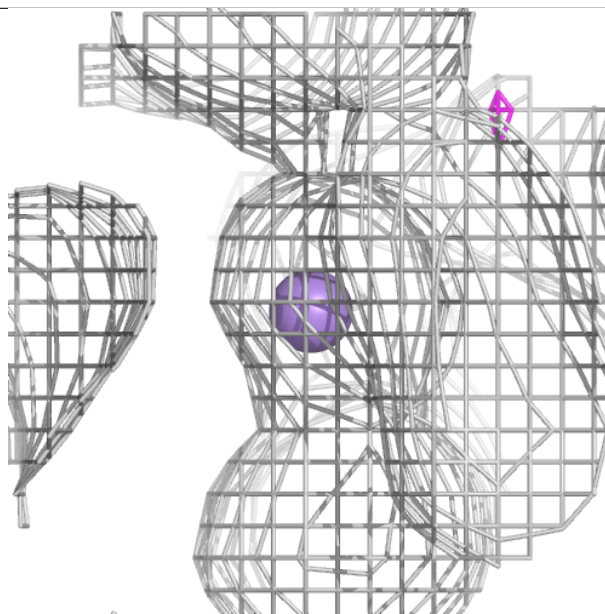
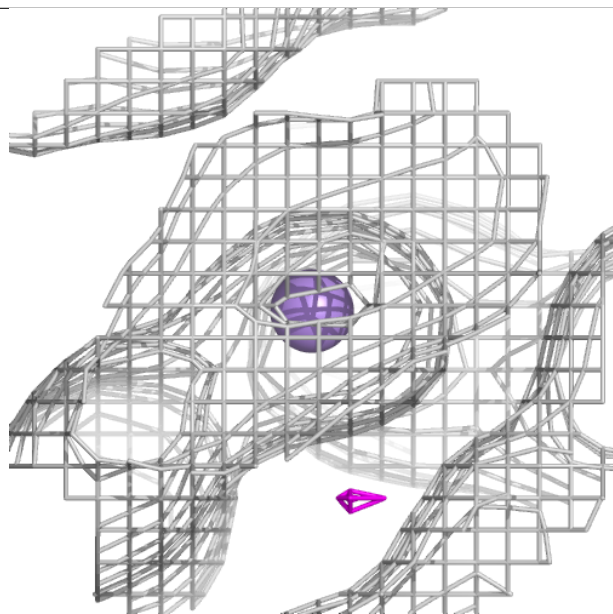
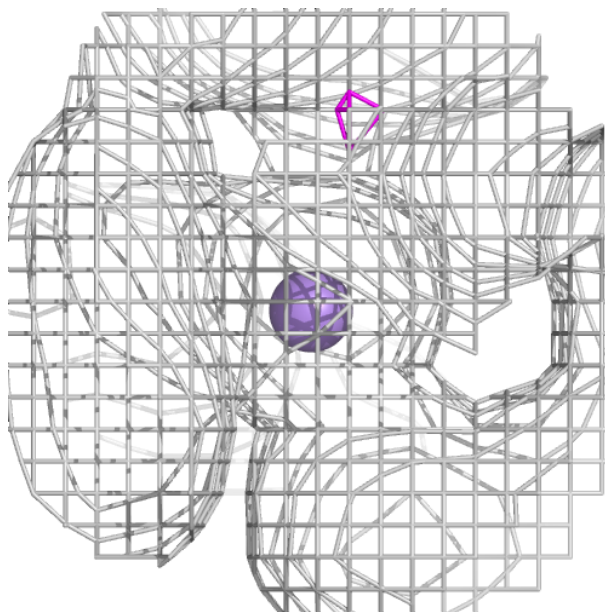
Electron density around MN H 403:

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



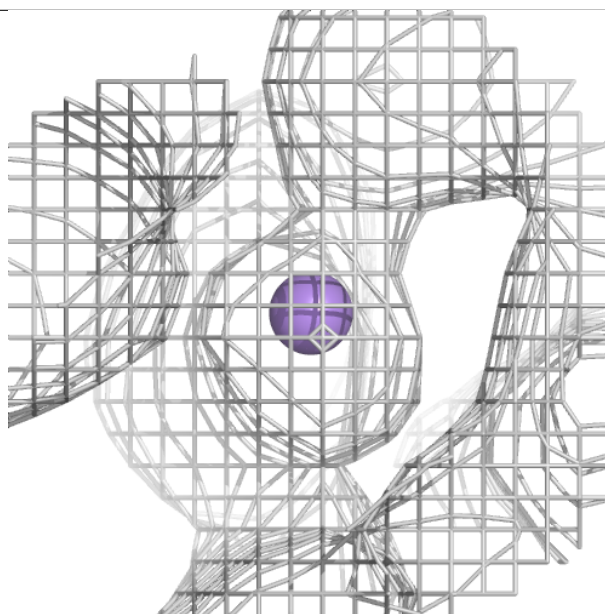
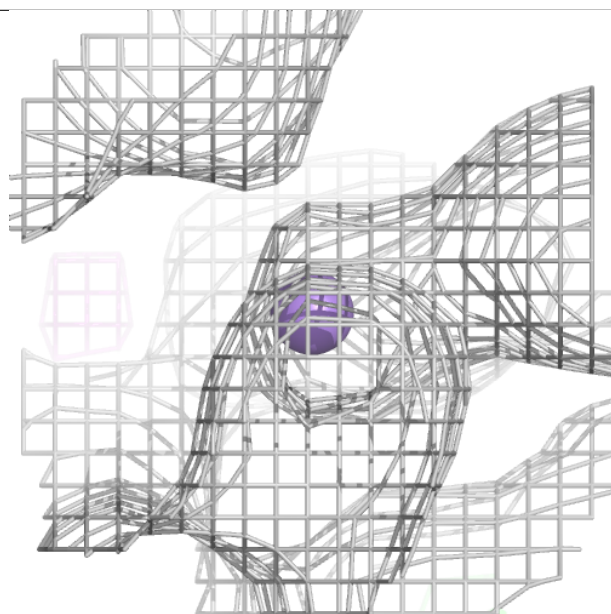
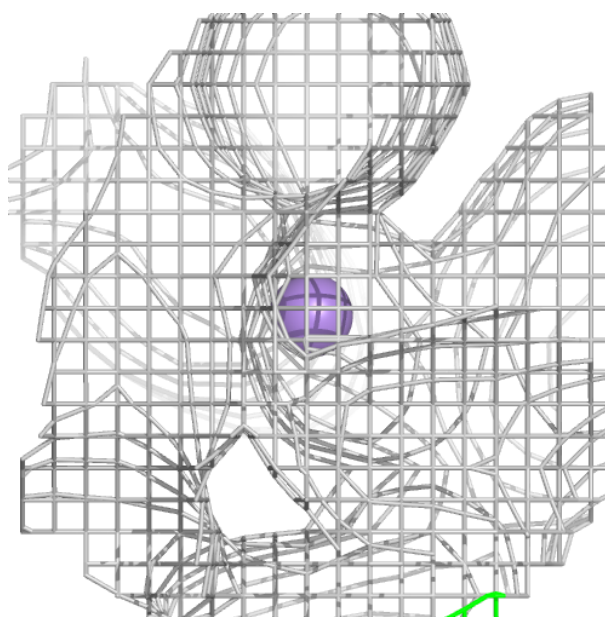
Electron density around MN I 403:

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



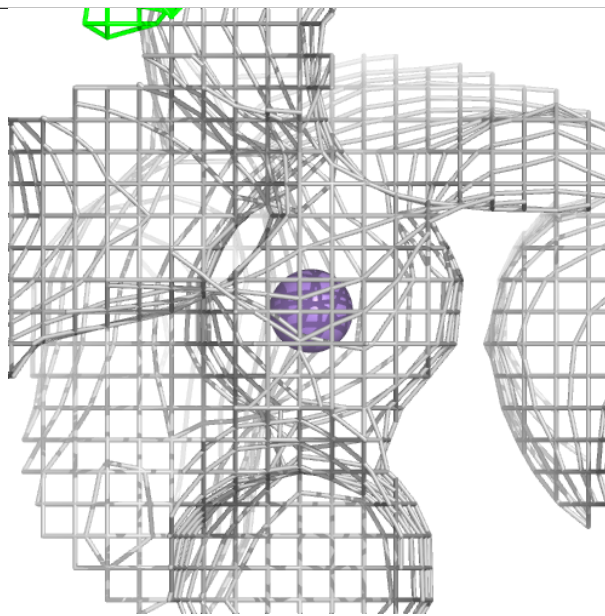
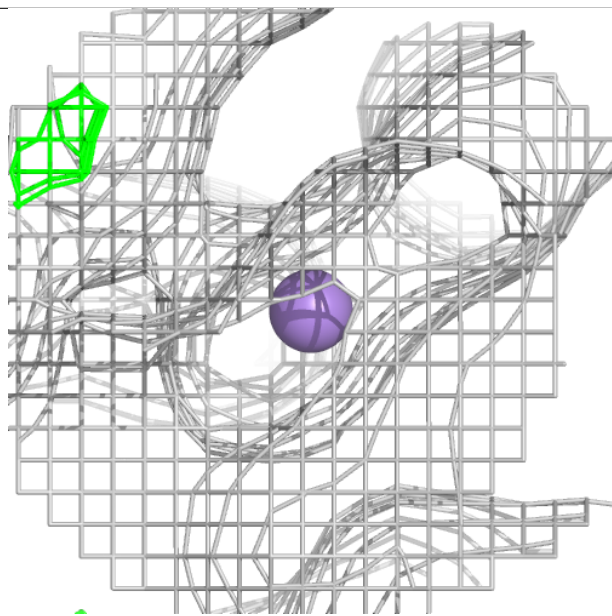
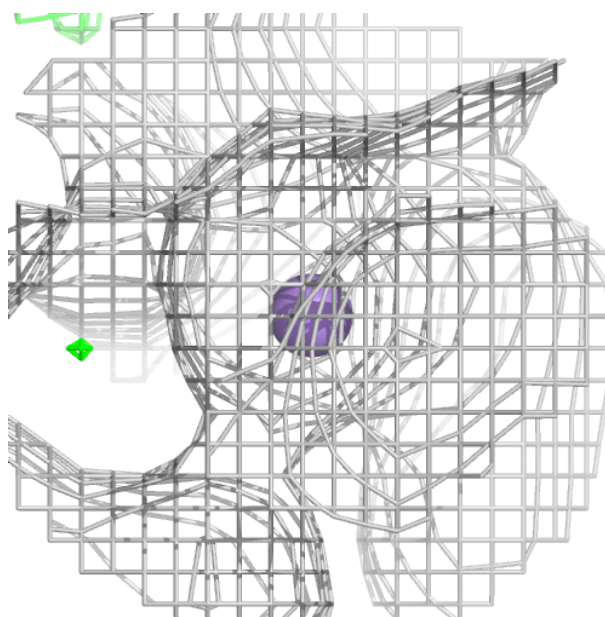
Electron density around MN J 403:

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



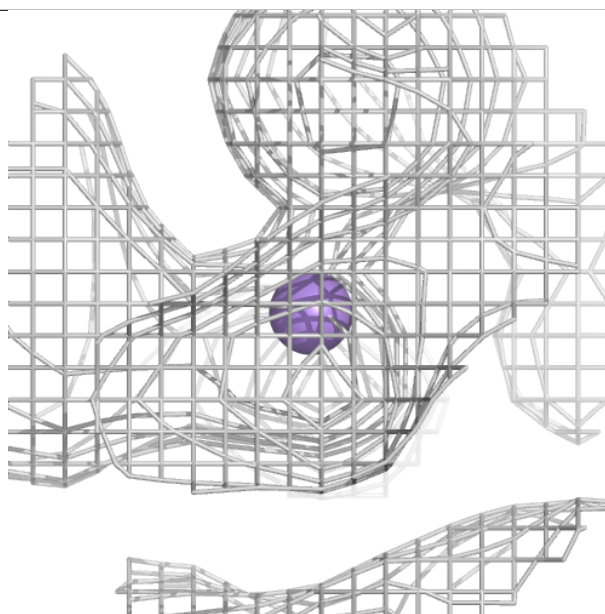
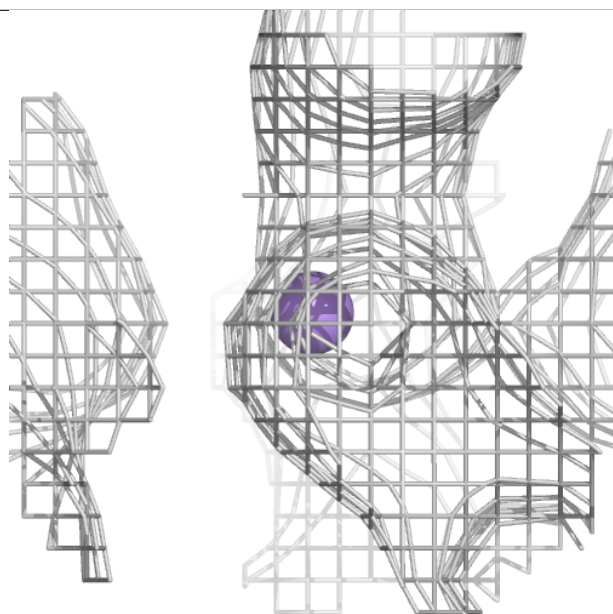
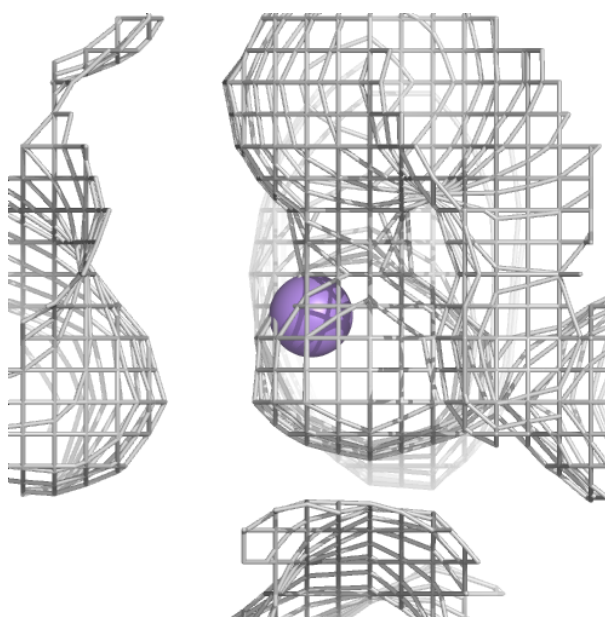
Electron density around MN K 403:

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



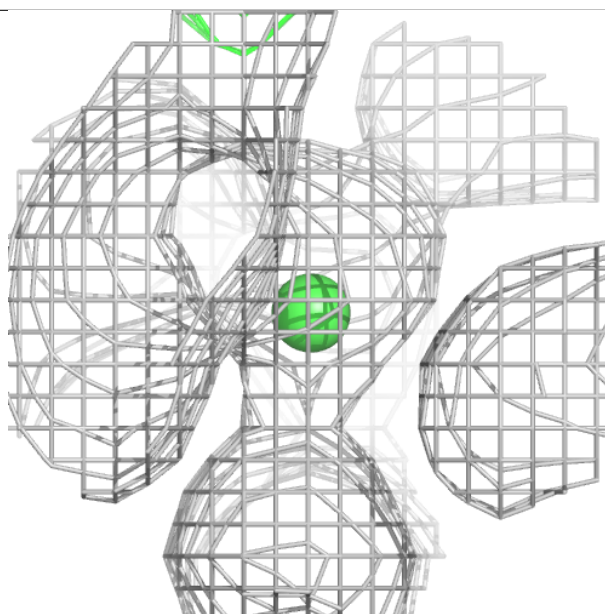
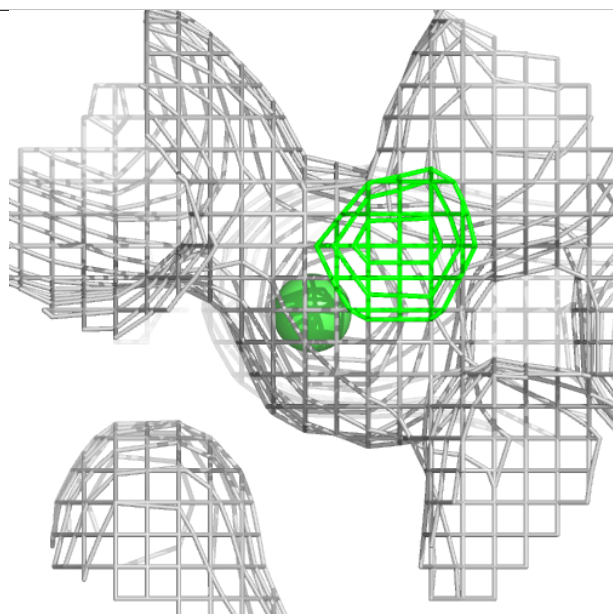
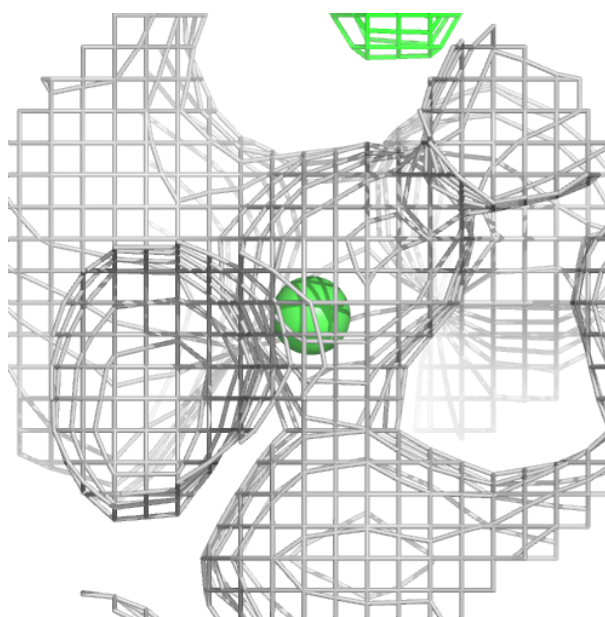
Electron density around MN L 403:

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



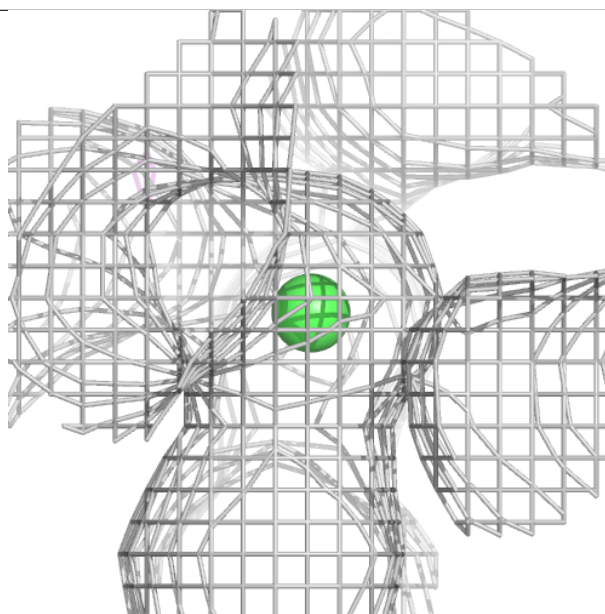
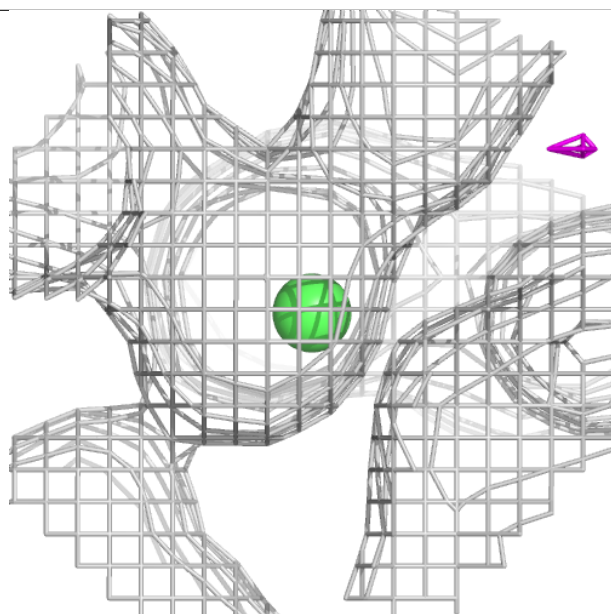
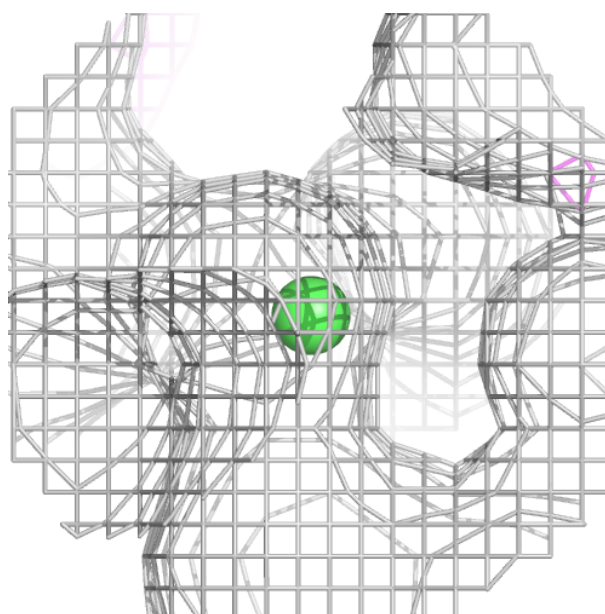
Electron density around NI E 404:

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



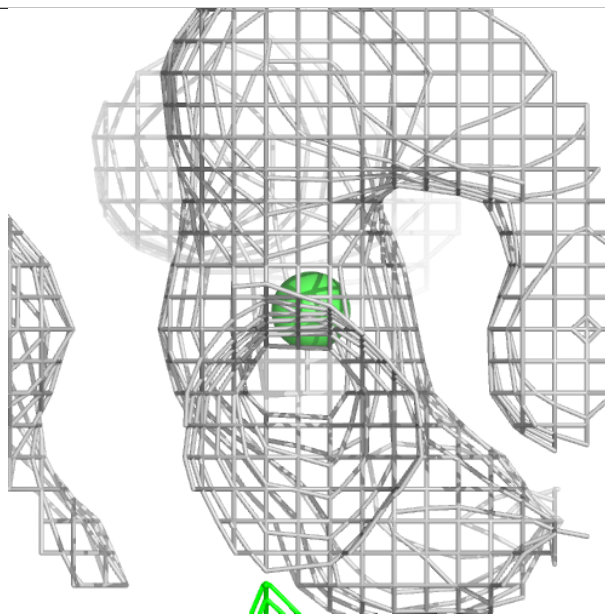
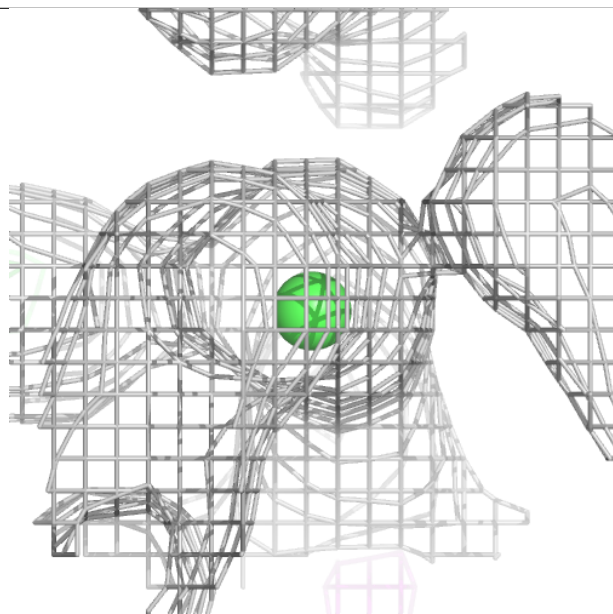
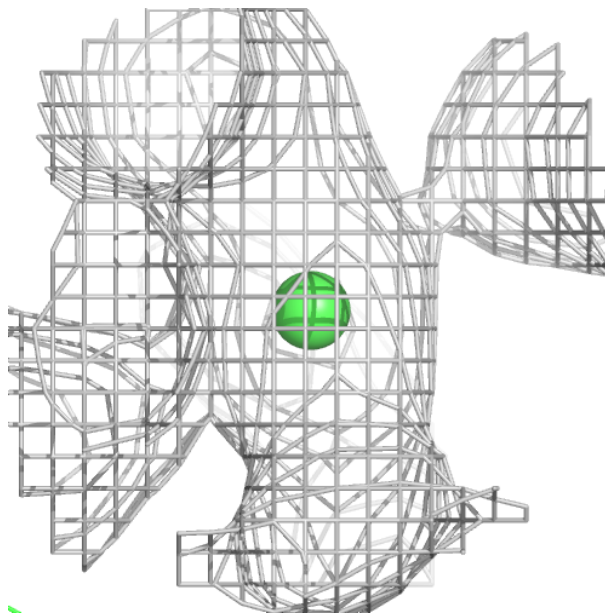
Electron density around NI I 404:

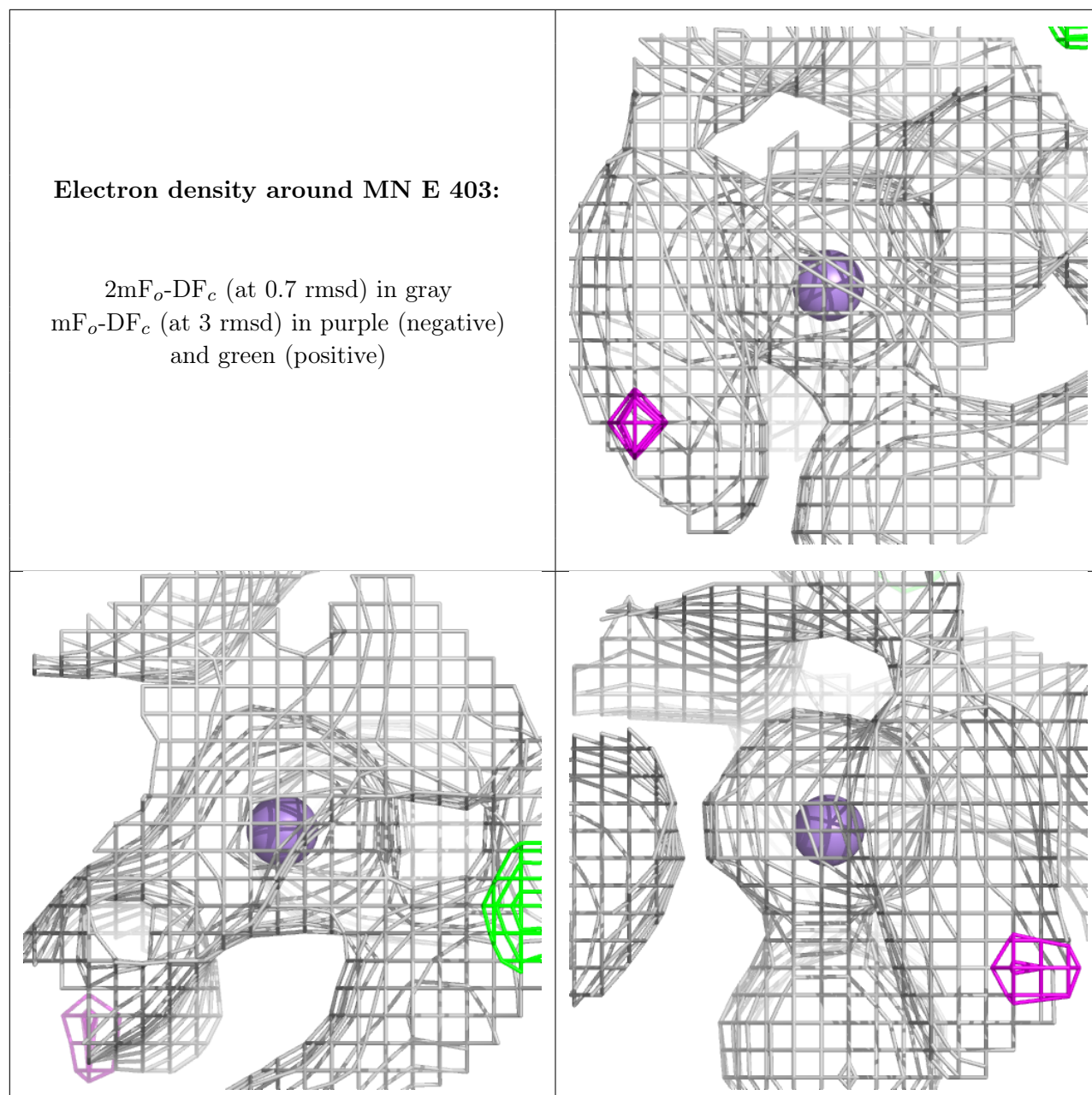
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI J 404:

$2mF_o-DF_c$ (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.