



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:44 PM UTC

PDB ID : 9LKK / pdb_00009lkk
Title : Crystal structure of C1ql1-gC1q hexamer
Authors : Liao, L.; Niu, F.; Wei, Z.
Deposited on : 2025-01-16
Resolution : 2.22 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

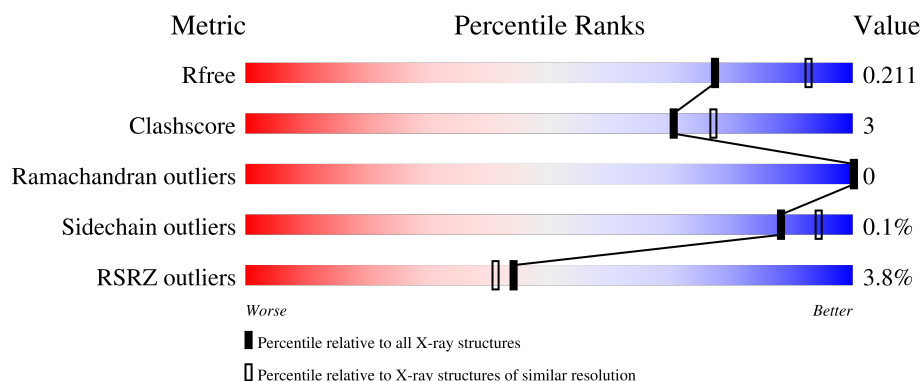
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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.



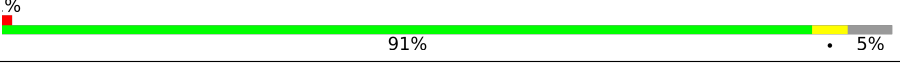
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	140	4% 84% 9% 7%
1	B	140	6% 87% 6% 6%
1	C	140	3% 84% 10% 6%
1	D	140	92% 6%
1	E	140	% 89% 6% 6%

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Mol	Chain	Length	Quality of chain
1	F	140	 91% 5%
1	G	140	 79% 13% 9%
1	H	140	 81% 8% 10%
1	I	140	 84% 7% 9%

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
3	CAC	B	505	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9706 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 Clq-related factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	6	0
			1022	646	171	201	4			
1	B	131	Total	C	N	O	S	0	4	0
			1029	650	172	203	4			
1	C	131	Total	C	N	O	S	0	7	0
			1040	657	176	203	4			
1	D	132	Total	C	N	O	S	0	0	0
			1016	643	170	199	4			
1	E	132	Total	C	N	O	S	0	0	0
			1014	641	170	199	4			
1	F	133	Total	C	N	O	S	0	2	0
			1034	654	175	201	4			
1	G	128	Total	C	N	O	S	0	1	0
			991	630	166	191	4			
1	H	126	Total	C	N	O	S	0	1	0
			977	622	161	190	4			
1	I	127	Total	C	N	O	S	0	3	0
			996	633	165	194	4			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP O88992
A	120	PRO	-	expression tag	UNP O88992
A	121	GLY	-	expression tag	UNP O88992
A	122	SER	-	expression tag	UNP O88992
A	123	GLU	-	expression tag	UNP O88992
A	124	PHE	-	expression tag	UNP O88992
B	119	GLY	-	expression tag	UNP O88992
B	120	PRO	-	expression tag	UNP O88992
B	121	GLY	-	expression tag	UNP O88992
B	122	SER	-	expression tag	UNP O88992
B	123	GLU	-	expression tag	UNP O88992

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Chain	Residue	Modelled	Actual	Comment	Reference
B	124	PHE	-	expression tag	UNP O88992
C	119	GLY	-	expression tag	UNP O88992
C	120	PRO	-	expression tag	UNP O88992
C	121	GLY	-	expression tag	UNP O88992
C	122	SER	-	expression tag	UNP O88992
C	123	GLU	-	expression tag	UNP O88992
C	124	PHE	-	expression tag	UNP O88992
D	119	GLY	-	expression tag	UNP O88992
D	120	PRO	-	expression tag	UNP O88992
D	121	GLY	-	expression tag	UNP O88992
D	122	SER	-	expression tag	UNP O88992
D	123	GLU	-	expression tag	UNP O88992
D	124	PHE	-	expression tag	UNP O88992
E	119	GLY	-	expression tag	UNP O88992
E	120	PRO	-	expression tag	UNP O88992
E	121	GLY	-	expression tag	UNP O88992
E	122	SER	-	expression tag	UNP O88992
E	123	GLU	-	expression tag	UNP O88992
E	124	PHE	-	expression tag	UNP O88992
F	119	GLY	-	expression tag	UNP O88992
F	120	PRO	-	expression tag	UNP O88992
F	121	GLY	-	expression tag	UNP O88992
F	122	SER	-	expression tag	UNP O88992
F	123	GLU	-	expression tag	UNP O88992
F	124	PHE	-	expression tag	UNP O88992
G	119	GLY	-	expression tag	UNP O88992
G	120	PRO	-	expression tag	UNP O88992
G	121	GLY	-	expression tag	UNP O88992
G	122	SER	-	expression tag	UNP O88992
G	123	GLU	-	expression tag	UNP O88992
G	124	PHE	-	expression tag	UNP O88992
H	119	GLY	-	expression tag	UNP O88992
H	120	PRO	-	expression tag	UNP O88992
H	121	GLY	-	expression tag	UNP O88992
H	122	SER	-	expression tag	UNP O88992
H	123	GLU	-	expression tag	UNP O88992
H	124	PHE	-	expression tag	UNP O88992
I	119	GLY	-	expression tag	UNP O88992
I	120	PRO	-	expression tag	UNP O88992
I	121	GLY	-	expression tag	UNP O88992
I	122	SER	-	expression tag	UNP O88992
I	123	GLU	-	expression tag	UNP O88992

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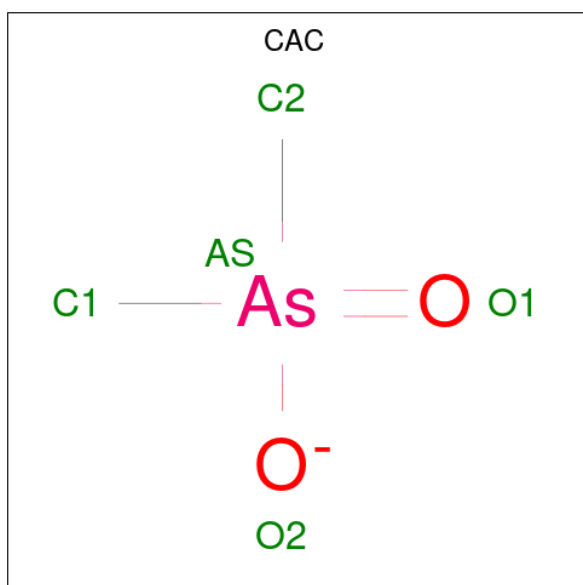
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Chain	Residue	Modelled	Actual	Comment	Reference
I	124	PHE	-	expression tag	UNP O88992

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

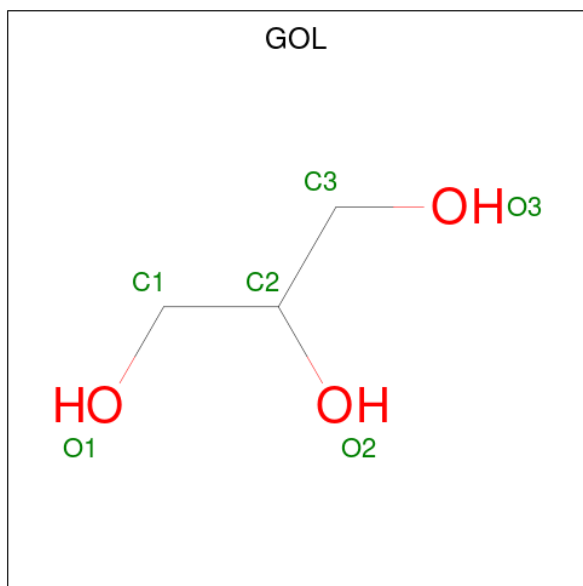
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Ca 5 5	0	0
2	B	4	Total Ca 4 4	0	0
2	C	4	Total Ca 4 4	0	0
2	D	5	Total Ca 5 5	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	C	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	I	1	Total Cl 1 1	0	0

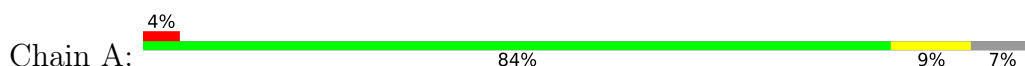
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	77	Total O 77 77	0	0
6	B	54	Total O 54 54	0	0
6	C	61	Total O 61 61	0	0
6	D	68	Total O 68 68	0	0
6	E	61	Total O 61 61	0	0
6	F	73	Total O 73 73	0	0
6	G	32	Total O 32 32	0	0
6	H	32	Total O 32 32	0	0
6	I	39	Total O 39 39	0	0

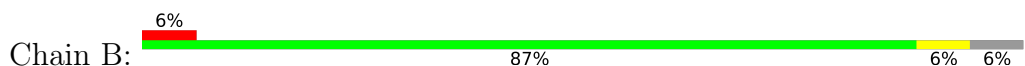
3 Residue-property plots [i](#)

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.

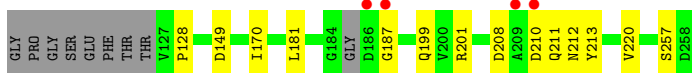
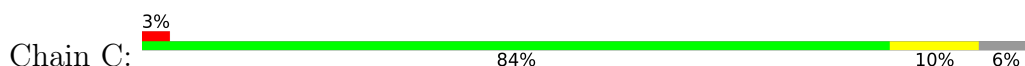
- Molecule 1: C1q-related factor



- Molecule 1: C1q-related factor



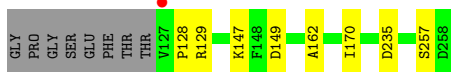
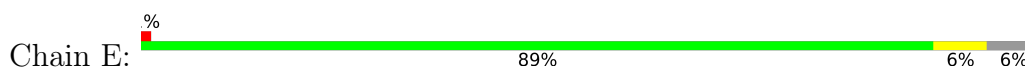
- Molecule 1: C1q-related factor



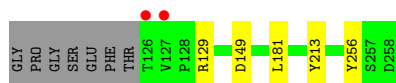
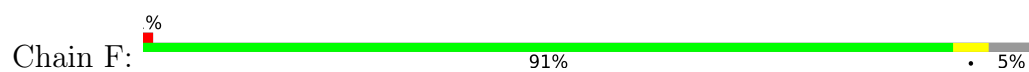
- Molecule 1: C1q-related factor



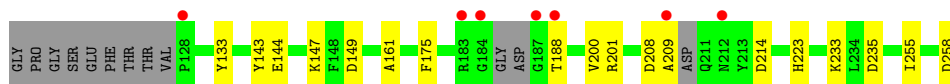
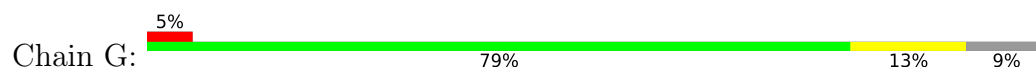
- Molecule 1: C1q-related factor



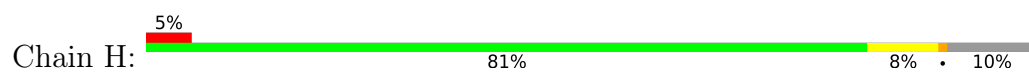
- Molecule 1: C1q-related factor



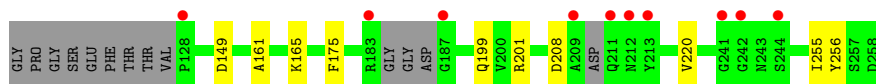
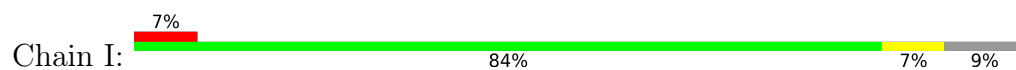
- Molecule 1: C1q-related factor



- Molecule 1: C1q-related factor



- Molecule 1: C1q-related factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.37Å 110.63Å 114.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.46 – 2.22 57.46 – 2.22	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.46-2.22) 100.0 (57.46-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.172 , 0.210 0.173 , 0.211	Depositor DCC
R_{free} test set	3340 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k 0.007 for -l,-k,-h 0.013 for k,h,-l 0.017 for k,l,h 0.017 for l,h,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9706	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CAC, CA, GOL

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	0.33	0/1045	0.56	0/1412
1	B	0.33	0/1052	0.54	0/1422
1	C	0.33	0/1065	0.55	0/1437
1	D	0.34	0/1041	0.52	0/1410
1	E	0.35	0/1039	0.53	0/1407
1	F	0.34	0/1065	0.54	0/1442
1	G	0.29	0/1017	0.49	0/1373
1	H	0.25	0/1000	0.47	0/1352
1	I	0.29	0/1022	0.46	0/1381
All	All	0.32	0/9346	0.52	0/12636

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1022	0	946	11	0
1	B	1029	0	953	8	0
1	C	1040	0	970	11	0
1	D	1016	0	946	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1014	0	939	6	0
1	F	1034	0	967	4	0
1	G	991	0	927	15	0
1	H	977	0	908	8	0
1	I	996	0	927	11	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	12	0	16	0	0
4	E	18	0	24	1	0
4	F	6	0	8	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	A	77	0	0	0	0
6	B	54	0	0	1	0
6	C	61	0	0	1	0
6	D	68	0	0	0	0
6	E	61	0	0	0	0
6	F	73	0	0	1	0
6	G	32	0	0	3	0
6	H	32	0	0	0	0
6	I	39	0	0	1	0
All	All	9706	0	8547	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (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)
1:C:212:ASN:HD21	1:G:209:ALA:HB3	1.50	0.74
1:B:212:ASN:ND2	1:I:208:ASP:OD2	2.23	0.71
1:I:199[A]:GLN:OE1	1:I:201:ARG:NH2	2.28	0.66
1:G:175:PHE:HB2	1:G:255:ILE:HD11	1.81	0.62
1:H:149:ASP:HA	1:H:161:ALA:HB1	1.82	0.62
1:E:128:PRO:HB3	1:E:170:ILE:HD13	1.82	0.61
1:G:143:TYR:O	1:G:233:LYS:NZ	2.36	0.59
1:C:199:GLN:NE2	6:C:602:HOH:O	2.34	0.59
1:B:129:ARG:NH2	1:C:257:SER:O	2.36	0.58
1:B:129:ARG:NH1	6:B:602:HOH:O	2.35	0.58
1:H:175:PHE:HB2	1:H:255:ILE:HD11	1.86	0.56
1:E:149:ASP:OD1	1:E:149:ASP:N	2.39	0.55
1:B:181:LEU:HD11	1:B:213:TYR:HB3	1.90	0.54
1:B:210[A]:ASP:N	1:I:208:ASP:OD1	2.41	0.53
1:A:181:LEU:HD11	1:A:213:TYR:HB3	1.89	0.53
1:A:143:TYR:O	1:A:233:LYS:HE2	2.10	0.51
1:C:181:LEU:HD11	1:C:213:TYR:HB3	1.93	0.50
1:I:175:PHE:HB2	1:I:255:ILE:HD11	1.93	0.50
1:B:143:TYR:O	1:B:233:LYS:HE2	2.11	0.50
1:H:133:TYR:CZ	1:I:220:VAL:HG12	2.48	0.49
1:A:212:ASN:ND2	1:G:208:ASP:OD2	2.47	0.48
1:F:129[A]:ARG:NH2	6:F:602:HOH:O	2.48	0.47
1:C:149:ASP:OD1	1:C:149:ASP:N	2.47	0.47
1:I:165:LYS:NZ	6:I:402:HOH:O	2.46	0.47
1:A:190:MET:HE2	1:A:190:MET:HB3	1.79	0.47
1:H:129:ARG:HA	1:I:256:TYR:CZ	2.50	0.46
1:G:147:LYS:NZ	6:G:401:HOH:O	2.47	0.46
1:A:210[A]:ASP:N	1:G:208:ASP:OD1	2.49	0.46
1:G:133:TYR:CZ	1:H:220:VAL:HG12	2.51	0.46
1:G:144:GLU:HB2	6:G:401:HOH:O	2.17	0.45
1:C:211[A]:GLN:CD	1:C:211[A]:GLN:N	2.75	0.44
1:G:188:THR:HA	6:G:424:HOH:O	2.16	0.44
1:F:181:LEU:HD11	1:F:213:TYR:HB3	1.98	0.44
1:G:200:VAL:O	1:G:201[B]:ARG:HD2	2.17	0.44
1:E:128:PRO:HG2	1:E:257:SER:HB3	1.98	0.44
1:B:133:TYR:CZ	1:C:220:VAL:HG12	2.53	0.44
1:E:147:LYS:HD2	1:E:162:ALA:O	2.17	0.44
1:A:175:PHE:HB2	1:A:255:ILE:HD11	1.99	0.44
1:G:223:HIS:NE2	1:G:258:ASP:OD2	2.36	0.44
1:E:235:ASP:OD2	4:E:404:GOL:H31	2.18	0.43
1:I:201:ARG:HD3	1:I:201:ARG:HA	1.83	0.43
1:E:129:ARG:HA	1:F:256:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:ASP:HA	1:I:161:ALA:HB1	2.01	0.42
1:A:133:TYR:CZ	1:B:220:VAL:HG12	2.55	0.42
1:H:147:LYS:HB2	1:H:147:LYS:HE2	1.31	0.42
1:A:212:ASN:HB2	1:G:208:ASP:OD2	2.20	0.42
1:I:199[A]:GLN:CD	1:I:201:ARG:HH12	2.28	0.42
1:C:128:PRO:HB3	1:C:170:ILE:HD13	2.02	0.42
1:C:187[A]:GLY:HA2	1:C:211[A]:GLN:HE22	1.85	0.42
1:I:199[A]:GLN:CD	1:I:201:ARG:HH22	2.25	0.41
1:C:208:ASP:OD1	1:C:210[B]:ASP:N	2.53	0.41
1:F:149:ASP:OD1	1:F:149:ASP:N	2.51	0.41
1:A:191:TRP:HB2	1:G:235:ASP:HB3	2.02	0.41
1:C:201:ARG:HD3	1:C:201:ARG:HA	1.86	0.41
1:H:170:ILE:O	1:H:174:TYR:OH	2.33	0.41
1:A:191:TRP:CE2	1:A:205:ILE:HD12	2.55	0.41
1:H:206:ALA:HB1	1:H:214:ASP:HB3	2.03	0.41
1:G:149:ASP:HA	1:G:161:ALA:HB1	2.03	0.41
1:A:206:ALA:HB1	1:G:214:ASP:HB3	2.02	0.41
1:D:149:ASP:OD1	1:D:149:ASP:N	2.51	0.40
1:D:127:VAL:HA	1:D:128:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	128/140 (91%)	124 (97%)	4 (3%)	0	100	100
1	B	129/140 (92%)	126 (98%)	3 (2%)	0	100	100
1	C	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
1	D	130/140 (93%)	128 (98%)	2 (2%)	0	100	100
1	E	130/140 (93%)	127 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	133/140 (95%)	131 (98%)	2 (2%)	0	100	100
1	G	123/140 (88%)	119 (97%)	4 (3%)	0	100	100
1	H	120/140 (86%)	116 (97%)	4 (3%)	0	100	100
1	I	123/140 (88%)	119 (97%)	4 (3%)	0	100	100
All	All	1145/1260 (91%)	1115 (97%)	30 (3%)	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	106/111 (96%)	106 (100%)	0	100	100
1	B	107/111 (96%)	107 (100%)	0	100	100
1	C	108/111 (97%)	108 (100%)	0	100	100
1	D	105/111 (95%)	105 (100%)	0	100	100
1	E	104/111 (94%)	104 (100%)	0	100	100
1	F	107/111 (96%)	107 (100%)	0	100	100
1	G	102/111 (92%)	102 (100%)	0	100	100
1	H	101/111 (91%)	100 (99%)	1 (1%)	68	80
1	I	103/111 (93%)	103 (100%)	0	100	100
All	All	943/999 (94%)	942 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	147	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	240	HIS
1	C	212	ASN
1	C	245	ASN
1	G	240	HIS
1	I	158	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 38 ligands modelled in this entry, 27 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CAC	B	505	-	2,4,4	2.71	2 (100%)	4,6,6	2.13	2 (50%)
3	CAC	C	506	-	2,4,4	2.66	2 (100%)	4,6,6	2.39	1 (25%)
4	GOL	E	403	-	5,5,5	1.24	0	5,5,5	0.81	0
4	GOL	D	506	-	5,5,5	1.02	0	5,5,5	1.02	0
4	GOL	C	507	-	5,5,5	0.90	0	5,5,5	1.04	0
4	GOL	D	507	-	5,5,5	1.16	0	5,5,5	1.17	0
4	GOL	E	401	-	5,5,5	1.31	1 (20%)	5,5,5	0.85	0
4	GOL	E	404	-	5,5,5	0.78	0	5,5,5	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CAC	A	406	-	2,4,4	2.75	2 (100%)	4,6,6	1.00	0
4	GOL	B	506	-	5,5,5	0.72	0	5,5,5	1.07	0
4	GOL	F	503	-	5,5,5	0.90	0	5,5,5	1.09	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	GOL	E	403	-	-	2/4/4/4	-
4	GOL	D	506	-	-	0/4/4/4	-
4	GOL	D	507	-	-	0/4/4/4	-
4	GOL	C	507	-	-	3/4/4/4	-
4	GOL	E	401	-	-	2/4/4/4	-
4	GOL	E	404	-	-	0/4/4/4	-
4	GOL	B	506	-	-	2/4/4/4	-
4	GOL	F	503	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	506	CAC	AS-C1	2.92	1.97	1.90
3	A	406	CAC	AS-C2	2.84	1.97	1.90
3	B	505	CAC	AS-C1	2.72	1.96	1.90
3	B	505	CAC	AS-C2	2.69	1.96	1.90
3	A	406	CAC	AS-C1	2.66	1.96	1.90
3	C	506	CAC	AS-C2	2.38	1.96	1.90
4	E	401	GOL	C1-C2	2.08	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	506	CAC	O1-AS-C2	-4.17	106.32	111.50
3	B	505	CAC	O1-AS-C2	-3.15	107.58	111.50
3	B	505	CAC	O1-AS-C1	-2.07	108.92	111.50

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	401	GOL	C1-C2-C3-O3
4	E	401	GOL	O2-C2-C3-O3
4	B	506	GOL	C1-C2-C3-O3
4	C	507	GOL	C1-C2-C3-O3
4	C	507	GOL	O2-C2-C3-O3
4	C	507	GOL	O1-C1-C2-C3
4	E	403	GOL	C1-C2-C3-O3
4	B	506	GOL	O2-C2-C3-O3
4	E	403	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	404	GOL	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	130/140 (92%)	-0.13	6 (4%) 37 34	22, 34, 52, 67	8 (6%)
1	B	131/140 (93%)	-0.04	8 (6%) 27 24	23, 35, 58, 72	4 (3%)
1	C	131/140 (93%)	-0.36	4 (3%) 51 49	20, 33, 44, 70	8 (6%)
1	D	132/140 (94%)	-0.39	0 100 100	26, 36, 48, 72	0
1	E	132/140 (94%)	-0.37	1 (0%) 82 81	26, 35, 48, 68	0
1	F	133/140 (95%)	-0.37	2 (1%) 72 70	24, 35, 47, 84	2 (1%)
1	G	128/140 (91%)	0.48	7 (5%) 30 28	18, 51, 66, 78	2 (1%)
1	H	126/140 (90%)	0.60	7 (5%) 30 27	37, 51, 68, 72	1 (0%)
1	I	127/140 (90%)	0.53	10 (7%) 18 16	20, 49, 70, 78	3 (2%)
All	All	1170/1260 (92%)	-0.01	45 (3%) 44 41	18, 38, 63, 84	28 (2%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	188[A]	THR	6.2
1	B	210[A]	ASP	5.5
1	I	187[A]	GLY	4.7
1	A	210[A]	ASP	4.2
1	I	209	ALA	4.0
1	B	185	GLY	3.9
1	H	184	GLY	3.6
1	C	209[A]	ALA	3.4
1	C	187[A]	GLY	3.4
1	B	188	THR	3.4
1	G	209	ALA	3.2
1	H	128	PRO	3.1
1	I	183	ARG	3.1
1	I	213	TYR	3.1
1	G	184	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	209[B]	ALA	2.9
1	A	186[B]	ASP	2.9
1	B	211[A]	GLN	2.9
1	G	183	ARG	2.8
1	F	126	THR	2.7
1	A	204	ALA	2.7
1	G	212	ASN	2.7
1	B	127	VAL	2.7
1	B	186	ASP	2.7
1	C	210[B]	ASP	2.7
1	C	186[B]	ASP	2.6
1	F	127	VAL	2.5
1	I	128	PRO	2.5
1	G	187	GLY	2.5
1	I	242	GLY	2.5
1	A	206	ALA	2.4
1	G	128	PRO	2.4
1	I	212	ASN	2.3
1	A	208[B]	ASP	2.3
1	I	244	SER	2.3
1	H	136	LEU	2.2
1	I	241	GLY	2.2
1	B	191	TRP	2.2
1	I	211	GLN	2.2
1	H	183	ARG	2.1
1	H	209	ALA	2.1
1	G	188	THR	2.1
1	B	209[B]	ALA	2.1
1	H	244	SER	2.0
1	E	127	VAL	2.0

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.

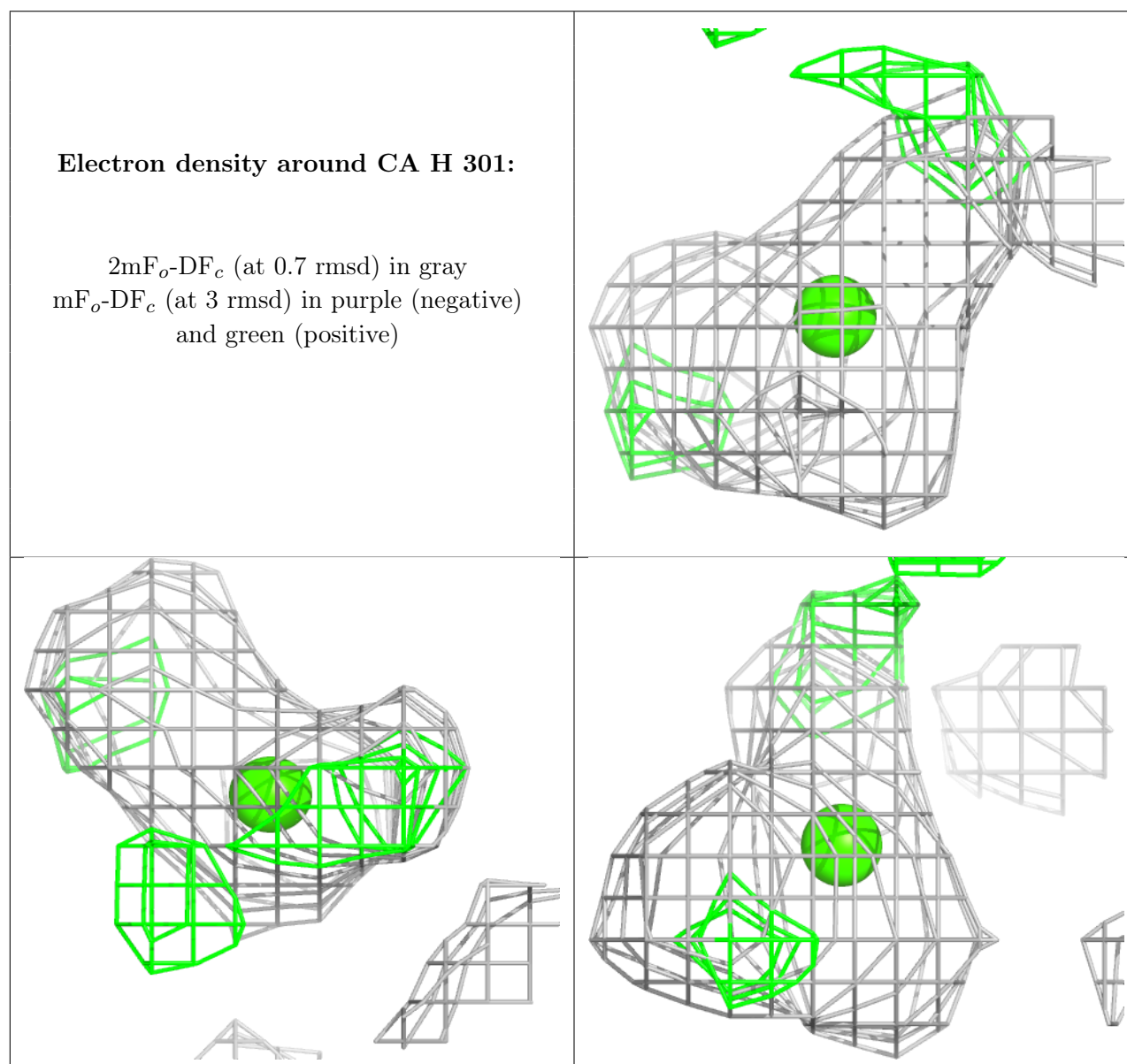
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	H	301	1/1	0.68	0.20	102,102,102,102	0
2	CA	D	504	1/1	0.72	0.16	88,88,88,88	0
4	GOL	E	404	6/6	0.77	0.14	54,56,61,65	0
3	CAC	A	406	5/5	0.79	0.26	31,40,45,65	5
2	CA	D	505	1/1	0.80	0.13	95,95,95,95	0
4	GOL	E	403	6/6	0.83	0.14	48,56,58,59	0
4	GOL	D	507	6/6	0.84	0.14	47,50,54,65	0
4	GOL	F	503	6/6	0.84	0.12	53,58,62,62	0
3	CAC	C	506	5/5	0.86	0.21	33,38,40,60	5
4	GOL	E	401	6/6	0.87	0.14	44,57,58,65	0
3	CAC	B	505	5/5	0.87	0.23	32,37,47,66	5
4	GOL	D	506	6/6	0.88	0.13	48,54,59,61	0
2	CA	B	504	1/1	0.89	0.12	88,88,88,88	0
2	CA	A	405	1/1	0.91	0.10	89,89,89,89	0
4	GOL	B	506	6/6	0.91	0.11	49,51,55,56	0
2	CA	F	501	1/1	0.92	0.11	78,78,78,78	0
2	CA	B	502	1/1	0.93	0.10	67,67,67,67	0
2	CA	C	504	1/1	0.94	0.07	77,77,77,77	0
2	CA	A	404	1/1	0.94	0.08	66,66,66,66	0
2	CA	C	501	1/1	0.94	0.06	61,61,61,61	0
2	CA	E	402	1/1	0.94	0.11	69,69,69,69	0
5	CL	F	502	1/1	0.94	0.12	58,58,58,58	0
5	CL	G	302	1/1	0.94	0.10	55,55,55,55	0
5	CL	I	302	1/1	0.94	0.13	60,60,60,60	0
4	GOL	C	507	6/6	0.95	0.09	44,50,52,52	0
2	CA	C	503	1/1	0.96	0.10	62,62,62,62	0
2	CA	B	503	1/1	0.96	0.07	57,57,57,57	0
5	CL	C	505	1/1	0.96	0.07	62,62,62,62	0
2	CA	G	301	1/1	0.98	0.10	60,60,60,60	0
2	CA	B	501	1/1	0.98	0.04	36,36,36,36	0
2	CA	I	301	1/1	0.98	0.11	62,62,62,62	0
2	CA	A	402	1/1	0.99	0.02	37,37,37,37	0
2	CA	A	401	1/1	0.99	0.03	32,32,32,32	0
2	CA	C	502	1/1	0.99	0.03	33,33,33,33	0
2	CA	D	502	1/1	1.00	0.01	33,33,33,33	0
2	CA	D	503	1/1	1.00	0.05	48,48,48,48	0
2	CA	A	403	1/1	1.00	0.02	33,33,33,33	0

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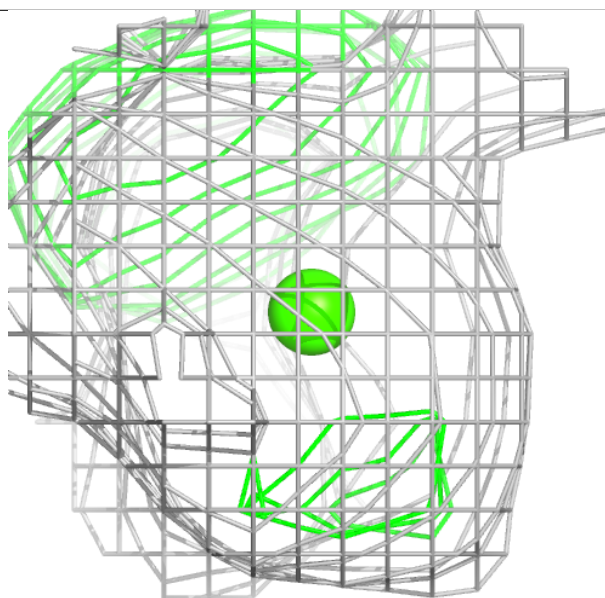
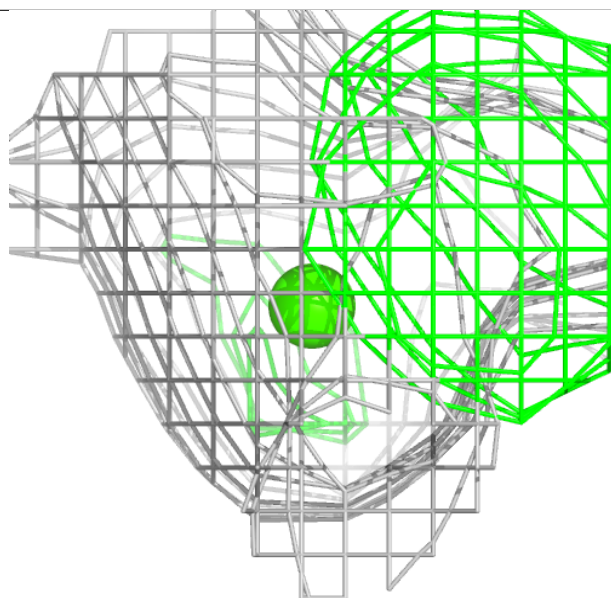
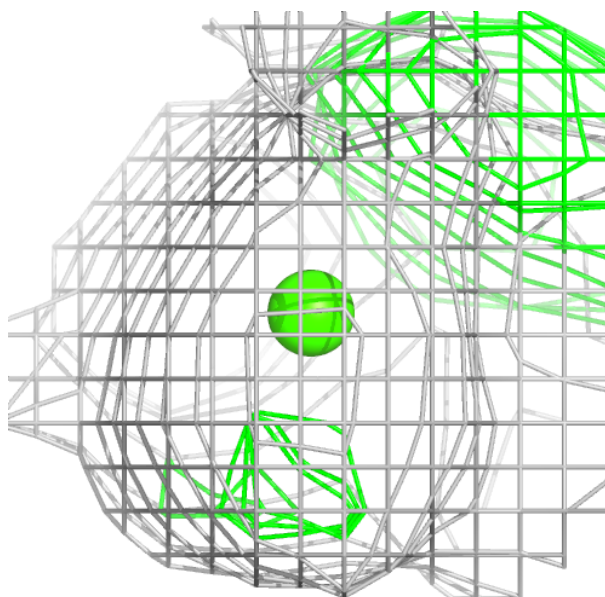
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	D	501	1/1	1.00	0.01	35,35,35,35	0

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.



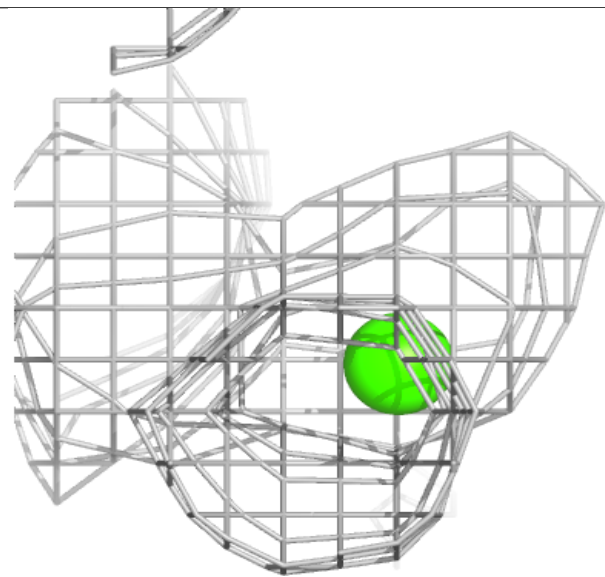
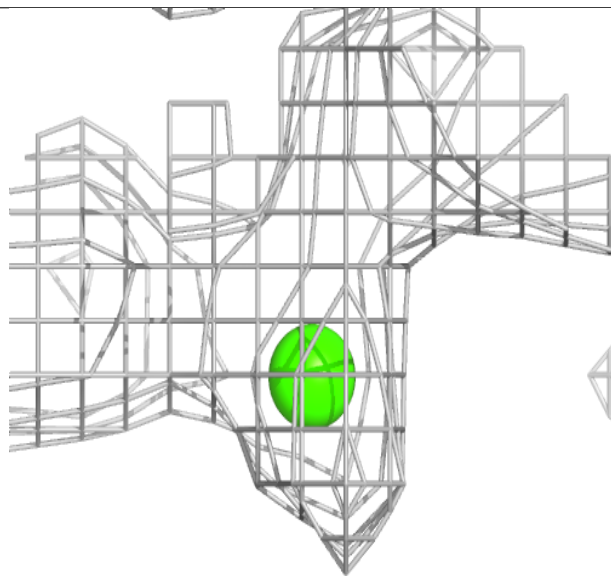
Electron density around CA D 504:

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



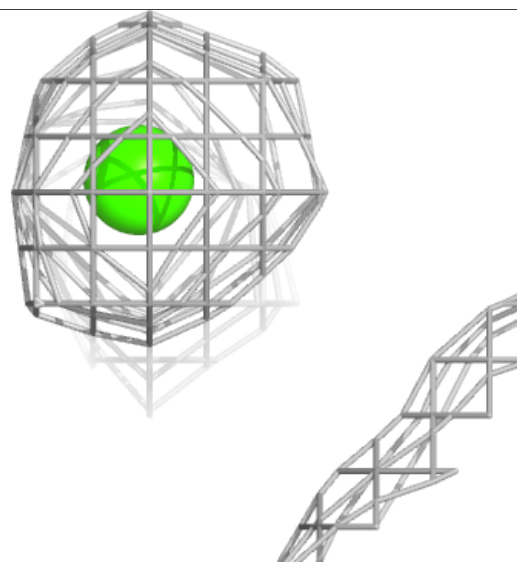
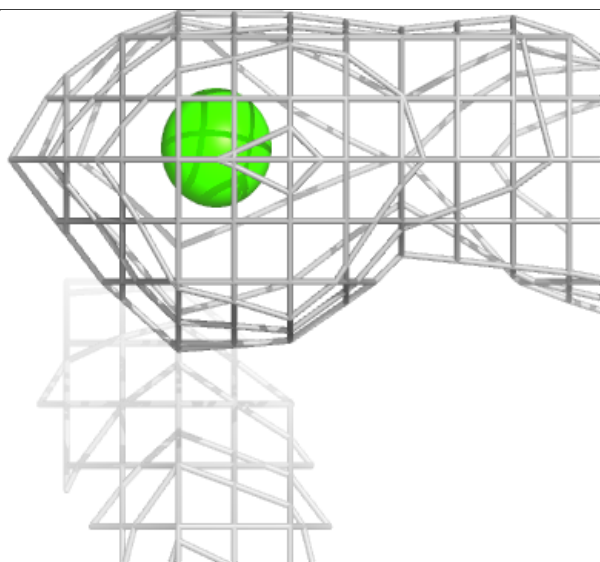
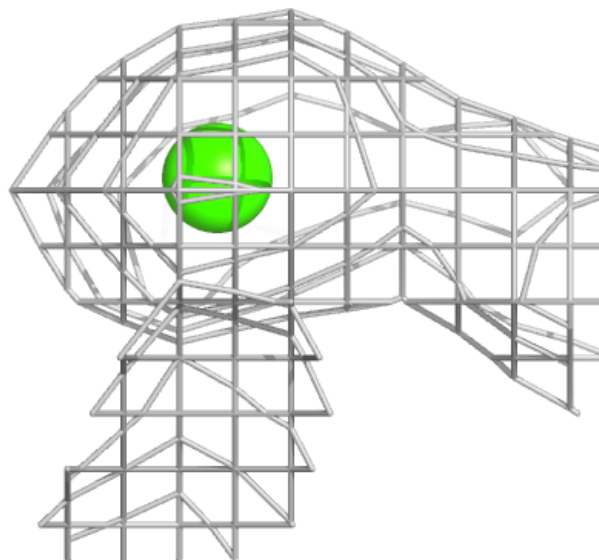
Electron density around CA D 505:

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



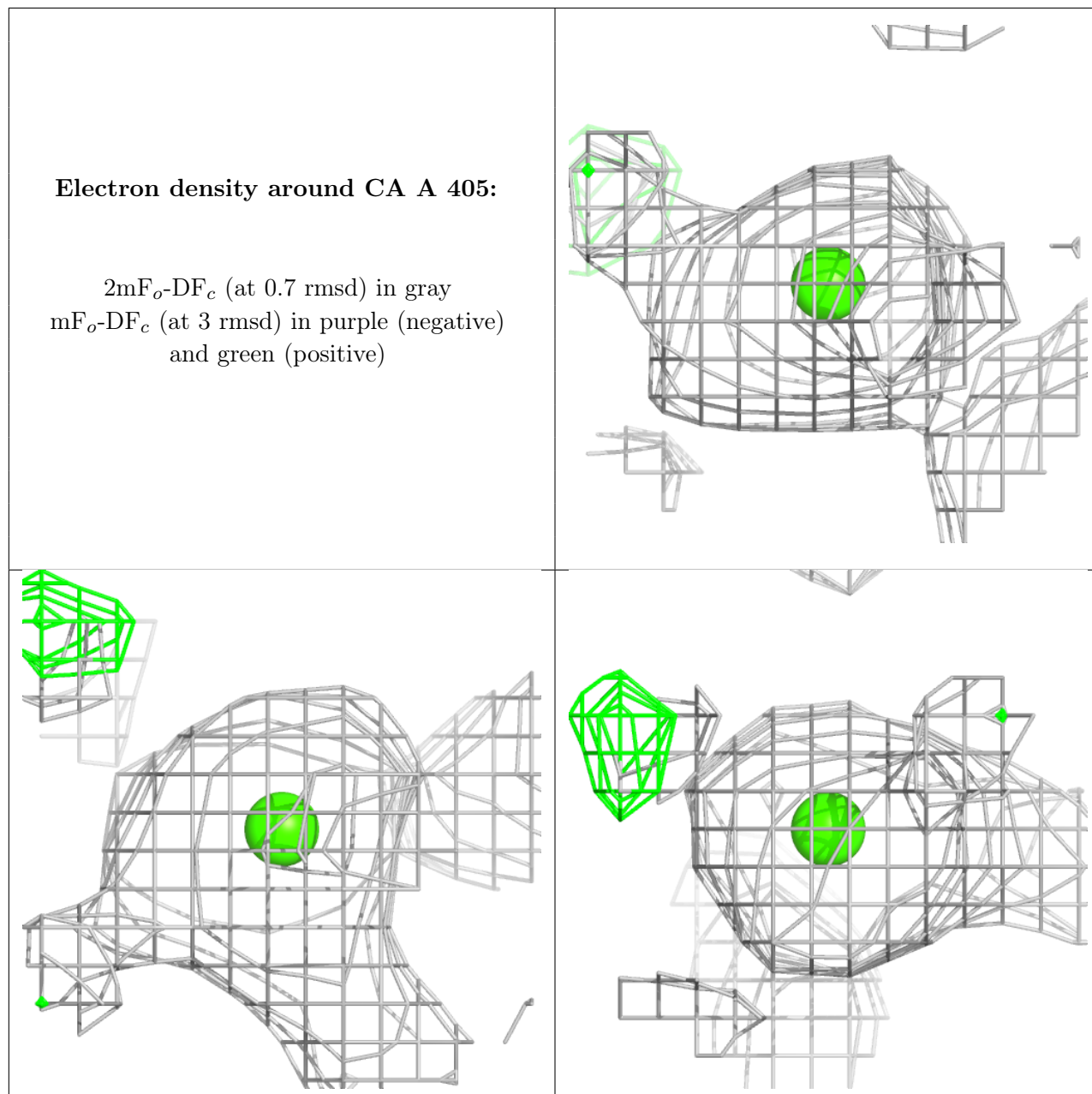
Electron density around CA B 504:

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



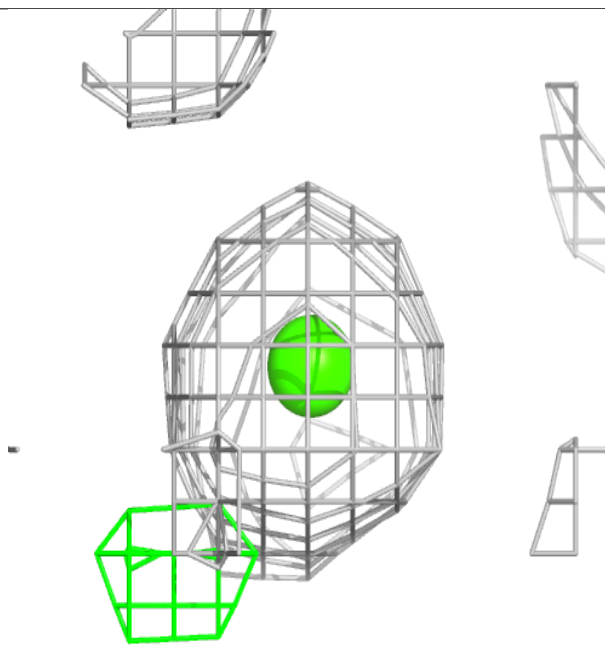
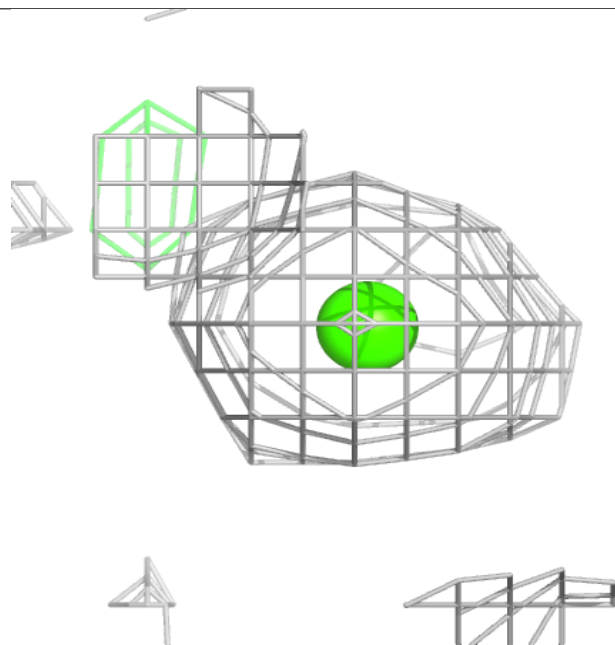
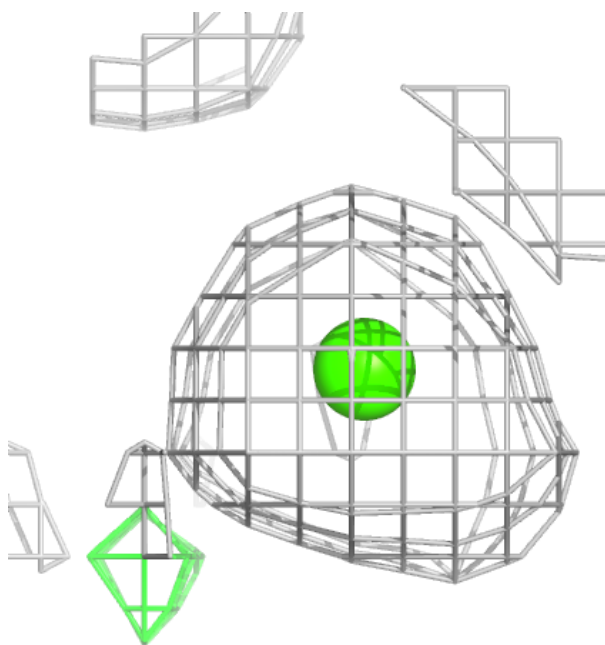
Electron density around CA A 405:

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



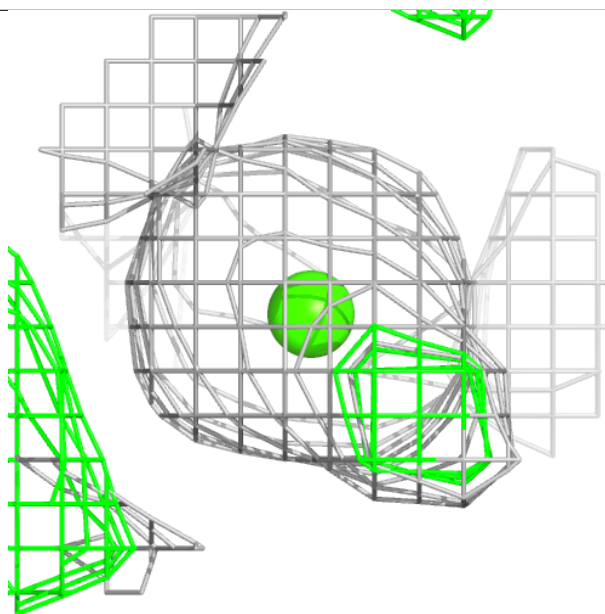
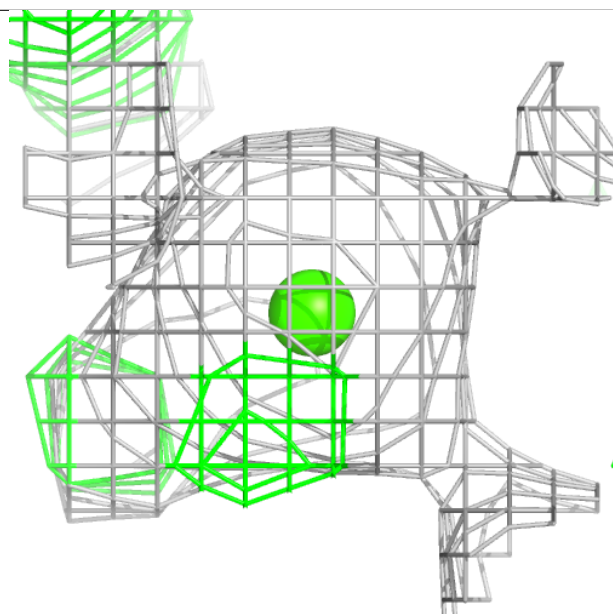
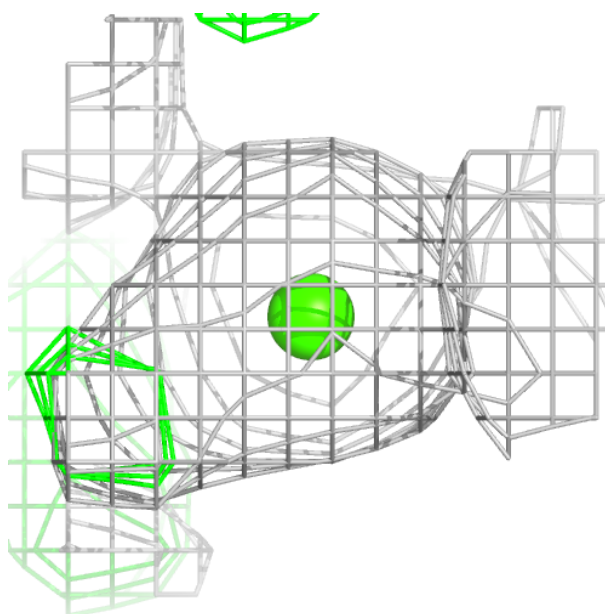
Electron density around CA F 501:

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



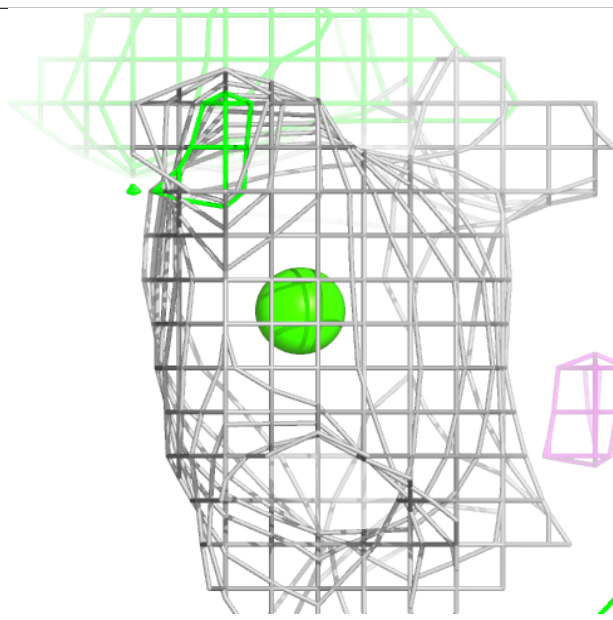
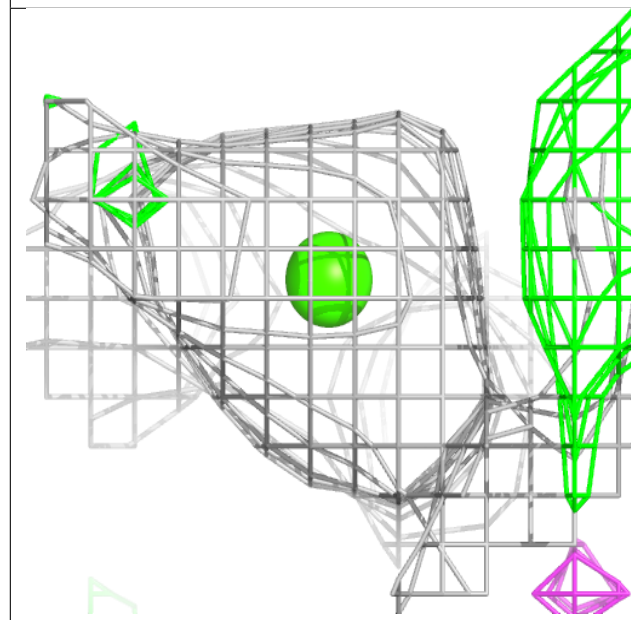
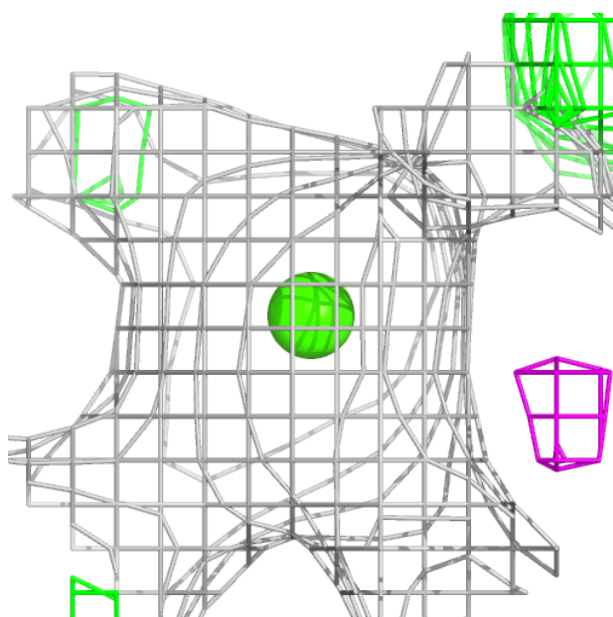
Electron density around CA B 502:

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



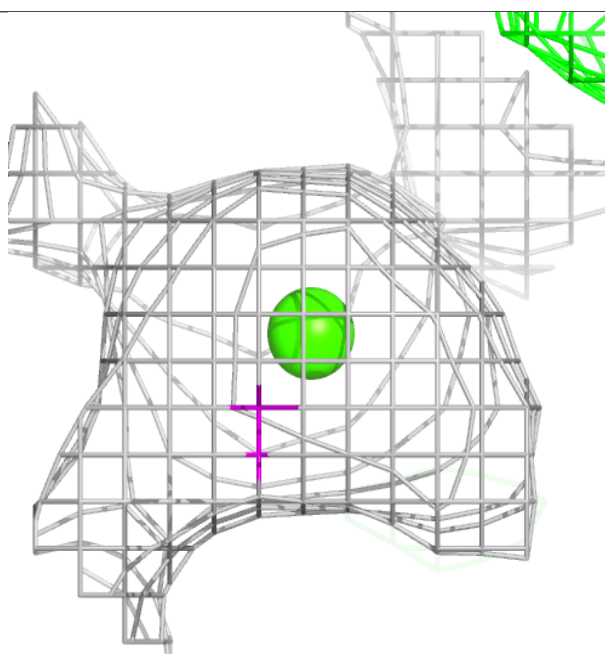
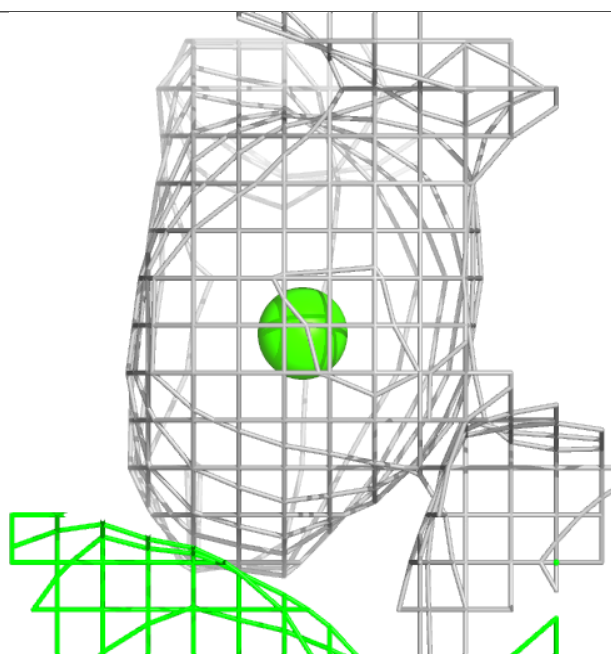
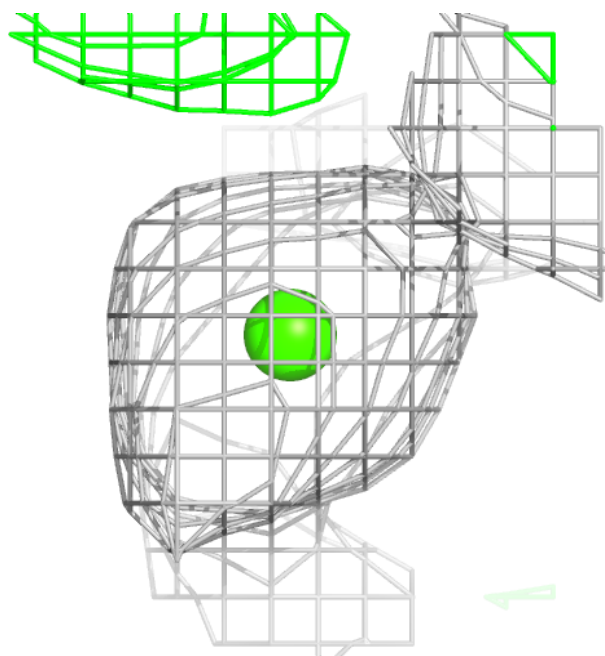
Electron density around CA C 504:

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



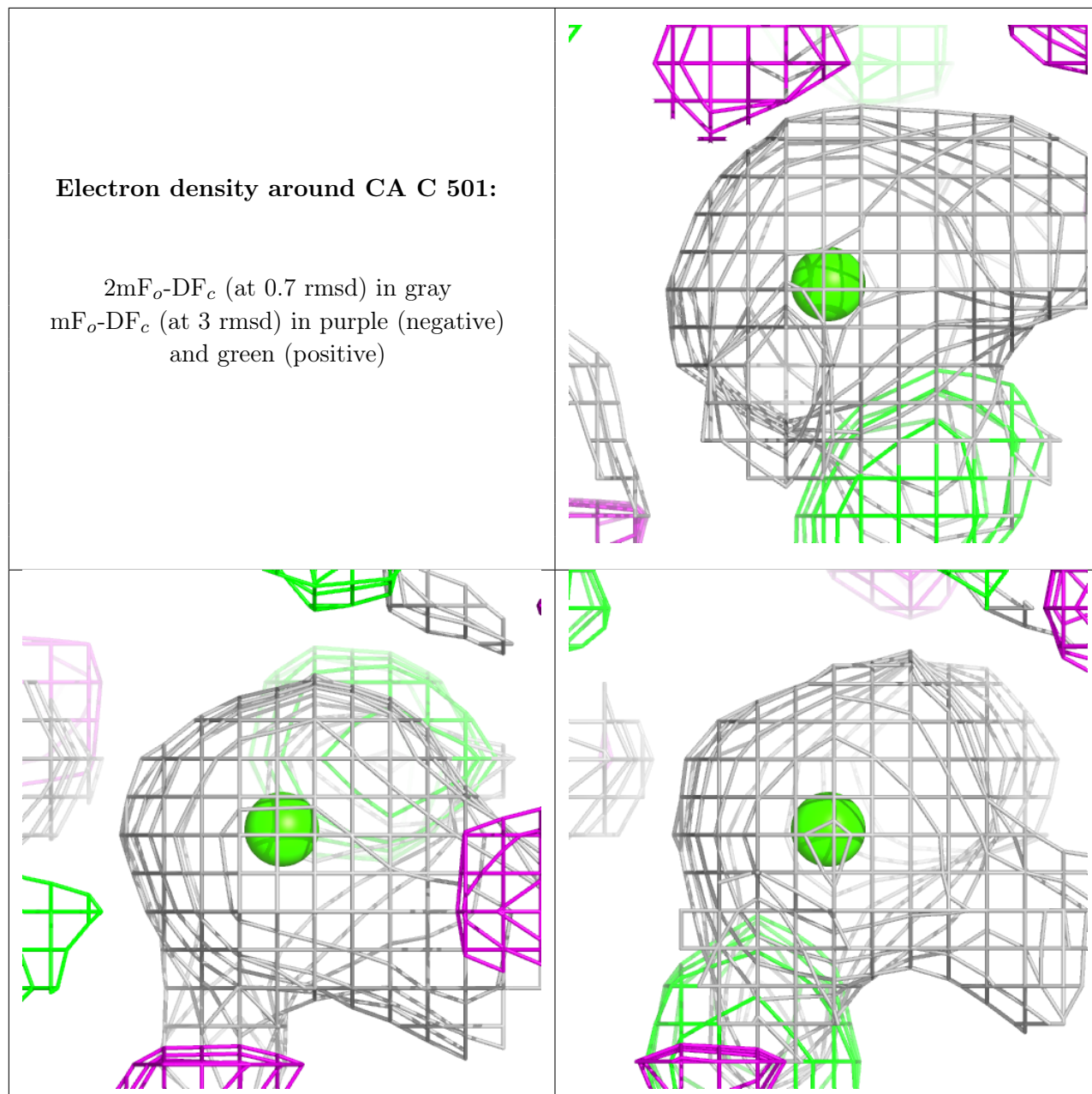
Electron density around CA A 404:

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



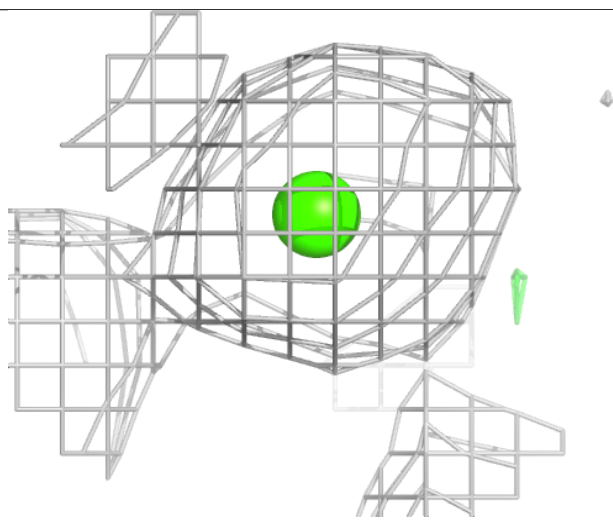
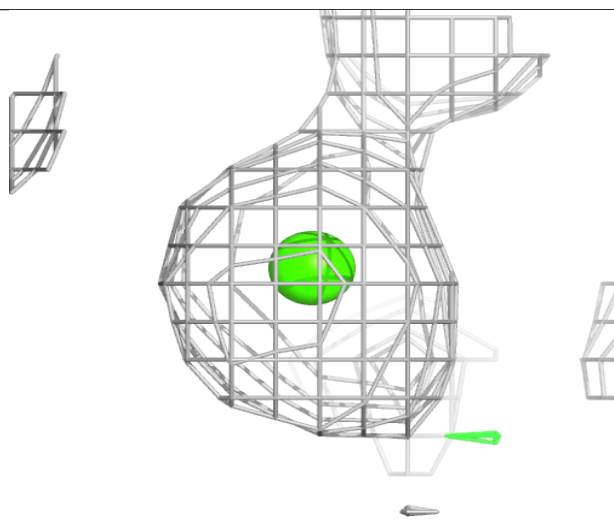
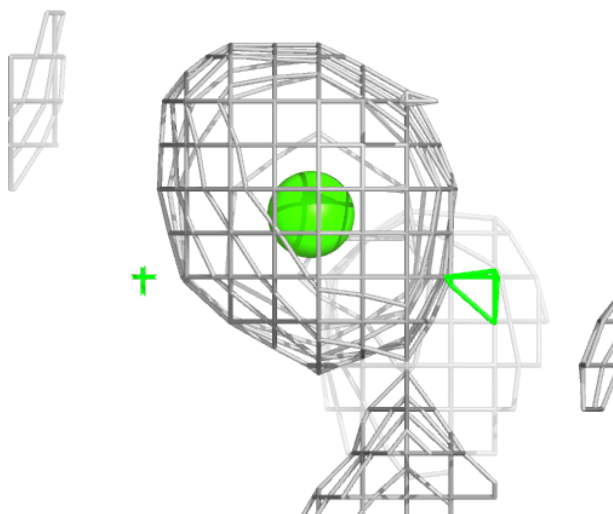
Electron density around CA C 501:

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



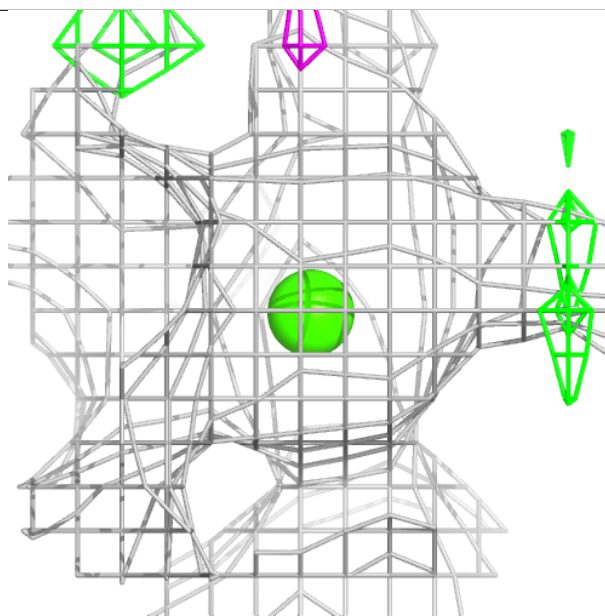
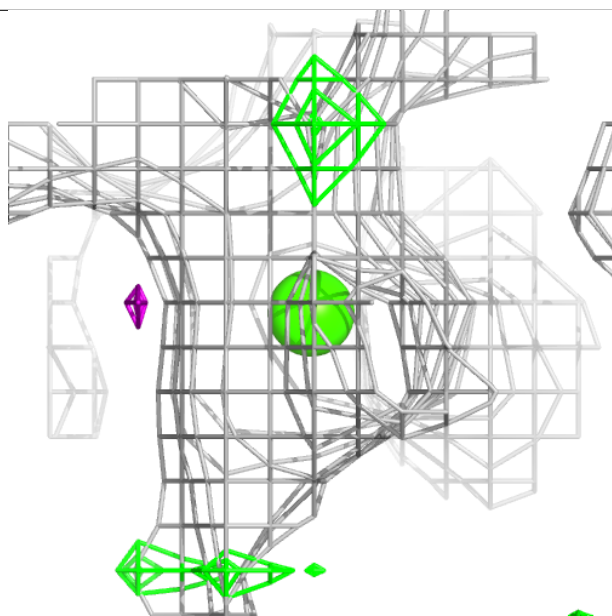
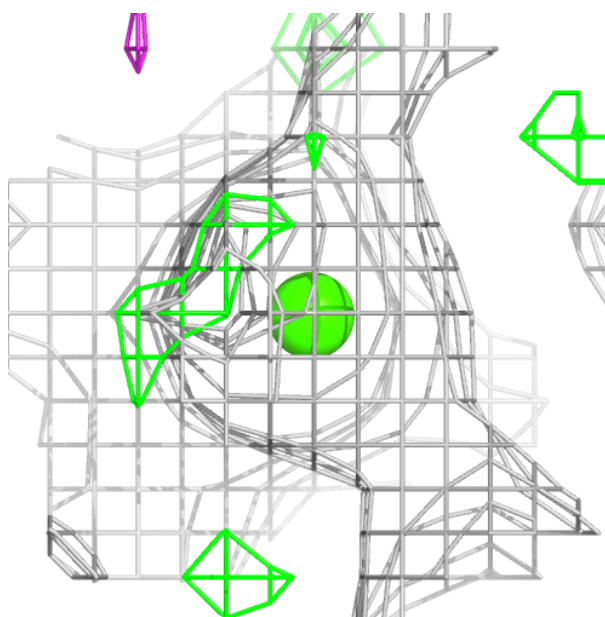
Electron density around CA E 402:

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



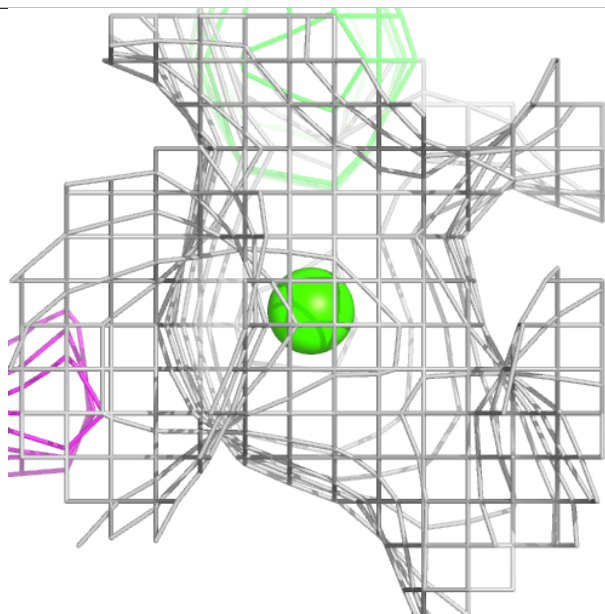
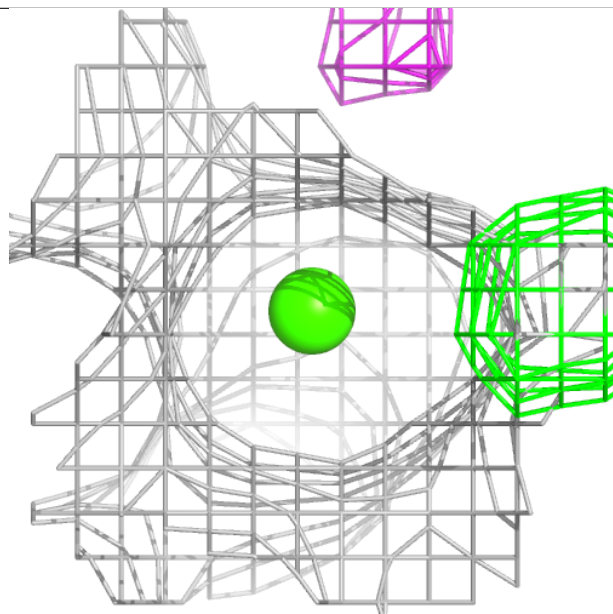
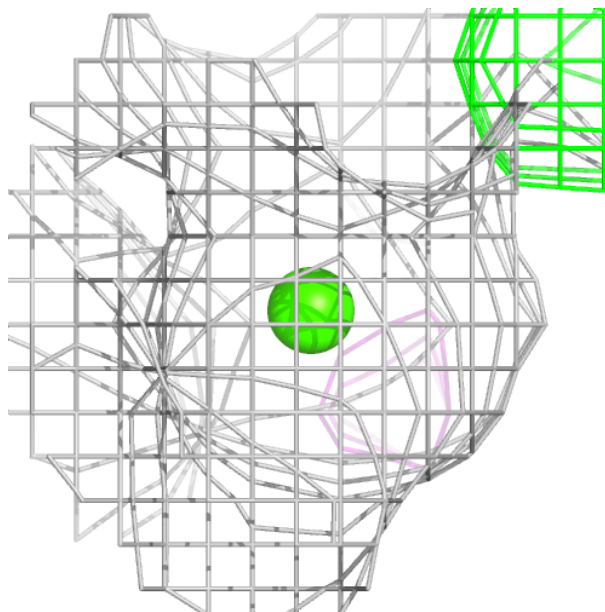
Electron density around CA C 503:

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



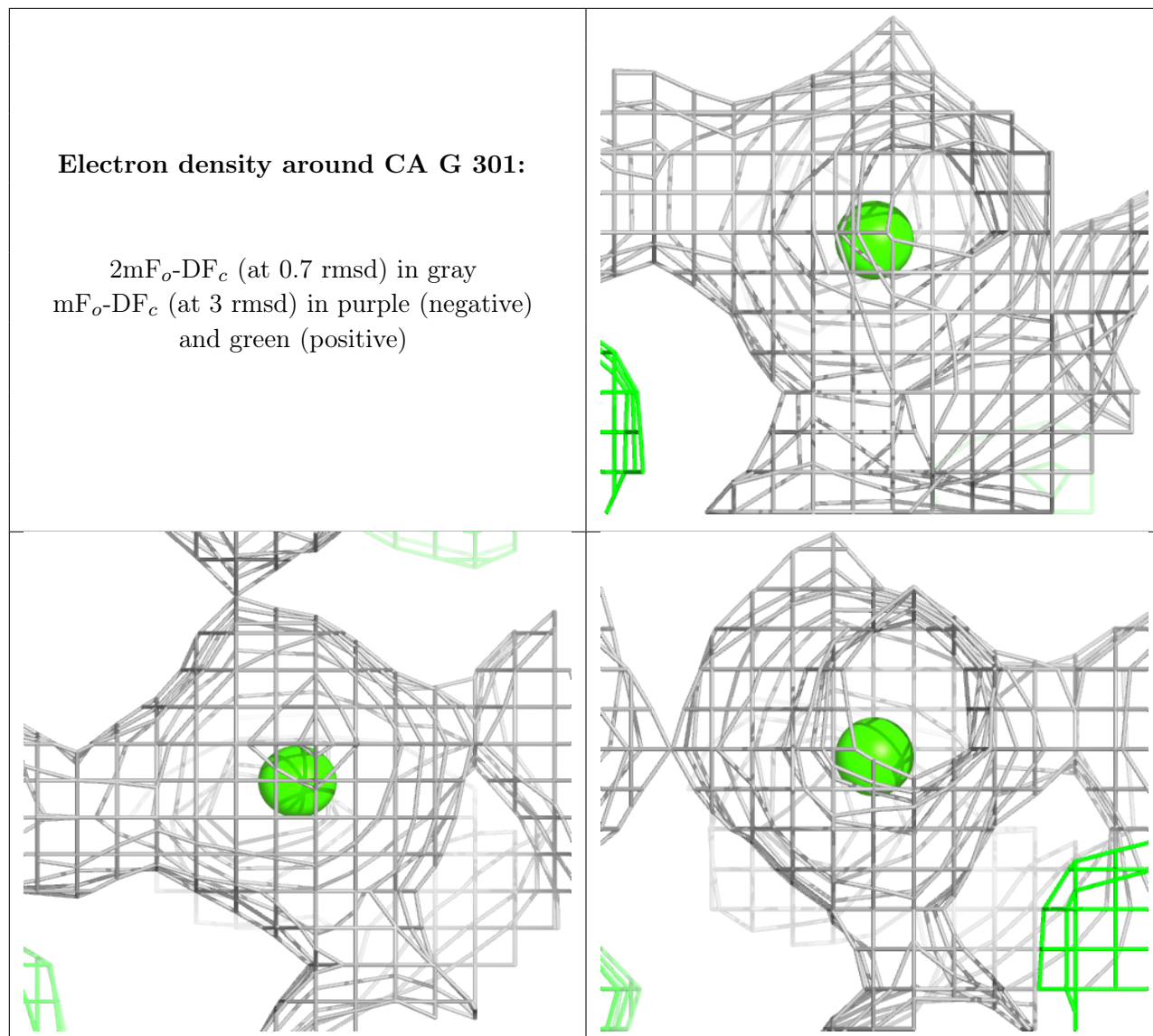
Electron density around CA B 503:

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



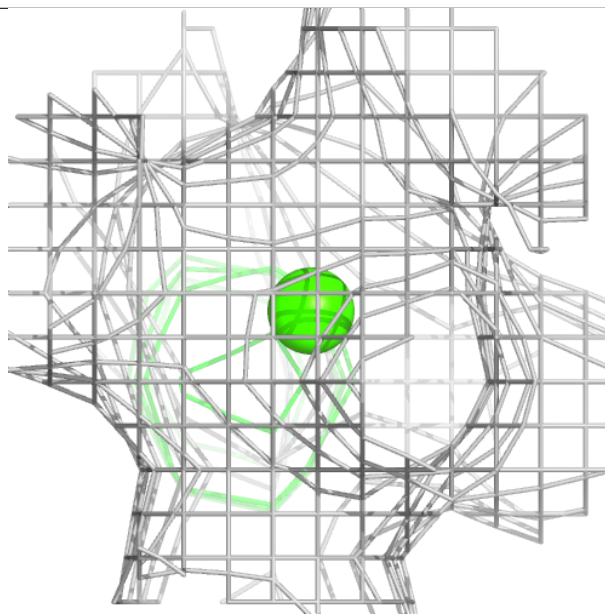
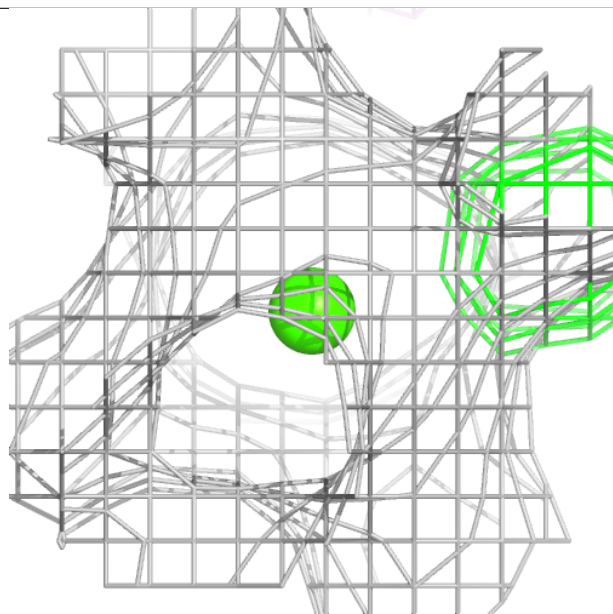
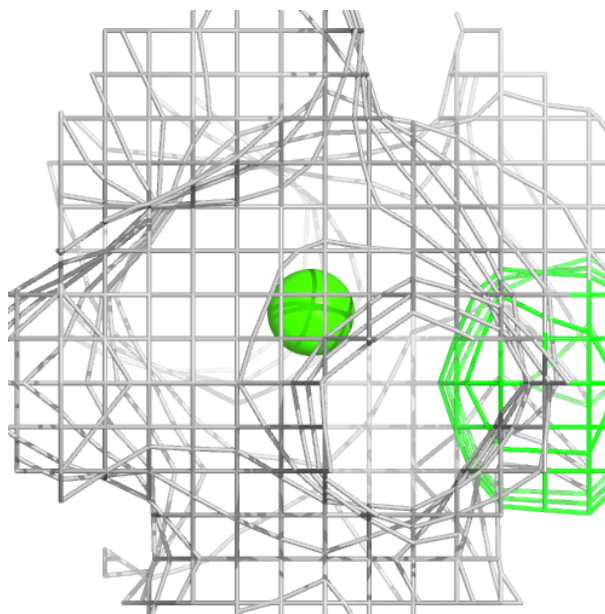
Electron density around CA G 301:

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



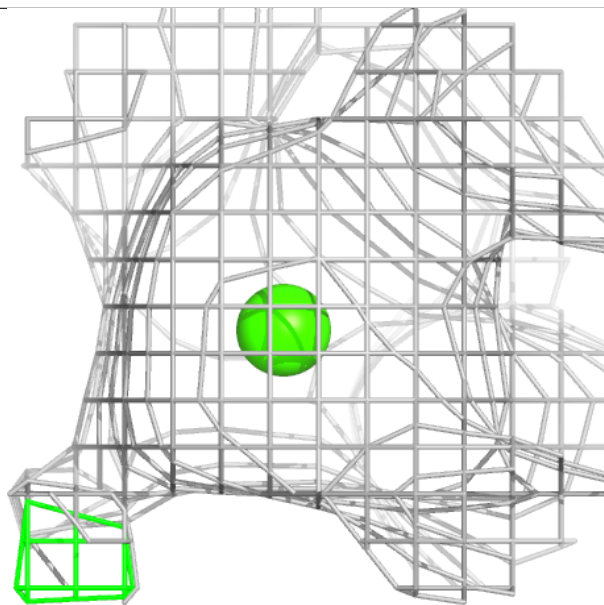
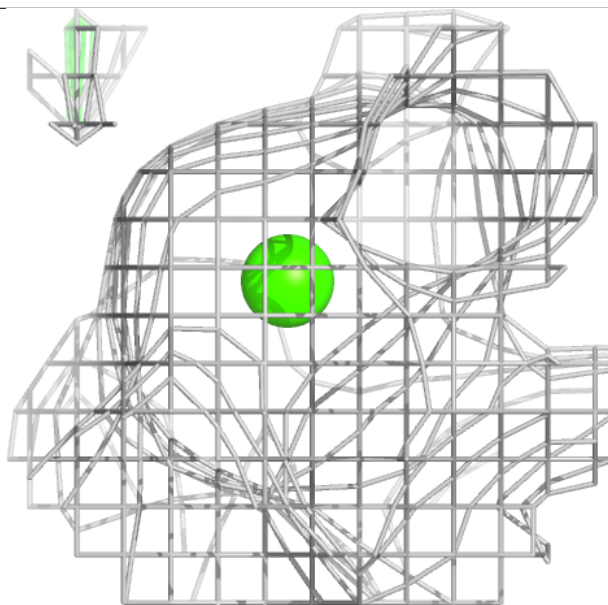
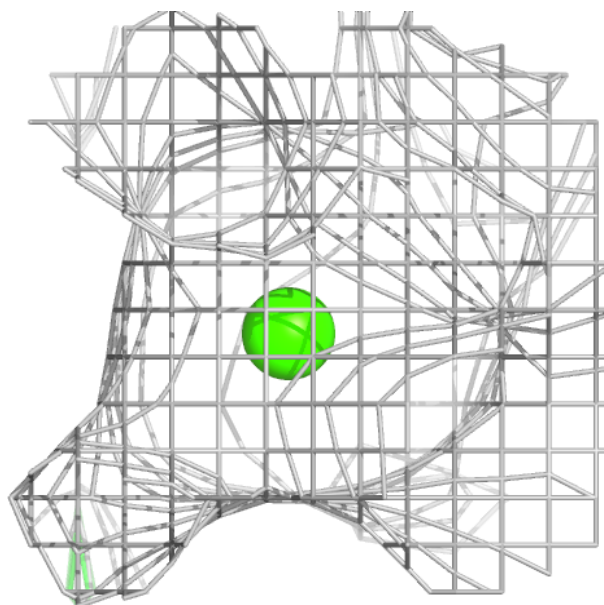
Electron density around CA B 501:

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



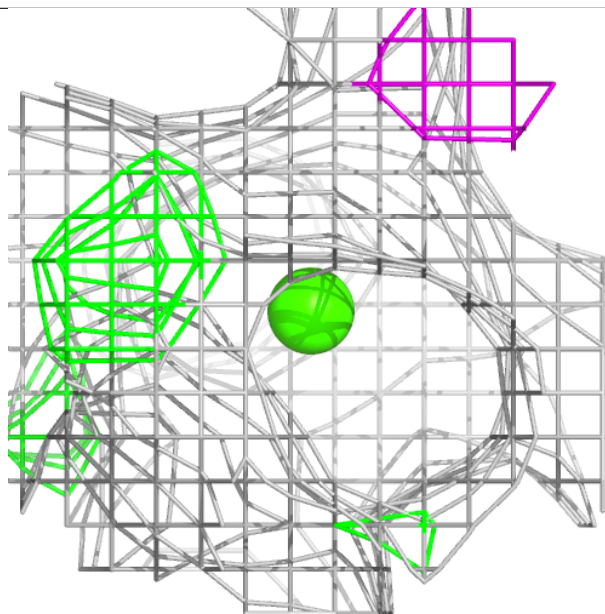
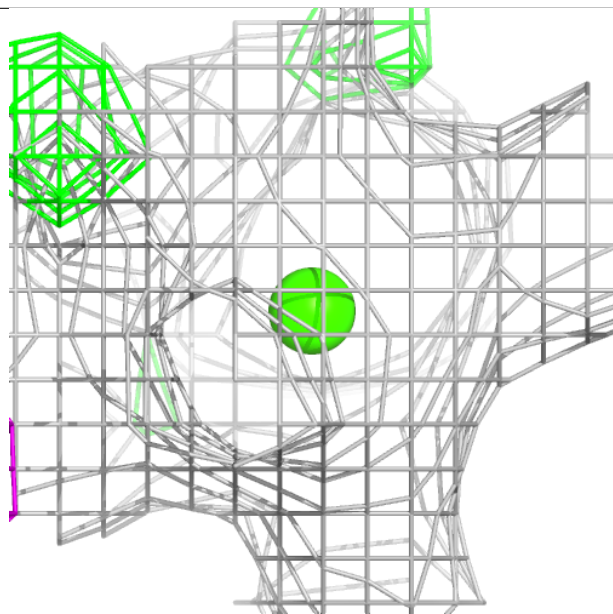
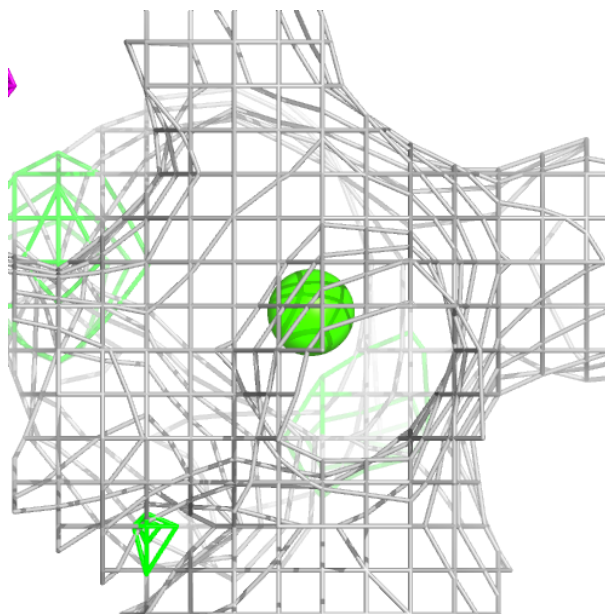
Electron density around CA I 301:

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



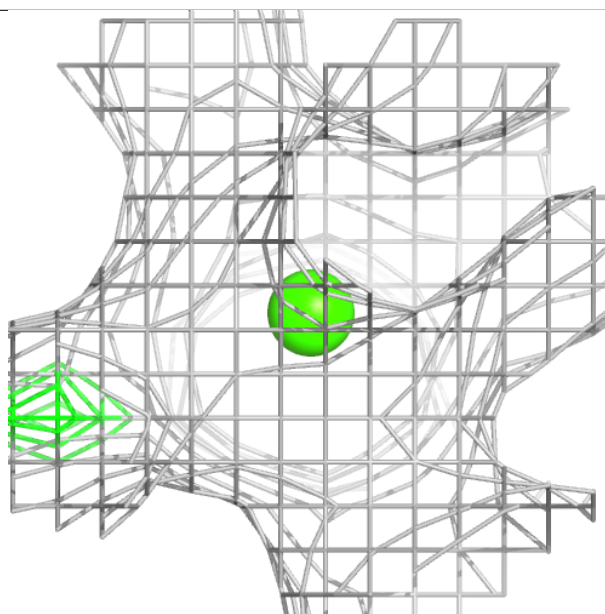
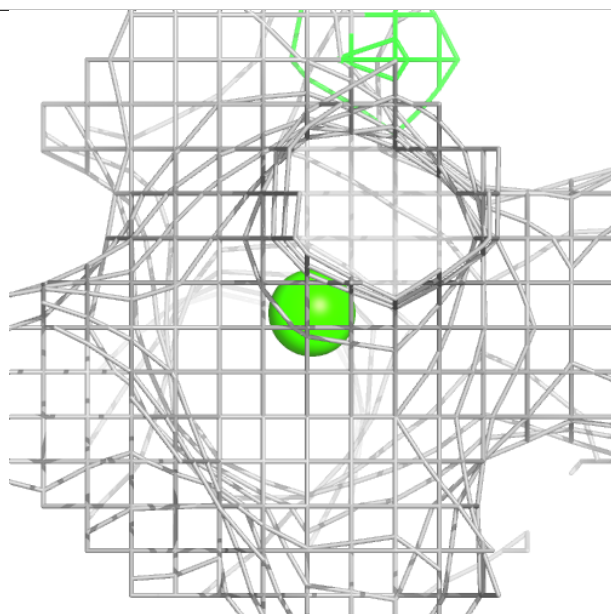
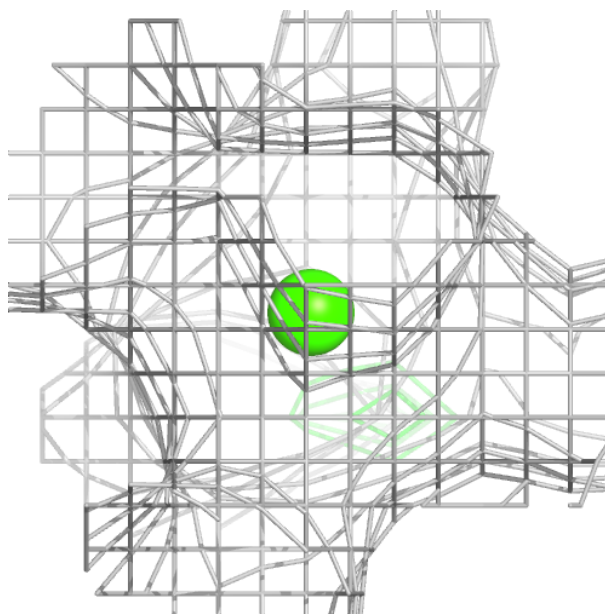
Electron density around CA A 402:

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



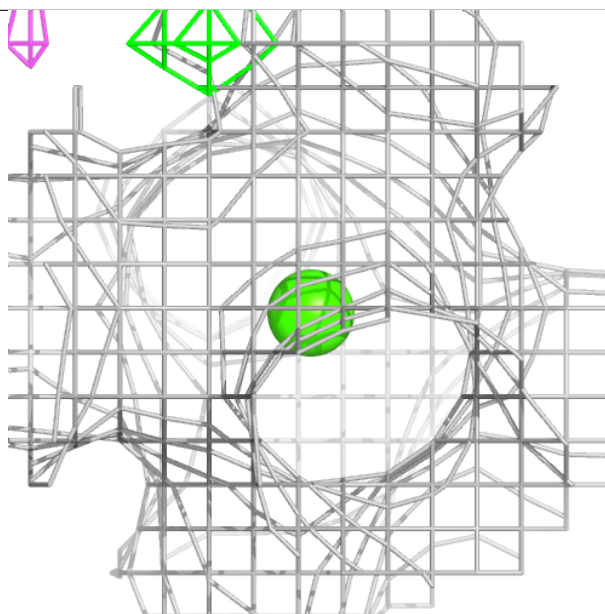
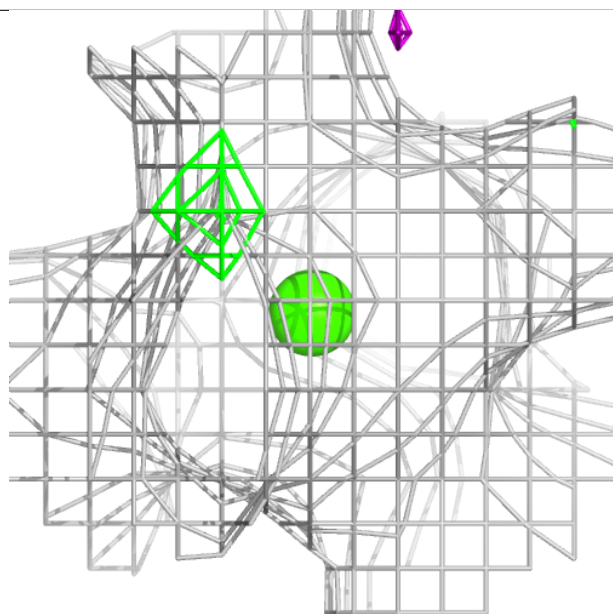
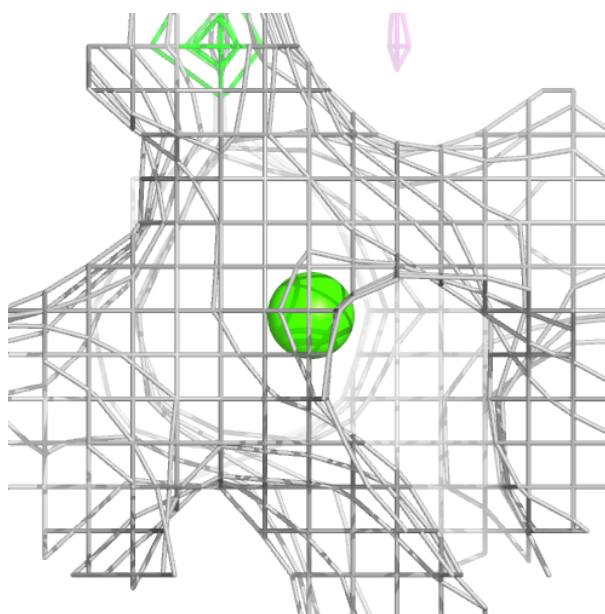
Electron density around CA A 401:

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



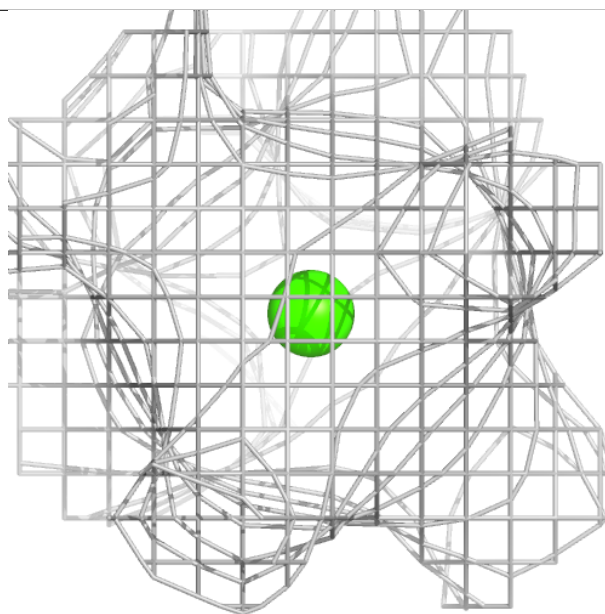
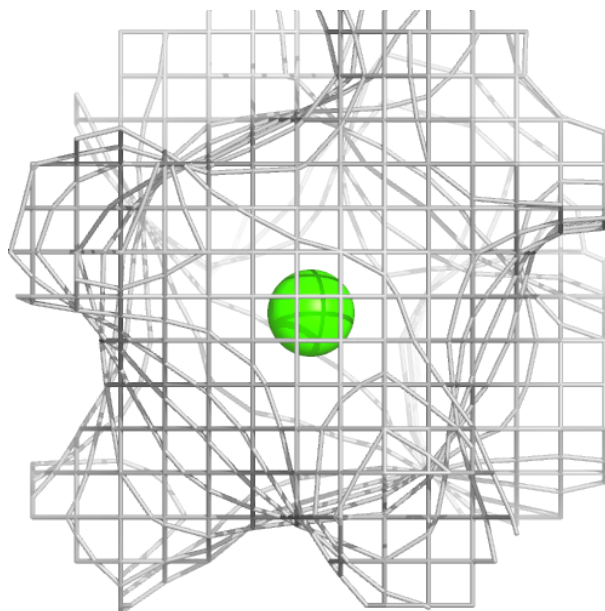
Electron density around CA C 502:

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



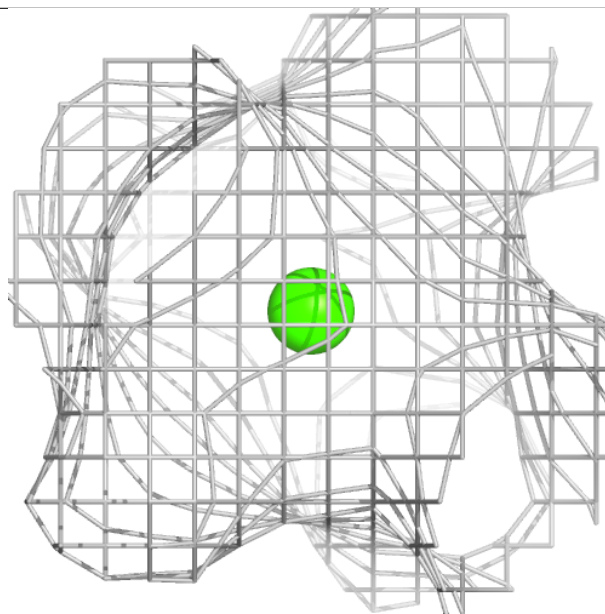
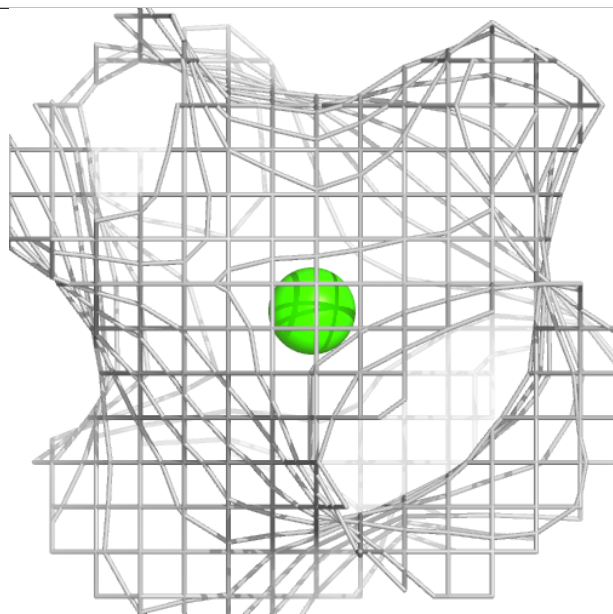
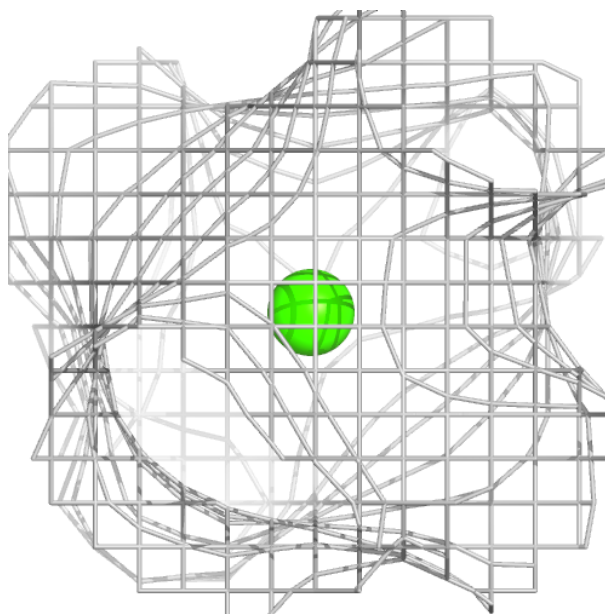
Electron density around CA D 502:

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



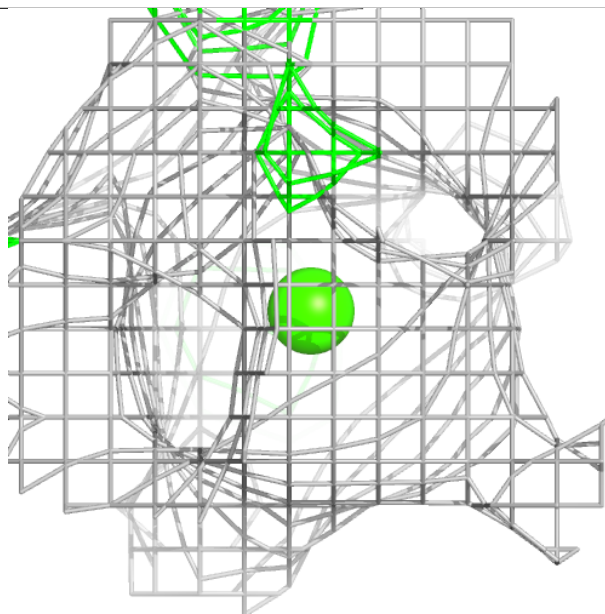
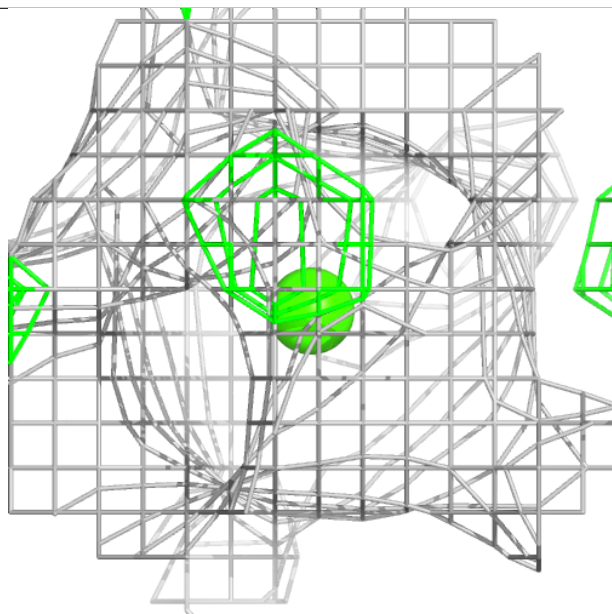
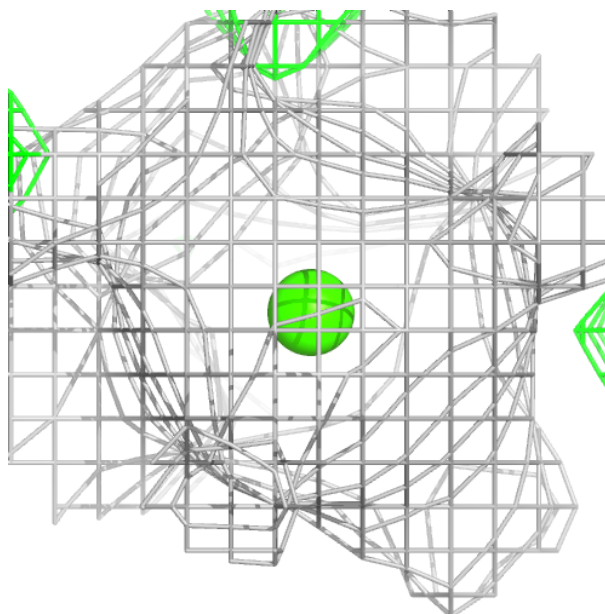
Electron density around CA D 503:

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



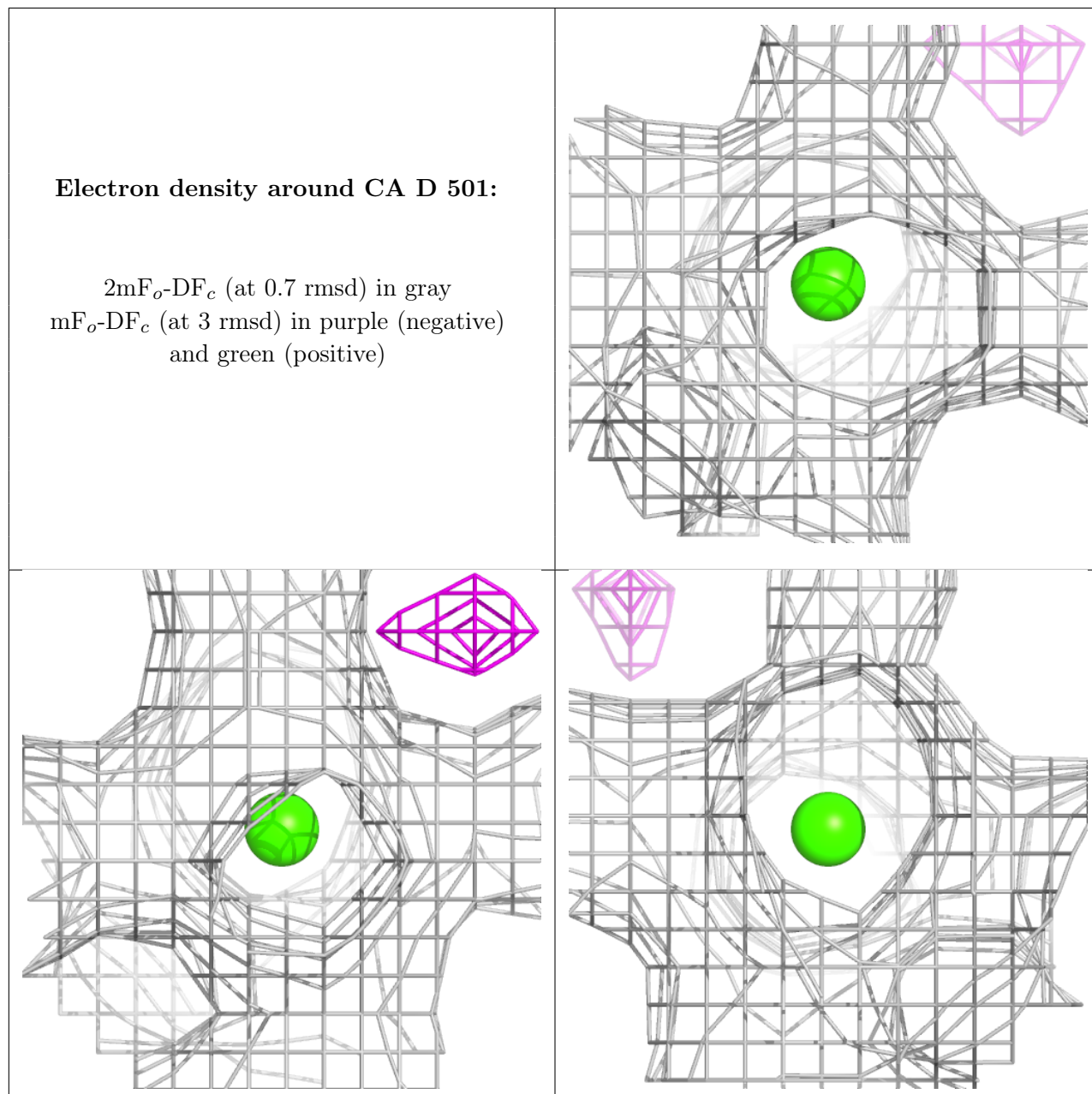
Electron density around CA A 403:

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



Electron density around CA D 501:

$2mF_o-DF_c$ (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.