



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:14 AM UTC

PDB ID : 9Y9W / pdb_00009y9w
Title : Vibrio cholerae protein FrhA peptid-binding domain and adjacent split domain (S1127-F1439) in complex with peptide AGWTD X-ray crystallography structure
Authors : Wang, M.; Guo, S.; Kinrade, B.; Davies, P.
Deposited on : 2025-09-15
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

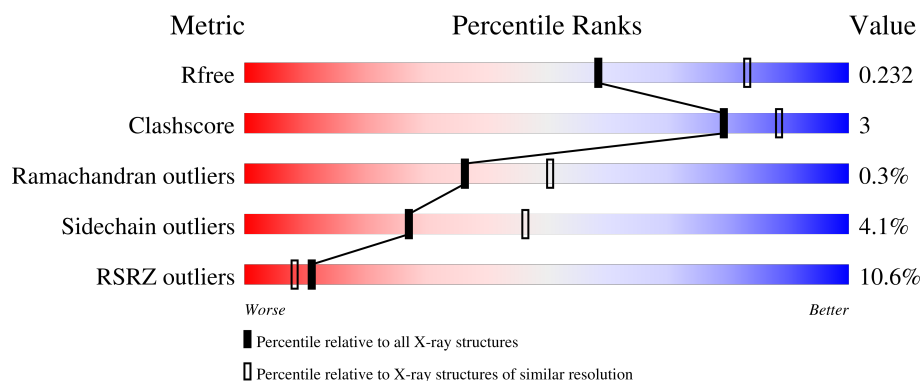
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	363	8% 75% 8% 17%
1	B	363	9% 78% 9% 13%
1	E	363	8% 76% 7% 17%
1	G	363	7% 76% 8% 16%
1	I	363	12% 78% 9% 13%

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Mol	Chain	Length	Quality of chain
1	K	363	
2	M	5	
2	N	5	
2	O	5	
2	P	5	
2	Q	5	
2	R	5	

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
4	PEG	B	407	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15182 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cadherin domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2216	1370	368	473	5			
1	B	316	Total	C	N	O	S	0	0	0
			2312	1430	382	495	5			
1	E	301	Total	C	N	O	S	0	1	0
			2225	1377	369	475	4			
1	G	305	Total	C	N	O	S	0	0	0
			2246	1389	372	480	5			
1	I	316	Total	C	N	O	S	0	0	0
			2318	1433	385	495	5			
1	K	303	Total	C	N	O	S	0	0	0
			2227	1379	369	475	4			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0H3AMP4
A	-18	ALA	-	expression tag	UNP A0A0H3AMP4
A	-17	SER	-	expression tag	UNP A0A0H3AMP4
A	-16	SER	-	expression tag	UNP A0A0H3AMP4
A	-15	HIS	-	expression tag	UNP A0A0H3AMP4
A	-14	HIS	-	expression tag	UNP A0A0H3AMP4
A	-13	HIS	-	expression tag	UNP A0A0H3AMP4
A	-12	HIS	-	expression tag	UNP A0A0H3AMP4
A	-11	HIS	-	expression tag	UNP A0A0H3AMP4
A	-10	HIS	-	expression tag	UNP A0A0H3AMP4
A	-9	SER	-	expression tag	UNP A0A0H3AMP4
A	-8	SER	-	expression tag	UNP A0A0H3AMP4
A	-7	GLY	-	expression tag	UNP A0A0H3AMP4
A	-6	LEU	-	expression tag	UNP A0A0H3AMP4
A	-5	VAL	-	expression tag	UNP A0A0H3AMP4
A	-4	PRO	-	expression tag	UNP A0A0H3AMP4
A	-3	ARG	-	expression tag	UNP A0A0H3AMP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A0H3AMP4
A	-1	SER	-	expression tag	UNP A0A0H3AMP4
A	0	HIS	-	expression tag	UNP A0A0H3AMP4
A	1	MET	-	expression tag	UNP A0A0H3AMP4
A	37	ALA	VAL	conflict	UNP A0A0H3AMP4
B	-19	MET	-	initiating methionine	UNP A0A0H3AMP4
B	-18	ALA	-	expression tag	UNP A0A0H3AMP4
B	-17	SER	-	expression tag	UNP A0A0H3AMP4
B	-16	SER	-	expression tag	UNP A0A0H3AMP4
B	-15	HIS	-	expression tag	UNP A0A0H3AMP4
B	-14	HIS	-	expression tag	UNP A0A0H3AMP4
B	-13	HIS	-	expression tag	UNP A0A0H3AMP4
B	-12	HIS	-	expression tag	UNP A0A0H3AMP4
B	-11	HIS	-	expression tag	UNP A0A0H3AMP4
B	-10	HIS	-	expression tag	UNP A0A0H3AMP4
B	-9	SER	-	expression tag	UNP A0A0H3AMP4
B	-8	SER	-	expression tag	UNP A0A0H3AMP4
B	-7	GLY	-	expression tag	UNP A0A0H3AMP4
B	-6	LEU	-	expression tag	UNP A0A0H3AMP4
B	-5	VAL	-	expression tag	UNP A0A0H3AMP4
B	-4	PRO	-	expression tag	UNP A0A0H3AMP4
B	-3	ARG	-	expression tag	UNP A0A0H3AMP4
B	-2	GLY	-	expression tag	UNP A0A0H3AMP4
B	-1	SER	-	expression tag	UNP A0A0H3AMP4
B	0	HIS	-	expression tag	UNP A0A0H3AMP4
B	1	MET	-	expression tag	UNP A0A0H3AMP4
B	37	ALA	VAL	conflict	UNP A0A0H3AMP4
E	-19	MET	-	initiating methionine	UNP A0A0H3AMP4
E	-18	ALA	-	expression tag	UNP A0A0H3AMP4
E	-17	SER	-	expression tag	UNP A0A0H3AMP4
E	-16	SER	-	expression tag	UNP A0A0H3AMP4
E	-15	HIS	-	expression tag	UNP A0A0H3AMP4
E	-14	HIS	-	expression tag	UNP A0A0H3AMP4
E	-13	HIS	-	expression tag	UNP A0A0H3AMP4
E	-12	HIS	-	expression tag	UNP A0A0H3AMP4
E	-11	HIS	-	expression tag	UNP A0A0H3AMP4
E	-10	HIS	-	expression tag	UNP A0A0H3AMP4
E	-9	SER	-	expression tag	UNP A0A0H3AMP4
E	-8	SER	-	expression tag	UNP A0A0H3AMP4
E	-7	GLY	-	expression tag	UNP A0A0H3AMP4
E	-6	LEU	-	expression tag	UNP A0A0H3AMP4
E	-5	VAL	-	expression tag	UNP A0A0H3AMP4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	PRO	-	expression tag	UNP A0A0H3AMP4
E	-3	ARG	-	expression tag	UNP A0A0H3AMP4
E	-2	GLY	-	expression tag	UNP A0A0H3AMP4
E	-1	SER	-	expression tag	UNP A0A0H3AMP4
E	0	HIS	-	expression tag	UNP A0A0H3AMP4
E	1	MET	-	expression tag	UNP A0A0H3AMP4
E	37	ALA	VAL	conflict	UNP A0A0H3AMP4
G	-19	MET	-	initiating methionine	UNP A0A0H3AMP4
G	-18	ALA	-	expression tag	UNP A0A0H3AMP4
G	-17	SER	-	expression tag	UNP A0A0H3AMP4
G	-16	SER	-	expression tag	UNP A0A0H3AMP4
G	-15	HIS	-	expression tag	UNP A0A0H3AMP4
G	-14	HIS	-	expression tag	UNP A0A0H3AMP4
G	-13	HIS	-	expression tag	UNP A0A0H3AMP4
G	-12	HIS	-	expression tag	UNP A0A0H3AMP4
G	-11	HIS	-	expression tag	UNP A0A0H3AMP4
G	-10	HIS	-	expression tag	UNP A0A0H3AMP4
G	-9	SER	-	expression tag	UNP A0A0H3AMP4
G	-8	SER	-	expression tag	UNP A0A0H3AMP4
G	-7	GLY	-	expression tag	UNP A0A0H3AMP4
G	-6	LEU	-	expression tag	UNP A0A0H3AMP4
G	-5	VAL	-	expression tag	UNP A0A0H3AMP4
G	-4	PRO	-	expression tag	UNP A0A0H3AMP4
G	-3	ARG	-	expression tag	UNP A0A0H3AMP4
G	-2	GLY	-	expression tag	UNP A0A0H3AMP4
G	-1	SER	-	expression tag	UNP A0A0H3AMP4
G	0	HIS	-	expression tag	UNP A0A0H3AMP4
G	1	MET	-	expression tag	UNP A0A0H3AMP4
G	37	ALA	VAL	conflict	UNP A0A0H3AMP4
I	-19	MET	-	initiating methionine	UNP A0A0H3AMP4
I	-18	ALA	-	expression tag	UNP A0A0H3AMP4
I	-17	SER	-	expression tag	UNP A0A0H3AMP4
I	-16	SER	-	expression tag	UNP A0A0H3AMP4
I	-15	HIS	-	expression tag	UNP A0A0H3AMP4
I	-14	HIS	-	expression tag	UNP A0A0H3AMP4
I	-13	HIS	-	expression tag	UNP A0A0H3AMP4
I	-12	HIS	-	expression tag	UNP A0A0H3AMP4
I	-11	HIS	-	expression tag	UNP A0A0H3AMP4
I	-10	HIS	-	expression tag	UNP A0A0H3AMP4
I	-9	SER	-	expression tag	UNP A0A0H3AMP4
I	-8	SER	-	expression tag	UNP A0A0H3AMP4
I	-7	GLY	-	expression tag	UNP A0A0H3AMP4

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP A0A0H3AMP4
I	-5	VAL	-	expression tag	UNP A0A0H3AMP4
I	-4	PRO	-	expression tag	UNP A0A0H3AMP4
I	-3	ARG	-	expression tag	UNP A0A0H3AMP4
I	-2	GLY	-	expression tag	UNP A0A0H3AMP4
I	-1	SER	-	expression tag	UNP A0A0H3AMP4
I	0	HIS	-	expression tag	UNP A0A0H3AMP4
I	1	MET	-	expression tag	UNP A0A0H3AMP4
I	37	ALA	VAL	conflict	UNP A0A0H3AMP4
K	-19	MET	-	initiating methionine	UNP A0A0H3AMP4
K	-18	ALA	-	expression tag	UNP A0A0H3AMP4
K	-17	SER	-	expression tag	UNP A0A0H3AMP4
K	-16	SER	-	expression tag	UNP A0A0H3AMP4
K	-15	HIS	-	expression tag	UNP A0A0H3AMP4
K	-14	HIS	-	expression tag	UNP A0A0H3AMP4
K	-13	HIS	-	expression tag	UNP A0A0H3AMP4
K	-12	HIS	-	expression tag	UNP A0A0H3AMP4
K	-11	HIS	-	expression tag	UNP A0A0H3AMP4
K	-10	HIS	-	expression tag	UNP A0A0H3AMP4
K	-9	SER	-	expression tag	UNP A0A0H3AMP4
K	-8	SER	-	expression tag	UNP A0A0H3AMP4
K	-7	GLY	-	expression tag	UNP A0A0H3AMP4
K	-6	LEU	-	expression tag	UNP A0A0H3AMP4
K	-5	VAL	-	expression tag	UNP A0A0H3AMP4
K	-4	PRO	-	expression tag	UNP A0A0H3AMP4
K	-3	ARG	-	expression tag	UNP A0A0H3AMP4
K	-2	GLY	-	expression tag	UNP A0A0H3AMP4
K	-1	SER	-	expression tag	UNP A0A0H3AMP4
K	0	HIS	-	expression tag	UNP A0A0H3AMP4
K	1	MET	-	expression tag	UNP A0A0H3AMP4
K	37	ALA	VAL	conflict	UNP A0A0H3AMP4

- Molecule 2 is a protein called Ala-Gly-Trp-Thr-Asp (AGWTD).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	5	Total	C	N	O	0	0	0
			39	24	6	9			
2	N	5	Total	C	N	O	0	0	0
			39	24	6	9			
2	O	5	Total	C	N	O	0	0	0
			39	24	6	9			
2	P	4	Total	C	N	O	0	0	0
			34	21	5	8			

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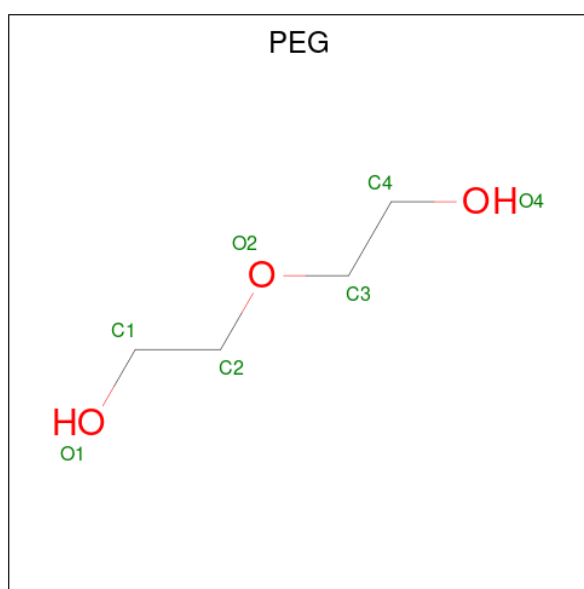
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	4	Total	C	N	O	0	0	0
			34	21	5	8			
2	R	4	Total	C	N	O	0	0	0
			34	21	5	8			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Ca	0	0
			6	6		
3	B	6	Total	Ca	0	0
			6	6		
3	E	6	Total	Ca	0	0
			6	6		
3	G	6	Total	Ca	0	0
			6	6		
3	I	6	Total	Ca	0	0
			6	6		
3	K	6	Total	Ca	0	0
			6	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



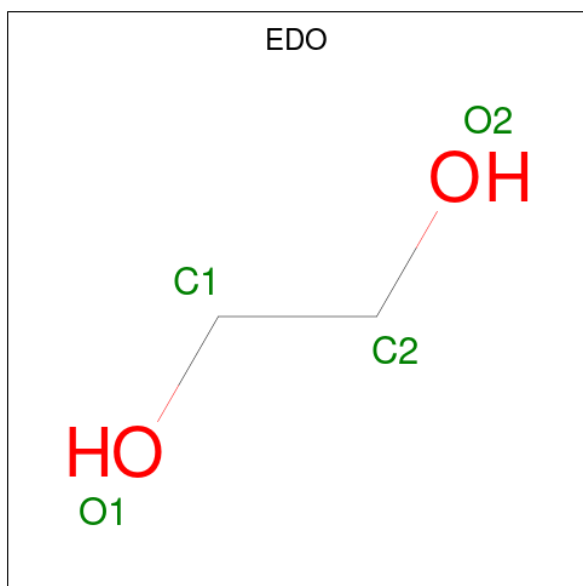
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	240	Total	O	0	1
			241	241		
6	B	209	Total	O	0	0
			209	209		
6	E	245	Total	O	0	0
			245	245		

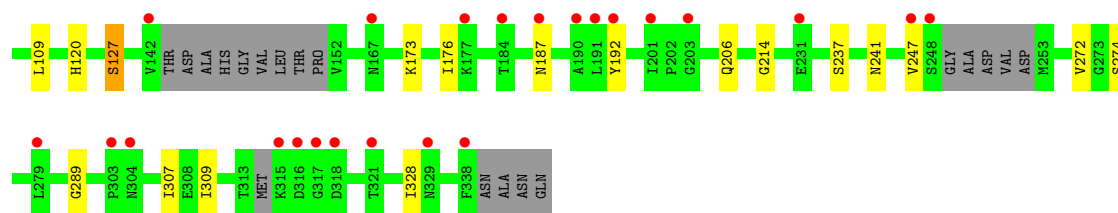
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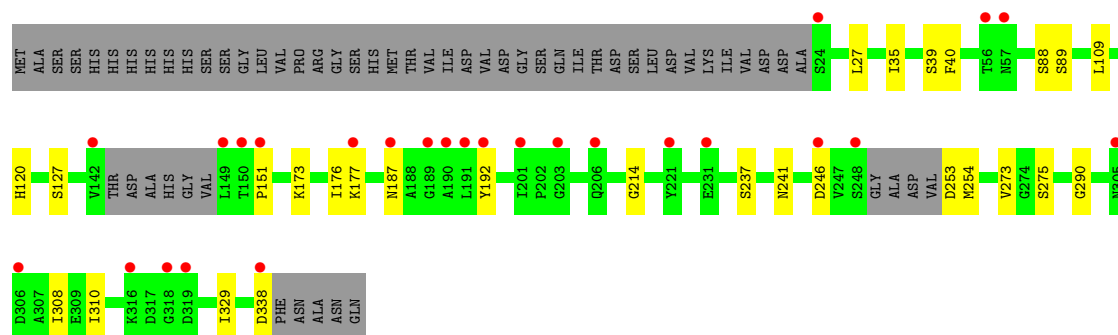
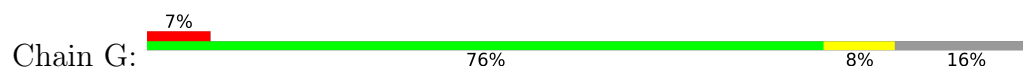
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	256	Total 256	O 256	0	0
6	I	198	Total 198	O 198	0	0
6	K	177	Total 177	O 177	0	0
6	M	5	Total 5	O 5	0	0
6	N	4	Total 4	O 4	0	0
6	O	3	Total 3	O 3	0	0
6	P	2	Total 2	O 2	0	0
6	Q	4	Total 4	O 4	0	0
6	R	5	Total 5	O 5	0	0

- Molecule 1: Cadherin domain protein

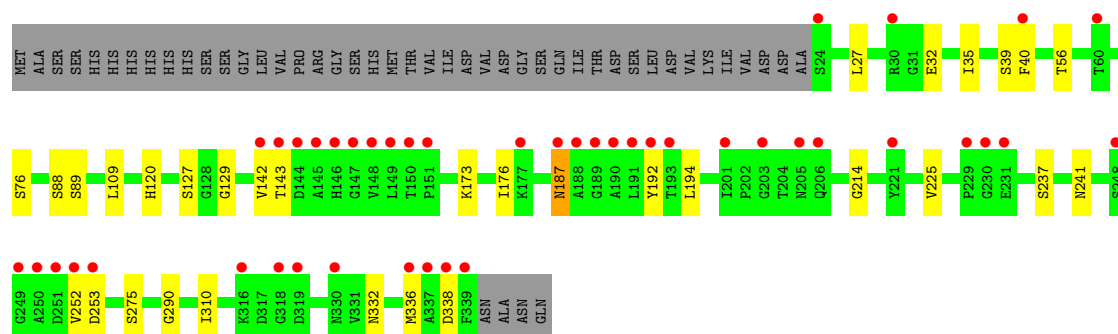
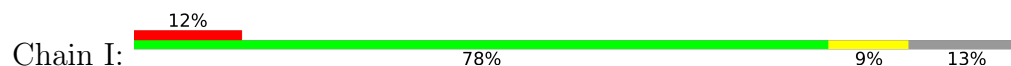




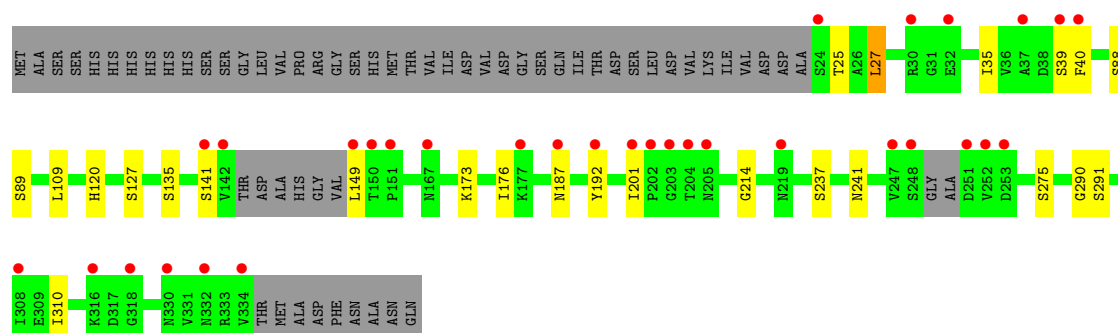
● Molecule 1: Cadherin domain protein



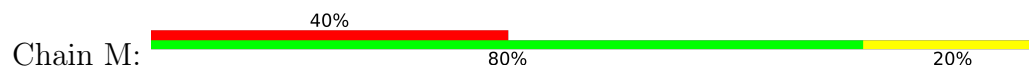
● Molecule 1: Cadherin domain protein



● Molecule 1: Cadherin domain protein



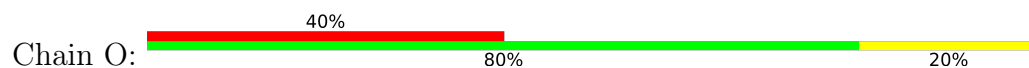
- Molecule 2: Ala-Gly-Trp-Thr-Asp (AGWTD)



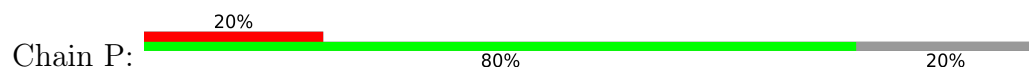
- Molecule 2: Ala-Gly-Trp-Thr-Asp (AGWTD)



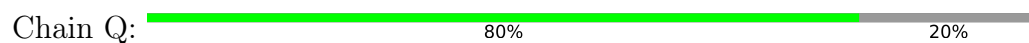
- Molecule 2: Ala-Gly-Trp-Thr-Asp (AGWTD)



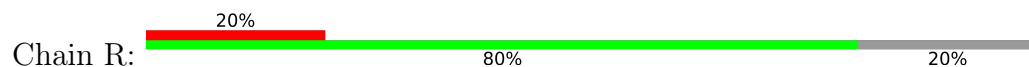
- Molecule 2: Ala-Gly-Trp-Thr-Asp (AGWTD)



- Molecule 2: Ala-Gly-Trp-Thr-Asp (AGWTD)



- Molecule 2: Ala-Gly-Trp-Thr-Asp (AGWTD)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.27Å 118.73Å 118.71Å 60.03° 85.62° 76.70°	Depositor
Resolution (Å)	102.72 – 2.40 102.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (102.72-2.40) 98.7 (102.72-2.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.227 , 0.232 0.229 , 0.232	Depositor DCC
R_{free} test set	2041 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15182	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, CA

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	0.66	0/2254	0.84	0/3076
1	B	0.64	0/2354	0.78	0/3219
1	E	0.58	0/2262	0.70	0/3086
1	G	0.61	0/2284	0.75	0/3119
1	I	0.64	0/2360	0.82	0/3226
1	K	0.62	0/2265	0.76	0/3094
2	M	0.86	0/40	0.94	0/53
2	N	1.13	0/40	1.34	0/53
2	O	0.58	0/40	0.68	0/53
2	P	0.52	0/35	0.81	0/46
2	Q	0.53	0/35	0.80	0/46
2	R	0.52	0/35	0.81	0/46
All	All	0.63	0/14004	0.78	0/19117

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	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	333	ARG	Sidechain
1	A	82	ARG	Sidechain

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	2216	0	2086	12	0
1	B	2312	0	2160	19	0
1	E	2225	0	2090	14	0
1	G	2246	0	2116	12	0
1	I	2318	0	2171	12	0
1	K	2227	0	2093	8	0
2	M	39	0	28	1	0
2	N	39	0	28	0	0
2	O	39	0	28	1	0
2	P	34	0	23	0	0
2	Q	34	0	23	0	0
2	R	34	0	23	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	E	6	0	0	0	0
3	G	6	0	0	0	0
3	I	6	0	0	0	0
3	K	6	0	0	0	0
4	B	7	0	10	4	0
4	G	7	0	10	0	0
5	B	12	0	18	3	0
5	E	4	0	6	0	0
5	I	4	0	6	0	0
6	A	241	0	0	1	0
6	B	209	0	0	4	0
6	E	245	0	0	1	0
6	G	256	0	0	0	0
6	I	198	0	0	1	0
6	K	177	0	0	0	0
6	M	5	0	0	0	0
6	N	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	3	0	0	0	0
6	P	2	0	0	0	0
6	Q	4	0	0	0	0
6	R	5	0	0	0	0
All	All	15182	0	12919	73	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.

The worst 5 of 73 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:B:126:TYR:HB2	4:B:407:PEG:H42	1.61	0.83
1:A:151:PRO:HG3	1:B:291:SER:HB2	1.71	0.71
1:B:126:TYR:HB2	4:B:407:PEG:C4	2.23	0.69
1:E:206:GLN:HG3	6:E:619:HOH:O	1.94	0.67
1:B:120:HIS:CG	1:B:176:ILE:HD11	2.33	0.64

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	295/363 (81%)	290 (98%)	4 (1%)	1 (0%)	36	50
1	B	314/363 (86%)	308 (98%)	5 (2%)	1 (0%)	36	50
1	E	294/363 (81%)	288 (98%)	5 (2%)	1 (0%)	36	50
1	G	299/363 (82%)	293 (98%)	5 (2%)	1 (0%)	36	50
1	I	314/363 (86%)	306 (98%)	7 (2%)	1 (0%)	36	50
1	K	297/363 (82%)	290 (98%)	6 (2%)	1 (0%)	36	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	3/5 (60%)	3 (100%)	0	0	100	100
2	N	3/5 (60%)	3 (100%)	0	0	100	100
2	O	3/5 (60%)	3 (100%)	0	0	100	100
2	P	2/5 (40%)	2 (100%)	0	0	100	100
2	Q	2/5 (40%)	2 (100%)	0	0	100	100
2	R	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1828/2208 (83%)	1790 (98%)	32 (2%)	6 (0%)	36	50

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	SER
1	B	89	SER
1	E	89	SER
1	G	89	SER
1	I	89	SER

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	244/296 (82%)	236 (97%)	8 (3%)	33	55
1	B	252/296 (85%)	243 (96%)	9 (4%)	31	52
1	E	245/296 (83%)	236 (96%)	9 (4%)	30	51
1	G	248/296 (84%)	238 (96%)	10 (4%)	28	47
1	I	253/296 (86%)	240 (95%)	13 (5%)	21	37
1	K	245/296 (83%)	233 (95%)	12 (5%)	22	39
2	M	3/3 (100%)	3 (100%)	0	100	100
2	N	3/3 (100%)	3 (100%)	0	100	100
2	O	3/3 (100%)	3 (100%)	0	100	100
2	P	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	3/3 (100%)	3 (100%)	0	100	100
2	R	3/3 (100%)	3 (100%)	0	100	100
All	All	1505/1794 (84%)	1444 (96%)	61 (4%)	27	46

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	88	SER
1	K	149	LEU
1	G	338	ASP
1	K	141	SER
1	K	275	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	85	GLN
1	G	295	GLN
1	I	85	GLN
1	I	146	HIS
1	I	332	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 36 are monoatomic - leaving 7 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	$\# Z > 2$
4	PEG	G	407	-	6,6,6	0.12	0	5,5,5	0.26	0
5	EDO	B	408	-	3,3,3	0.34	0	2,2,2	0.14	0
5	EDO	E	407	-	3,3,3	0.31	0	2,2,2	0.03	0
4	PEG	B	407	-	6,6,6	0.24	0	5,5,5	0.79	0
5	EDO	B	409	-	3,3,3	0.36	0	2,2,2	0.59	0
5	EDO	B	410	-	3,3,3	0.33	0	2,2,2	0.09	0
5	EDO	I	407	-	3,3,3	0.18	0	2,2,2	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	G	407	-	-	3/4/4/4	-
5	EDO	B	408	-	-	0/1/1/1	-
5	EDO	E	407	-	-	0/1/1/1	-
4	PEG	B	407	-	-	0/4/4/4	-
5	EDO	B	409	-	-	1/1/1/1	-
5	EDO	B	410	-	-	0/1/1/1	-
5	EDO	I	407	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	407	PEG	O1-C1-C2-O2
5	B	409	EDO	O1-C1-C2-O2
4	G	407	PEG	C1-C2-O2-C3
4	G	407	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	408	EDO	2	0
4	B	407	PEG	4	0
5	B	410	EDO	1	0

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	301/363 (82%)	0.53	30 (9%) 12 9	17, 29, 61, 102	0
1	B	316/363 (87%)	0.62	31 (9%) 13 10	17, 29, 67, 142	0
1	E	301/363 (82%)	0.61	28 (9%) 14 11	11, 29, 59, 88	1 (0%)
1	G	305/363 (84%)	0.58	26 (8%) 16 13	17, 29, 61, 111	0
1	I	316/363 (87%)	0.84	44 (13%) 6 5	17, 29, 84, 145	0
1	K	303/363 (83%)	0.70	32 (10%) 11 8	17, 29, 64, 119	0
2	M	5/5 (100%)	1.59	2 (40%) 1 0	22, 26, 51, 67	0
2	N	5/5 (100%)	2.36	1 (20%) 3 2	22, 26, 51, 104	0
2	O	5/5 (100%)	1.52	2 (40%) 1 0	26, 31, 76, 85	0
2	P	4/5 (80%)	0.55	1 (25%) 2 1	25, 31, 39, 52	0
2	Q	4/5 (80%)	0.43	0 100 100	25, 31, 39, 52	0
2	R	4/5 (80%)	0.85	1 (25%) 2 1	25, 31, 39, 52	0
All	All	1869/2208 (84%)	0.66	198 (10%) 11 8	11, 29, 66, 145	1 (0%)

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	VAL	8.2
1	B	150	THR	7.7
1	I	150	THR	7.5
1	K	150	THR	6.3
1	I	148	VAL	5.8

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	PEG	G	407	7/7	0.70	0.26	36,44,70,98	0
5	EDO	I	407	4/4	0.77	0.25	27,60,66,84	0
5	EDO	B	408	4/4	0.85	0.22	9,36,69,91	0
5	EDO	B	409	4/4	0.86	0.15	27,35,37,40	0
3	CA	G	403	1/1	0.86	0.08	26,26,26,26	0
5	EDO	E	407	4/4	0.87	0.26	42,56,64,77	0
5	EDO	B	410	4/4	0.87	0.14	39,49,58,62	0
3	CA	E	403	1/1	0.92	0.07	26,26,26,26	0
3	CA	K	406	1/1	0.93	0.04	25,25,25,25	0
4	PEG	B	407	7/7	0.93	0.18	22,47,114,115	0
3	CA	A	405	1/1	0.93	0.05	29,29,29,29	0
3	CA	B	406	1/1	0.93	0.08	25,25,25,25	0
3	CA	I	403	1/1	0.94	0.06	26,26,26,26	0
3	CA	I	405	1/1	0.96	0.04	29,29,29,29	0
3	CA	A	406	1/1	0.96	0.04	25,25,25,25	0
3	CA	B	405	1/1	0.96	0.04	29,29,29,29	0
3	CA	E	405	1/1	0.97	0.10	29,29,29,29	0
3	CA	K	404	1/1	0.97	0.04	20,20,20,20	0
3	CA	G	404	1/1	0.97	0.06	20,20,20,20	0
3	CA	I	401	1/1	0.97	0.04	18,18,18,18	0
3	CA	G	402	1/1	0.97	0.03	24,24,24,24	0
3	CA	K	401	1/1	0.98	0.06	18,18,18,18	0
3	CA	E	401	1/1	0.98	0.04	18,18,18,18	0
3	CA	A	404	1/1	0.98	0.04	20,20,20,20	0
3	CA	E	404	1/1	0.98	0.06	20,20,20,20	0
3	CA	G	406	1/1	0.98	0.03	25,25,25,25	0
3	CA	B	404	1/1	0.98	0.05	20,20,20,20	0
3	CA	I	402	1/1	0.98	0.06	24,24,24,24	0
3	CA	E	406	1/1	0.98	0.06	25,25,25,25	0
3	CA	G	401	1/1	0.98	0.07	18,18,18,18	0
3	CA	I	406	1/1	0.98	0.04	25,25,25,25	0
3	CA	A	402	1/1	0.99	0.03	24,24,24,24	0

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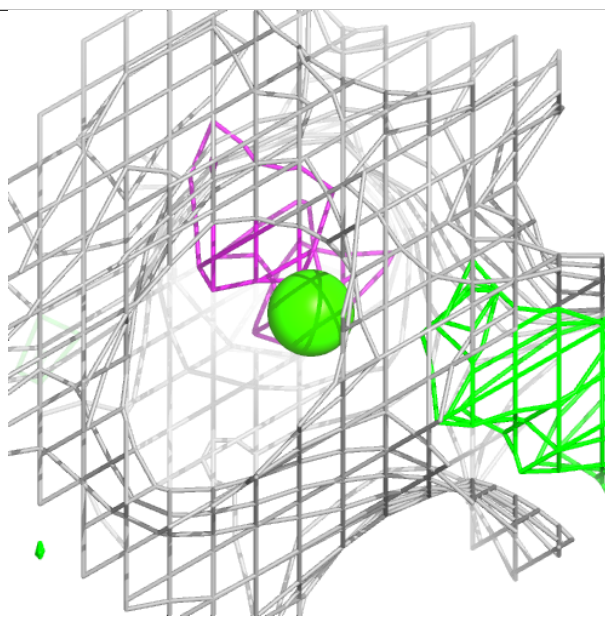
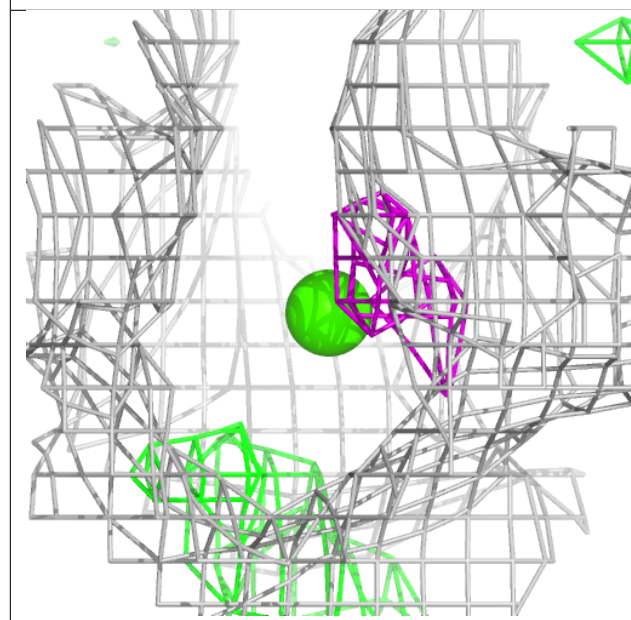
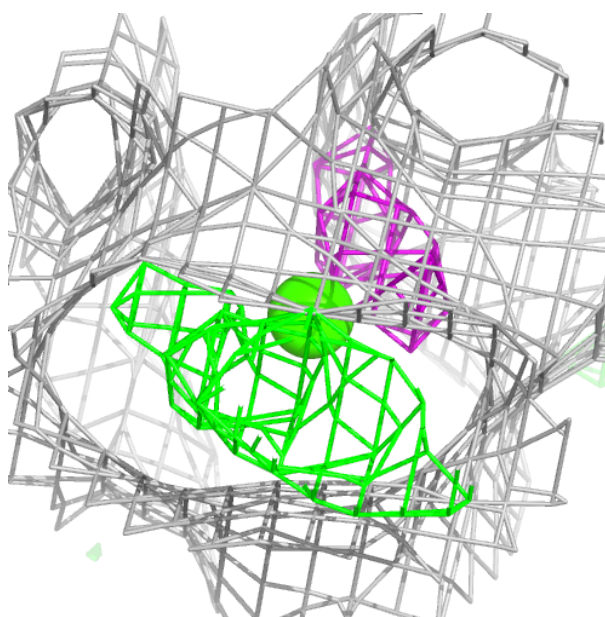
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	K	405	1/1	0.99	0.04	29,29,29,29	0
3	CA	A	403	1/1	0.99	0.03	26,26,26,26	0
3	CA	B	401	1/1	0.99	0.03	18,18,18,18	0
3	CA	E	402	1/1	0.99	0.02	24,24,24,24	0
3	CA	B	403	1/1	0.99	0.02	26,26,26,26	0
3	CA	A	401	1/1	0.99	0.02	18,18,18,18	0
3	CA	G	405	1/1	0.99	0.04	29,29,29,29	0
3	CA	K	402	1/1	0.99	0.02	24,24,24,24	0
3	CA	K	403	1/1	0.99	0.02	26,26,26,26	0
3	CA	I	404	1/1	1.00	0.03	20,20,20,20	0
3	CA	B	402	1/1	1.00	0.03	24,24,24,24	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.

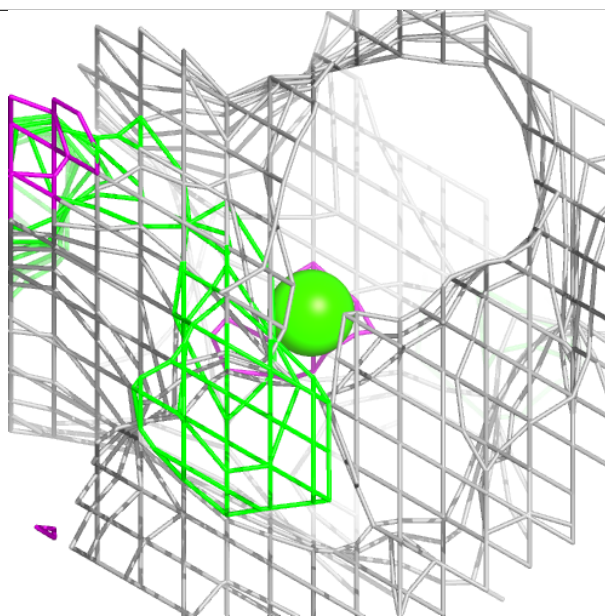
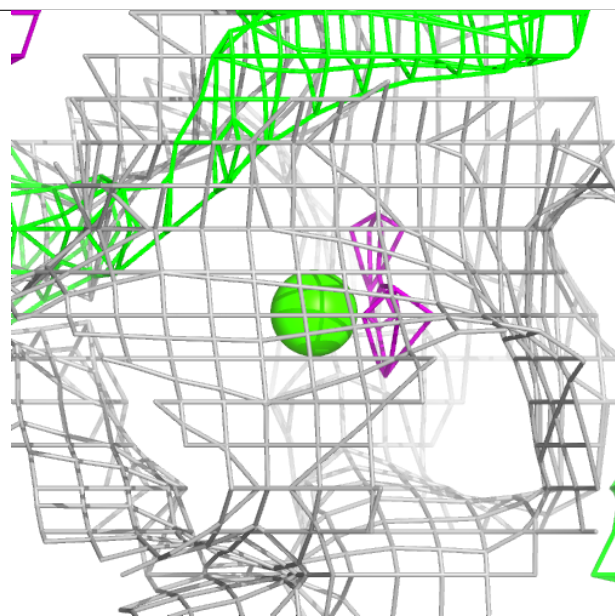
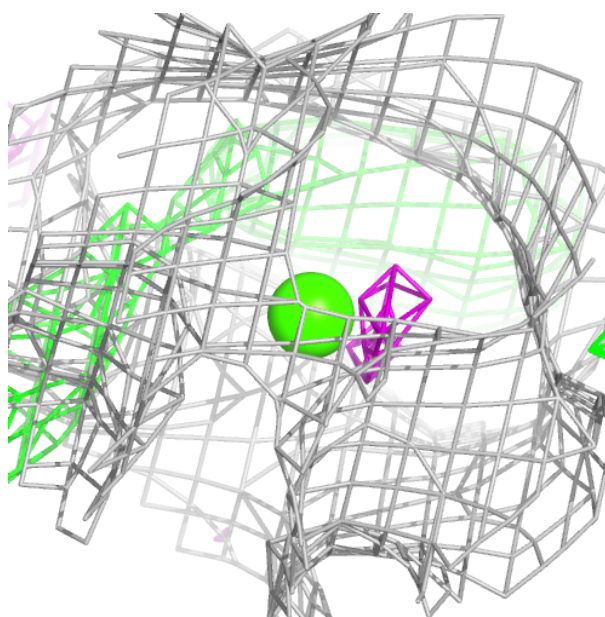
Electron density around CA G 403:

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



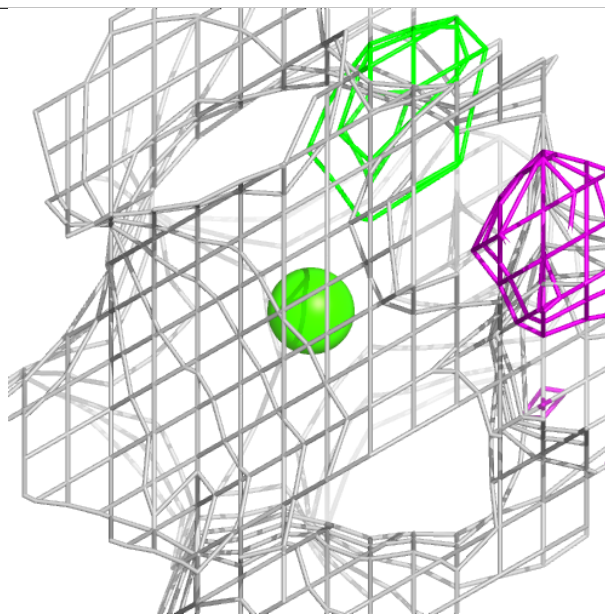
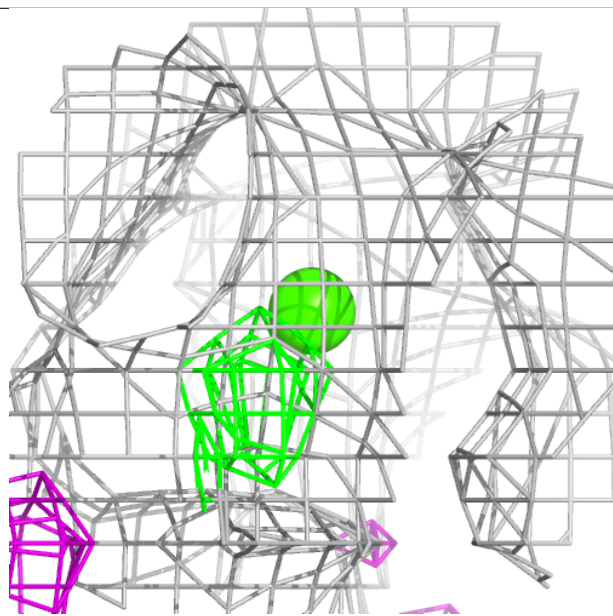
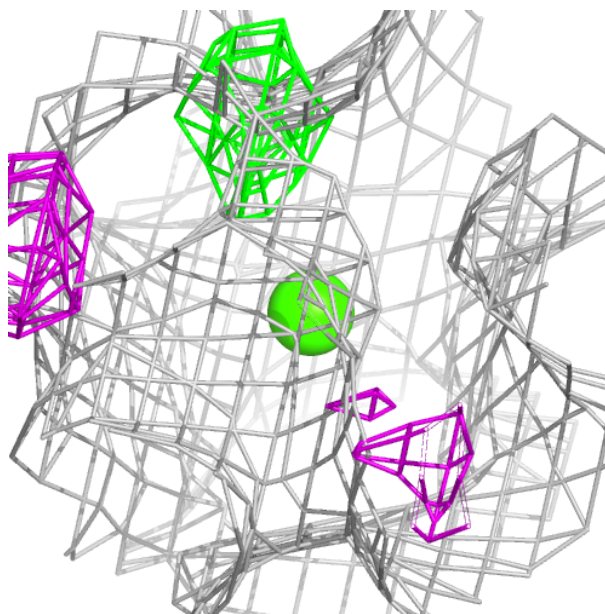
Electron density around CA E 403:

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



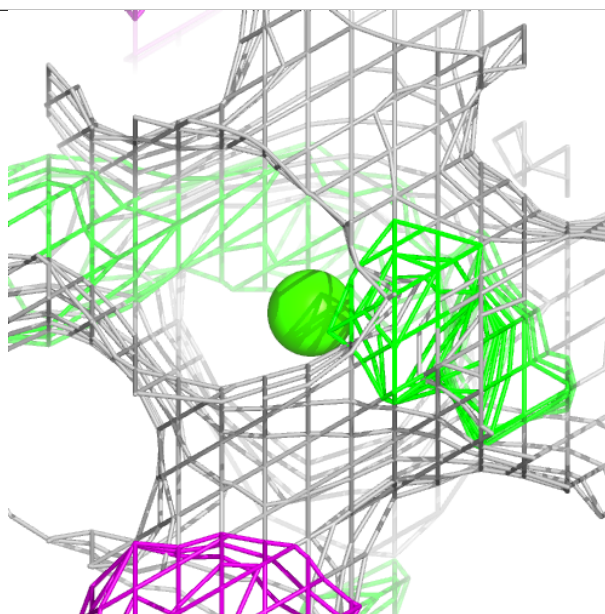
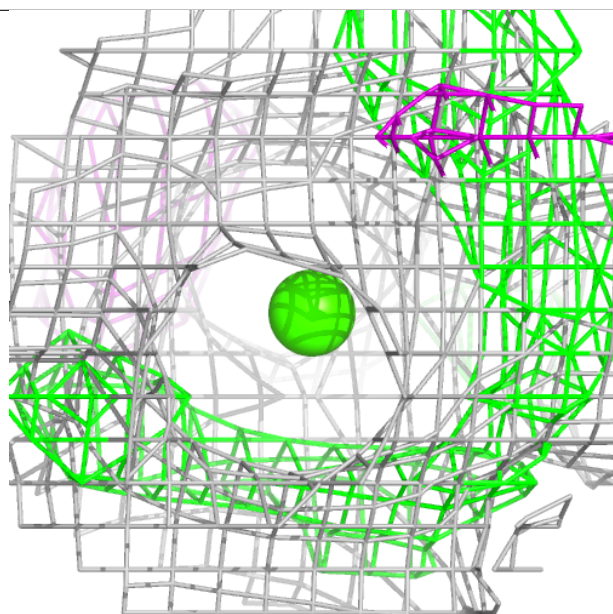
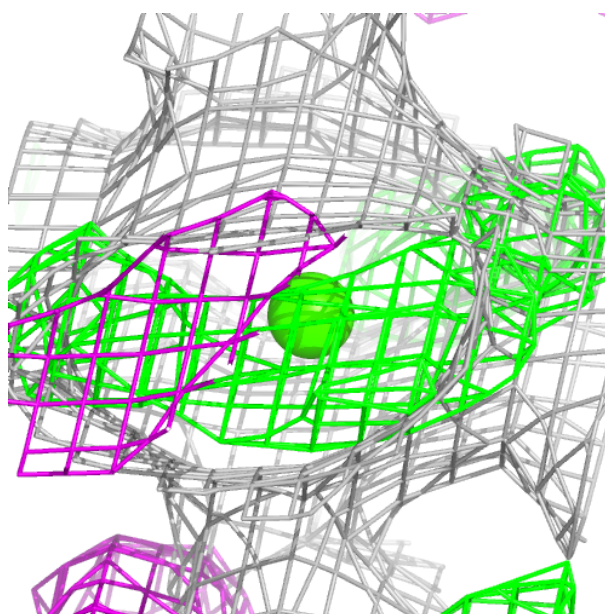
Electron density around CA K 406:

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and green (positive)



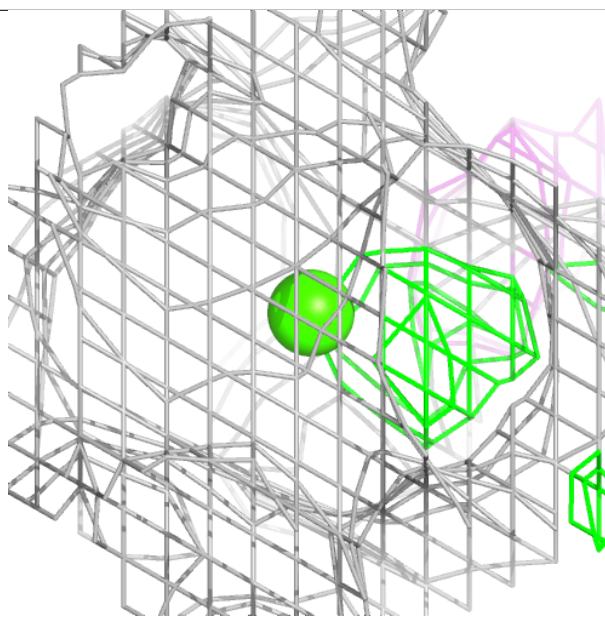
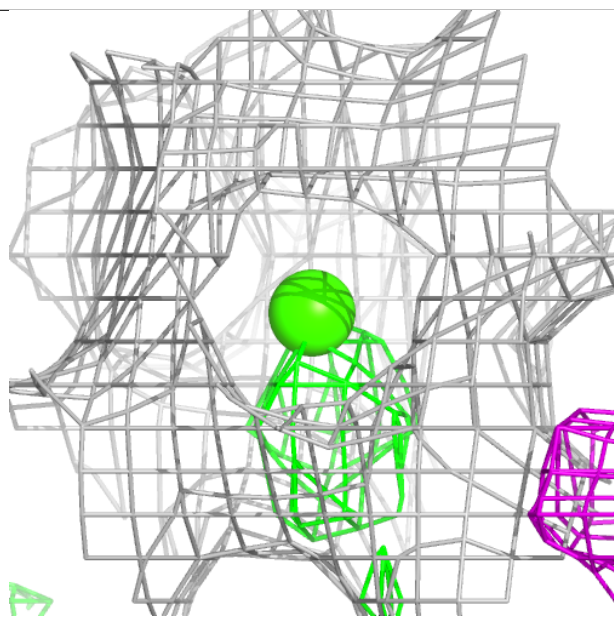
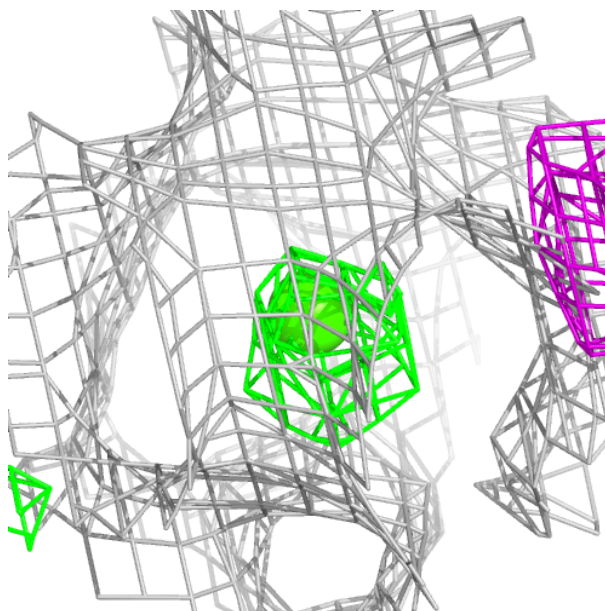
Electron density around CA A 405:

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and green (positive)



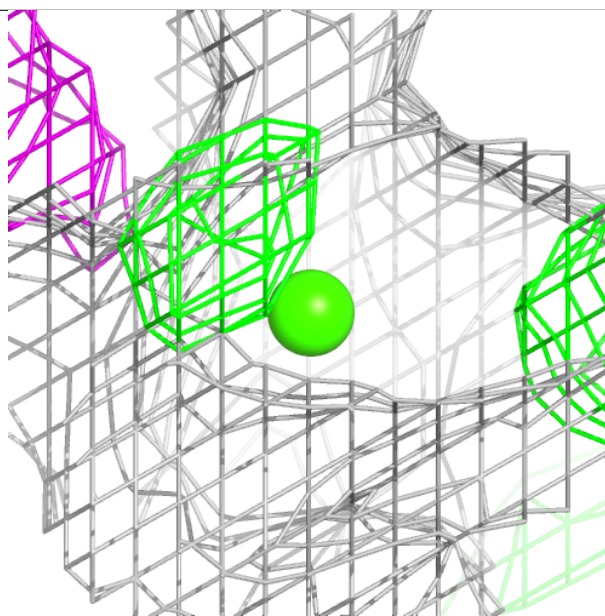
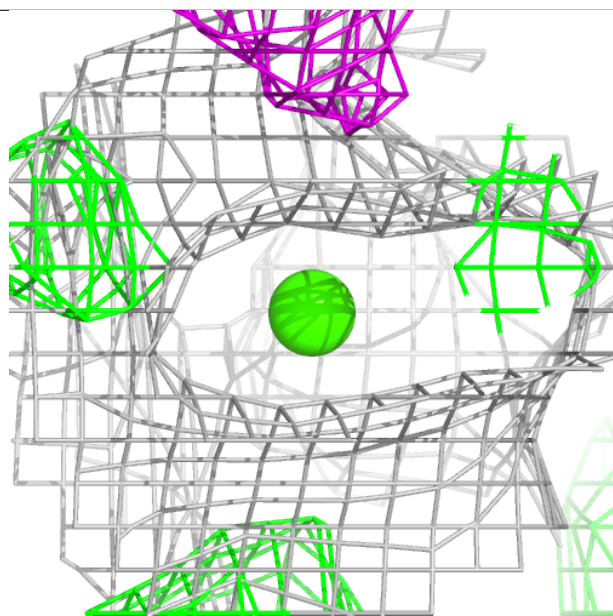
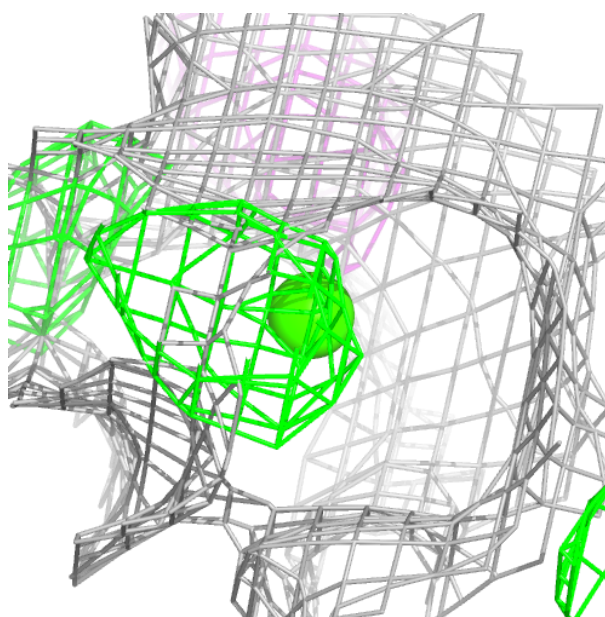
Electron density around CA B 406:

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



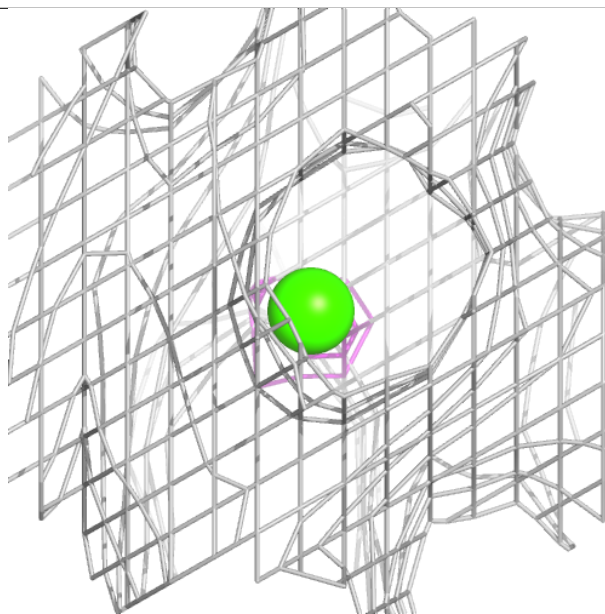
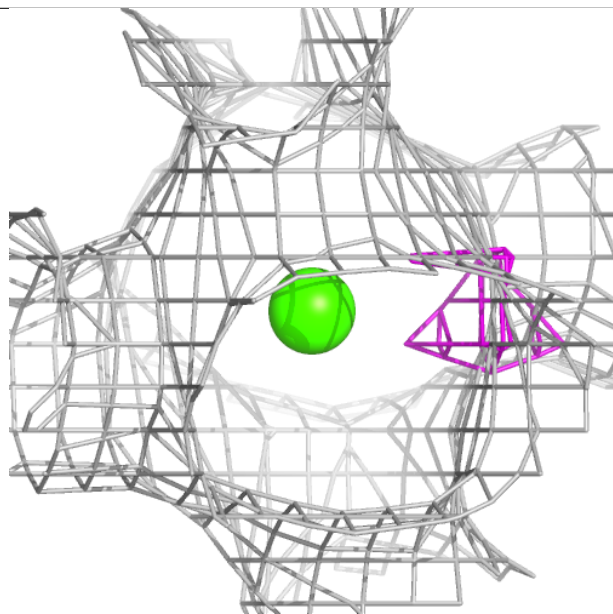
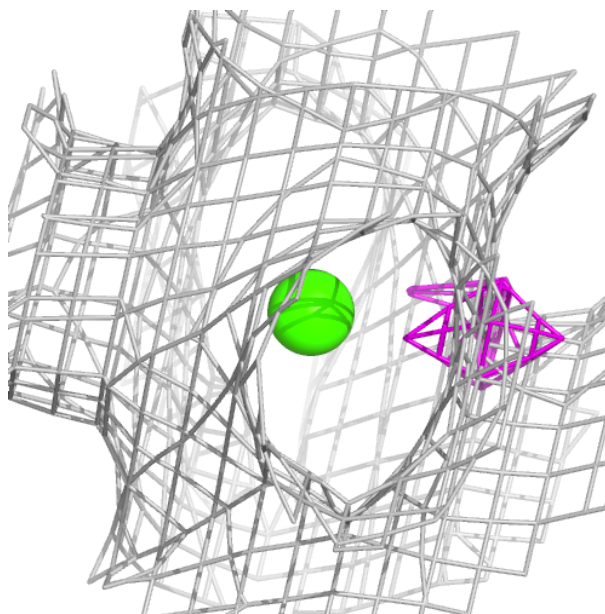
Electron density around CA I 403:

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



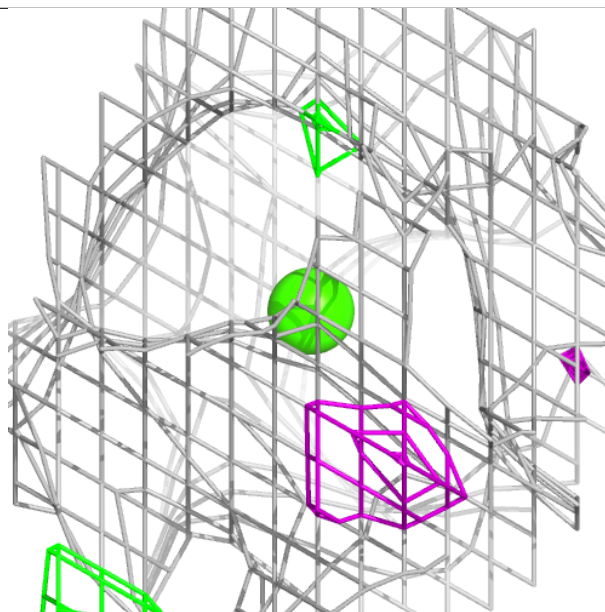
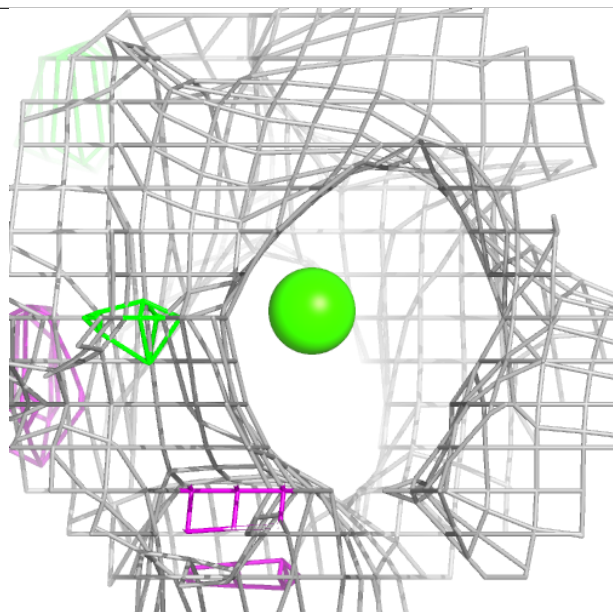
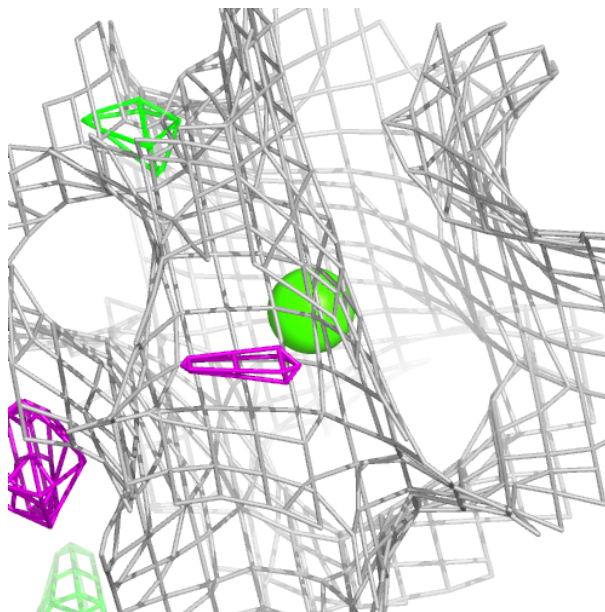
Electron density around CA I 405:

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



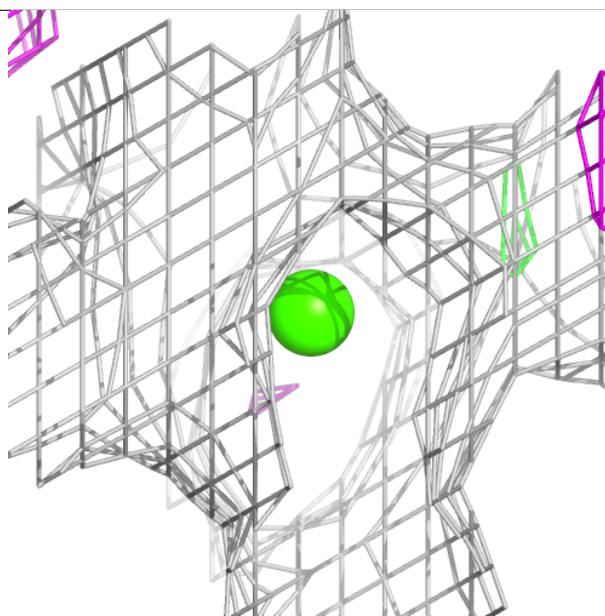
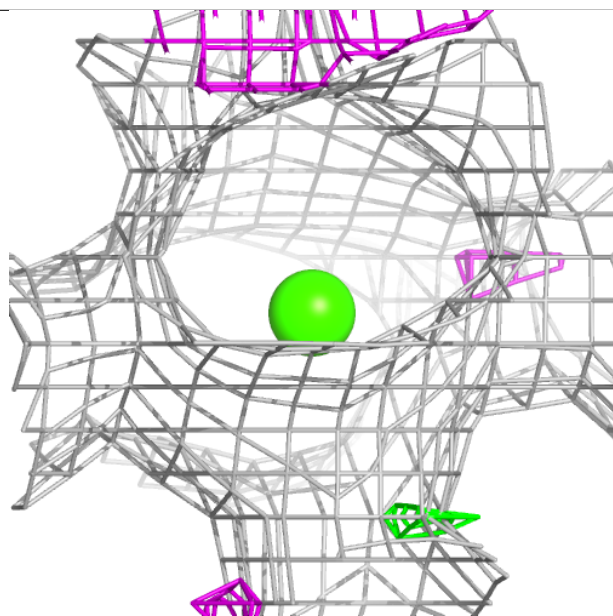
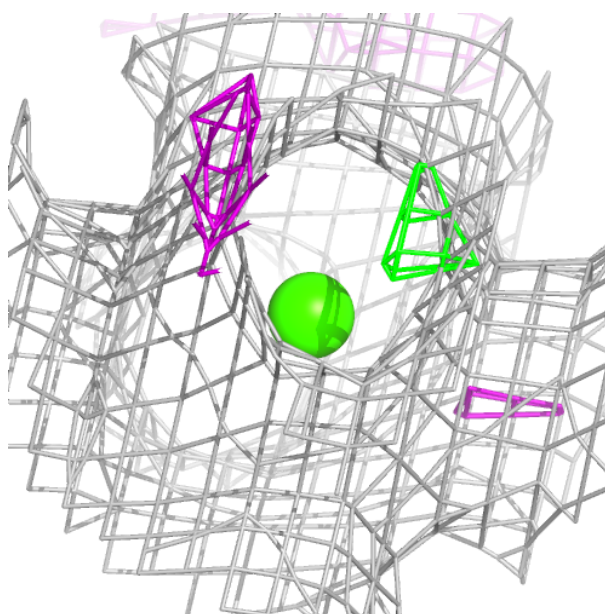
Electron density around CA A 406:

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



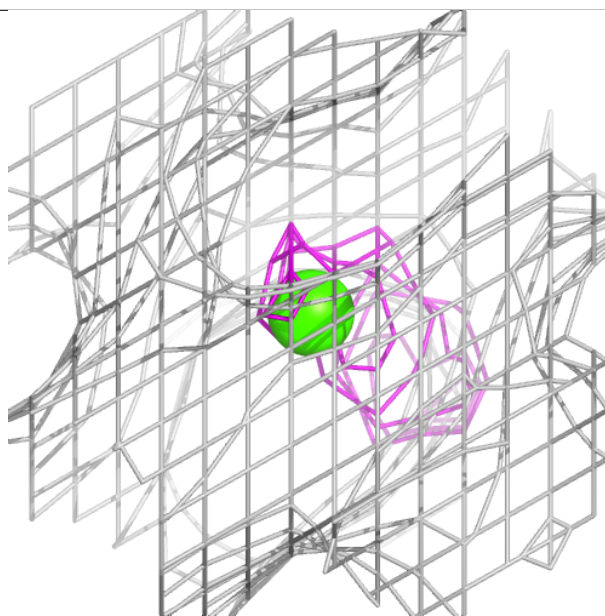
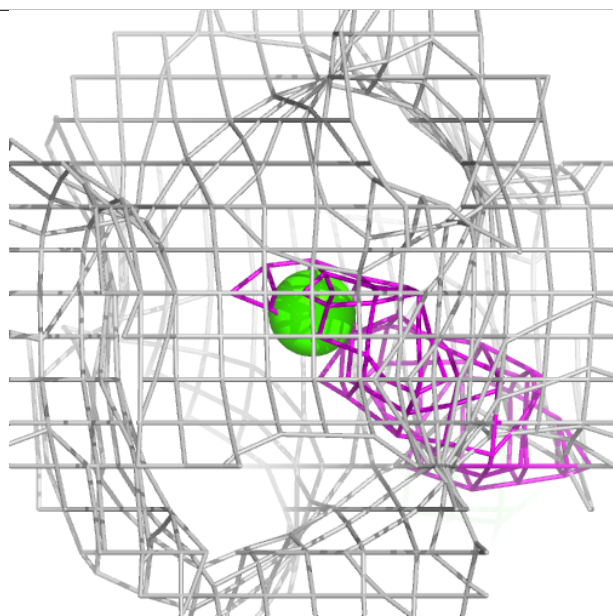
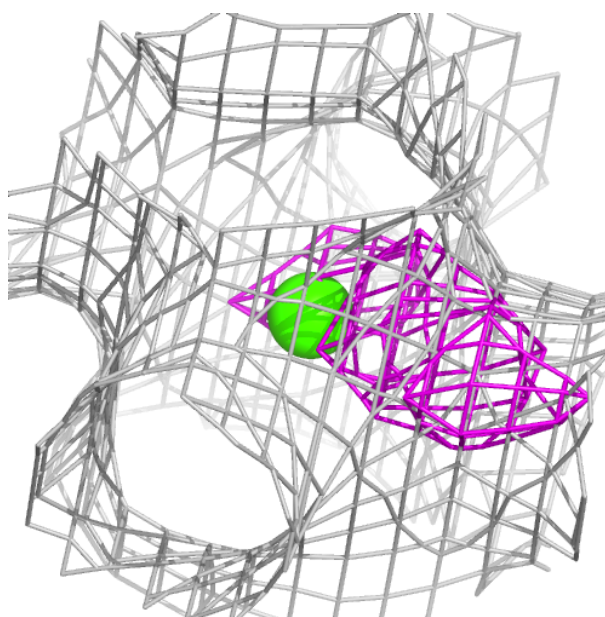
Electron density around CA B 405:

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



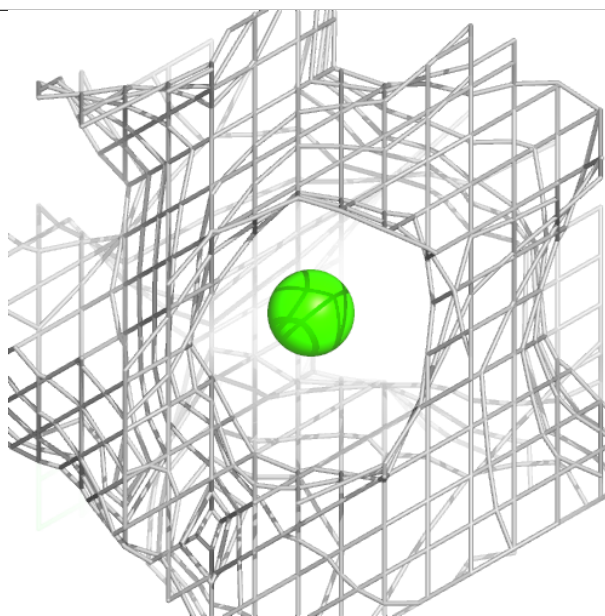
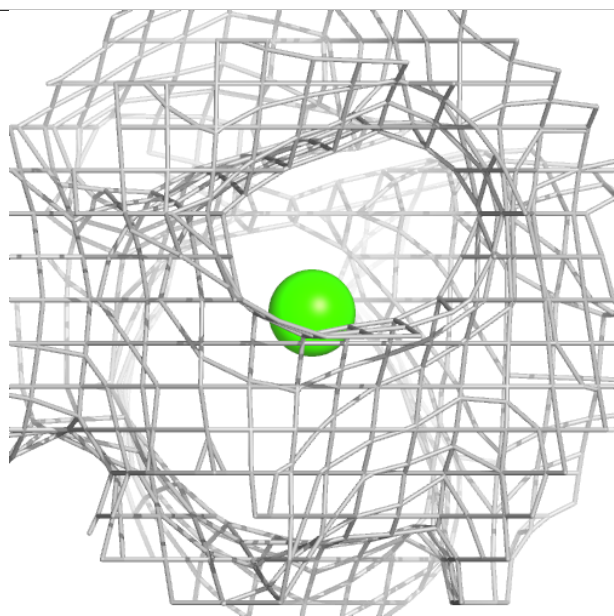
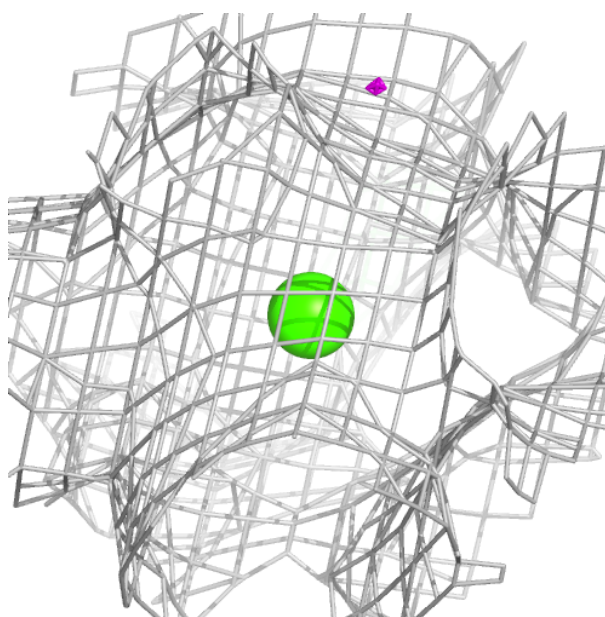
Electron density around CA E 405:

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



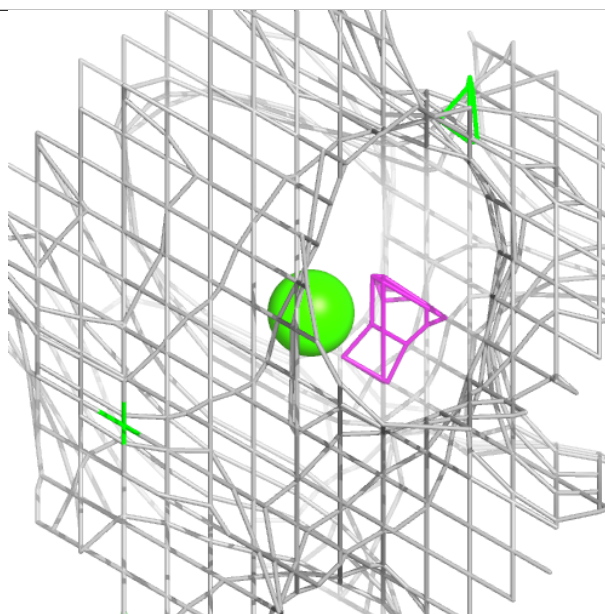
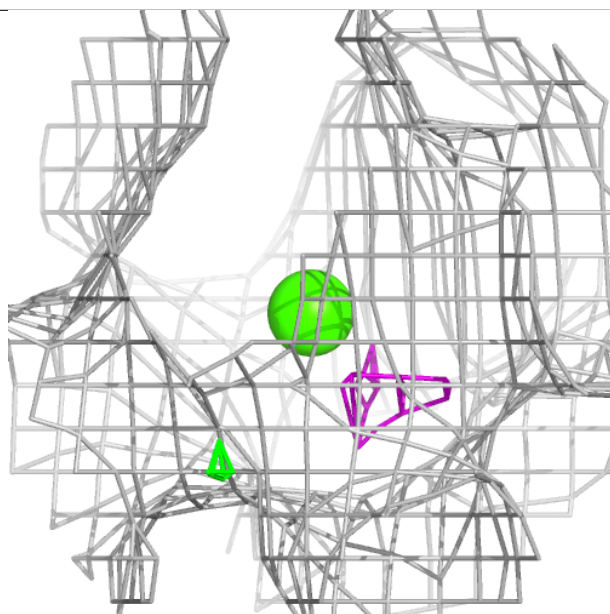
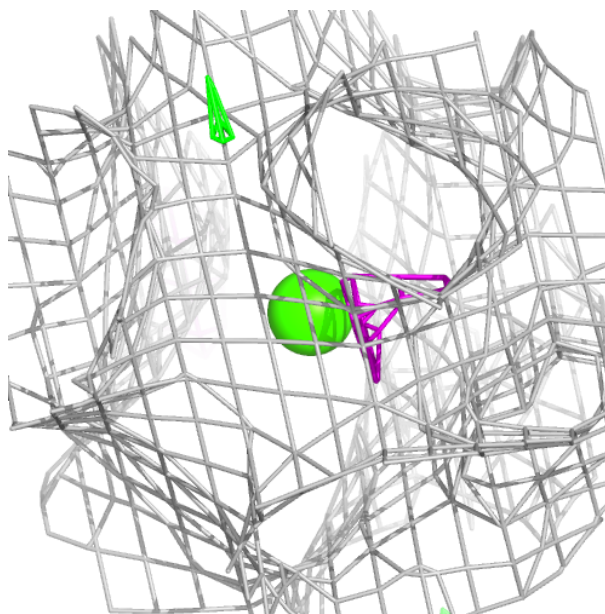
Electron density around CA K 404:

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



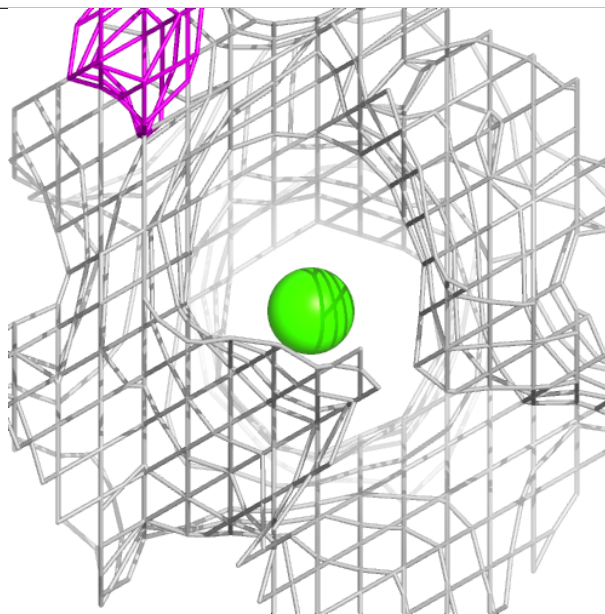
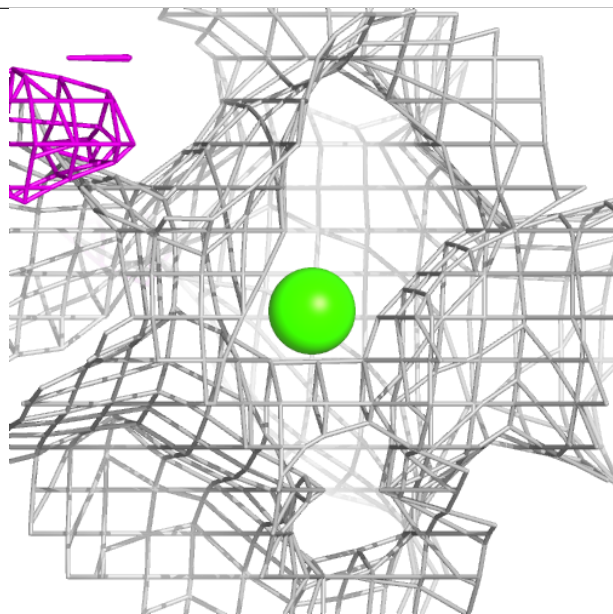
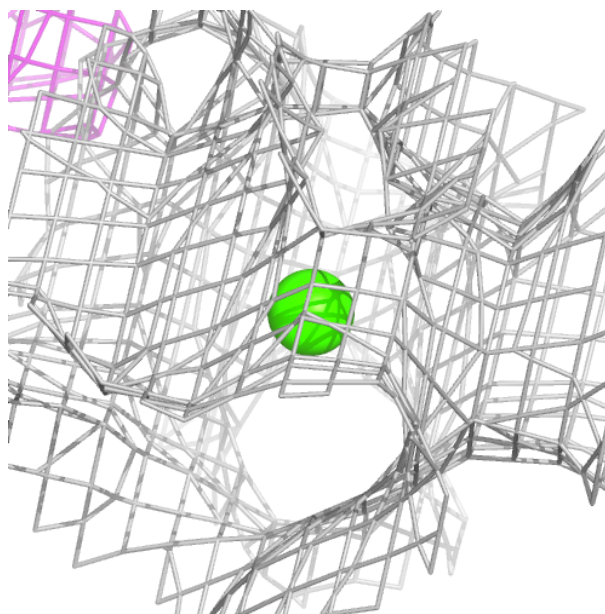
Electron density around CA G 404:

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



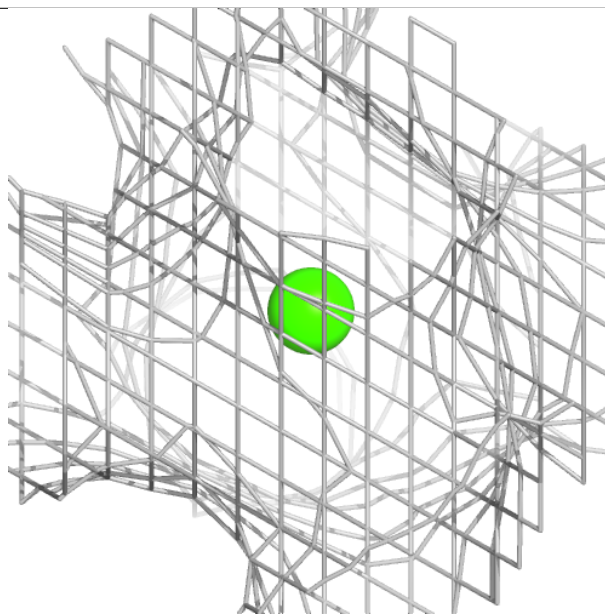
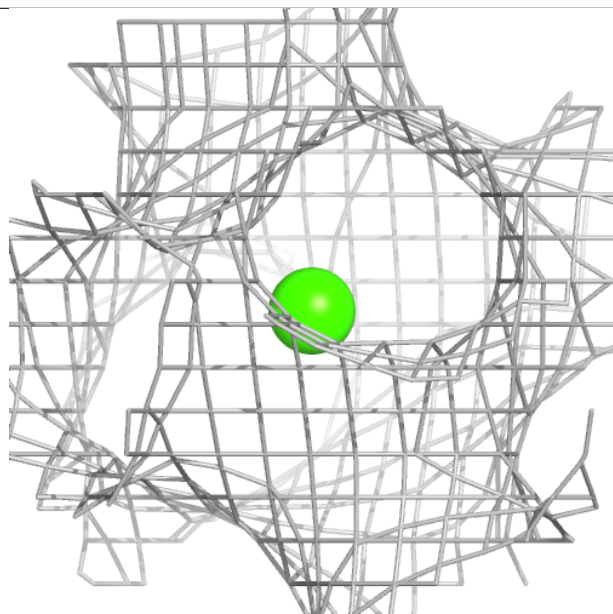
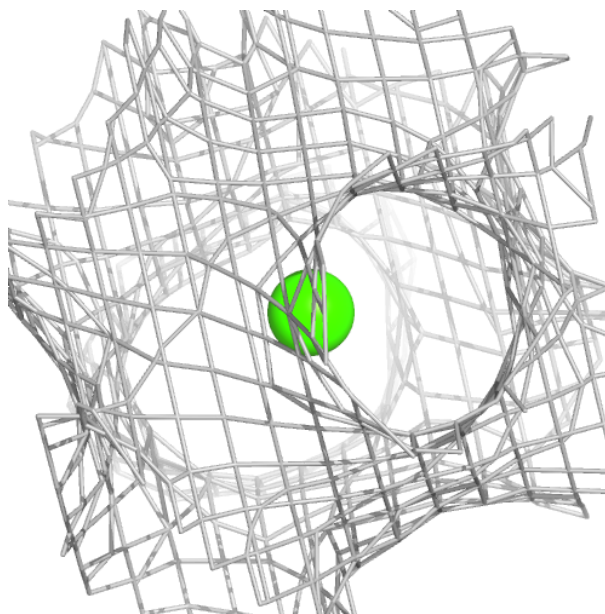
Electron density around CA I 401:

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



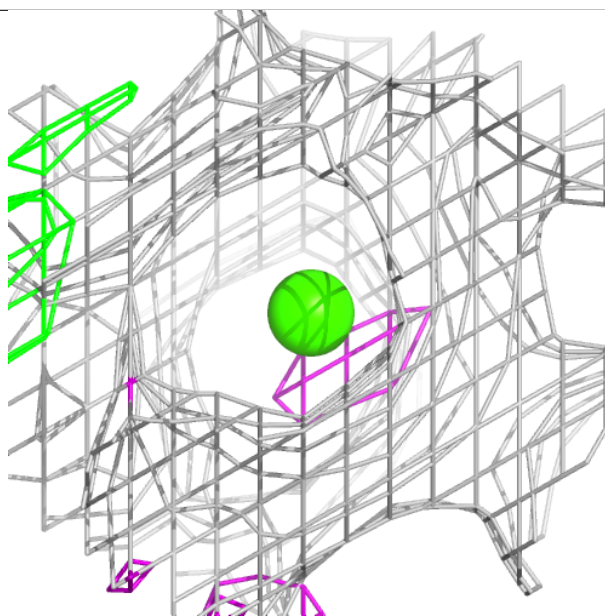
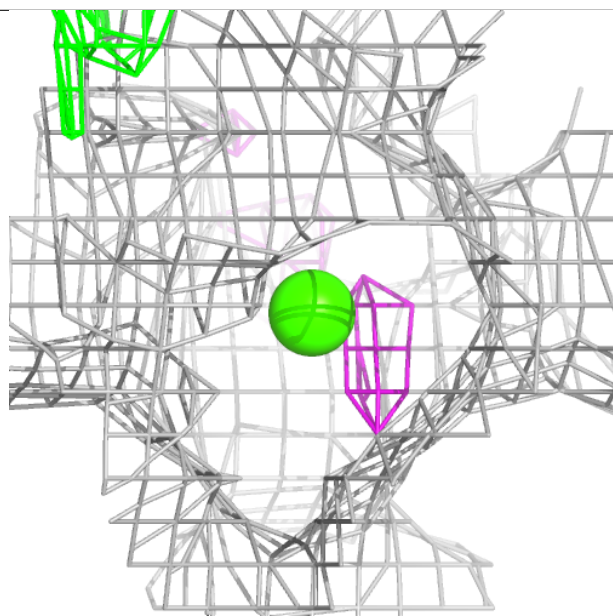
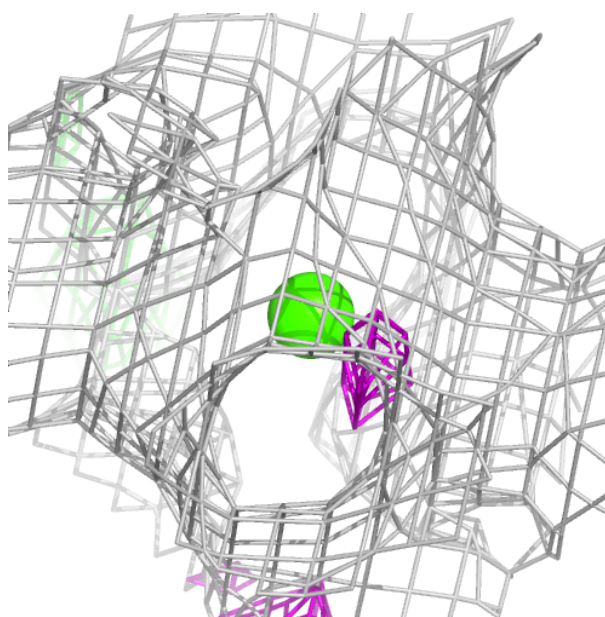
Electron density around CA G 402:

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



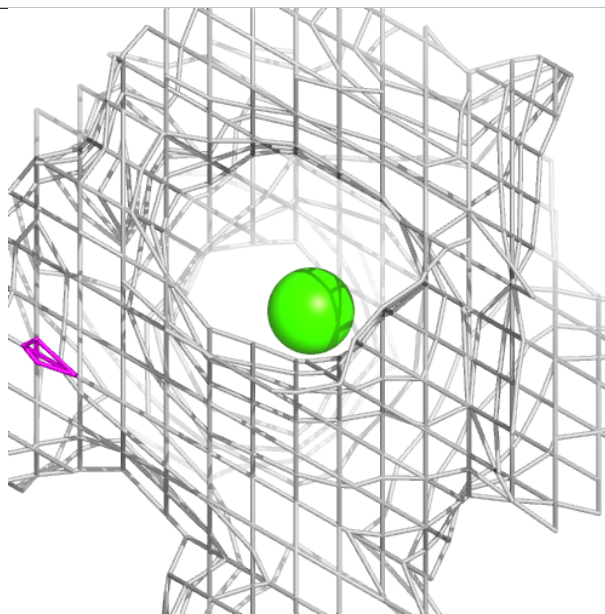
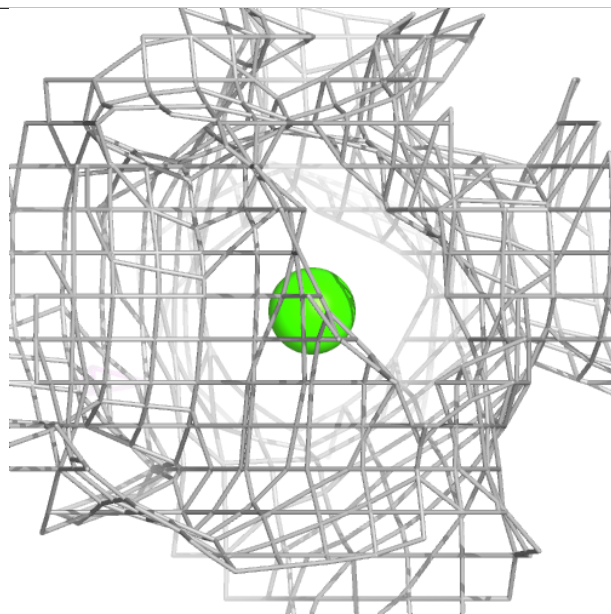
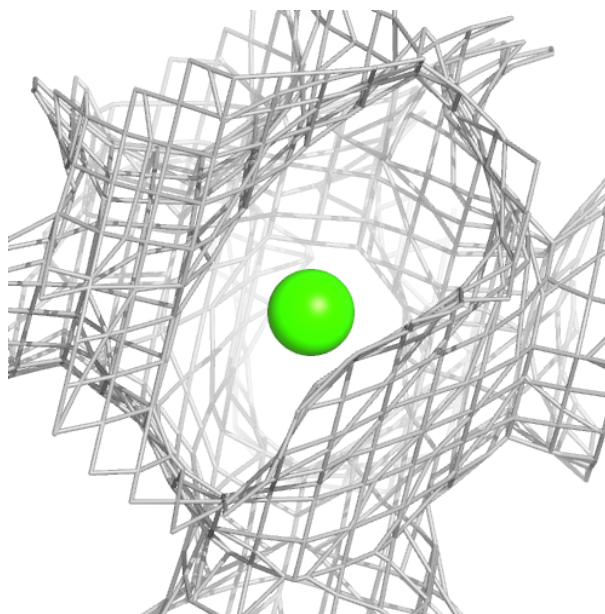
Electron density around CA K 401:

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



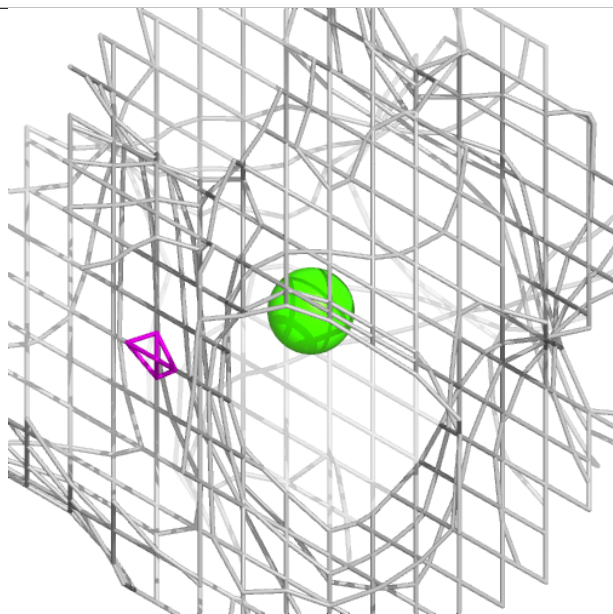
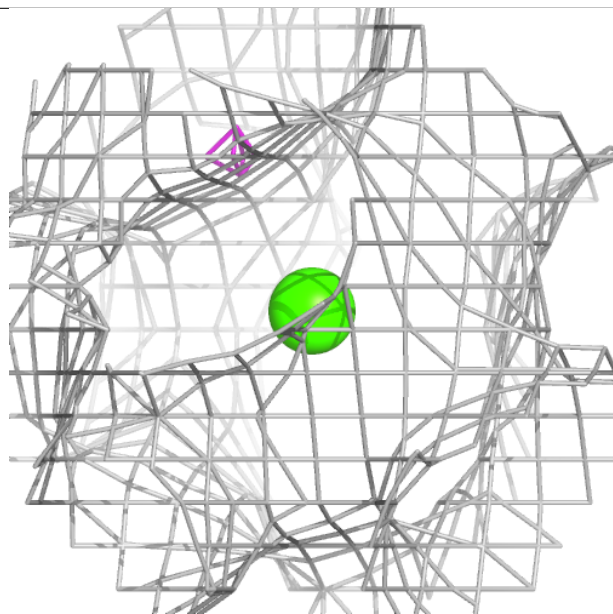
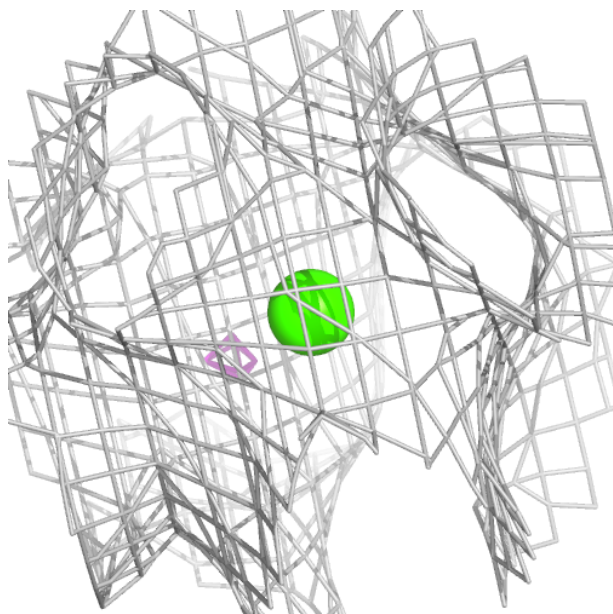
Electron density around CA E 401:

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



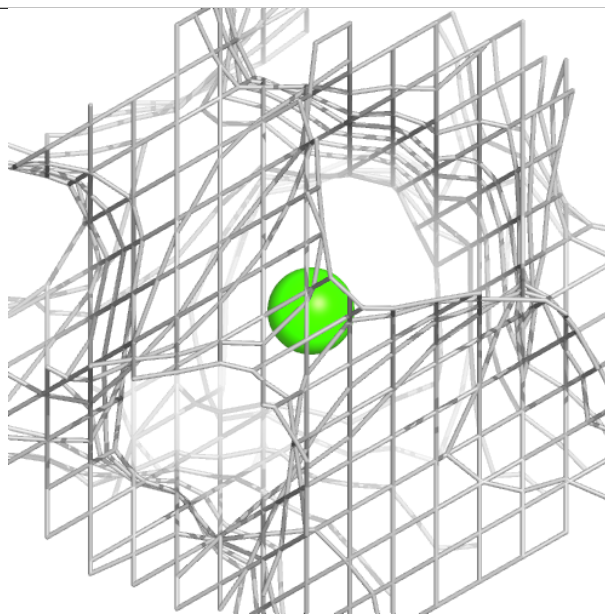
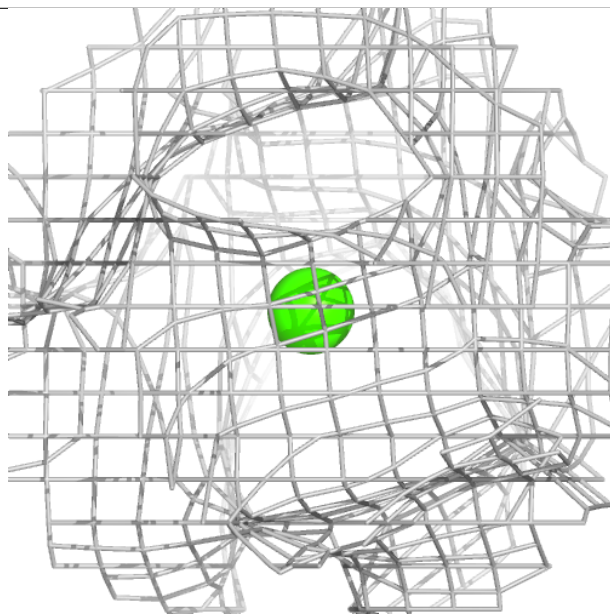
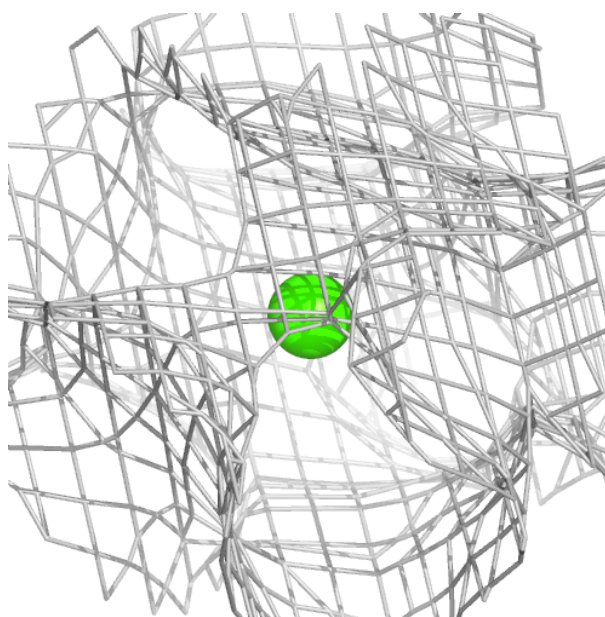
Electron density around CA A 404:

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



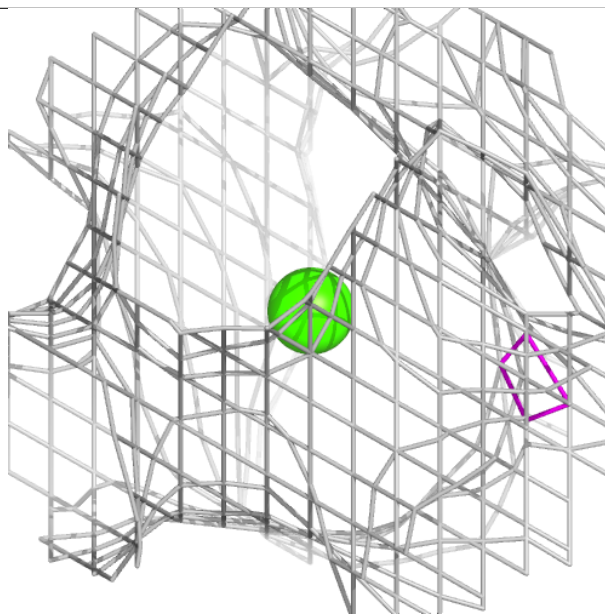
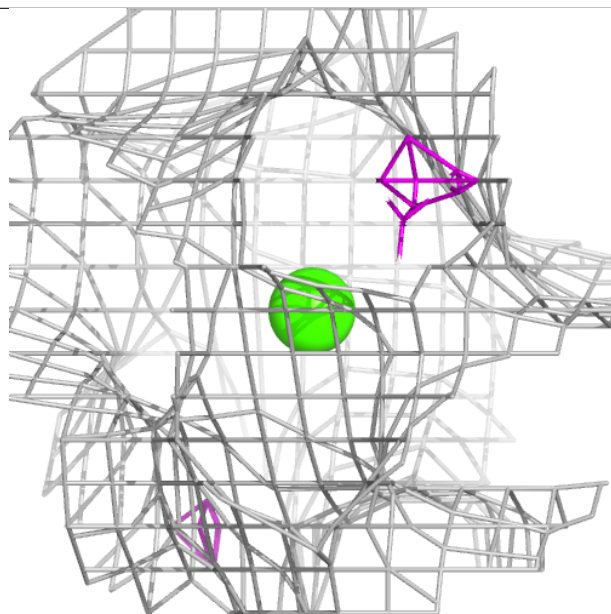
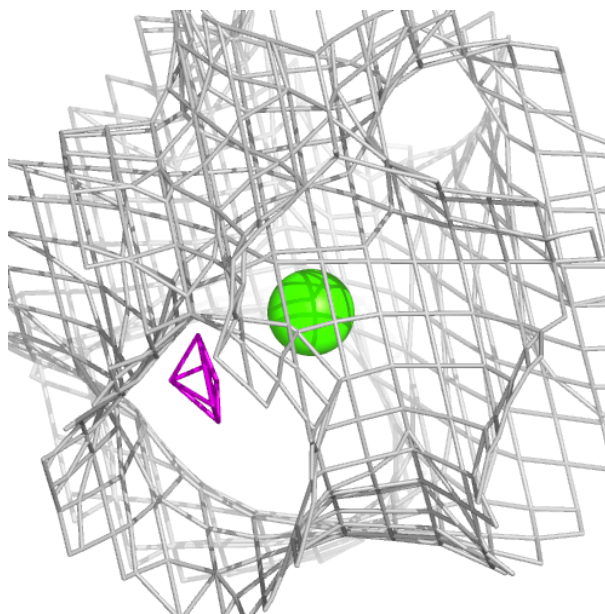
Electron density around CA E 404:

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



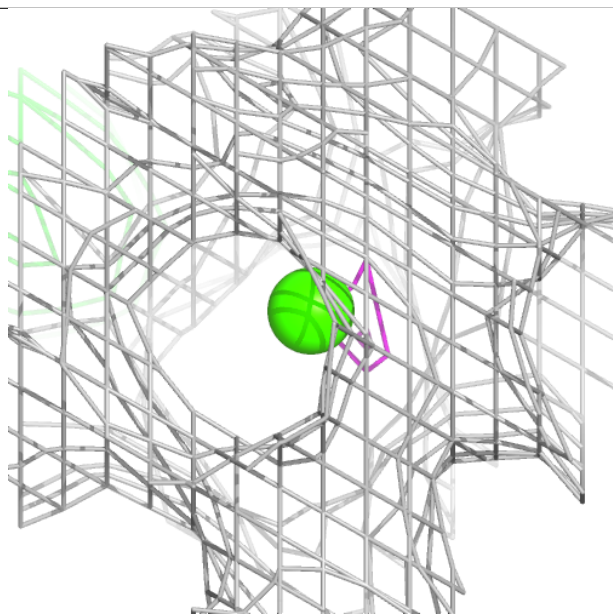
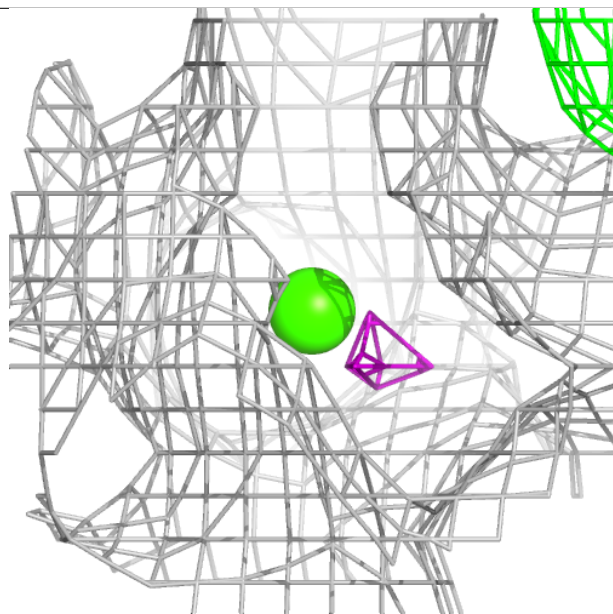
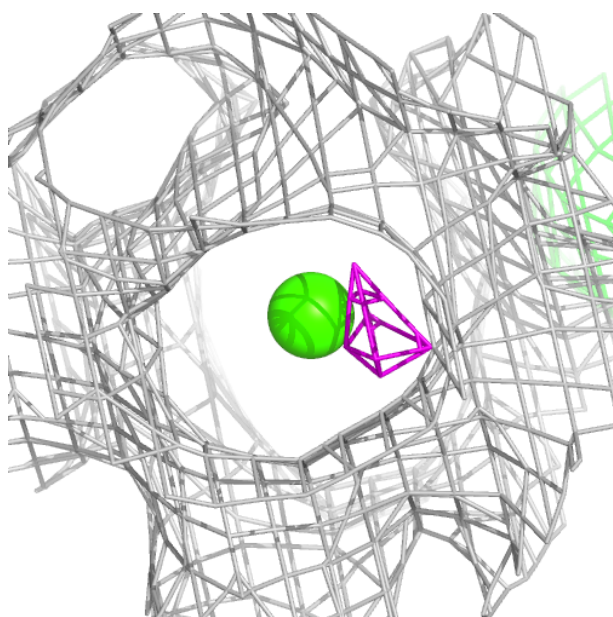
Electron density around CA G 406:

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



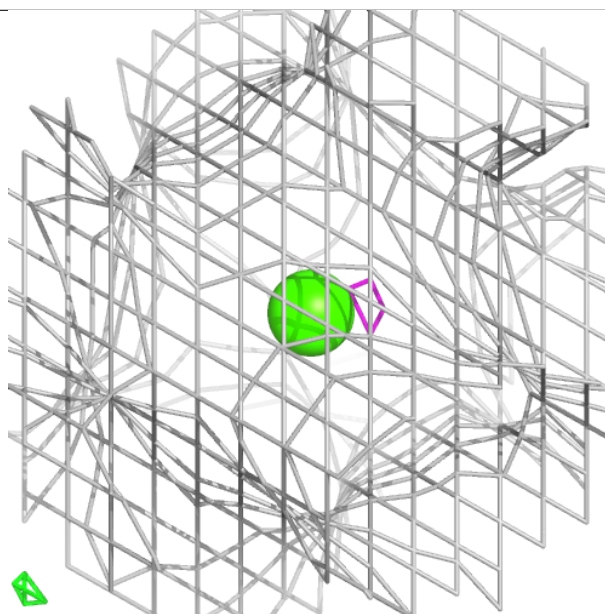
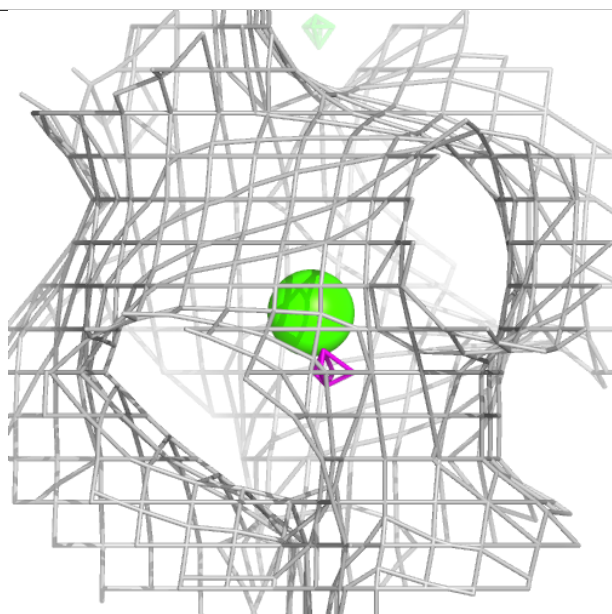
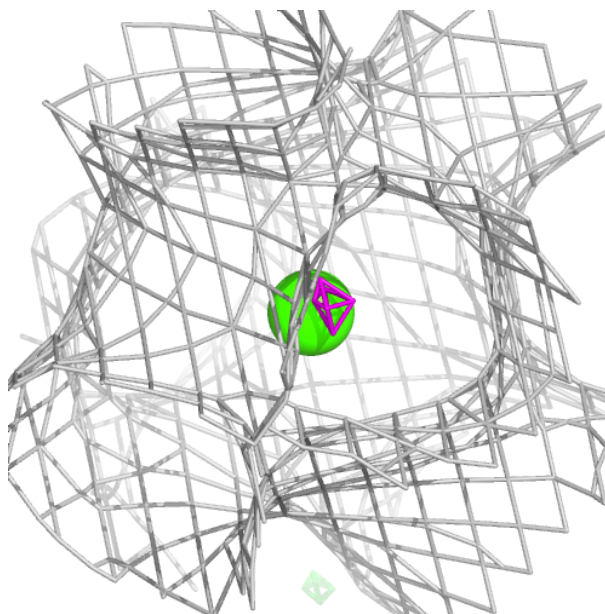
Electron density around CA B 404:

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



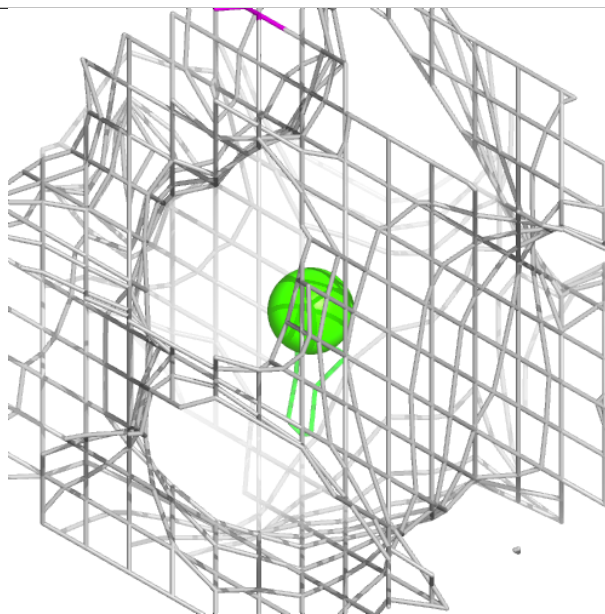
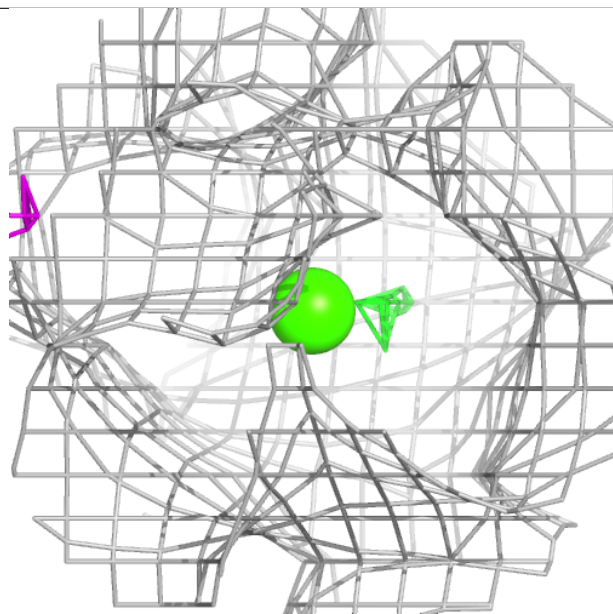
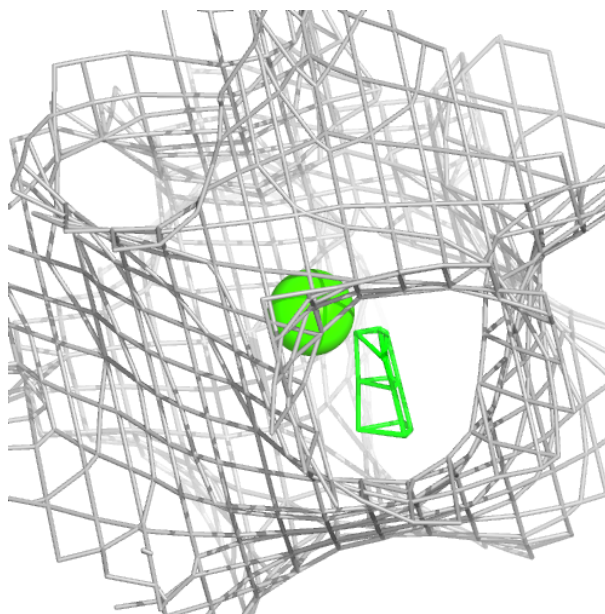
Electron density around CA I 402:

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



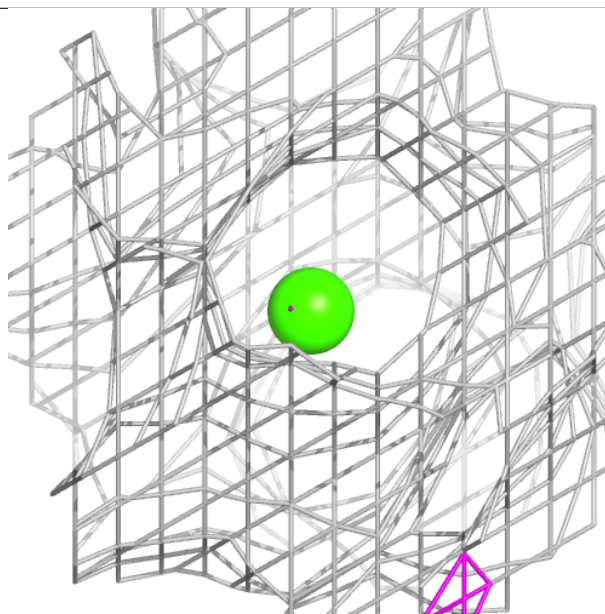
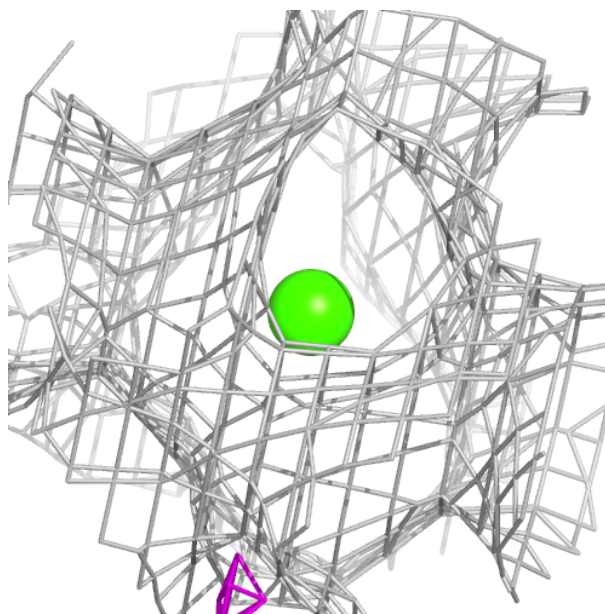
Electron density around CA E 406:

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



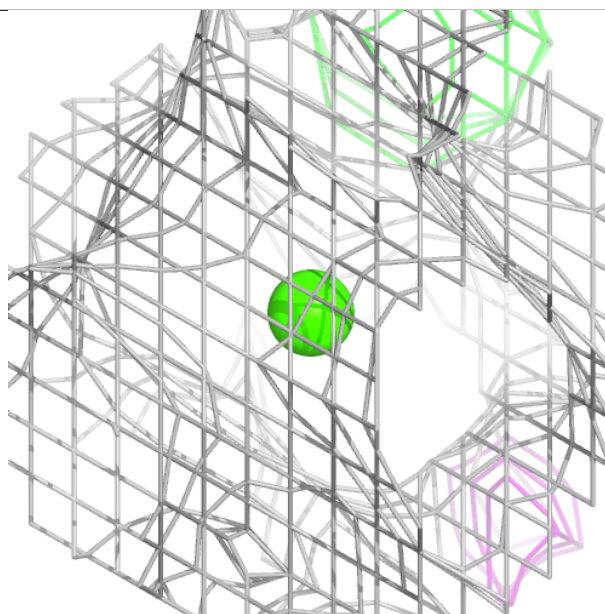
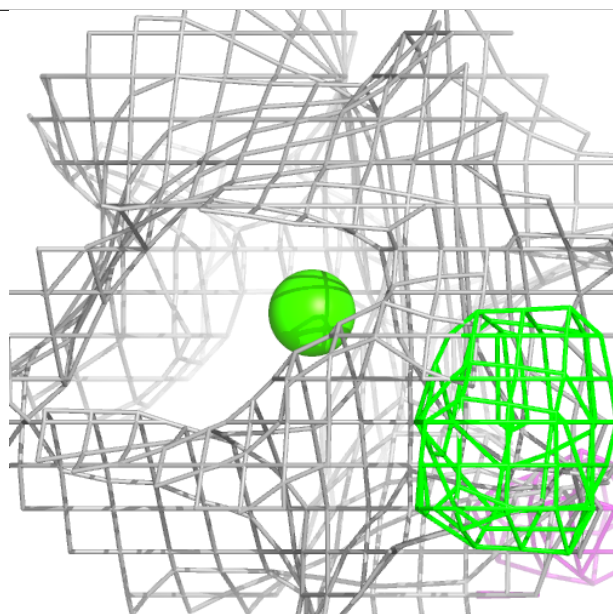
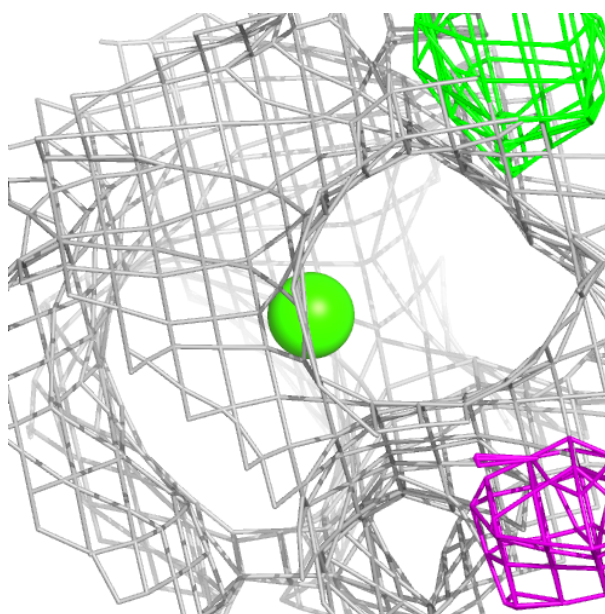
Electron density around CA G 401:

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



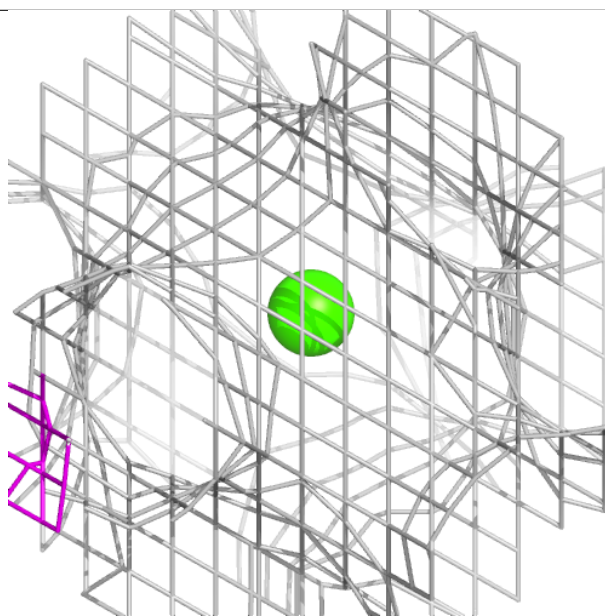
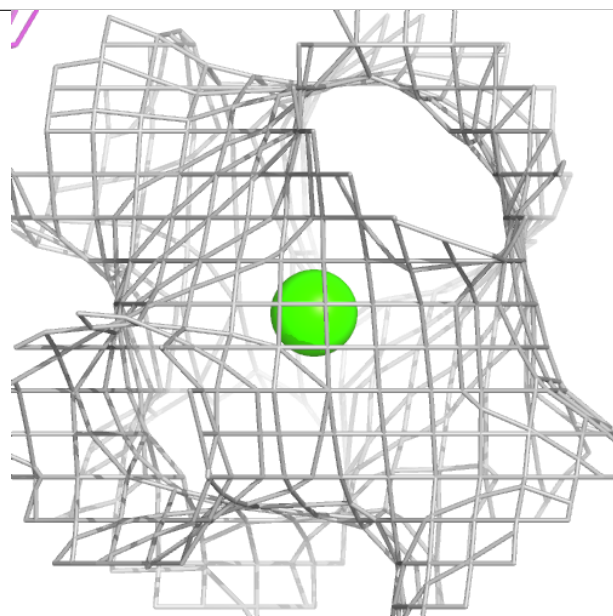
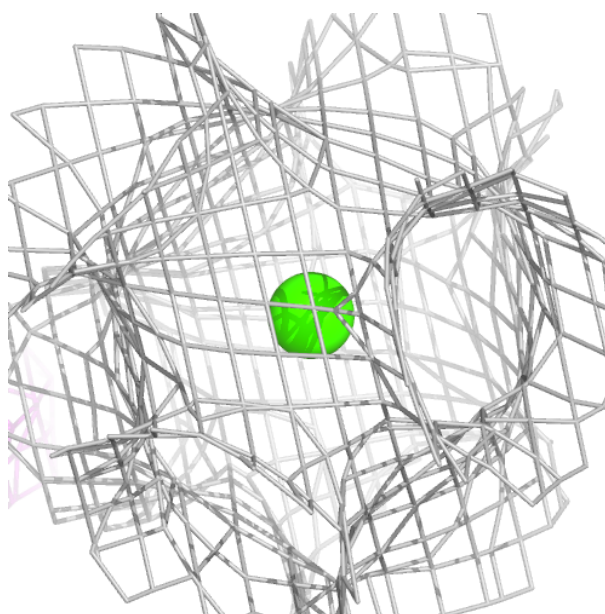
Electron density around CA I 406:

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



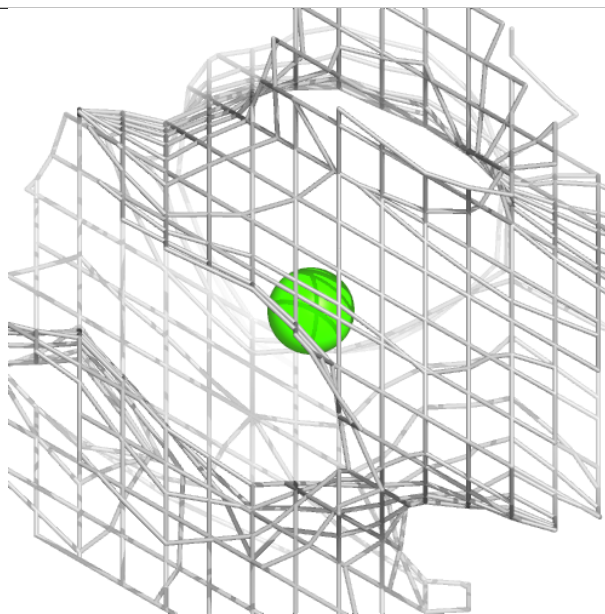
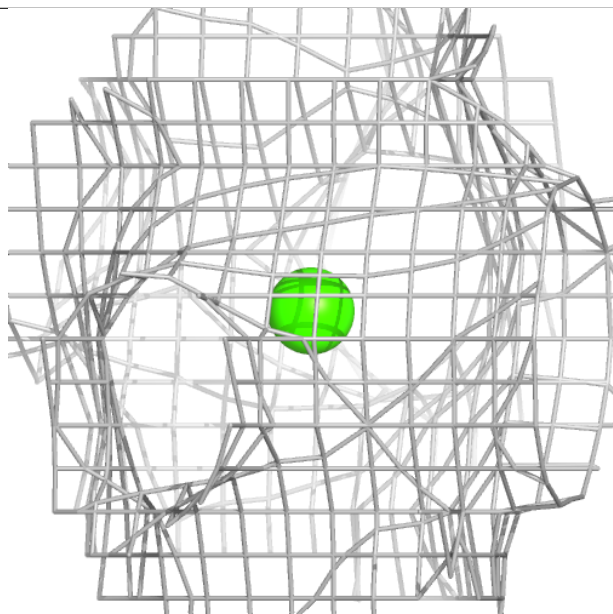
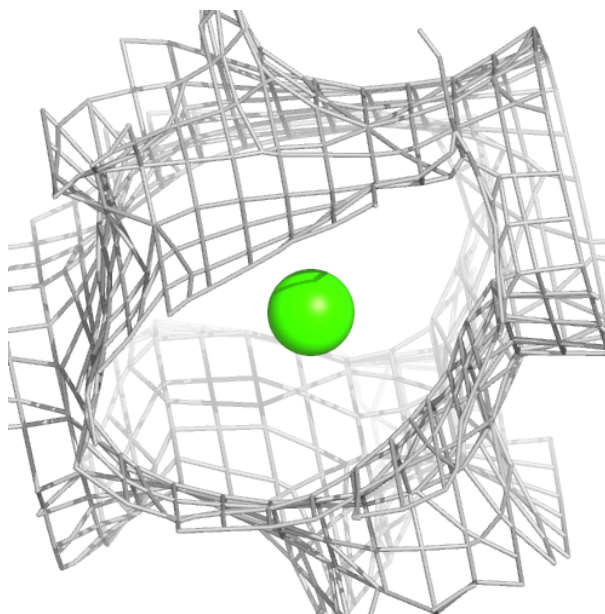
Electron density around CA A 402:

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



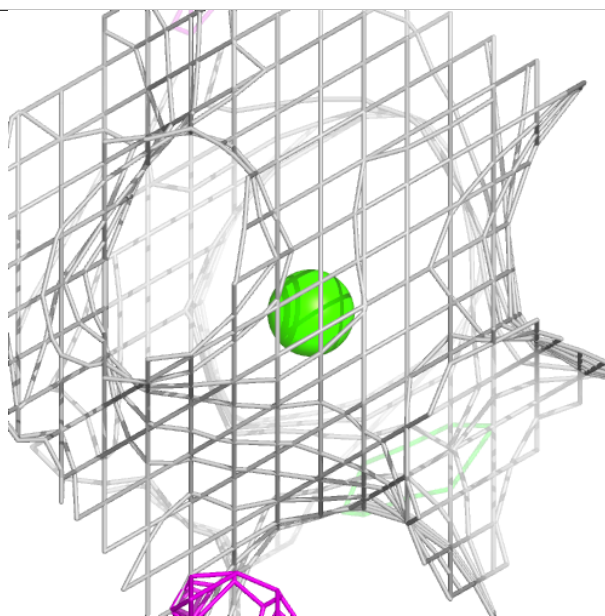
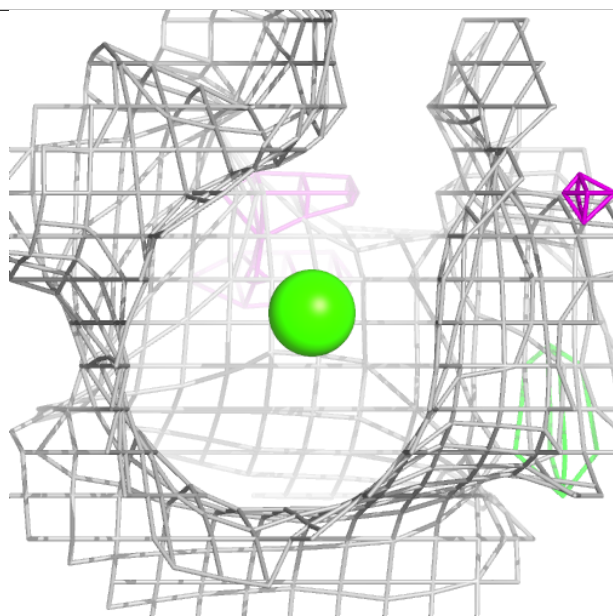
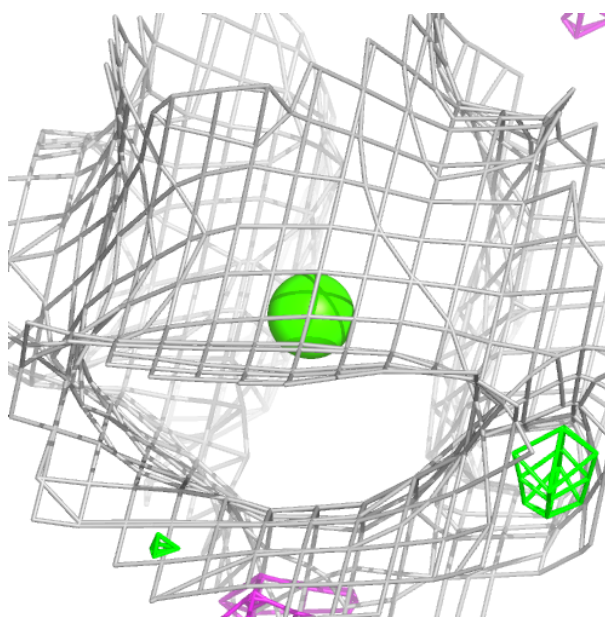
Electron density around CA K 405:

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



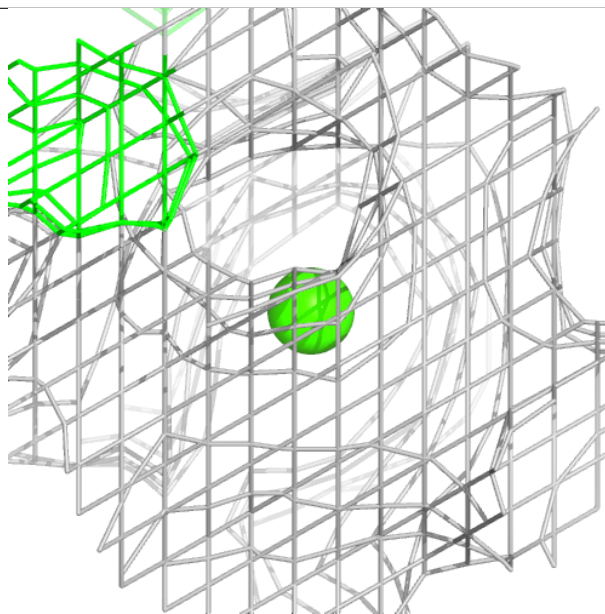
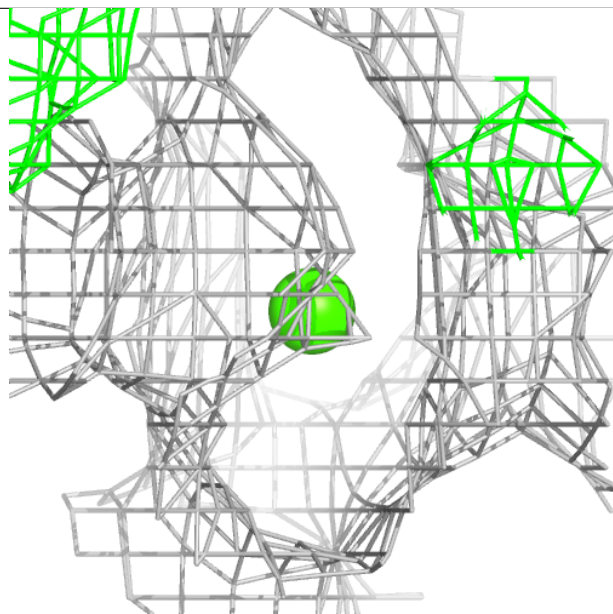
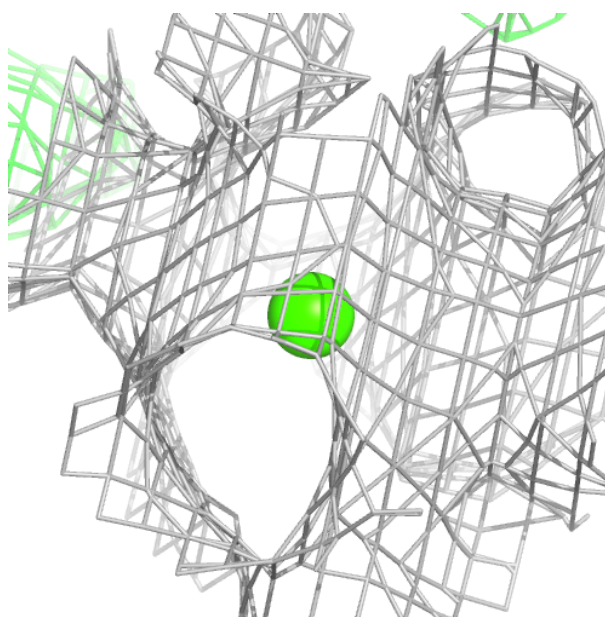
Electron density around CA A 403:

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



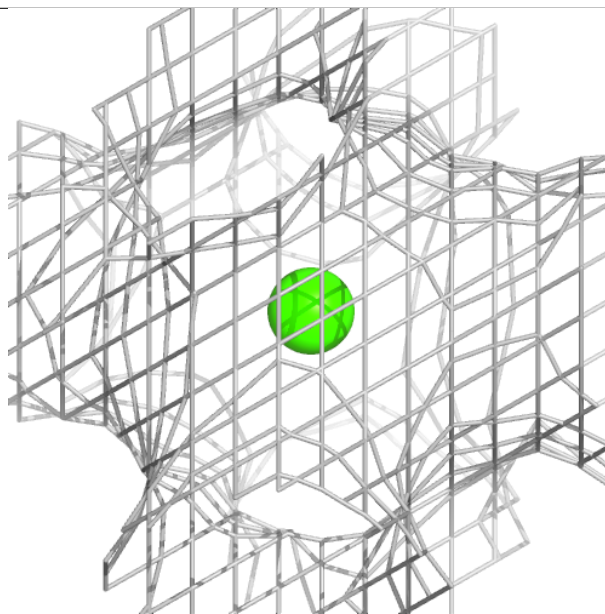
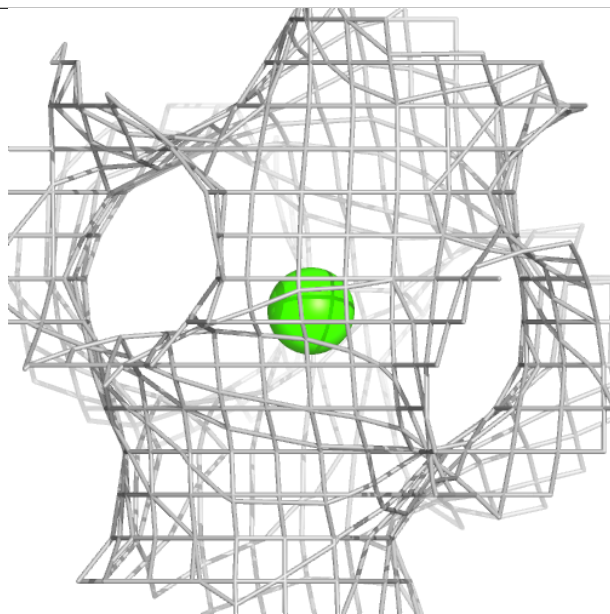
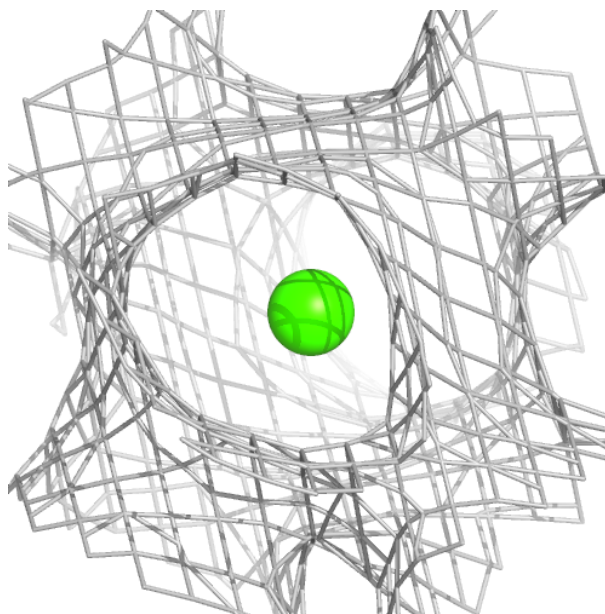
Electron density around CA B 401:

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



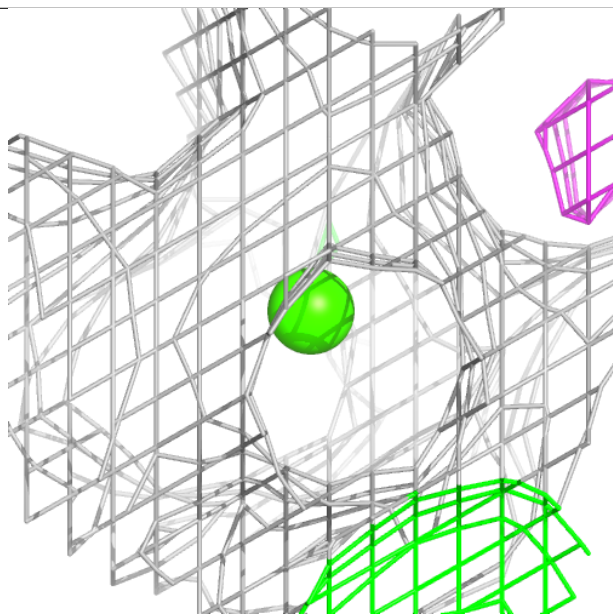
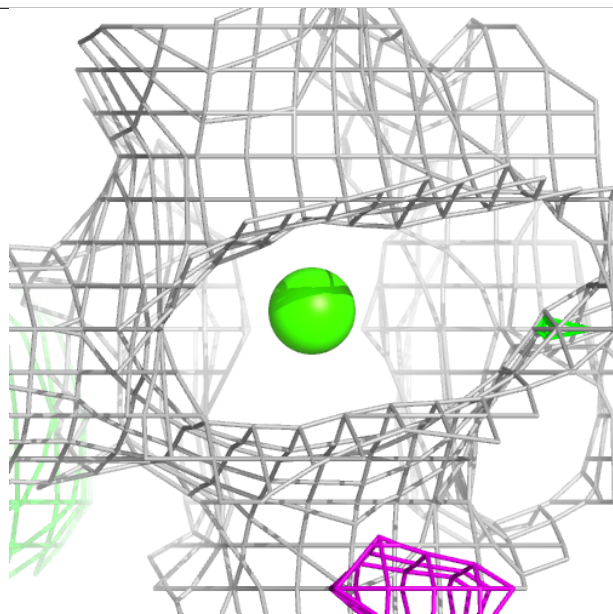
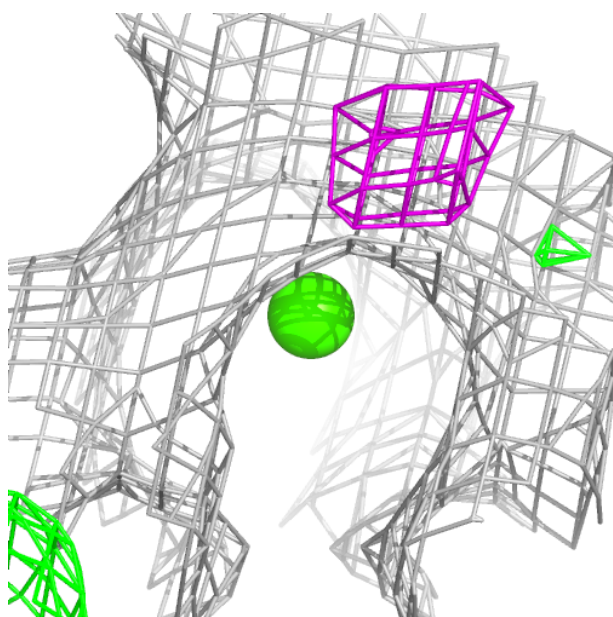
Electron density around CA E 402:

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



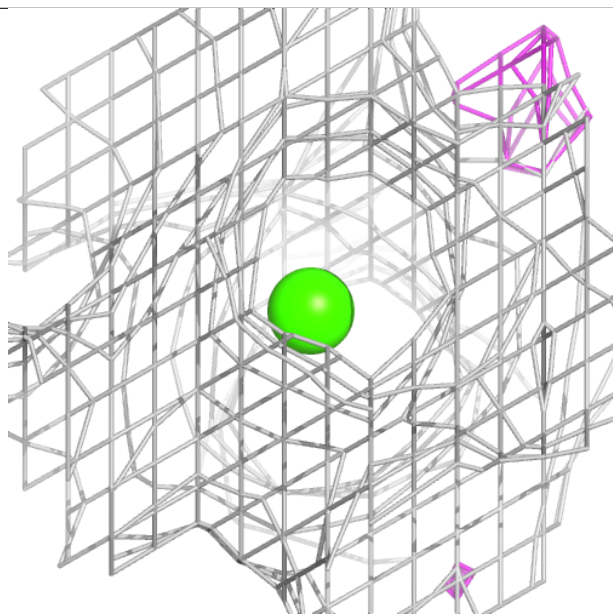
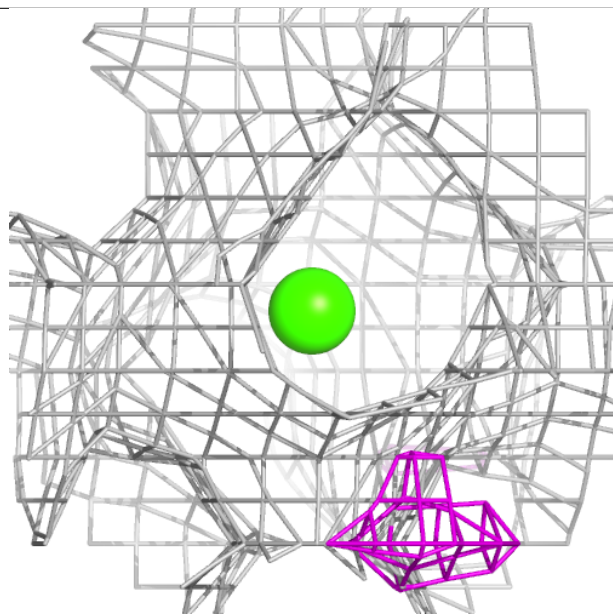
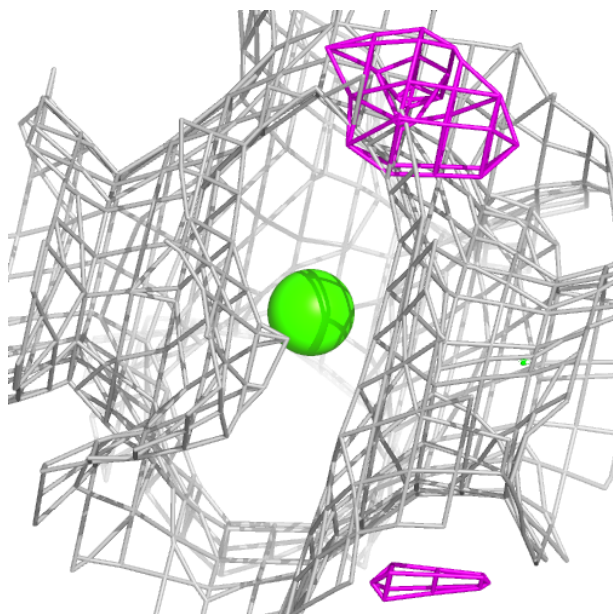
Electron density around CA B 403:

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



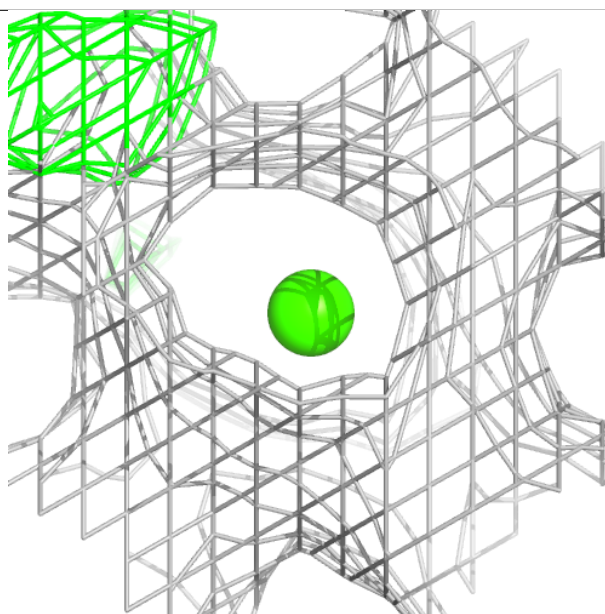
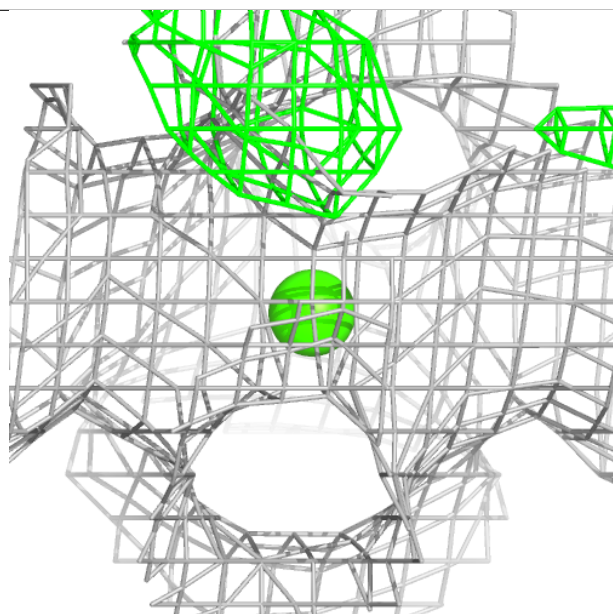
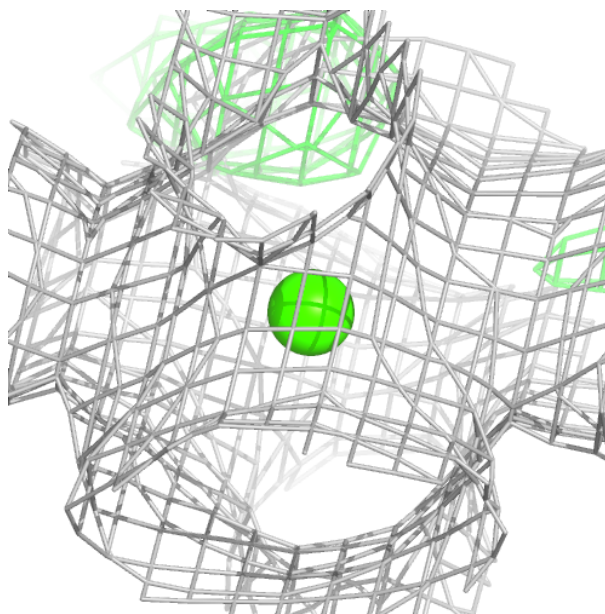
Electron density around CA A 401:

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



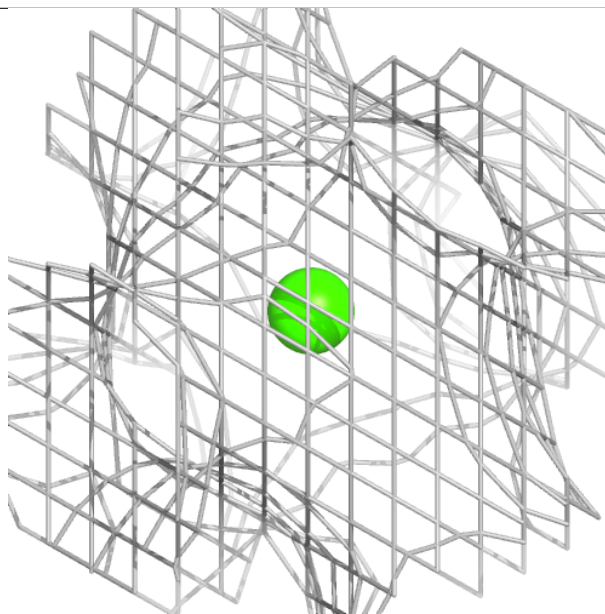
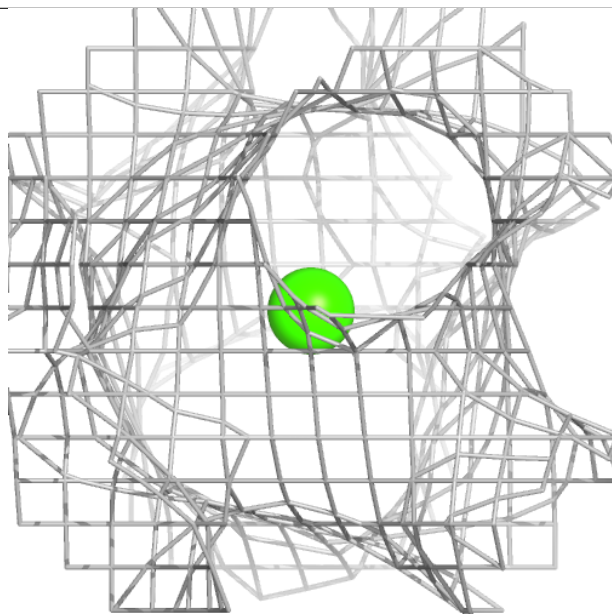
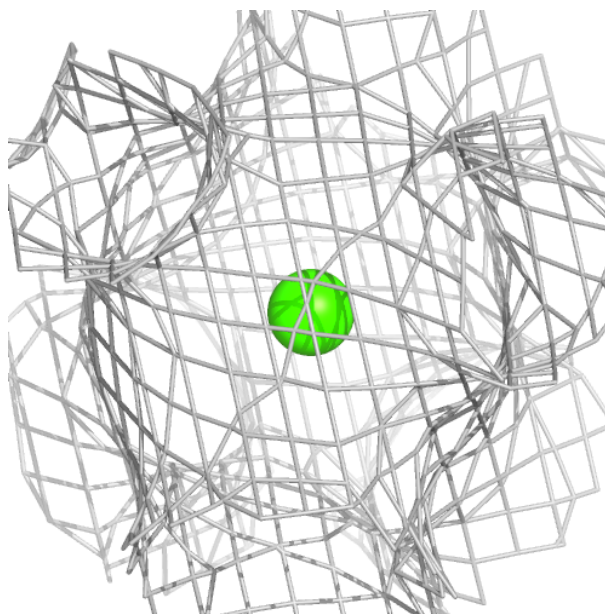
Electron density around CA G 405:

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



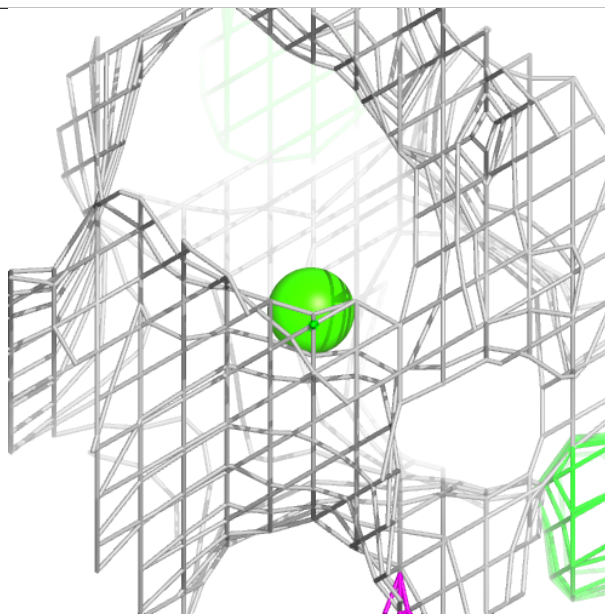
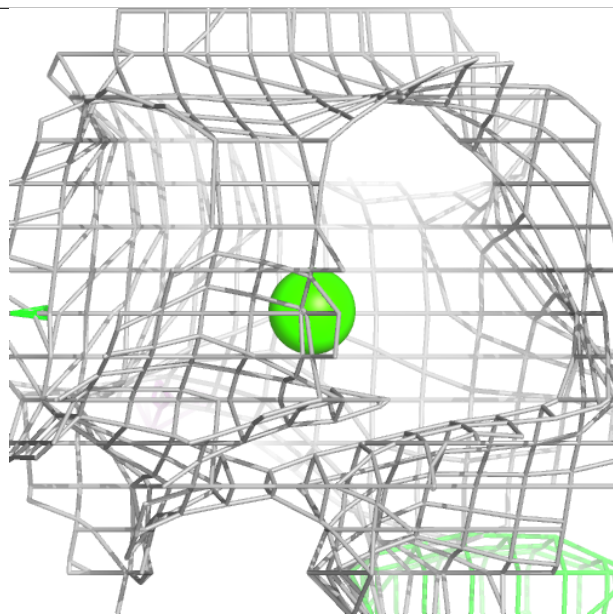
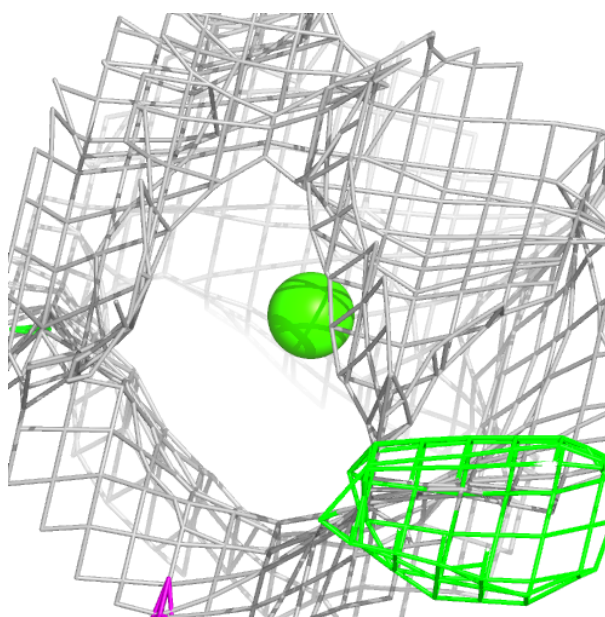
Electron density around CA K 402:

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



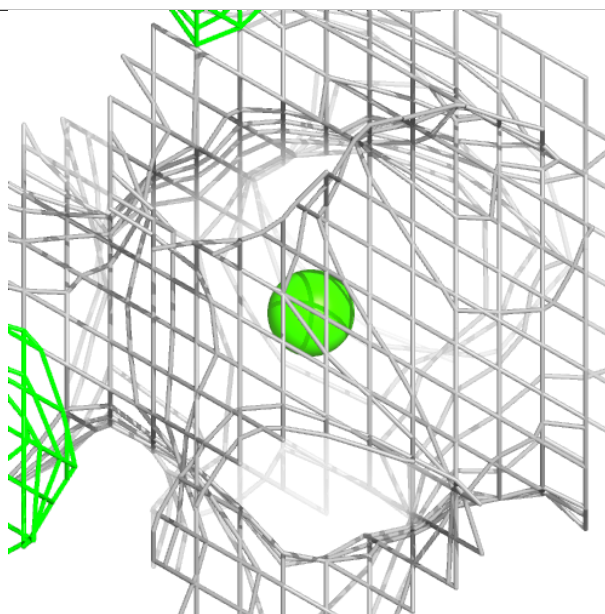
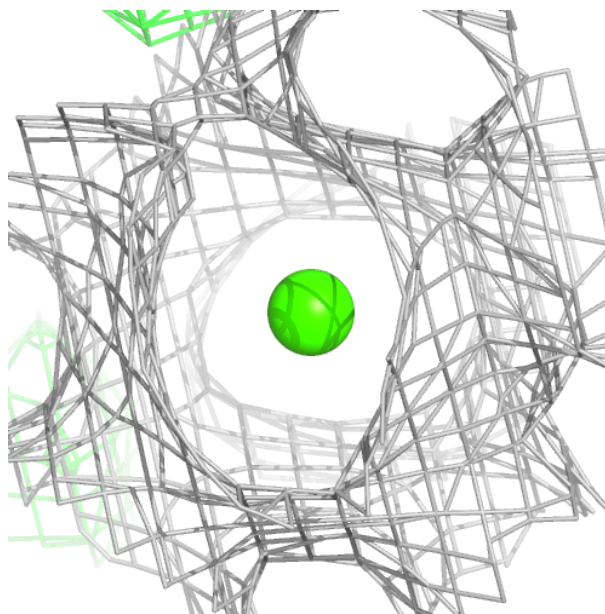
Electron density around CA K 403:

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



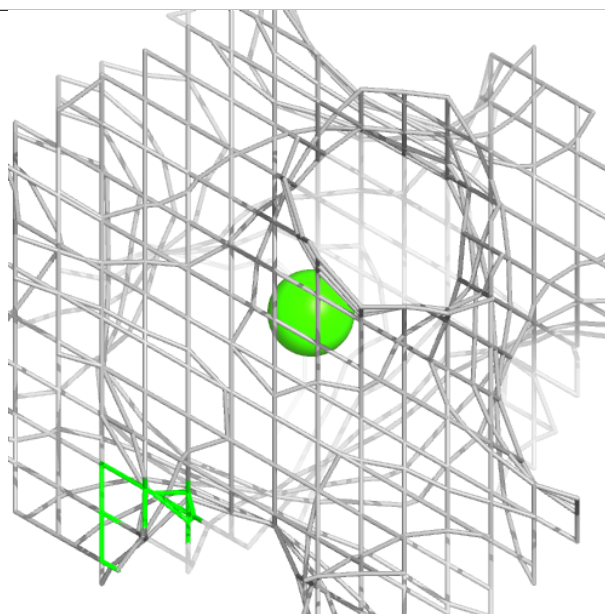
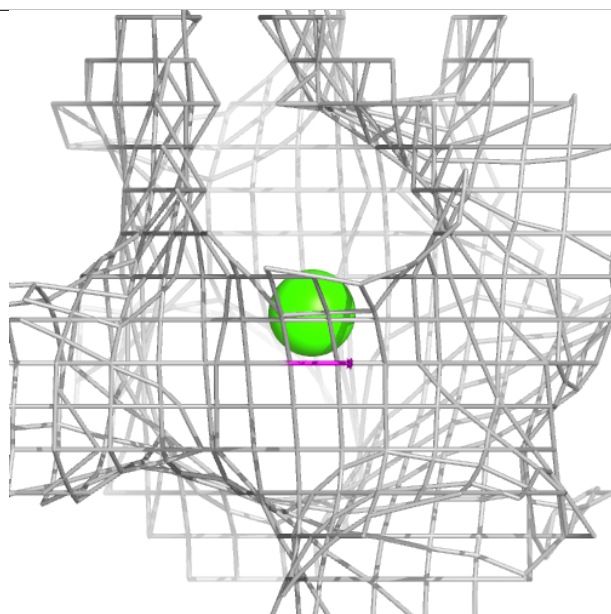
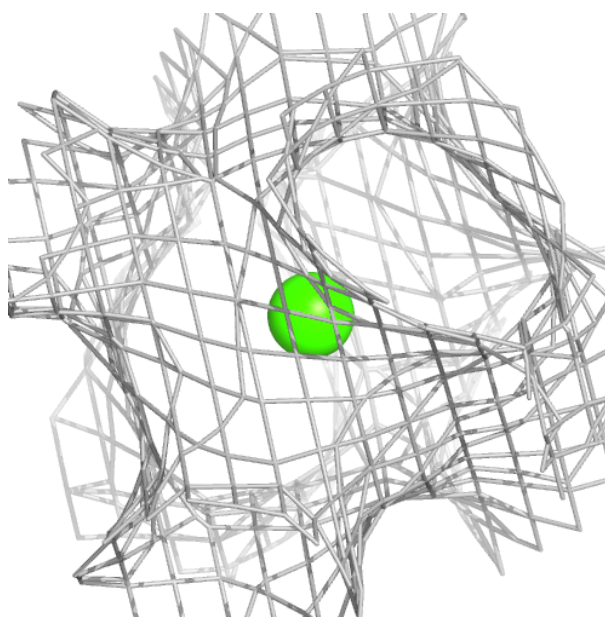
Electron density around CA I 404:

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



Electron density around CA B 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.