



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2026 – 11:29 PM JST

PDB ID : 9X9P / pdb_00009x9p
Title : crystal structure of Cd(II)Ca(II)Mg(II)-bound human calprotectin
Authors : Tao, X.
Deposited on : 2025-10-21
Resolution : 1.85 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 Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

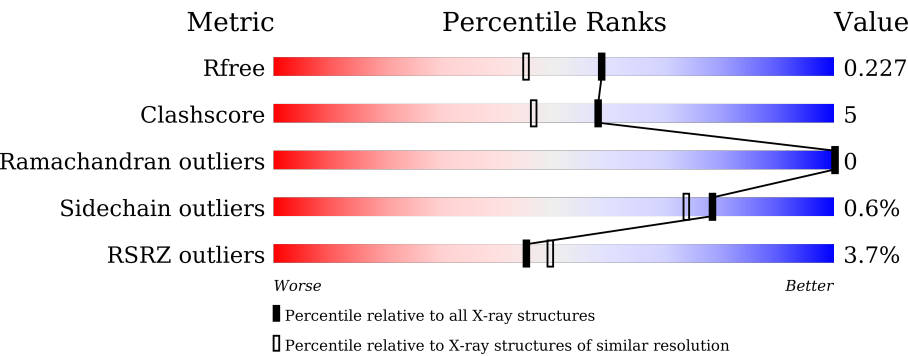
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	114	4% 84% 11% .
1	C	114	4% 85% 10% ..
1	E	114	3% 89% . 6%
1	G	114	4% 83% 11% 5%
2	B	94	3% 89% 5% ..
2	D	94	2% 87% 9% .

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Mol	Chain	Length	Quality of chain
2	F	94	4% 90% 5%
2	H	94	3% 87% 6% • 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
7	CL	C	207	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7537 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 Protein S100-A9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	2	0
			904	567	159	172	6			
1	C	109	Total	C	N	O	S	0	3	0
			911	572	159	174	6			
1	E	107	Total	C	N	O	S	0	2	0
			889	557	155	171	6			
1	G	108	Total	C	N	O	S	0	2	0
			901	566	160	170	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	CYS	conflict	UNP P06702
C	3	SER	CYS	conflict	UNP P06702
E	3	SER	CYS	conflict	UNP P06702
G	3	SER	CYS	conflict	UNP P06702

- Molecule 2 is a protein called Protein S100-A8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	S	0	4	0
			756	489	125	140	2			
2	D	90	Total	C	N	O	S	0	3	0
			749	484	125	138	2			
2	F	90	Total	C	N	O	S	0	2	0
			743	481	124	136	2			
2	H	89	Total	C	N	O	S	0	2	0
			733	475	121	135	2			

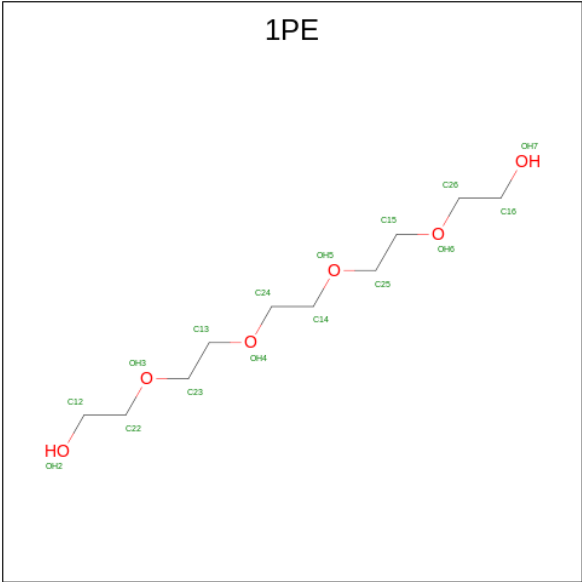
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P05109
B	42	SER	CYS	conflict	UNP P05109
D	0	GLY	-	expression tag	UNP P05109
D	42	SER	CYS	conflict	UNP P05109
F	0	GLY	-	expression tag	UNP P05109
F	42	SER	CYS	conflict	UNP P05109
H	0	GLY	-	expression tag	UNP P05109
H	42	SER	CYS	conflict	UNP P05109

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

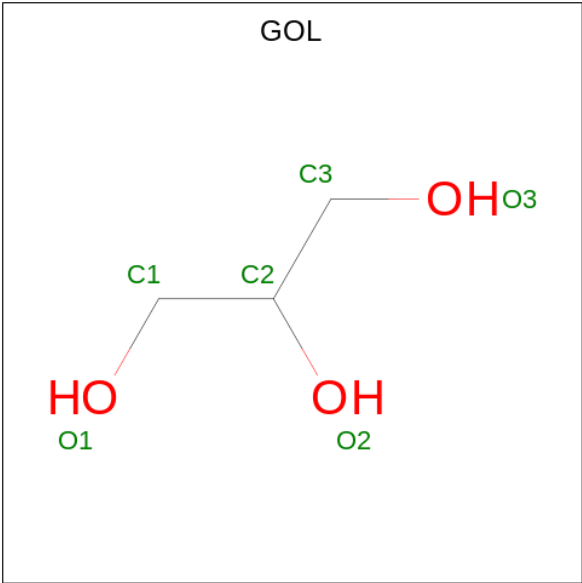
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0
3	E	2	Total Ca 2 2	0	0
3	F	2	Total Ca 2 2	0	0
3	G	2	Total Ca 2 2	0	0
3	H	2	Total Ca 2 2	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	G	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		

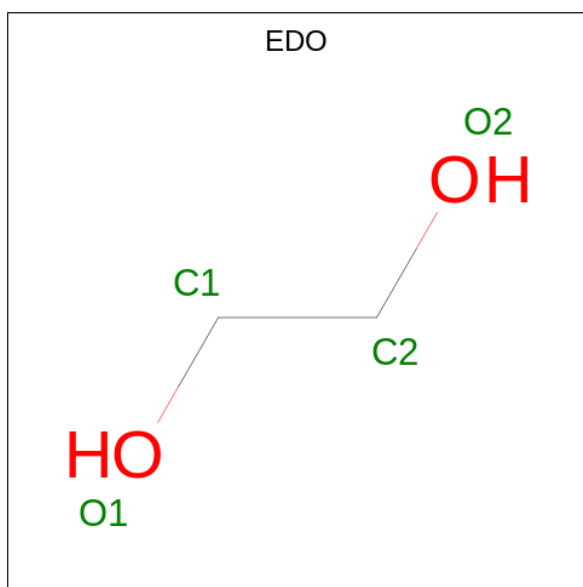
- Molecule 6 is CADMIUM ION (CCD ID: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Cd	0	0
			2	2		
6	C	2	Total	Cd	0	0
			2	2		
6	E	1	Total	Cd	0	0
			1	1		
6	G	1	Total	Cd	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		
7	E	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	G	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	1	Total	Mg	0	0
			1	1		
9	G	1	Total	Mg	0	0
			1	1		

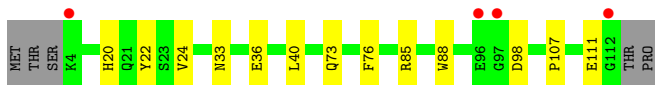
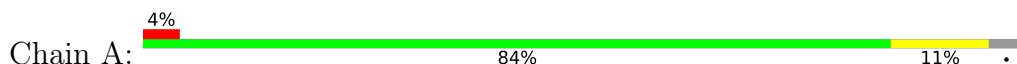
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	125	Total 125	O 125	0	0
10	B	100	Total 100	O 100	0	0
10	C	136	Total 136	O 136	0	0
10	D	86	Total 86	O 86	0	0
10	E	135	Total 135	O 135	0	0
10	F	67	Total 67	O 67	0	0
10	G	99	Total 99	O 99	0	0
10	H	77	Total 77	O 77	0	0

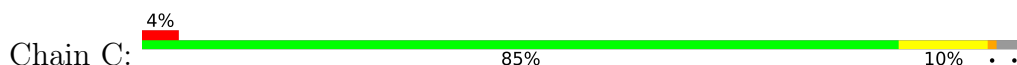
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

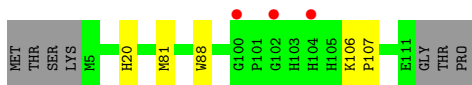
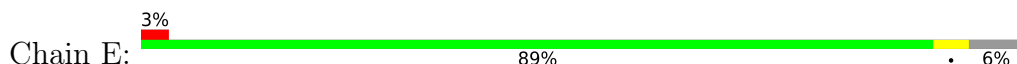
- Molecule 1: Protein S100-A9



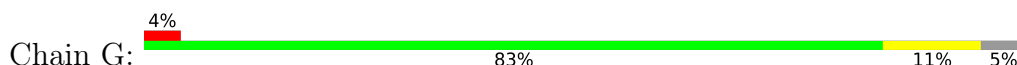
- Molecule 1: Protein S100-A9



- Molecule 1: Protein S100-A9



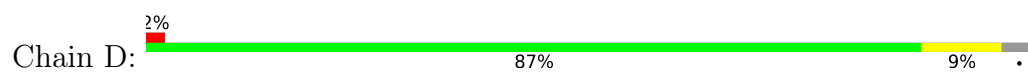
- Molecule 1: Protein S100-A9



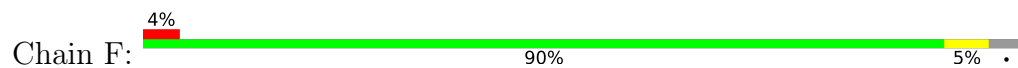
- Molecule 2: Protein S100-A8



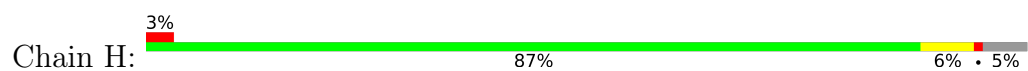
- Molecule 2: Protein S100-A8



• Molecule 2: Protein S100-A8



• Molecule 2: Protein S100-A8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.45Å 78.23Å 223.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.94 – 1.85 73.94 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (73.94-1.85) 98.7 (73.94-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.167 , 0.219 0.177 , 0.227	Depositor DCC
R_{free} test set	4355 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7537	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% 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: 1PE, CL, EDO, MG, CD, GOL, 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	0.62	0/925	1.07	2/1238 (0.2%)
1	C	0.62	0/935	1.04	2/1251 (0.2%)
1	E	0.62	0/913	1.04	0/1223
1	G	0.61	0/925	1.03	3/1238 (0.2%)
2	B	0.63	0/782	0.99	0/1050
2	D	0.63	0/772	1.05	0/1037
2	F	0.59	0/764	1.05	0/1026
2	H	0.66	0/753	1.02	1/1012 (0.1%)
All	All	0.62	0/6769	1.04	8/9075 (0.1%)

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	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ASP	CA-CB-CG	6.94	119.54	112.60
2	H	69	GLN	N-CA-CB	6.48	119.75	110.16
1	C	76	PHE	CA-CB-CG	-5.79	108.01	113.80
1	C	98	ASP	CA-CB-CG	5.66	118.25	112.60
1	G	14	THR	CA-CB-OG1	-5.53	101.31	109.60
1	G	18	THR	CA-CB-OG1	-5.40	101.50	109.60
1	G	98	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	76	PHE	CA-CB-CG	-5.05	108.75	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	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	904	0	882	13	0
1	C	911	0	891	8	0
1	E	889	0	862	4	0
1	G	901	0	886	7	0
2	B	756	0	775	6	0
2	D	749	0	767	7	0
2	F	743	0	757	5	0
2	H	733	0	750	13	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	16	0	22	1	0
4	G	16	0	22	0	0
5	A	6	0	8	0	0
5	B	6	0	8	2	0
5	C	6	0	8	0	0
5	E	6	0	8	0	0
5	G	6	0	8	2	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	C	4	0	6	0	0
8	D	12	0	18	1	0
8	E	12	0	18	1	0
8	G	4	0	6	0	0
8	H	4	0	6	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
10	A	125	0	0	6	0
10	B	100	0	0	6	0
10	C	136	0	0	2	0
10	D	86	0	0	5	0
10	E	135	0	0	2	1
10	F	67	0	0	0	0
10	G	99	0	0	2	1
10	H	77	0	0	4	0
All	All	7537	0	6708	61	1

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 5.

All (61) 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)
8:D:105:EDO:H11	10:D:214:HOH:O	1.60	1.01
7:C:207:CL:CL	2:H:69:GLN:CG	2.65	0.81
2:B:88:GLU:OE1	10:B:202:HOH:O	2.04	0.76
5:B:103:GOL:H2	10:B:221:HOH:O	1.86	0.76
2:B:39:GLU:OE2	10:B:203:HOH:O	2.05	0.75
1:A:73:GLN:HG2	10:A:301:HOH:O	1.91	0.70
2:D:44:GLN:HG3	10:D:255:HOH:O	1.92	0.69
7:C:207:CL:CL	2:H:69:GLN:HG2	2.31	0.68
7:C:207:CL:CL	2:H:69:GLN:HG3	2.31	0.67
2:D:57:GLU:OE1	10:D:201:HOH:O	2.13	0.66
2:D:14[A]:ASP:OD1	10:D:202:HOH:O	2.14	0.65
2:H:14[B]:ASP:OD1	10:H:201:HOH:O	2.16	0.62
2:B:69:GLN:HE21	2:B:69:GLN:H	1.47	0.62
8:E:206:EDO:O2	10:E:301:HOH:O	2.16	0.60
1:E:20:HIS:HE1	2:F:83:HIS:CD2	2.22	0.57
1:C:81[A]:MET:HG3	7:C:207:CL:CL	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:LEU:C	1:G:40:LEU:HD23	2.31	0.55
1:A:33:ASN:ND2	10:A:306:HOH:O	2.40	0.55
2:B:47:ARG:NH1	10:B:206:HOH:O	2.40	0.54
1:G:31:THR:OG1	1:G:73:GLN:NE2	2.41	0.53
2:H:31:ARG:NH2	10:H:205:HOH:O	2.42	0.52
2:F:37:LEU:C	2:F:37:LEU:HD23	2.35	0.52
2:B:57[B]:GLU:HG3	10:B:219:HOH:O	2.10	0.51
1:A:33:ASN:HB2	10:A:308:HOH:O	2.12	0.50
1:A:40:LEU:C	1:A:40:LEU:HD23	2.38	0.49
1:C:34:GLN:NE2	10:C:305:HOH:O	2.45	0.49
1:G:92:GLU:OE2	5:G:204:GOL:H11	2.12	0.48
1:A:22:TYR:CZ	1:A:40:LEU:HA	2.49	0.48
1:G:13:GLU:OE1	10:G:302:HOH:O	2.20	0.47
1:A:73:GLN:CG	10:A:301:HOH:O	2.57	0.46
2:H:37:LEU:C	2:H:37:LEU:HD23	2.40	0.46
2:H:69:GLN:N	2:H:69:GLN:CD	2.74	0.46
2:H:69:GLN:CD	2:H:69:GLN:H	2.24	0.46
2:D:52:ASP:OD1	10:D:203:HOH:O	2.21	0.46
1:E:106:LYS:HB3	1:E:107:PRO:CD	2.46	0.46
2:H:62[B]:THR:HG22	10:H:221:HOH:O	2.16	0.45
10:C:341:HOH:O	2:H:62[B]:THR:HG23	2.16	0.45
2:B:23:LYS:NZ	10:B:201:HOH:O	2.02	0.45
1:A:33:ASN:ND2	1:A:36:GLU:OE1	2.49	0.43
1:C:106:LYS:HB3	1:C:107:PRO:HD2	2.00	0.43
1:G:42[B]:ARG:NE	10:G:307:HOH:O	2.50	0.43
1:A:88:TRP:CE2	4:A:203:1PE:H151	2.54	0.43
1:C:106:LYS:HB3	1:C:107:PRO:CD	2.49	0.43
2:F:1:MET:HE3	2:F:7:LYS:NZ	2.34	0.43
1:A:33:ASN:HB2	10:A:353:HOH:O	2.18	0.43
1:A:33:ASN:CG	10:A:306:HOH:O	2.61	0.43
2:D:3:THR:O	2:D:7:LYS:HG3	2.19	0.42
1:E:88:TRP:HE3	10:E:373:HOH:O	2.00	0.42
1:E:20:HIS:HE1	2:F:83:HIS:NE2	2.17	0.42
1:A:107:PRO:HB3	1:A:111:GLU:HG3	2.00	0.42
2:D:80:VAL:HG11	2:H:62[B]:THR:CG2	2.50	0.42
1:C:69:ASN:O	1:C:70:ALA:HB3	2.19	0.41
1:G:20:HIS:HA	1:G:23:SER:OG	2.20	0.41
1:A:20:HIS:CG	1:C:24:VAL:HG11	2.55	0.41
5:B:103:GOL:H11	2:F:77:LYS:HE3	2.01	0.41
1:A:24[A]:VAL:HG21	1:C:20:HIS:CG	2.54	0.41
1:G:56:GLU:O	1:G:60:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:204:GOL:H31	2:H:27:HIS:CE1	2.56	0.41
2:H:57:GLU:OE1	10:H:202:HOH:O	2.22	0.41
1:C:74:LEU:HA	1:C:78[A]:GLU:OE1	2.20	0.41
2:D:37:LEU:HD23	2:D:37:LEU:C	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:339:HOH:O	10:G:375:HOH:O[2_554]	1.88	0.32

5.3 Torsion angles

5.3.1 Protein backbone

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	109/114 (96%)	109 (100%)	0	0	100	100
1	C	110/114 (96%)	108 (98%)	2 (2%)	0	100	100
1	E	107/114 (94%)	105 (98%)	2 (2%)	0	100	100
1	G	108/114 (95%)	107 (99%)	1 (1%)	0	100	100
2	B	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
2	D	91/94 (97%)	91 (100%)	0	0	100	100
2	F	90/94 (96%)	89 (99%)	1 (1%)	0	100	100
2	H	89/94 (95%)	89 (100%)	0	0	100	100
All	All	796/832 (96%)	789 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	100/103 (97%)	100 (100%)	0	100	100
1	C	101/103 (98%)	99 (98%)	2 (2%)	48	36
1	E	99/103 (96%)	97 (98%)	2 (2%)	48	36
1	G	100/103 (97%)	100 (100%)	0	100	100
2	B	83/83 (100%)	82 (99%)	1 (1%)	63	55
2	D	82/83 (99%)	82 (100%)	0	100	100
2	F	81/83 (98%)	81 (100%)	0	100	100
2	H	80/83 (96%)	79 (99%)	1 (1%)	61	51
All	All	726/744 (98%)	720 (99%)	6 (1%)	78	67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	69	GLN
1	C	81[A]	MET
1	C	81[B]	MET
1	E	81[A]	MET
1	E	81[B]	MET
2	H	69	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
2	B	10	ASN
1	C	11	ASN
1	C	34	GLN
2	D	10	ASN
1	E	61	HIS
1	E	73	GLN
2	F	10	ASN

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Mol	Chain	Res	Type
1	G	73	GLN
2	H	10	ASN
2	H	69	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 28 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	G	204	-	5,5,5	0.18	0	5,5,5	0.45	0
8	EDO	E	204	-	3,3,3	0.06	0	2,2,2	0.26	0
4	1PE	A	203	-	15,15,15	0.24	0	14,14,14	0.16	0
5	GOL	E	201	-	5,5,5	0.12	0	5,5,5	0.33	0
8	EDO	D	104	-	3,3,3	0.10	0	2,2,2	0.29	0
8	EDO	G	203	-	3,3,3	0.18	0	2,2,2	0.30	0
8	EDO	D	103	-	3,3,3	0.15	0	2,2,2	0.07	0
8	EDO	H	103	-	3,3,3	0.21	0	2,2,2	0.22	0
5	GOL	B	103	-	5,5,5	0.09	0	5,5,5	0.45	0
8	EDO	D	105	-	3,3,3	0.35	0	2,2,2	0.38	0
8	EDO	E	205	-	3,3,3	0.05	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	204	-	5,5,5	0.10	0	5,5,5	0.37	0
8	EDO	E	206	-	3,3,3	0.12	0	2,2,2	0.09	0
8	EDO	C	203	-	3,3,3	0.14	0	2,2,2	0.11	0
4	1PE	G	205	-	15,15,15	0.27	0	14,14,14	0.21	0
5	GOL	C	204	-	5,5,5	0.14	0	5,5,5	0.42	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
5	GOL	G	204	-	-	3/4/4/4	-
8	EDO	E	204	-	-	0/1/1/1	-
4	1PE	A	203	-	-	5/13/13/13	-
5	GOL	E	201	-	-	2/4/4/4	-
8	EDO	D	104	-	-	0/1/1/1	-
8	EDO	G	203	-	-	1/1/1/1	-
8	EDO	D	103	-	-	0/1/1/1	-
8	EDO	H	103	-	-	1/1/1/1	-
5	GOL	B	103	-	-	4/4/4/4	-
8	EDO	D	105	-	-	1/1/1/1	-
8	EDO	E	205	-	-	0/1/1/1	-
5	GOL	A	204	-	-	0/4/4/4	-
8	EDO	E	206	-	-	0/1/1/1	-
8	EDO	C	203	-	-	0/1/1/1	-
4	1PE	G	205	-	-	6/13/13/13	-
5	GOL	C	204	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	103	GOL	O1-C1-C2-C3
5	C	204	GOL	C1-C2-C3-O3
5	E	201	GOL	C1-C2-C3-O3
5	G	204	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	D	105	EDO	O1-C1-C2-O2
4	G	205	1PE	OH4-C13-C23-OH3
5	G	204	GOL	O1-C1-C2-O2
5	G	204	GOL	C1-C2-C3-O3
5	B	103	GOL	O1-C1-C2-O2
5	C	204	GOL	O2-C2-C3-O3
5	E	201	GOL	O2-C2-C3-O3
4	A	203	1PE	OH7-C16-C26-OH6
4	A	203	1PE	OH4-C13-C23-OH3
8	H	103	EDO	O1-C1-C2-O2
4	A	203	1PE	C15-C25-OH5-C14
4	G	205	1PE	C13-C23-OH3-C22
4	G	205	1PE	C25-C15-OH6-C26
5	B	103	GOL	C1-C2-C3-O3
4	G	205	1PE	OH5-C14-C24-OH4
8	G	203	EDO	O1-C1-C2-O2
5	B	103	GOL	O2-C2-C3-O3
4	G	205	1PE	C14-C24-OH4-C13
4	A	203	1PE	C14-C24-OH4-C13
4	G	205	1PE	OH6-C15-C25-OH5
4	A	203	1PE	C16-C26-OH6-C15

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	204	GOL	2	0
4	A	203	1PE	1	0
5	B	103	GOL	2	0
8	D	105	EDO	1	0
8	E	206	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	109/114 (95%)	0.16	4 (3%)	45	49	12, 30, 52, 69	2 (1%)
1	C	109/114 (95%)	-0.10	5 (4%)	37	40	9, 28, 48, 75	3 (2%)
1	E	107/114 (93%)	0.02	3 (2%)	55	58	14, 30, 44, 61	2 (1%)
1	G	108/114 (94%)	0.44	5 (4%)	37	40	15, 37, 53, 76	3 (2%)
2	B	90/94 (95%)	-0.28	3 (3%)	49	53	13, 22, 43, 89	4 (4%)
2	D	90/94 (95%)	-0.09	2 (2%)	62	66	17, 26, 42, 71	3 (3%)
2	F	90/94 (95%)	0.29	4 (4%)	39	42	21, 30, 55, 99	2 (2%)
2	H	89/94 (94%)	-0.09	3 (3%)	48	52	14, 24, 55, 88	3 (3%)
All	All	792/832 (95%)	0.05	29 (3%)	45	49	9, 28, 52, 99	22 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	LYS	4.0
2	H	0	GLY	3.3
1	C	102	GLY	3.1
2	F	1	MET	3.0
2	H	1	MET	3.0
2	F	87[A]	HIS	2.9
1	C	112	GLY	2.9
1	G	101	PRO	2.8
1	C	4	LYS	2.8
1	C	101	PRO	2.8
2	B	89	GLU	2.7
2	D	26	PHE	2.7
2	H	87	HIS	2.6
1	A	112	GLY	2.6
1	G	4	LYS	2.5
1	G	26	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	100	GLY	2.3
1	E	102	GLY	2.2
1	G	27	GLY	2.2
2	B	0	GLY	2.2
1	A	97	GLY	2.2
1	C	104	HIS	2.1
2	B	1	MET	2.1
1	A	96	GLU	2.1
2	F	0	GLY	2.1
1	E	104	HIS	2.1
1	G	104	HIS	2.1
2	F	89	GLU	2.1
2	D	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	EDO	E	205	4/4	0.79	0.19	67,68,70,72	0
8	EDO	D	104	4/4	0.81	0.18	50,61,64,64	0
8	EDO	H	103	4/4	0.81	0.18	54,55,55,58	0
8	EDO	E	206	4/4	0.82	0.17	56,60,60,62	0
5	GOL	E	201	6/6	0.82	0.17	44,57,59,66	0
8	EDO	C	203	4/4	0.83	0.15	40,50,53,54	0
5	GOL	G	204	6/6	0.84	0.15	32,51,53,53	0
8	EDO	G	203	4/4	0.84	0.13	58,61,64,64	0
5	GOL	A	204	6/6	0.84	0.17	65,69,70,72	0
5	GOL	B	103	6/6	0.85	0.17	49,52,53,57	0

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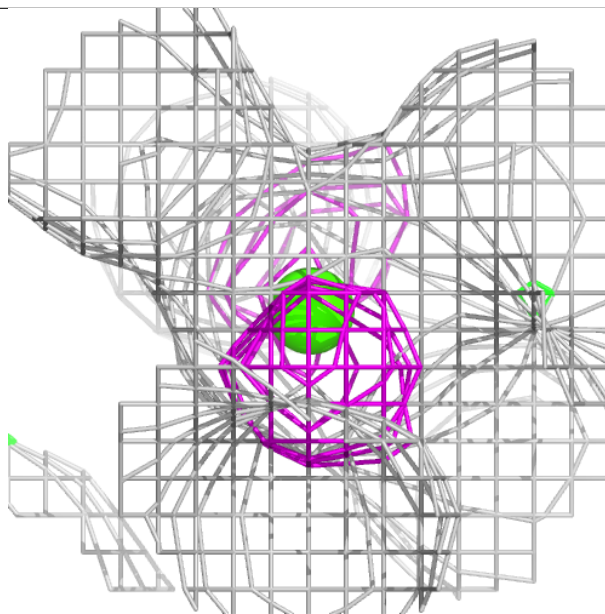
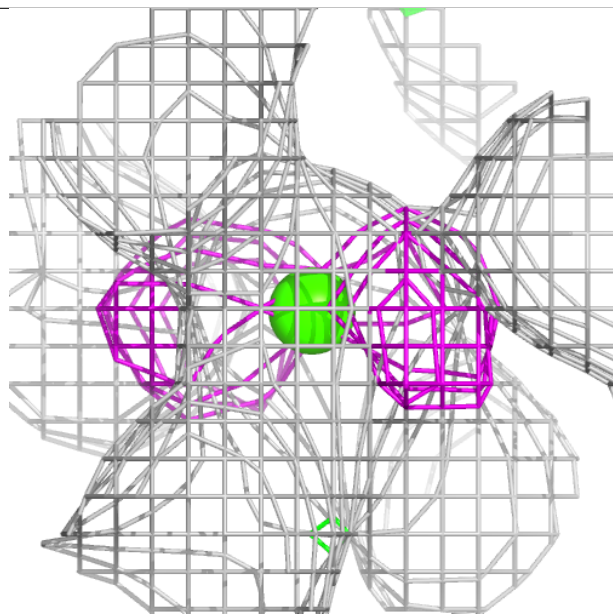
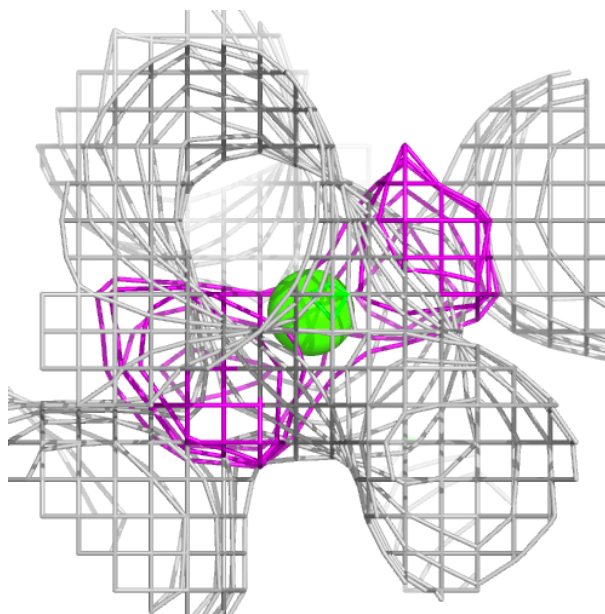
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	EDO	D	105	4/4	0.85	0.20	42,43,48,49	0
5	GOL	C	204	6/6	0.86	0.15	44,57,61,63	0
8	EDO	E	204	4/4	0.88	0.15	55,56,62,69	0
4	1PE	G	205	16/16	0.89	0.17	62,66,74,74	0
8	EDO	D	103	4/4	0.89	0.12	60,61,61,64	0
4	1PE	A	203	16/16	0.89	0.18	56,67,72,74	0
3	CA	D	102	1/1	0.92	0.14	32,32,32,32	1
7	CL	E	208	1/1	0.93	0.12	46,46,46,46	0
3	CA	G	202	1/1	0.93	0.09	34,34,34,34	0
9	MG	F	103	1/1	0.93	0.10	36,36,36,36	0
3	CA	G	201	1/1	0.94	0.08	41,41,41,41	0
3	CA	F	102	1/1	0.94	0.15	33,33,33,33	1
7	CL	C	207	1/1	0.95	0.13	51,51,51,51	0
9	MG	G	207	1/1	0.95	0.07	32,32,32,32	0
3	CA	A	201	1/1	0.96	0.06	34,34,34,34	0
3	CA	E	203	1/1	0.97	0.09	34,34,34,34	0
7	CL	D	106	1/1	0.97	0.08	41,41,41,41	0
3	CA	A	202	1/1	0.98	0.09	32,32,32,32	0
3	CA	E	202	1/1	0.98	0.04	28,28,28,28	0
3	CA	H	102	1/1	0.98	0.08	27,27,27,27	1
3	CA	C	202	1/1	0.98	0.05	32,32,32,32	0
3	CA	F	101	1/1	0.98	0.03	25,25,25,25	0
3	CA	D	101	1/1	0.98	0.04	27,27,27,27	0
6	CD	A	206	1/1	0.99	0.03	26,26,26,26	0
6	CD	C	205	1/1	0.99	0.03	25,25,25,25	0
6	CD	E	207	1/1	0.99	0.03	25,25,25,25	0
7	CL	A	207	1/1	0.99	0.08	37,37,37,37	0
3	CA	C	201	1/1	0.99	0.12	29,29,29,29	1
3	CA	B	102	1/1	0.99	0.13	27,27,27,27	1
3	CA	B	101	1/1	1.00	0.02	21,21,21,21	0
3	CA	H	101	1/1	1.00	0.01	19,19,19,19	0
6	CD	C	206	1/1	1.00	0.01	21,21,21,21	0
6	CD	A	205	1/1	1.00	0.01	19,19,19,19	0
6	CD	G	206	1/1	1.00	0.01	23,23,23,23	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.

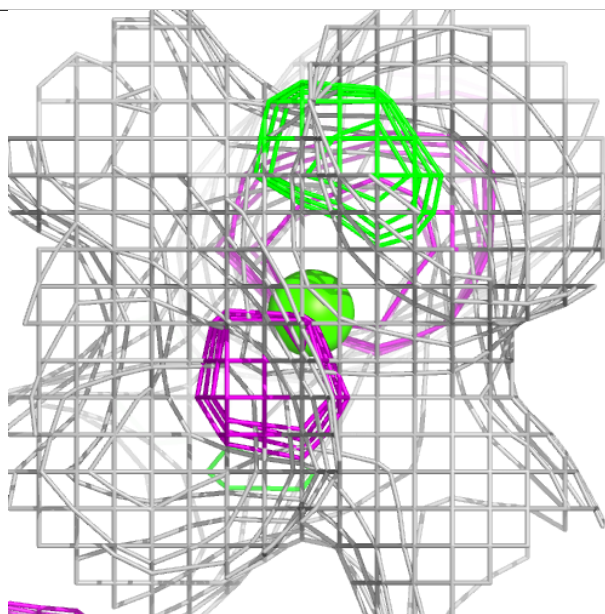
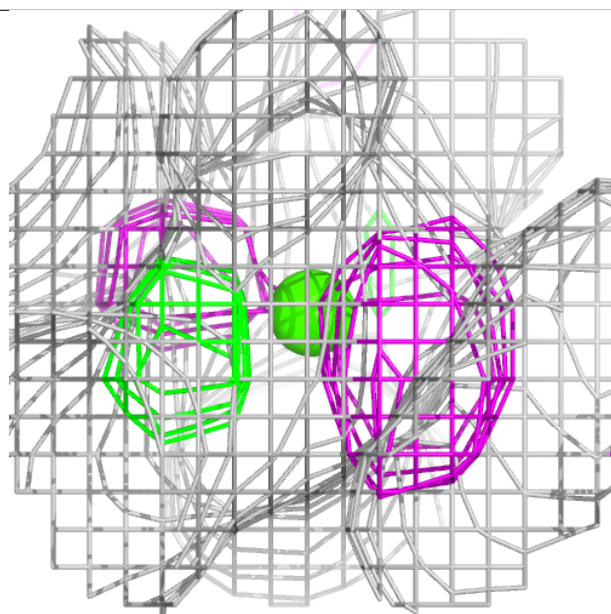
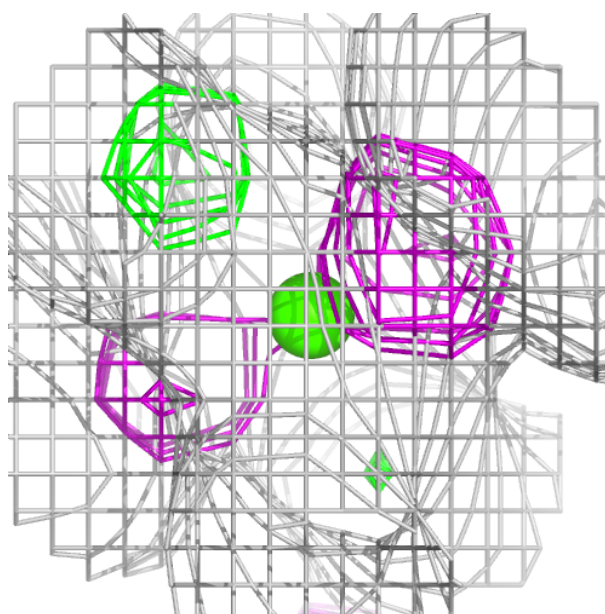
Electron density around CA D 102:

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



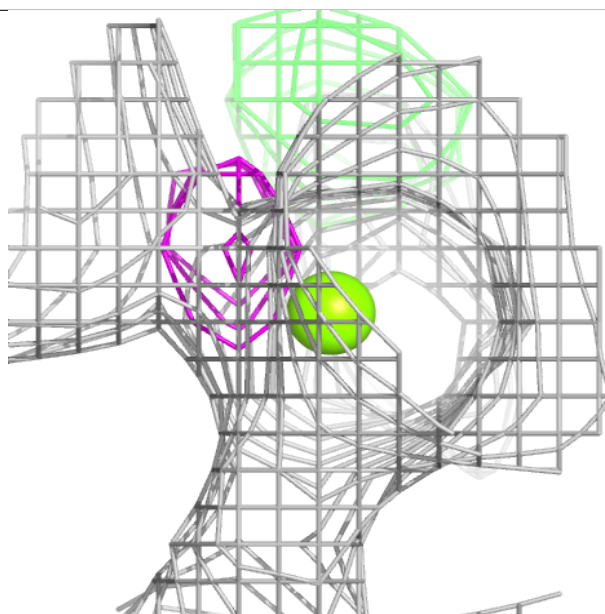
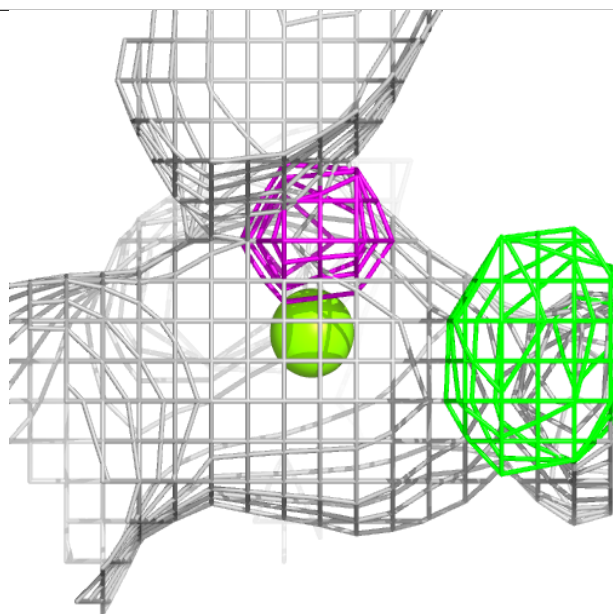
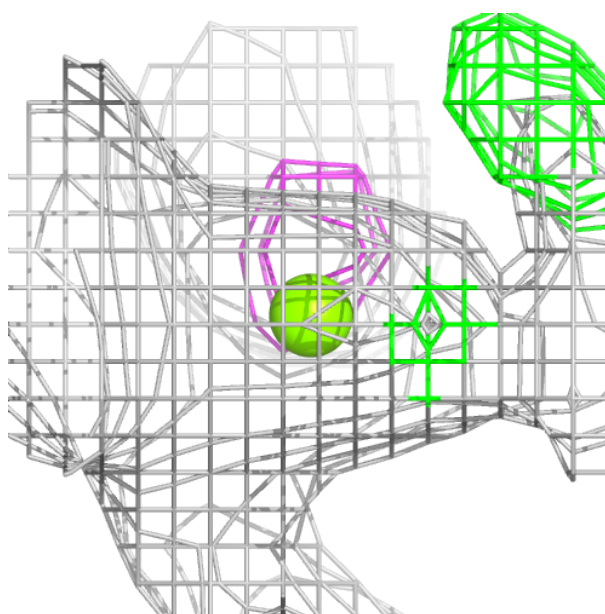
Electron density around CA G 202:

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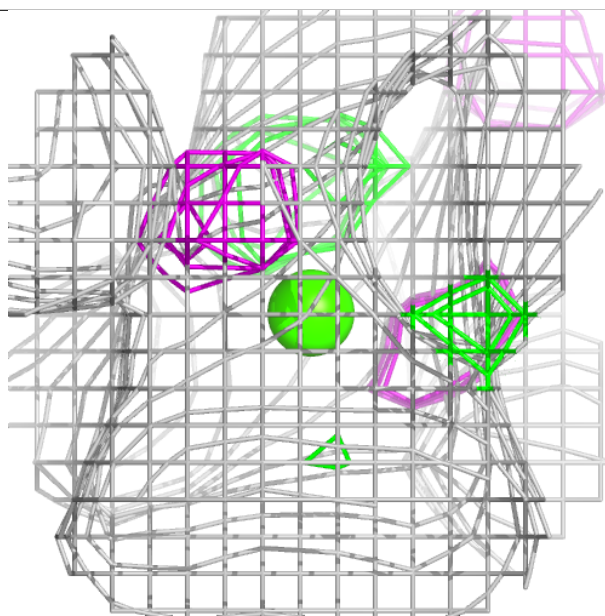
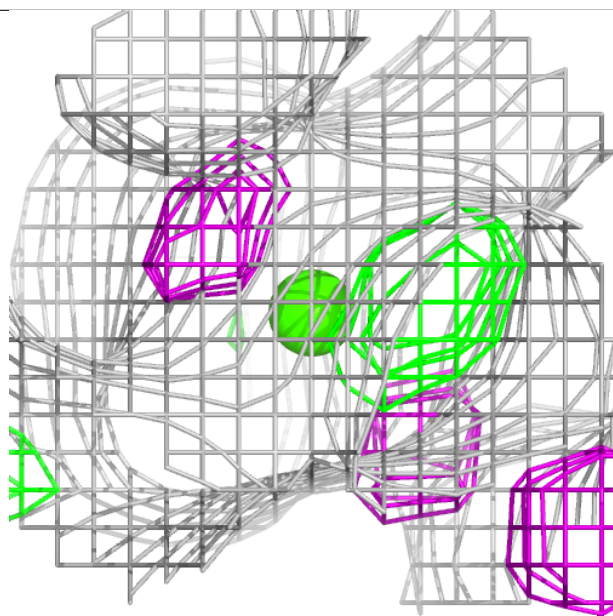
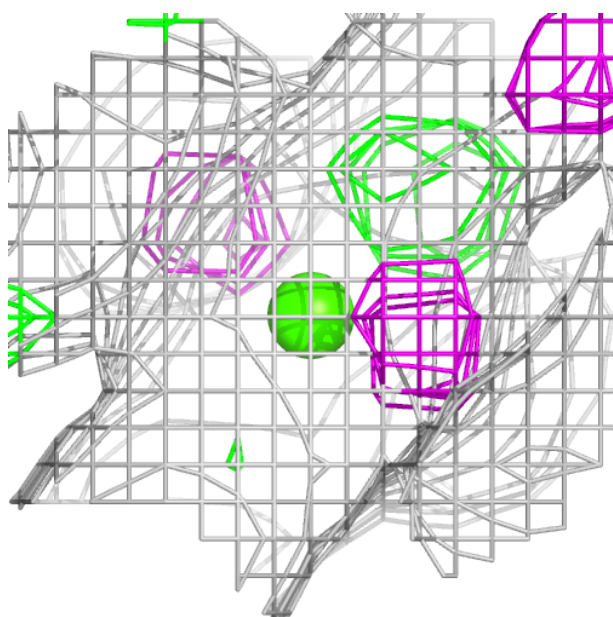
Electron density around MG F 103:

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



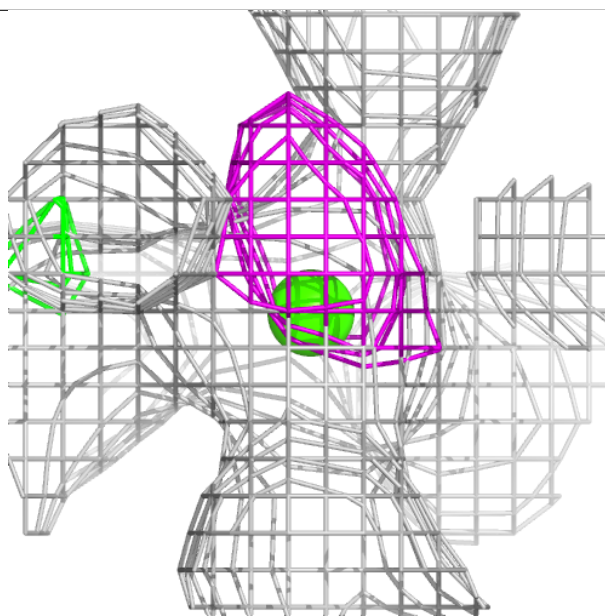
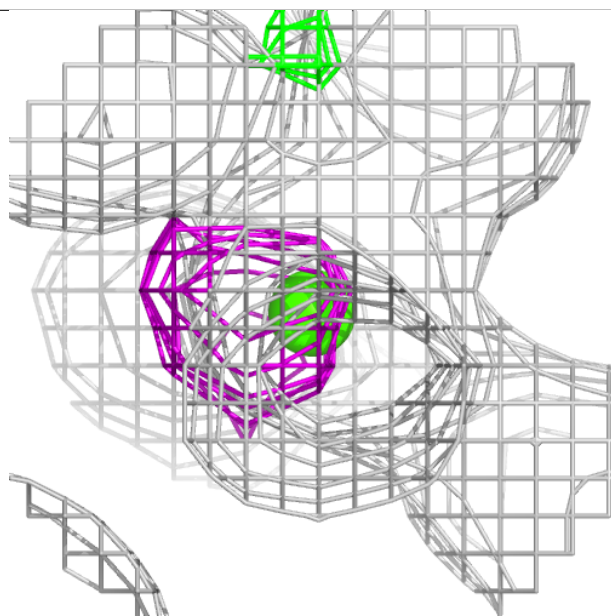
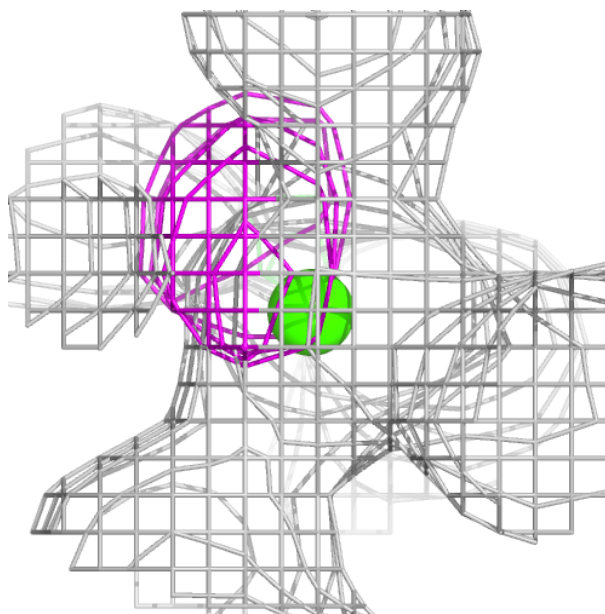
Electron density around CA G 201:

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



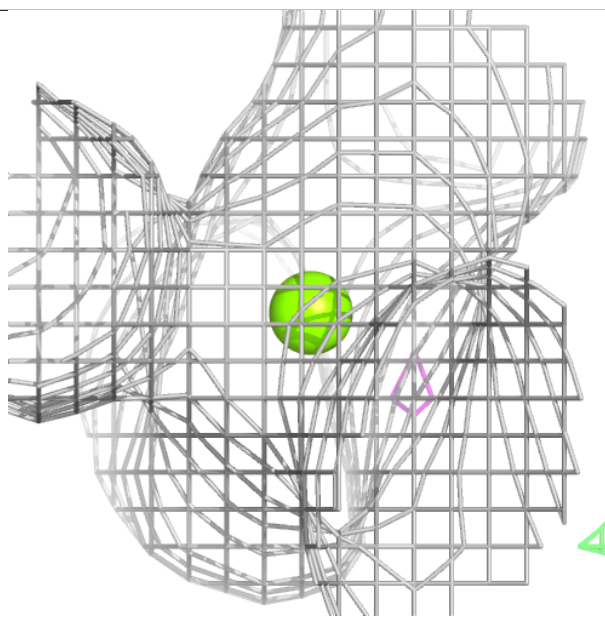
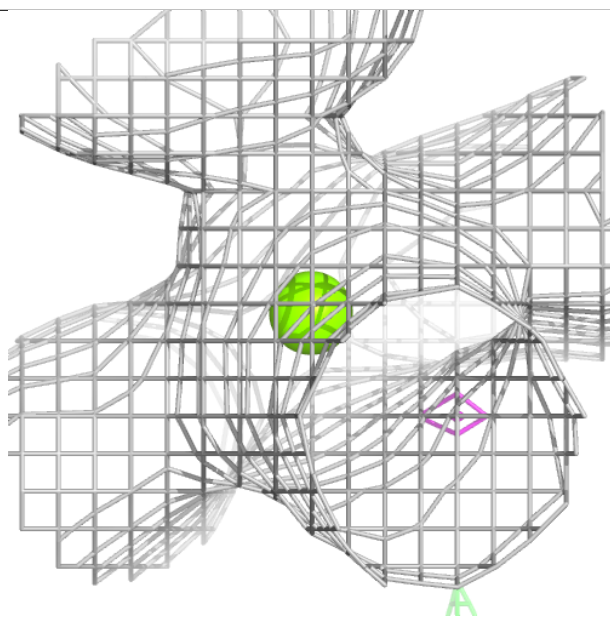
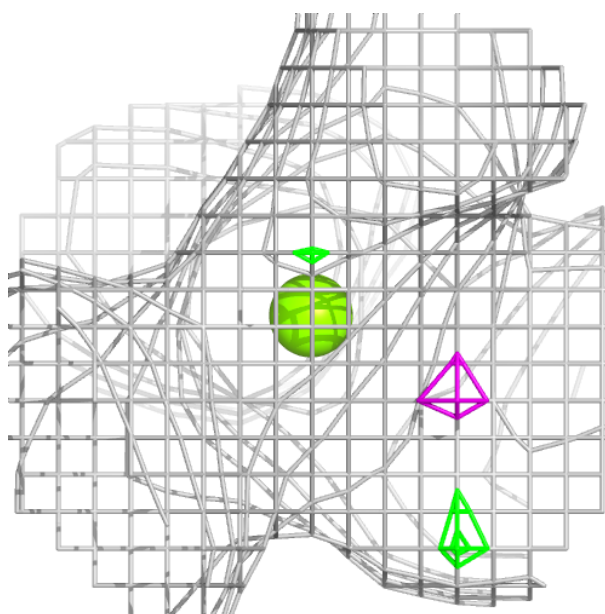
Electron density around CA F 102:

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



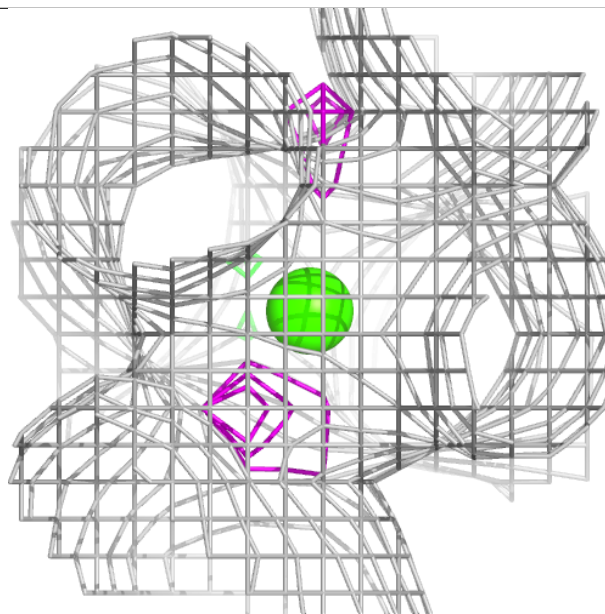
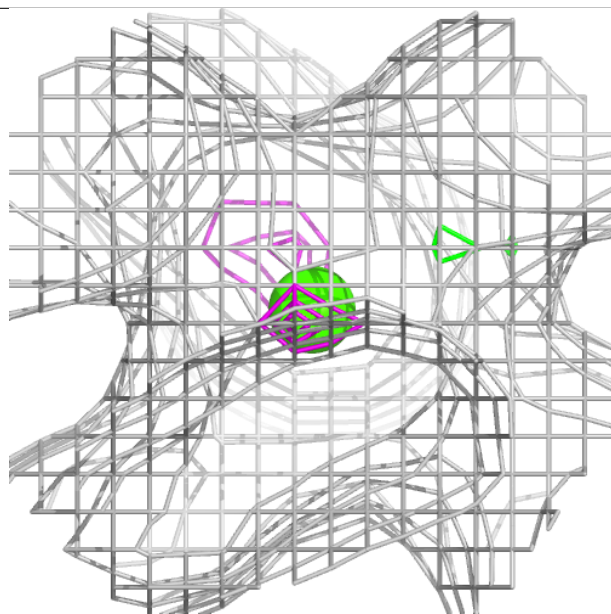
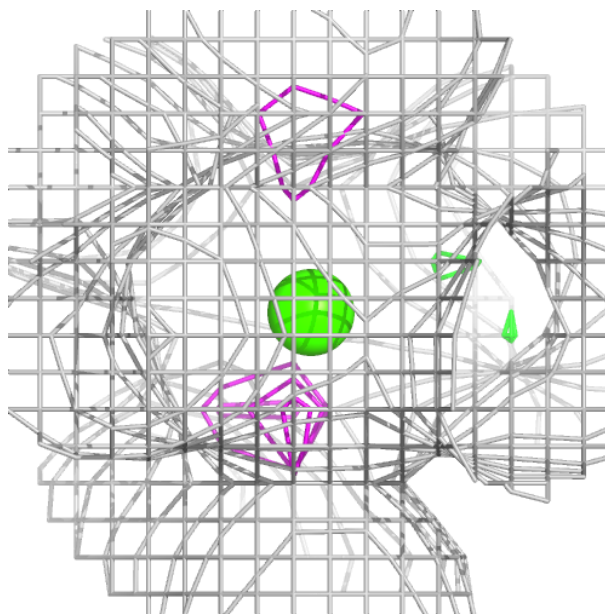
Electron density around MG G 207:

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



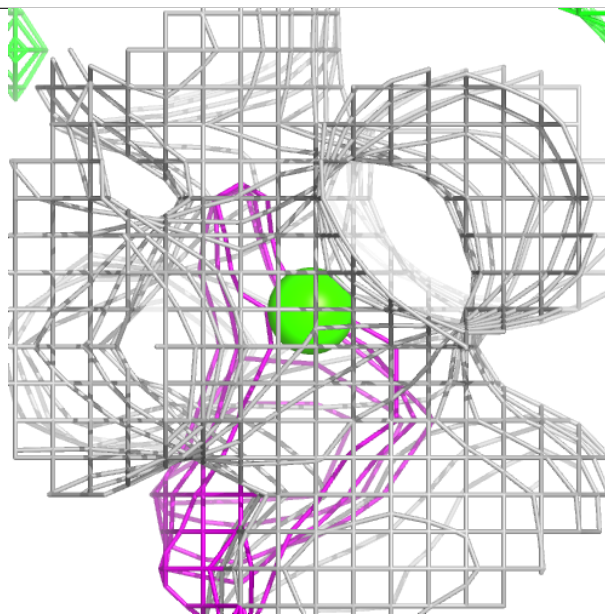
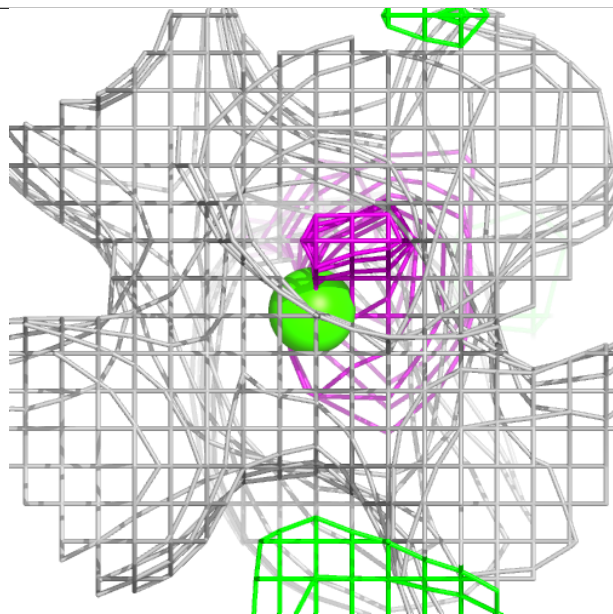
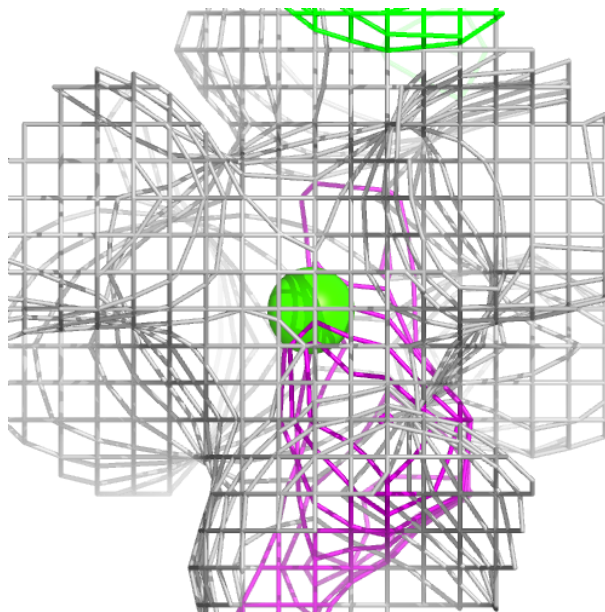
Electron density around CA A 201:

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



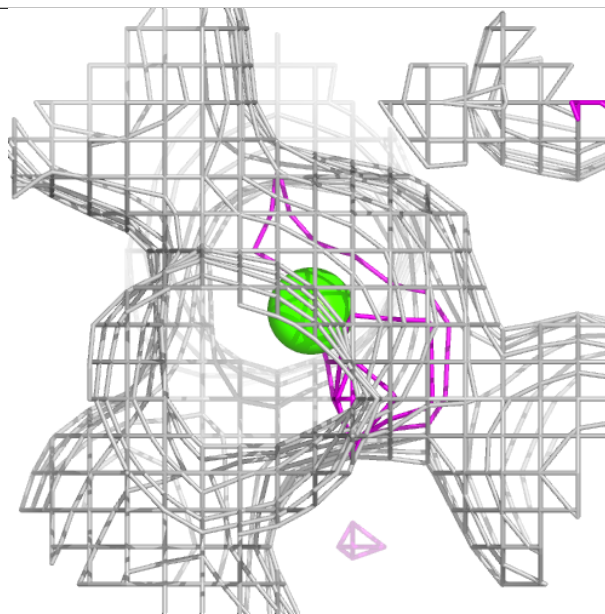
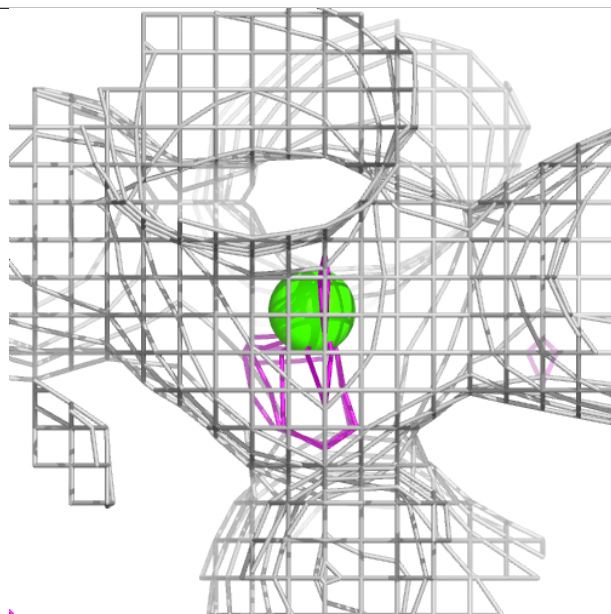
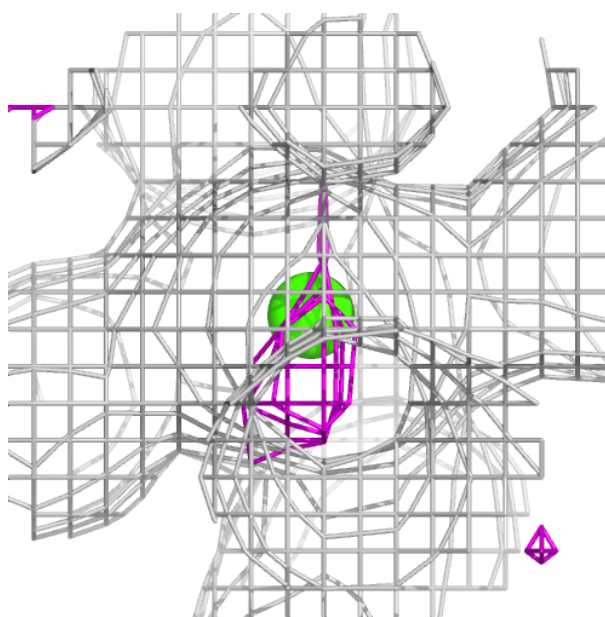
Electron density around CA E 203:

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



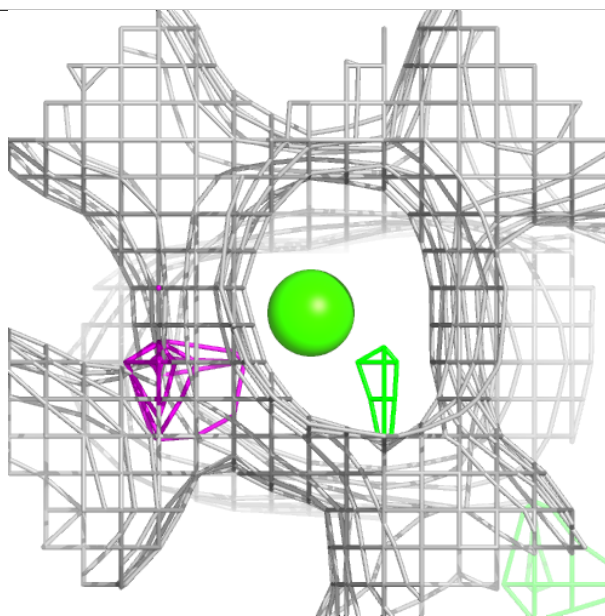
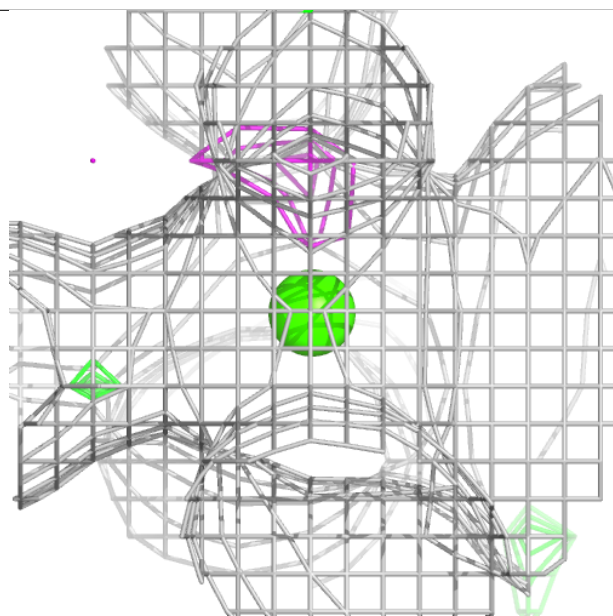
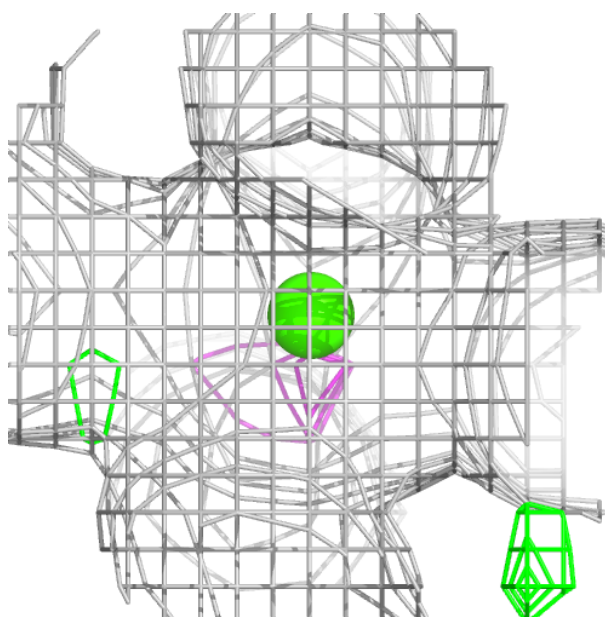
Electron density around CA A 202:

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



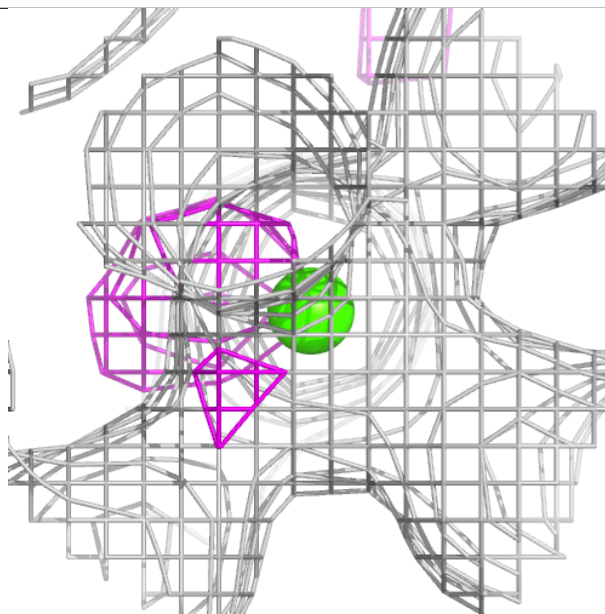
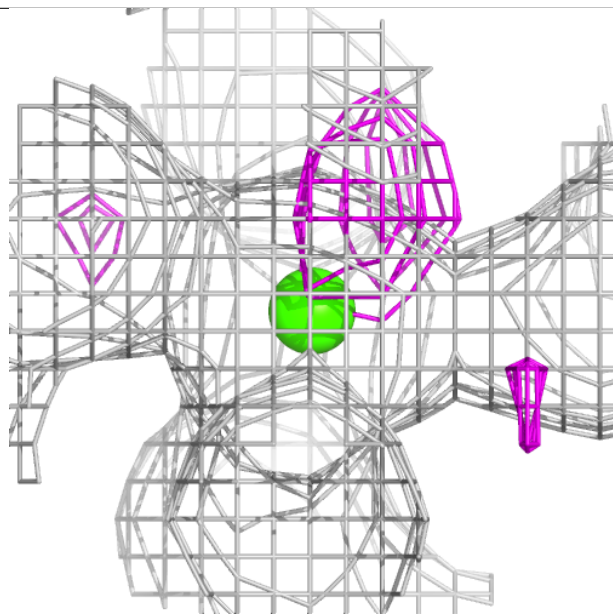
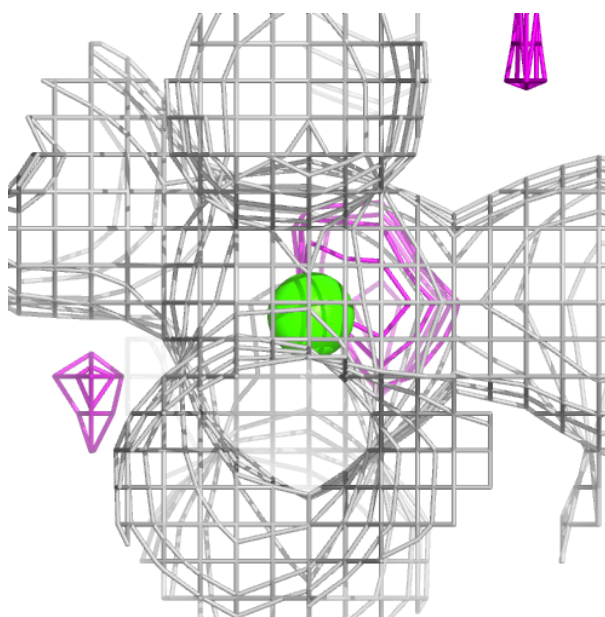
Electron density around CA E 202:

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



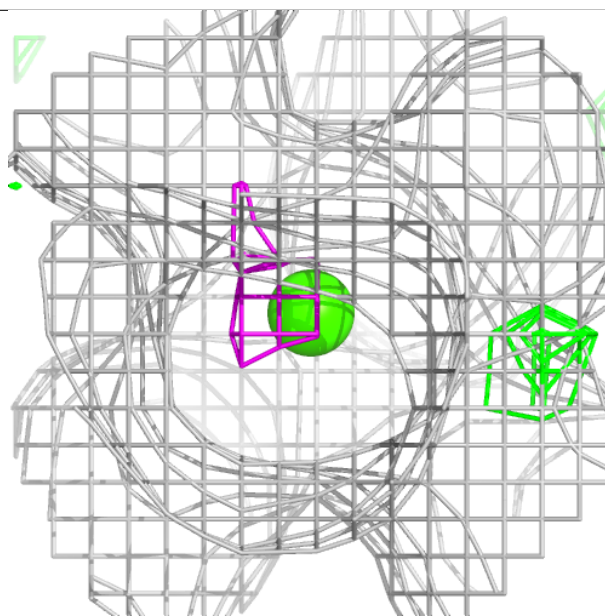
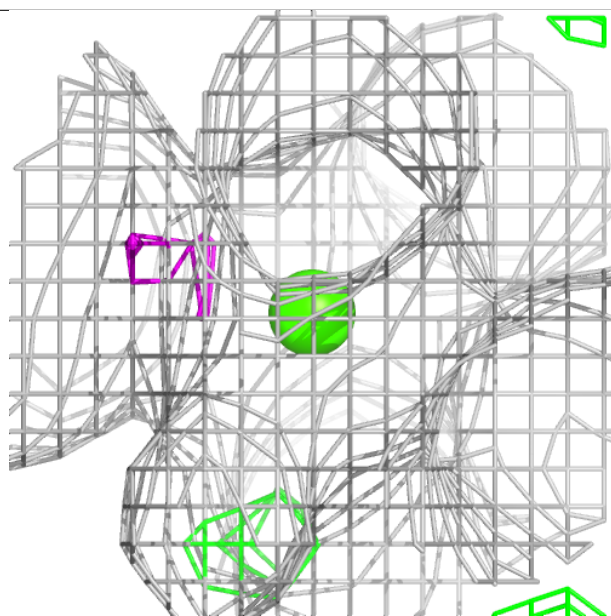
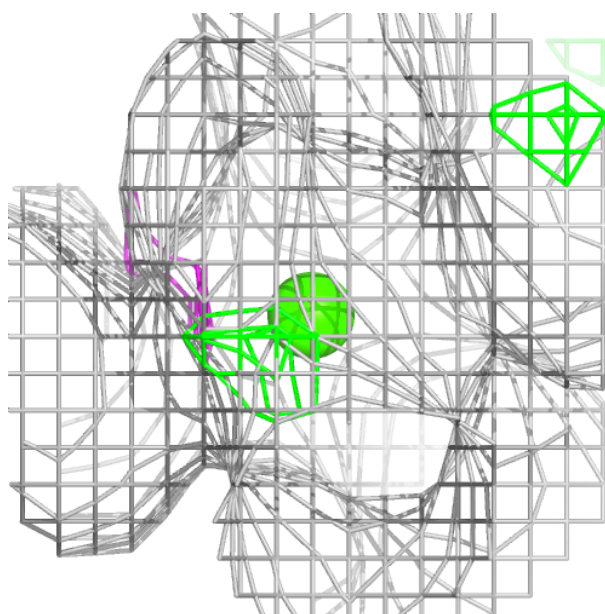
Electron density around CA H 102:

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



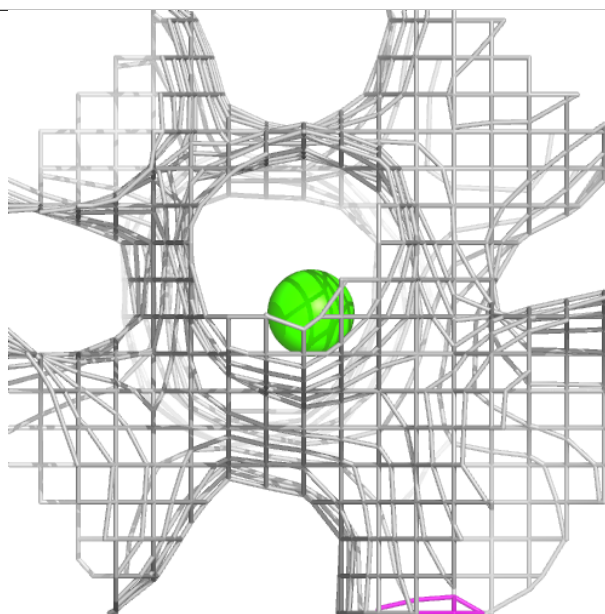
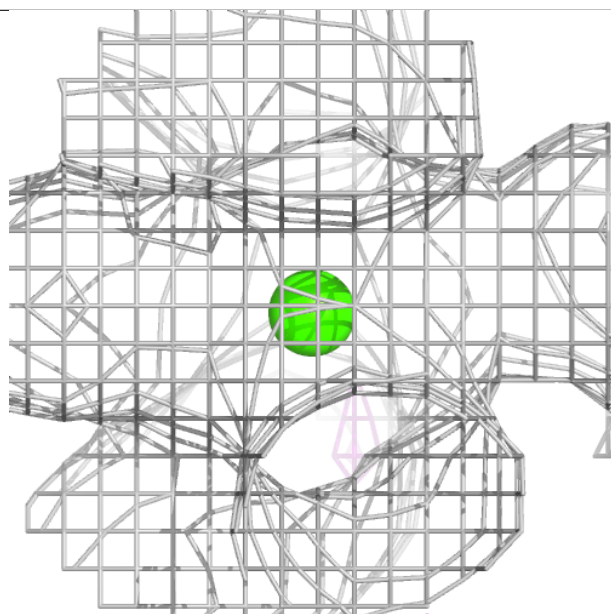
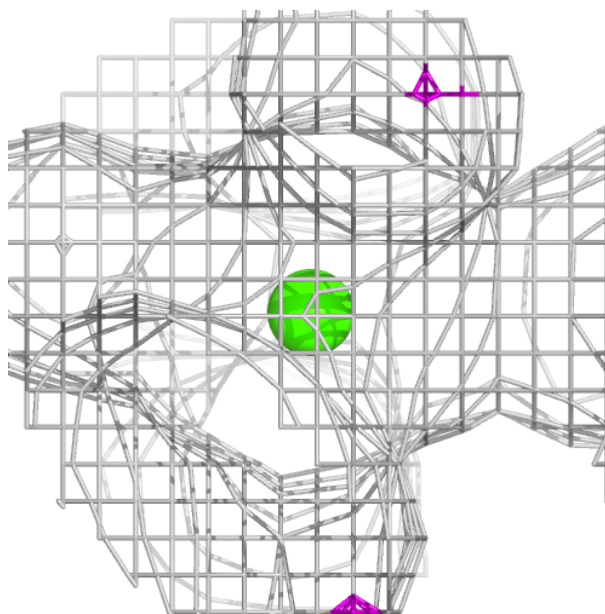
Electron density around CA C 202:

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



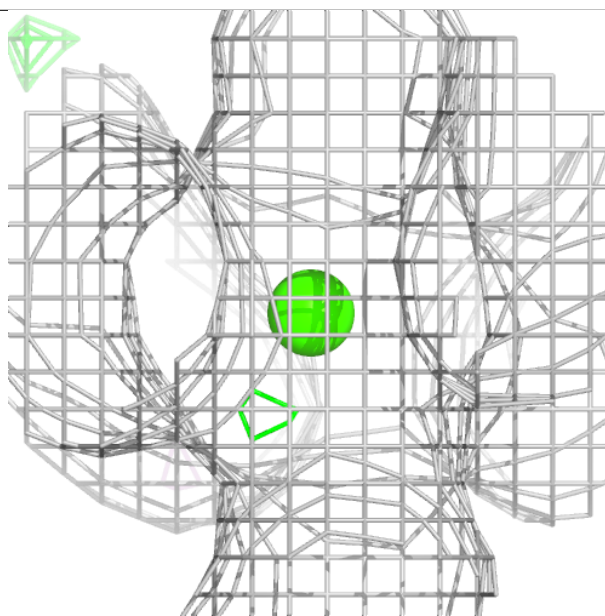
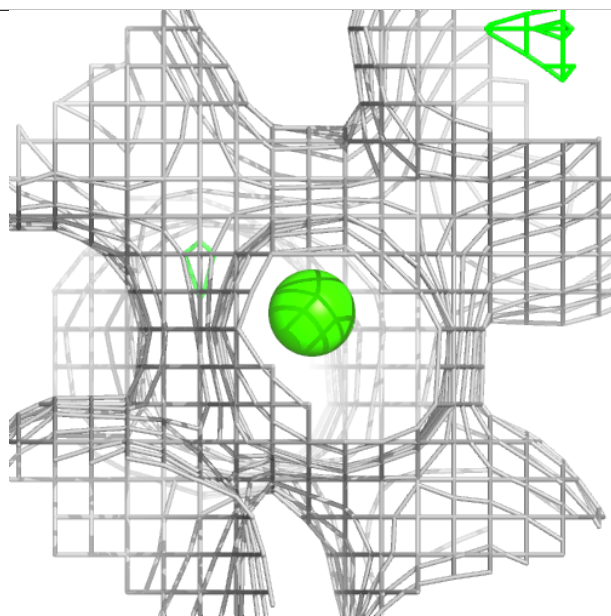
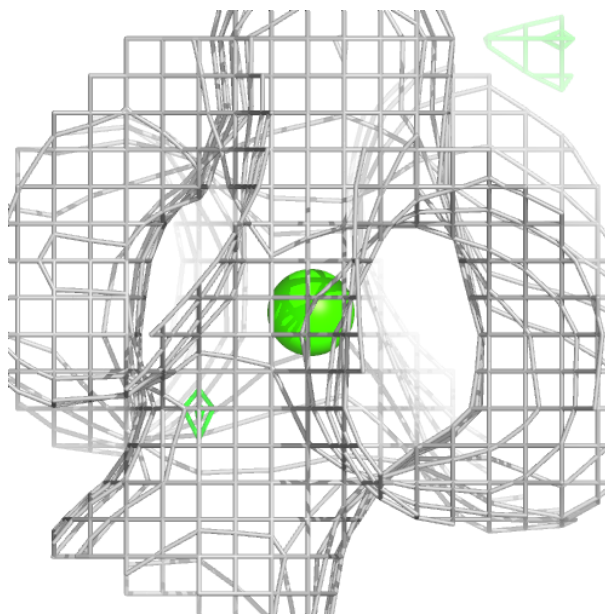
Electron density around CA F 101:

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



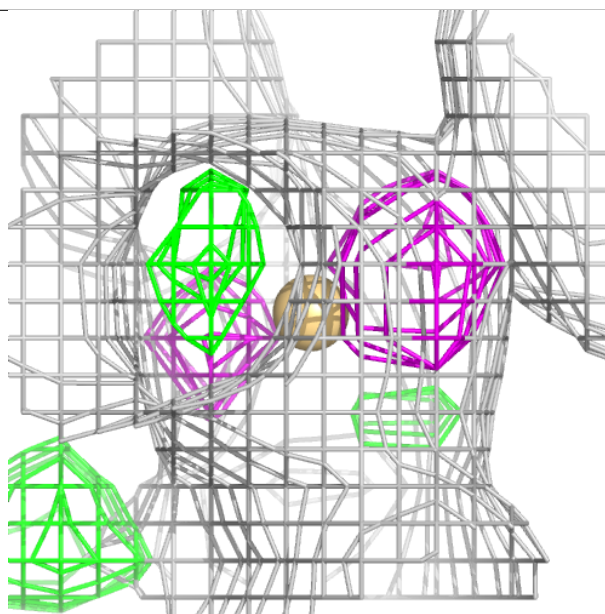
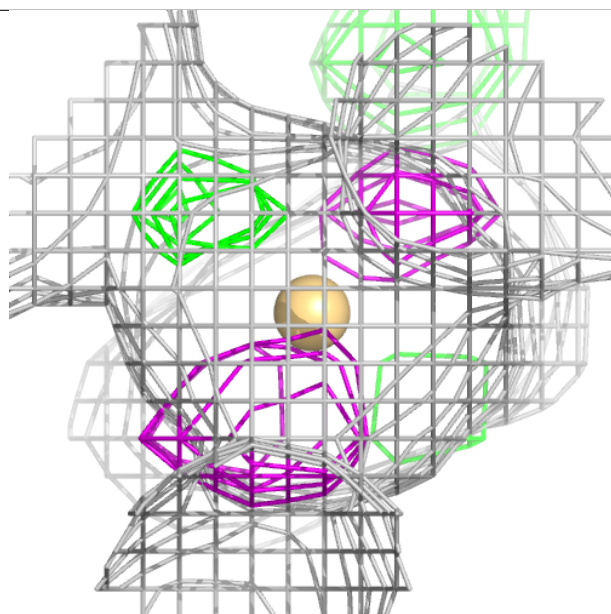
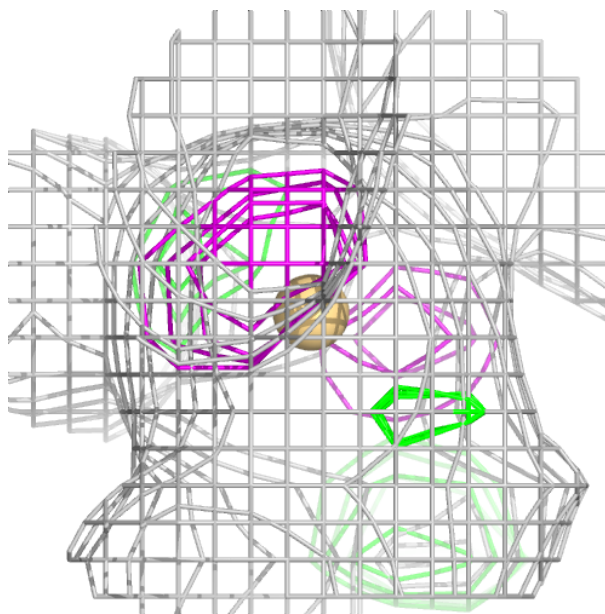
Electron density around CA D 101:

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



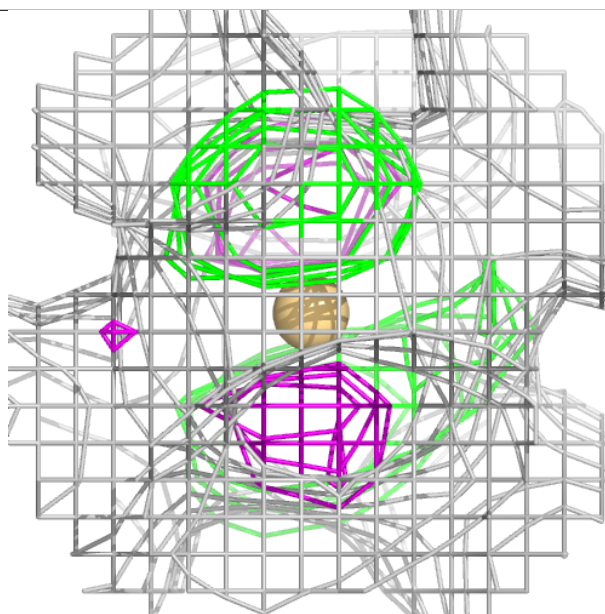
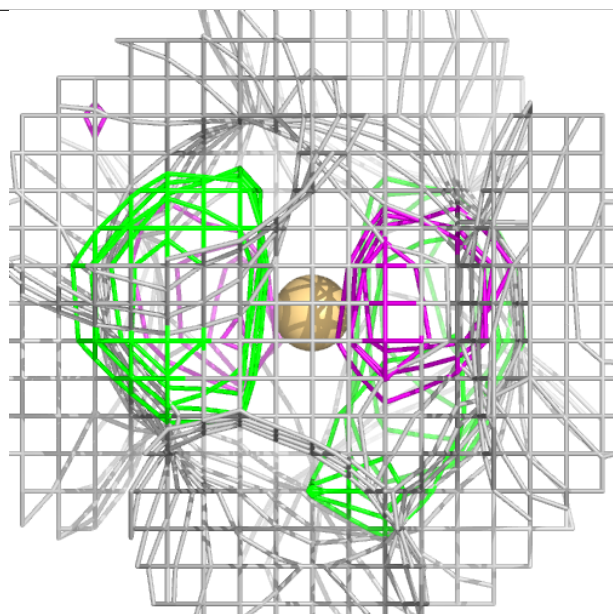
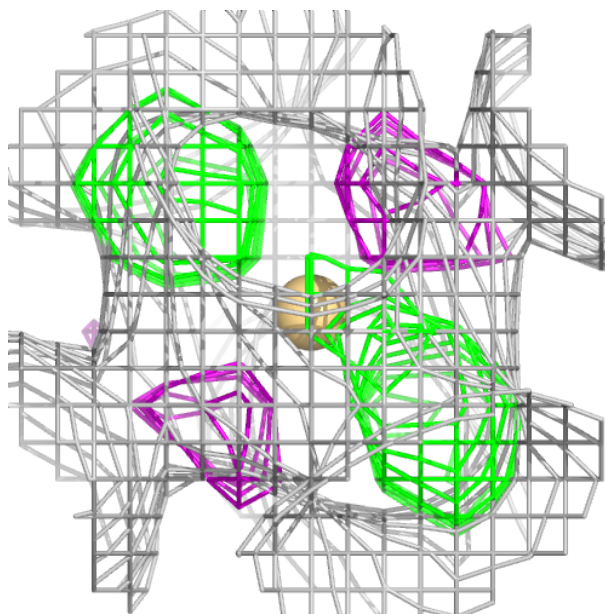
Electron density around CD A 206:

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



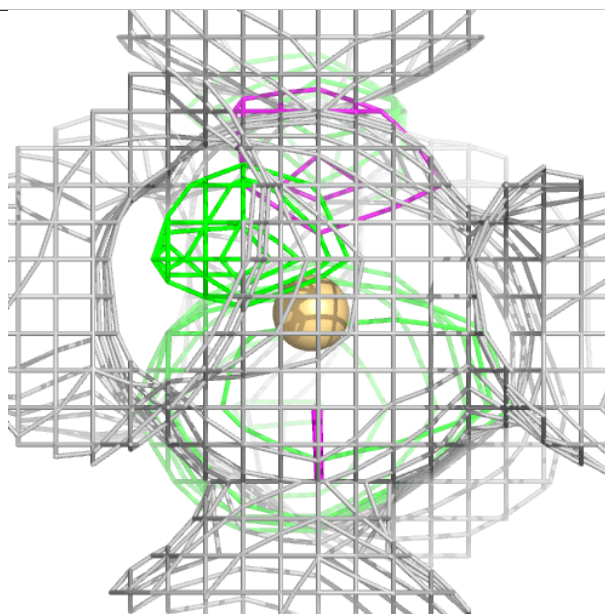
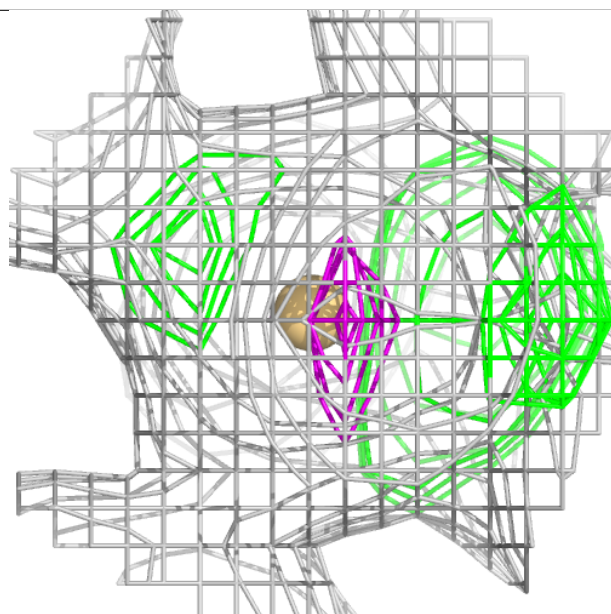
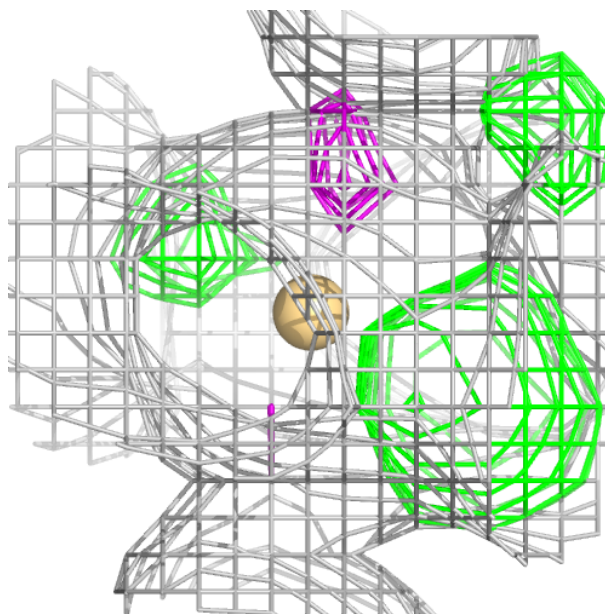
Electron density around CD C 205:

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



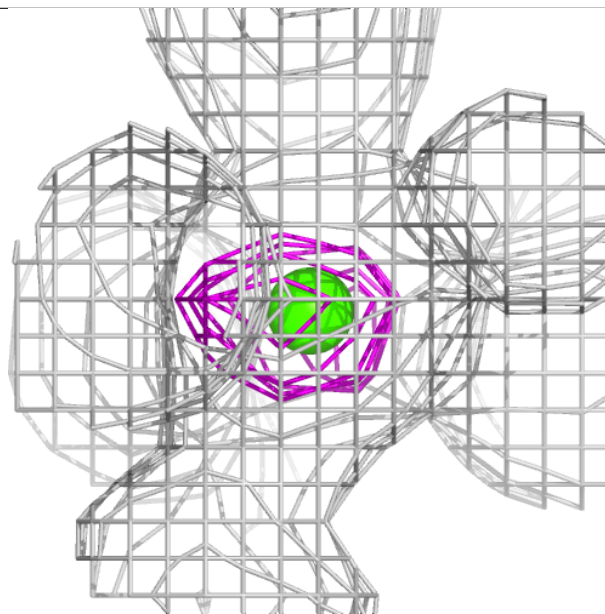
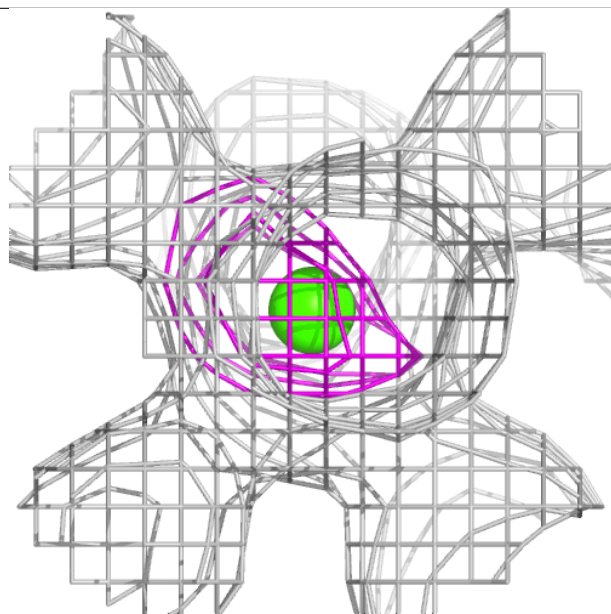
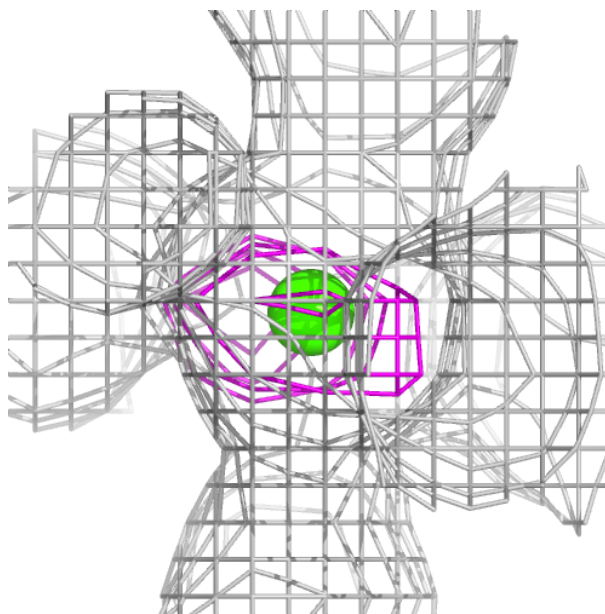
Electron density around CD E 207:

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



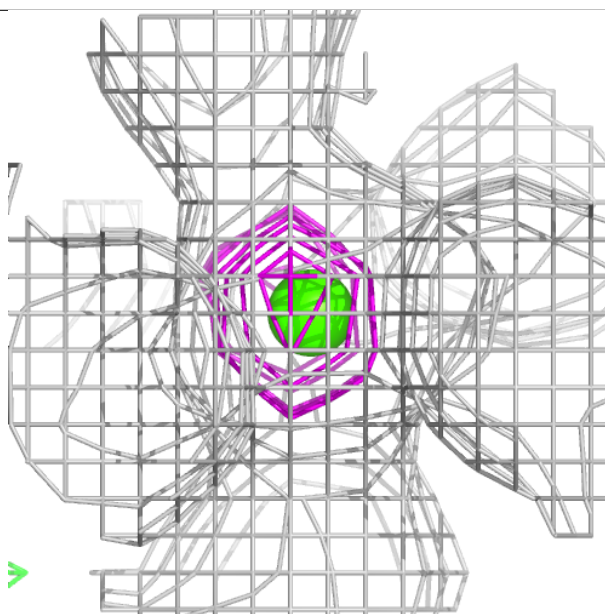
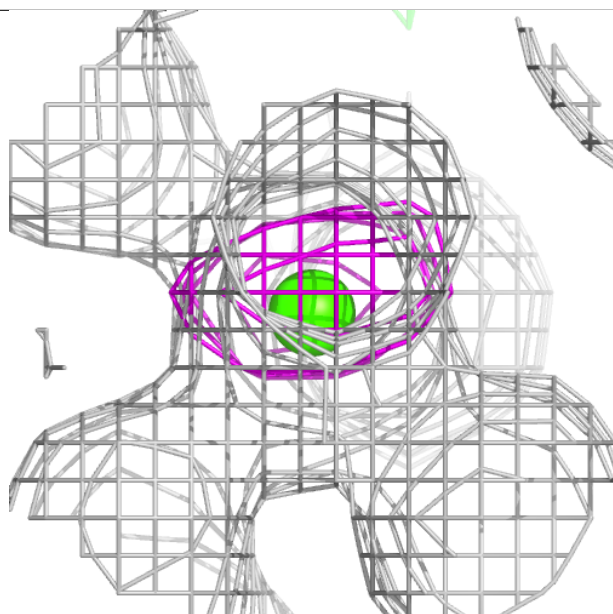
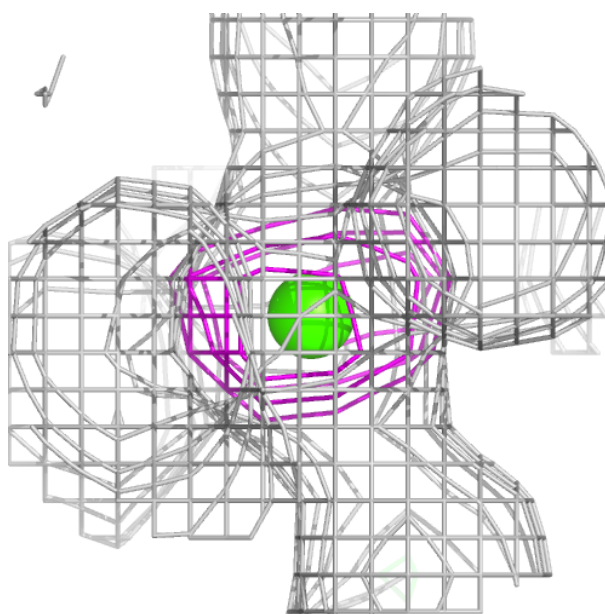
Electron density around CA C 201:

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



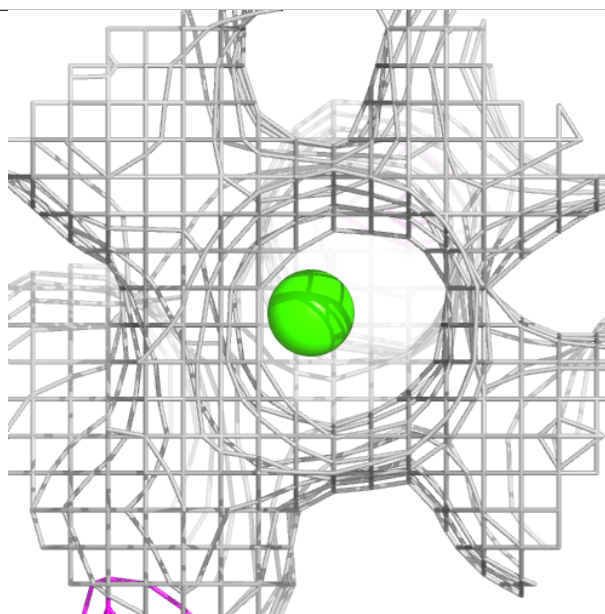
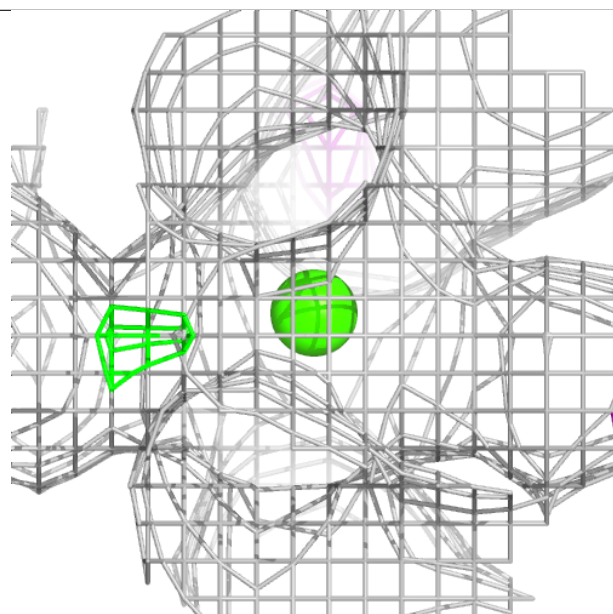
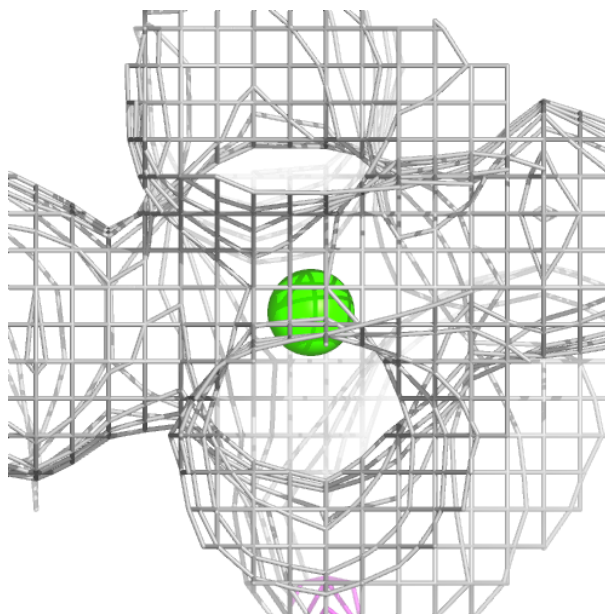
Electron density around CA B 102:

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



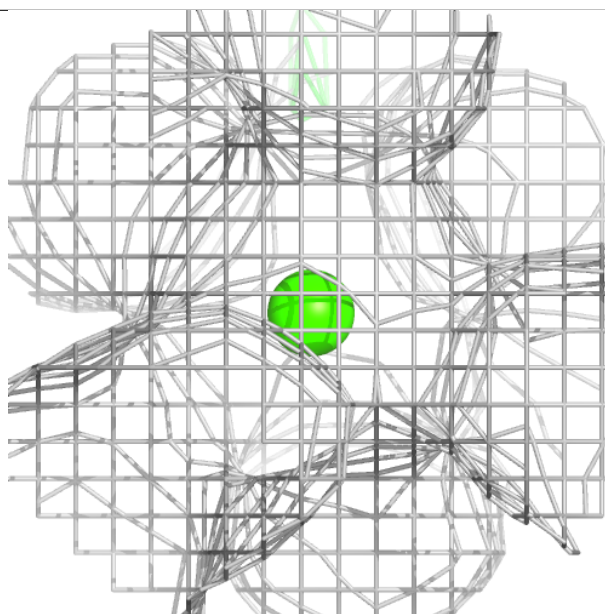
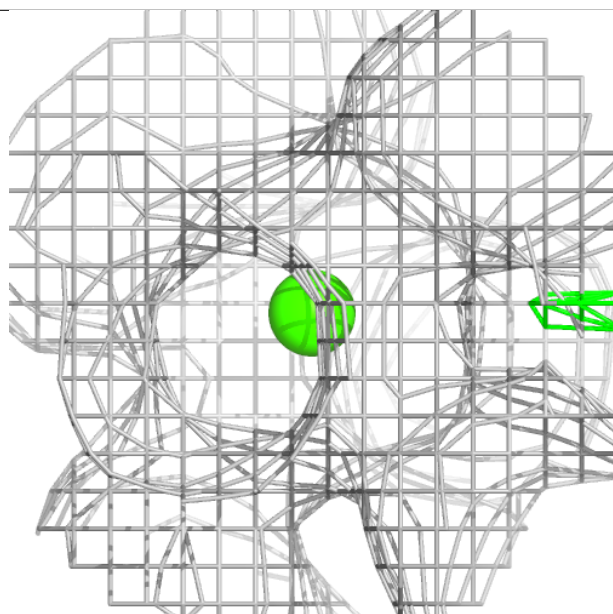
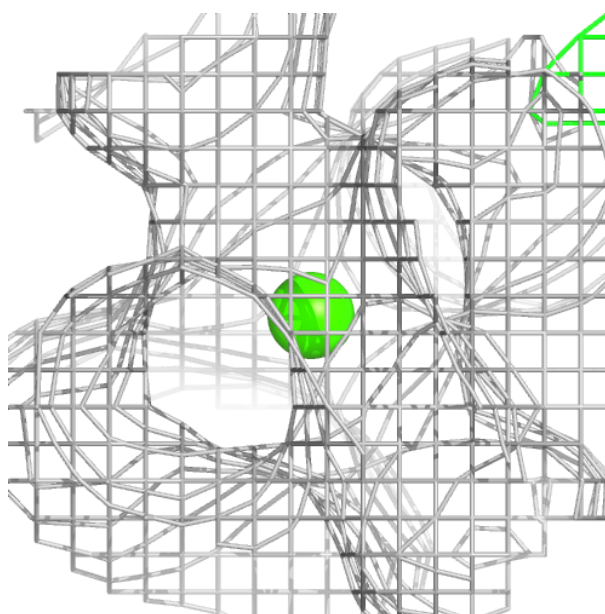
Electron density around CA B 101:

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



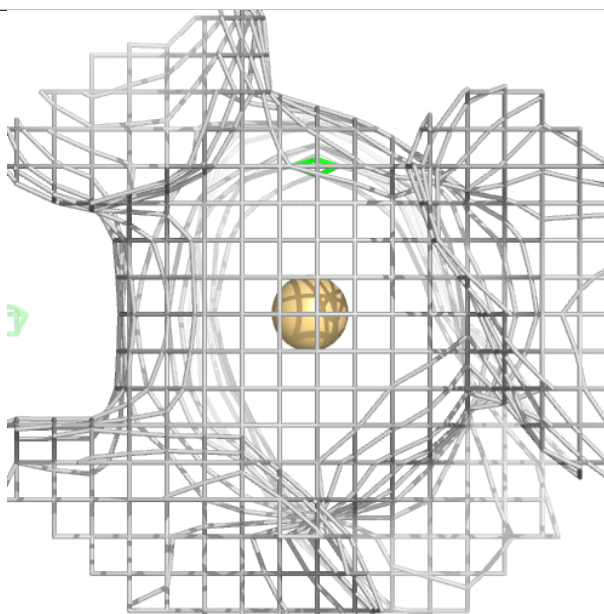
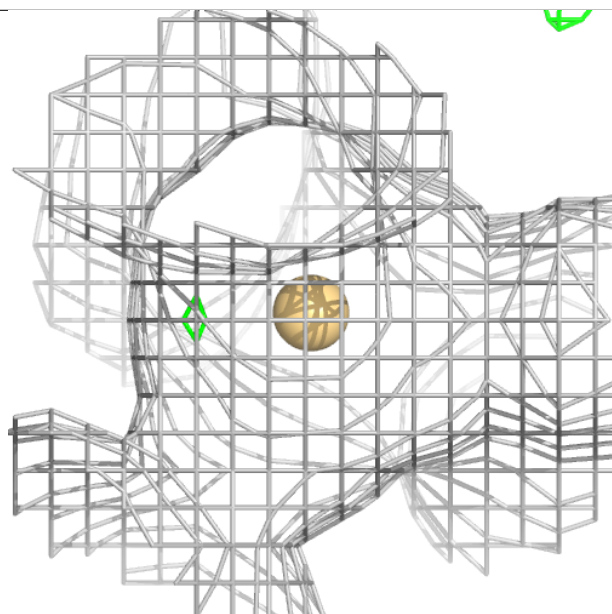
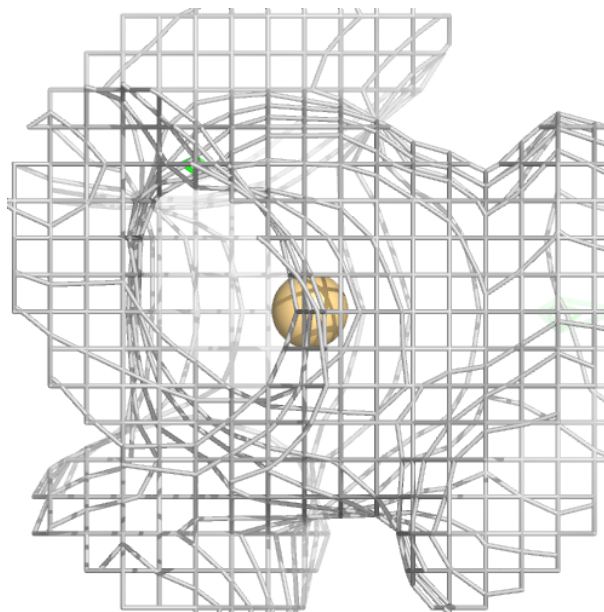
Electron density around CA H 101:

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



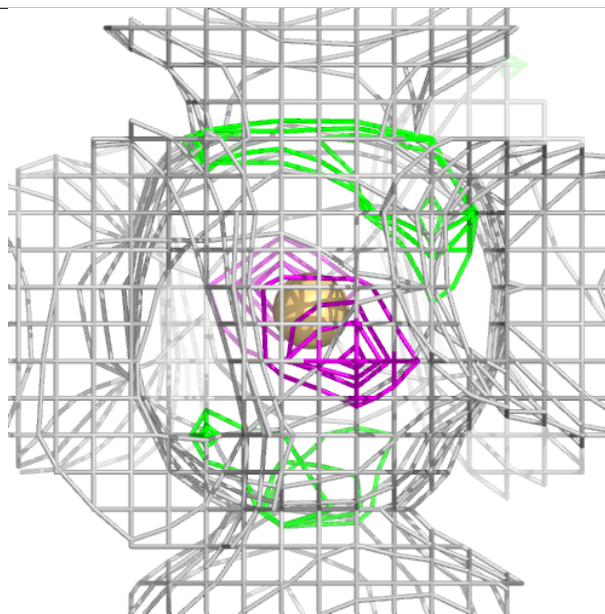
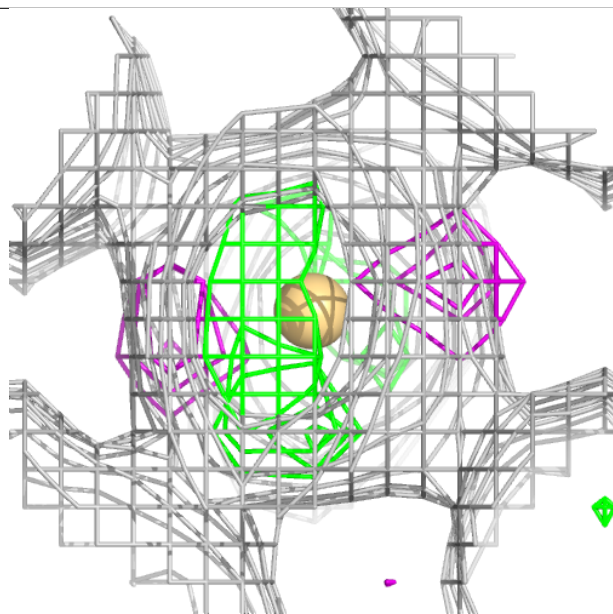
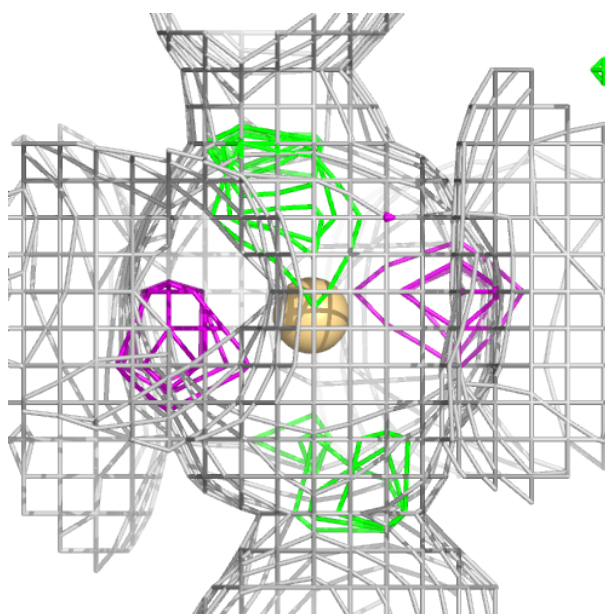
Electron density around CD C 206:

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



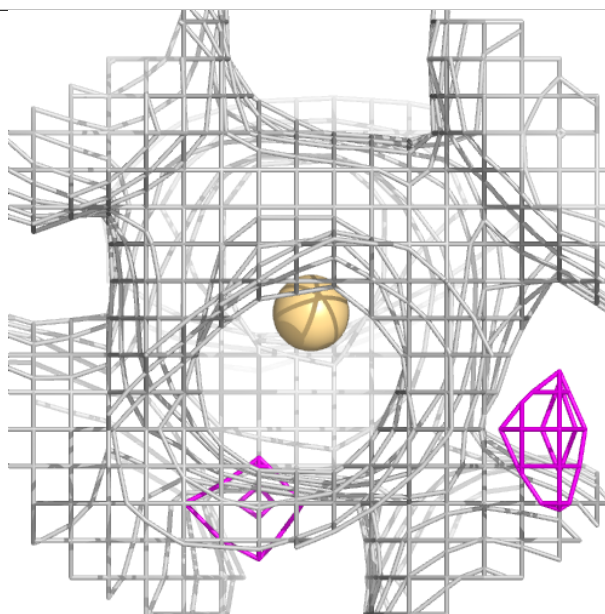
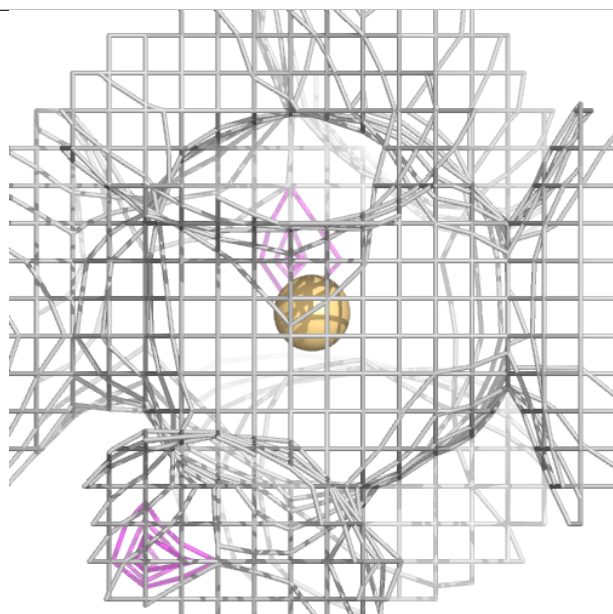
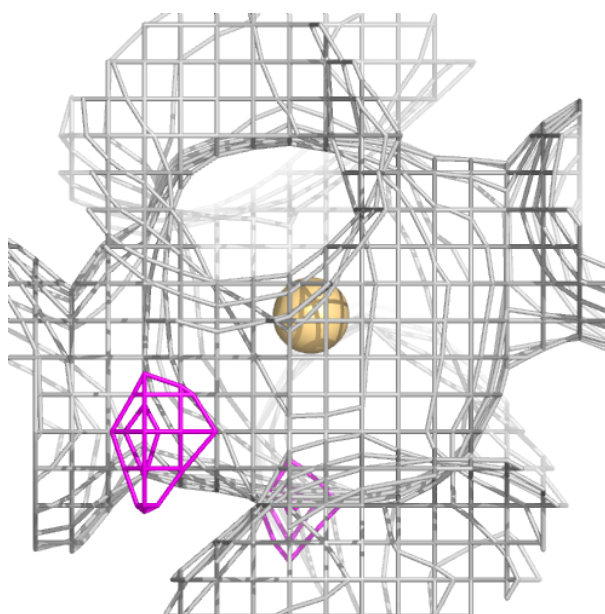
Electron density around CD A 205:

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



Electron density around CD G 206:

$2mF_o-DF_c$ (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.