



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:33 AM UTC

PDB ID : 6IM1 / pdb_00006im1
Title : Crystal structure of a highly thermostable carbonic anhydrase from *Persephonella marina* EX-H1
Authors : Jin, M.S.; Kim, S.; Sung, J.; Yeon, J.; Choi, S.H.
Deposited on : 2018-10-21
Resolution : 2.00 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:

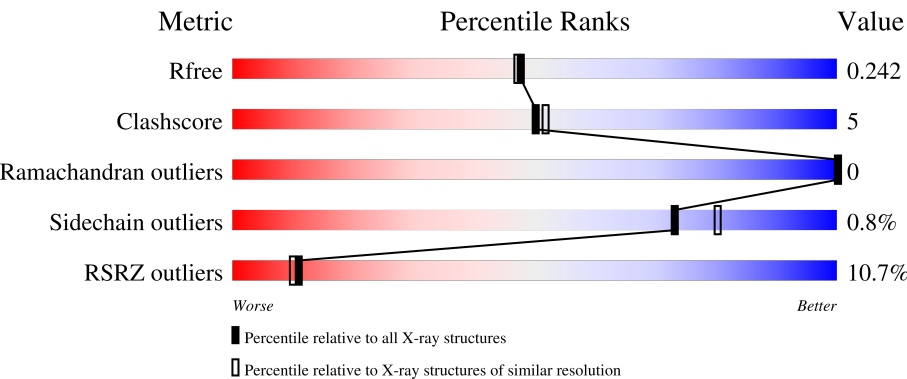
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	243	2% 78% 13% 9%
1	B	243	4% 81% 9% 9%
1	C	243	17% 79% 11% 9%
1	D	243	19% 83% 7% 9%
1	E	243	7% 75% 16% 9%

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Mol	Chain	Length	Quality of chain
1	F	243	10% 79% 12% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11390 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 Carbonic anhydrase (Carbonate dehydratase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1803	1152	315	326	10			
1	B	222	Total	C	N	O	S	0	0	0
			1803	1152	315	326	10			
1	C	222	Total	C	N	O	S	0	0	0
			1803	1152	315	326	10			
1	D	222	Total	C	N	O	S	0	0	0
			1803	1152	315	326	10			
1	E	222	Total	C	N	O	S	0	0	0
			1803	1152	315	326	10			
1	F	222	Total	C	N	O	S	0	0	0
			1802	1152	315	325	10			

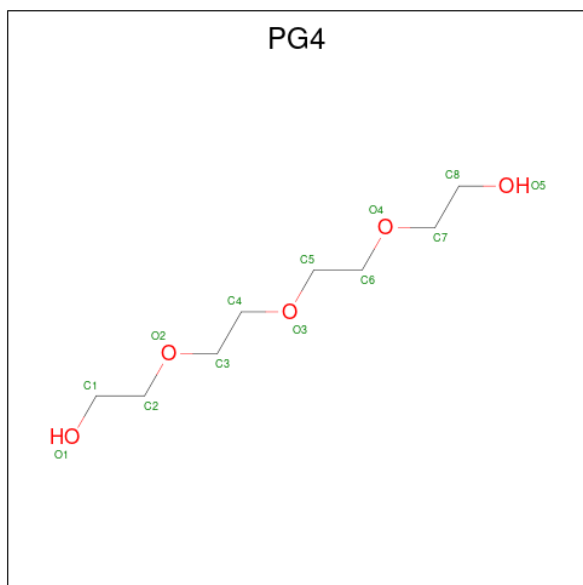
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- 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 6 6	0	0
3	B	6	Total Ca 6 6	0	0
3	D	3	Total Ca 3 3	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	E	1	Total C O 13 8 5	0	0
4	F	1	Total C O 13 8 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	141	Total O 141 141	0	0
5	B	126	Total O 126 126	0	0

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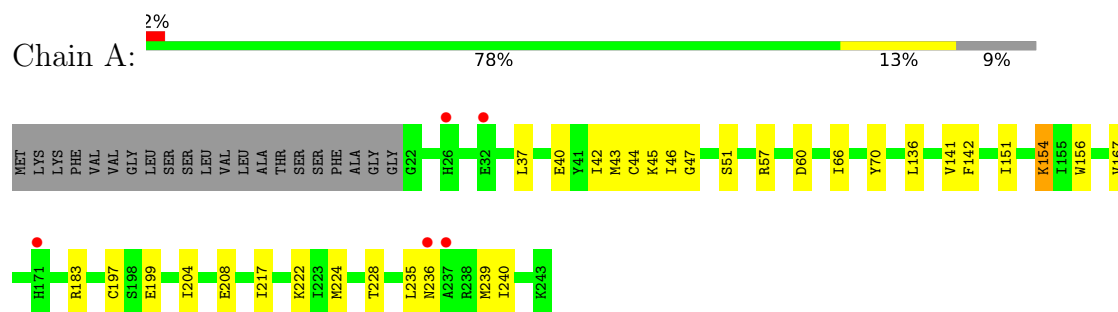
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	53	Total 53	O 53	0	0
5	D	54	Total 54	O 54	0	0
5	E	61	Total 61	O 61	0	0
5	F	65	Total 65	O 65	0	0

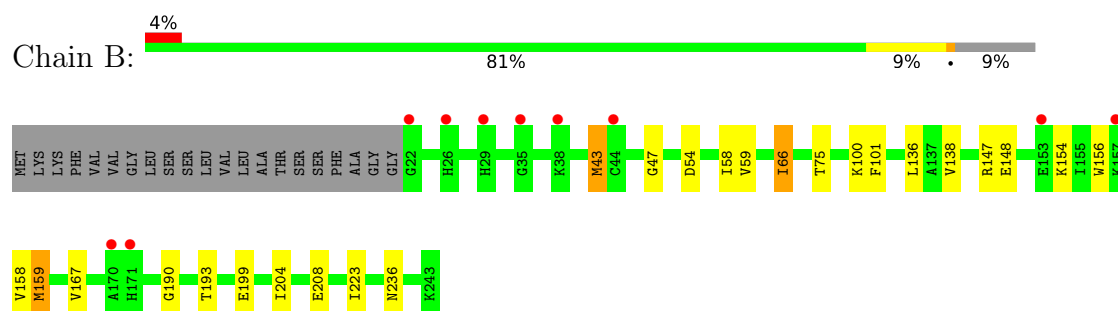
3 Residue-property plots [i](#)

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.

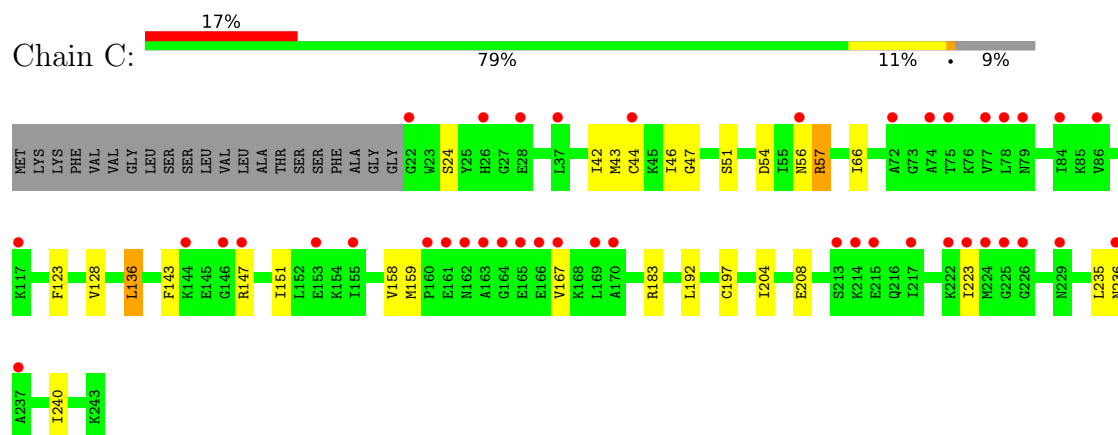
- Molecule 1: Carbonic anhydrase (Carbonate dehydratase)



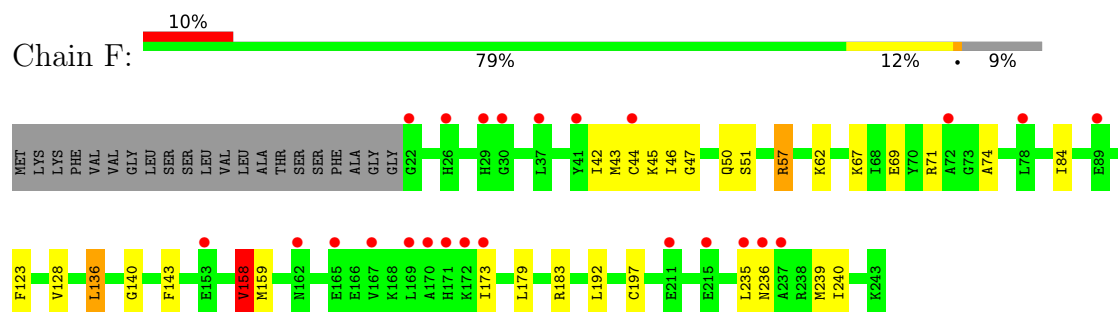
- Molecule 1: Carbonic anhydrase (Carbonate dehydratase)



- Molecule 1: Carbonic anhydrase (Carbonate dehydratase)



- Molecule 1: Carbonic anhydrase (Carbonate dehydratase)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.92Å 120.07Å 124.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.07 – 2.00 124.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (124.07-2.00) 99.5 (124.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.204 , 0.236 0.214 , 0.242	Depositor DCC
R_{free} test set	5670 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h 0.000 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11390	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7186e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PG4, ZN

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	1.50	7/1852 (0.4%)	1.16	7/2494 (0.3%)
1	B	1.45	10/1852 (0.5%)	1.10	5/2494 (0.2%)
1	C	1.25	2/1852 (0.1%)	1.08	9/2494 (0.4%)
1	D	1.22	4/1852 (0.2%)	1.05	5/2494 (0.2%)
1	E	1.32	1/1852 (0.1%)	1.07	8/2494 (0.3%)
1	F	1.33	4/1851 (0.2%)	1.08	10/2492 (0.4%)
All	All	1.35	28/11111 (0.3%)	1.09	44/14962 (0.3%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	57	ARG	C-N	8.16	1.45	1.33
1	D	55	ILE	C-N	-7.06	1.23	1.33
1	C	56	ASN	C-N	-6.74	1.23	1.33
1	A	70	TYR	C-N	-6.57	1.24	1.33
1	B	236	ASN	C-O	-6.36	1.18	1.24
1	F	140	GLY	CA-C	6.23	1.56	1.52
1	A	156	TRP	C-O	-6.06	1.17	1.24
1	A	217	ILE	C-O	-5.84	1.17	1.24
1	A	47	GLY	C-O	-5.78	1.17	1.23
1	B	156	TRP	CA-C	5.76	1.60	1.52
1	C	57	ARG	C-N	-5.76	1.25	1.33
1	A	142	PHE	CA-C	5.68	1.60	1.52
1	D	203	TRP	N-CA	5.38	1.52	1.46
1	B	59	VAL	C-O	-5.32	1.18	1.24
1	F	51	SER	C-O	-5.22	1.18	1.24
1	B	147	ARG	N-CA	-5.17	1.39	1.45
1	B	138	VAL	C-O	-5.14	1.18	1.24
1	B	101	PHE	N-CA	5.13	1.52	1.46
1	B	190	GLY	N-CA	-5.12	1.41	1.46
1	D	143	PHE	N-CA	5.07	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	ASN	C-O	-5.07	1.20	1.24
1	E	239	MET	N-CA	5.06	1.52	1.45
1	F	128	VAL	C-O	-5.05	1.18	1.24
1	B	66	ILE	C-O	-5.05	1.18	1.24
1	A	154	LYS	C-O	-5.04	1.18	1.24
1	B	43	MET	SD-CE	-5.03	1.67	1.79
1	A	141	VAL	N-CA	5.02	1.52	1.46
1	B	159	MET	SD-CE	-5.01	1.67	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	37	LEU	N-CA-C	9.56	121.70	111.28
1	F	183	ARG	N-CA-C	9.36	124.00	112.59
1	C	46	ILE	N-CA-C	7.67	120.42	112.83
1	C	51	SER	C-N-CD	6.93	135.85	120.60
1	A	51	SER	C-N-CD	6.91	135.81	120.60
1	A	37	LEU	N-CA-C	6.90	118.88	111.36
1	C	42	ILE	N-CA-C	6.66	117.41	110.62
1	F	46	ILE	N-CA-C	6.61	120.64	113.43
1	A	45	LYS	N-CA-C	6.54	118.20	111.14
1	F	71	ARG	N-CA-C	-6.53	99.40	109.52
1	D	46	ILE	N-CA-C	6.24	119.00	112.83
1	C	136	LEU	N-CA-C	6.13	120.04	110.17
1	C	128	VAL	N-CA-C	6.03	116.99	108.36
1	E	46	ILE	N-CA-C	6.03	118.95	113.10
1	E	45	LYS	N-CA-C	6.00	117.89	111.36
1	A	46	ILE	N-CA-C	5.93	118.59	112.90
1	B	136	LEU	N-CA-C	5.87	119.28	109.95
1	D	136	LEU	N-CA-C	5.87	119.28	109.95
1	F	158	VAL	N-CA-CB	-5.76	104.68	112.16
1	F	136	LEU	N-CA-C	5.70	119.11	109.76
1	B	58	ILE	N-CA-C	5.59	116.54	108.48
1	F	50	GLN	N-CA-C	5.59	118.09	110.55
1	A	42	ILE	N-CA-C	5.58	118.02	111.05
1	F	42	ILE	N-CA-C	5.57	116.30	110.62
1	A	136	LEU	N-CA-C	5.51	118.46	109.59
1	C	54	ASP	N-CA-C	-5.45	100.30	108.96
1	D	45	LYS	N-CA-C	5.42	118.01	111.40
1	E	136	LEU	N-CA-C	5.42	118.64	109.76
1	D	147	ARG	CB-CA-C	-5.30	100.59	109.65
1	E	211	GLU	N-CA-C	5.18	117.90	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	138	VAL	N-CA-C	5.17	115.34	108.11
1	E	147	ARG	CB-CG-CD	-5.15	99.44	111.30
1	B	148	GLU	CB-CA-C	-5.15	102.12	109.84
1	B	54	ASP	N-CA-C	-5.15	100.78	108.96
1	E	183	ARG	CA-CB-CG	-5.15	103.81	114.10
1	C	183	ARG	CA-CB-CG	-5.13	103.83	114.10
1	C	56	ASN	N-CA-C	5.13	120.67	113.02
1	A	183	ARG	CA-CB-CG	-5.12	103.86	114.10
1	F	179	LEU	CA-C-N	-5.11	114.69	119.85
1	F	179	LEU	C-N-CA	-5.11	114.69	119.85
1	F	45	LYS	N-CA-C	5.08	116.63	111.14
1	C	183	ARG	N-CA-C	5.06	118.94	112.26
1	B	75	THR	N-CA-C	5.03	119.89	113.55
1	D	158	VAL	N-CA-CB	-5.02	105.64	112.16

There are no chirality outliers.

There are no planarity outliers.

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	1803	0	1777	14	0
1	B	1803	0	1777	18	0
1	C	1803	0	1777	24	0
1	D	1803	0	1777	11	0
1	E	1803	0	1777	29	0
1	F	1802	0	1777	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	13	0	18	0	0
4	B	13	0	18	0	0
4	E	13	0	18	0	0
4	F	13	0	18	0	0
5	A	141	0	0	4	0
5	B	126	0	0	4	0
5	C	53	0	0	1	0
5	D	54	0	0	0	0
5	E	61	0	0	4	0
5	F	65	0	0	0	0
All	All	11390	0	10734	112	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 5.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:MET:HE2	1:E:223:ILE:HD12	1.22	1.17
1:E:159:MET:HE2	1:E:223:ILE:CD1	1.74	1.16
1:C:159:MET:HE2	1:C:223:ILE:HD12	1.22	1.10
1:C:159:MET:CE	1:C:223:ILE:HD12	1.82	1.08
1:E:159:MET:CE	1:E:223:ILE:HD12	1.84	1.06
1:C:159:MET:HE2	1:C:223:ILE:CD1	1.87	1.05
1:B:159:MET:HE2	1:B:223:ILE:CD1	1.98	0.93
1:B:159:MET:HE2	1:B:223:ILE:HD12	1.52	0.92
1:C:44:CYS:HG	1:C:197:CYS:HG	1.03	0.88
1:E:44:CYS:HG	1:E:197:CYS:HG	1.16	0.80
1:E:159:MET:HE2	1:E:223:ILE:HD13	1.63	0.80
1:D:44:CYS:HG	1:D:197:CYS:HG	0.81	0.78
1:B:159:MET:CE	1:B:223:ILE:HD12	2.13	0.78
1:A:154:LYS:HE3	5:A:529:HOH:O	1.85	0.76
1:F:44:CYS:HG	1:F:197:CYS:HG	1.33	0.72
1:A:224:MET:HE2	1:A:228:THR:HG21	1.72	0.71
1:C:43:MET:HE1	1:C:47:GLY:HA2	1.74	0.69
1:F:57:ARG:NH1	1:F:236:ASN:O	2.26	0.68
1:B:159:MET:HE2	1:B:223:ILE:HD13	1.75	0.68
1:F:235:LEU:HD21	1:F:240:ILE:HD11	1.76	0.68
1:D:43:MET:HE1	1:D:47:GLY:HA2	1.75	0.67
1:E:32:GLU:HG2	5:E:452:HOH:O	1.92	0.67
1:A:44:CYS:HG	1:A:197:CYS:HG	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:ILE:HG13	1:F:159:MET:HE3	1.78	0.66
1:A:235:LEU:HD21	1:A:240:ILE:HD11	1.79	0.65
1:B:154:LYS:HE3	5:B:513:HOH:O	1.96	0.65
1:E:235:LEU:HD21	1:E:240:ILE:HD11	1.80	0.64
1:B:158:VAL:HG12	1:B:158:VAL:O	1.97	0.63
1:C:235:LEU:HD21	1:C:240:ILE:HD11	1.81	0.63
1:C:158:VAL:HG12	1:C:158:VAL:O	1.99	0.62
1:E:158:VAL:CG1	1:E:167:VAL:HG11	2.29	0.62
1:B:158:VAL:CG1	1:B:167:VAL:HG11	2.29	0.62
1:E:43:MET:HE2	1:E:199:GLU:CD	2.24	0.62
1:E:158:VAL:O	1:E:158:VAL:HG12	1.99	0.61
1:C:159:MET:HE1	1:C:223:ILE:HD12	1.78	0.61
1:C:159:MET:CE	1:C:223:ILE:CD1	2.61	0.59
1:E:57:ARG:NH1	1:E:236:ASN:O	2.35	0.58
1:C:158:VAL:CG1	1:C:167:VAL:HG11	2.34	0.58
1:E:215:GLU:H	1:E:215:GLU:CD	2.12	0.57
1:A:44:CYS:SG	1:A:197:CYS:SG	3.02	0.57
1:E:159:MET:CE	1:E:223:ILE:CD1	2.58	0.57
1:F:43:MET:CE	1:F:47:GLY:HA2	2.35	0.57
1:F:84:ILE:CG1	1:F:159:MET:HE3	2.34	0.56
1:C:147:ARG:HD2	5:C:449:HOH:O	2.04	0.56
1:A:43:MET:HE2	1:A:199:GLU:CD	2.31	0.56
1:F:43:MET:HE1	1:F:47:GLY:HA2	1.88	0.55
1:F:43:MET:CE	1:F:47:GLY:CA	2.85	0.55
1:C:43:MET:CE	1:C:47:GLY:CA	2.85	0.55
1:E:214:LYS:HB3	1:E:215:GLU:OE2	2.07	0.55
1:C:57:ARG:NH1	1:C:236:ASN:O	2.36	0.55
1:D:52:PRO:HG3	1:D:113:GLU:HB3	1.88	0.54
1:D:43:MET:CE	1:D:47:GLY:CA	2.85	0.54
1:E:159:MET:HE1	1:E:223:ILE:HD12	1.83	0.53
1:C:43:MET:CE	1:C:47:GLY:HA2	2.38	0.53
1:D:43:MET:CE	1:D:47:GLY:HA2	2.37	0.52
1:E:32:GLU:CG	5:E:452:HOH:O	2.53	0.52
1:F:43:MET:HE3	1:F:47:GLY:CA	2.41	0.51
1:A:40:GLU:O	1:A:40:GLU:HG2	2.11	0.51
1:A:57:ARG:NH1	1:A:236:ASN:O	2.40	0.49
1:D:55:ILE:HG22	1:D:58:ILE:HD11	1.95	0.48
1:C:43:MET:HE3	1:C:47:GLY:CA	2.44	0.48
1:B:43:MET:HE2	1:B:199:GLU:CD	2.38	0.48
1:C:151:ILE:H	1:C:151:ILE:HD12	1.79	0.47
1:C:159:MET:HE2	1:C:223:ILE:HD13	1.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:MET:HE3	1:E:47:GLY:CA	2.44	0.47
1:B:66:ILE:HD11	1:B:204:ILE:HD12	1.95	0.47
1:C:158:VAL:HG11	1:C:167:VAL:HG11	1.97	0.47
1:D:66:ILE:HD11	1:D:204:ILE:HD12	1.96	0.46
1:B:159:MET:CE	1:B:223:ILE:CD1	2.80	0.46
1:E:212:MET:HG3	1:E:217:ILE:HG13	1.97	0.46
1:C:66:ILE:HD11	1:C:204:ILE:HD12	1.97	0.46
1:D:43:MET:HE3	1:D:47:GLY:CA	2.46	0.45
1:E:22:GLY:N	5:E:410:HOH:O	2.50	0.45
1:F:136:LEU:CD1	1:F:192:LEU:HD21	2.47	0.45
1:E:66:ILE:HD11	1:E:204:ILE:HD12	1.98	0.45
1:B:43:MET:HE1	1:B:47:GLY:HA2	1.99	0.45
1:E:224:MET:HE2	1:E:228:THR:HG21	1.99	0.45
1:B:43:MET:HE3	1:B:47:GLY:CA	2.48	0.44
1:B:158:VAL:HG11	1:B:167:VAL:HG11	1.97	0.44
1:B:158:VAL:O	1:B:158:VAL:CG1	2.65	0.44
1:E:43:MET:HE3	1:E:47:GLY:HA3	2.00	0.44
1:E:123:PHE:HB3	1:E:143:PHE:HB2	2.00	0.43
1:F:74:ALA:HB3	1:F:173:ILE:HB	2.01	0.43
1:E:158:VAL:HG11	1:E:167:VAL:HG11	2.00	0.43
1:C:136:LEU:HD12	1:C:192:LEU:HD21	1.99	0.43
1:B:43:MET:CE	1:B:47:GLY:HA2	2.49	0.42
1:F:123:PHE:HB3	1:F:143:PHE:HB2	2.01	0.42
1:F:67:LYS:HE2	1:F:69:GLU:CG	2.50	0.42
1:A:208:GLU:OE1	5:A:401:HOH:O	2.21	0.42
1:E:43:MET:CE	1:E:47:GLY:HA2	2.49	0.42
1:E:208:GLU:OE2	5:E:401:HOH:O	2.21	0.42
1:A:224:MET:HE2	1:A:228:THR:CG2	2.47	0.42
1:F:158:VAL:O	1:F:158:VAL:CG1	2.68	0.42
1:C:43:MET:HE3	1:C:47:GLY:HA3	2.02	0.42
1:B:100:LYS:HE3	5:B:516:HOH:O	2.20	0.41
1:E:224:MET:HE3	1:E:224:MET:HA	2.00	0.41
1:D:156:TRP:CD2	1:D:159:MET:HE1	2.55	0.41
1:D:123:PHE:HB3	1:D:143:PHE:HB2	2.03	0.41
1:C:123:PHE:HB3	1:C:143:PHE:HB2	2.02	0.41
1:E:158:VAL:CG1	1:E:158:VAL:O	2.67	0.41
1:E:41:TYR:CD1	1:E:41:TYR:N	2.86	0.41
1:A:60:ASP:OD1	5:A:402:HOH:O	2.22	0.41
1:C:43:MET:CE	1:C:47:GLY:HA3	2.50	0.41
1:C:208:GLU:OE2	1:F:62:LYS:HE2	2.21	0.41
1:B:193:THR:OG1	5:B:402:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ARG:HG2	1:F:239:MET:HE3	2.02	0.40
1:B:208:GLU:CD	5:B:403:HOH:O	2.64	0.40
1:D:158:VAL:O	1:D:158:VAL:CG1	2.68	0.40
1:F:239:MET:HE2	1:F:239:MET:HB3	1.95	0.40
1:A:57:ARG:HG2	1:A:239:MET:HE3	2.03	0.40
1:A:66:ILE:HD11	1:A:204:ILE:HD12	2.03	0.40
1:A:167:VAL:HG21	5:A:485:HOH:O	2.21	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	220/243 (90%)	215 (98%)	5 (2%)	0	100	100
1	B	220/243 (90%)	214 (97%)	6 (3%)	0	100	100
1	C	220/243 (90%)	214 (97%)	6 (3%)	0	100	100
1	D	220/243 (90%)	214 (97%)	6 (3%)	0	100	100
1	E	220/243 (90%)	215 (98%)	5 (2%)	0	100	100
1	F	220/243 (90%)	217 (99%)	3 (1%)	0	100	100
All	All	1320/1458 (90%)	1289 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/209 (92%)	191 (99%)	2 (1%)	68	75
1	B	193/209 (92%)	193 (100%)	0	100	100
1	C	193/209 (92%)	192 (100%)	1 (0%)	81	87
1	D	193/209 (92%)	192 (100%)	1 (0%)	81	87
1	E	193/209 (92%)	189 (98%)	4 (2%)	47	52
1	F	193/209 (92%)	192 (100%)	1 (0%)	81	87
All	All	1158/1254 (92%)	1149 (99%)	9 (1%)	73	80

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ILE
1	A	222	LYS
1	C	24	SER
1	D	158	VAL
1	E	24	SER
1	E	100	LYS
1	E	181	LYS
1	E	222	LYS
1	F	158	VAL

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

Mol	Chain	Res	Type
1	A	82	HIS
1	A	119	GLN
1	A	133	HIS
1	D	82	HIS
1	D	236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 21 are monoatomic - leaving 4 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	PG4	A	305	-	12,12,12	0.73	0	11,11,11	0.80	0
4	PG4	B	306	-	12,12,12	0.89	0	11,11,11	0.83	0
4	PG4	E	302	-	12,12,12	0.85	0	11,11,11	0.85	1 (9%)
4	PG4	F	302	-	12,12,12	0.96	0	11,11,11	1.08	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	PG4	A	305	-	-	2/10/10/10	-
4	PG4	B	306	-	-	3/10/10/10	-
4	PG4	E	302	-	-	1/10/10/10	-
4	PG4	F	302	-	-	4/10/10/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	302	PG4	O3-C4-C3	2.16	120.18	110.35

There are no chirality outliers.

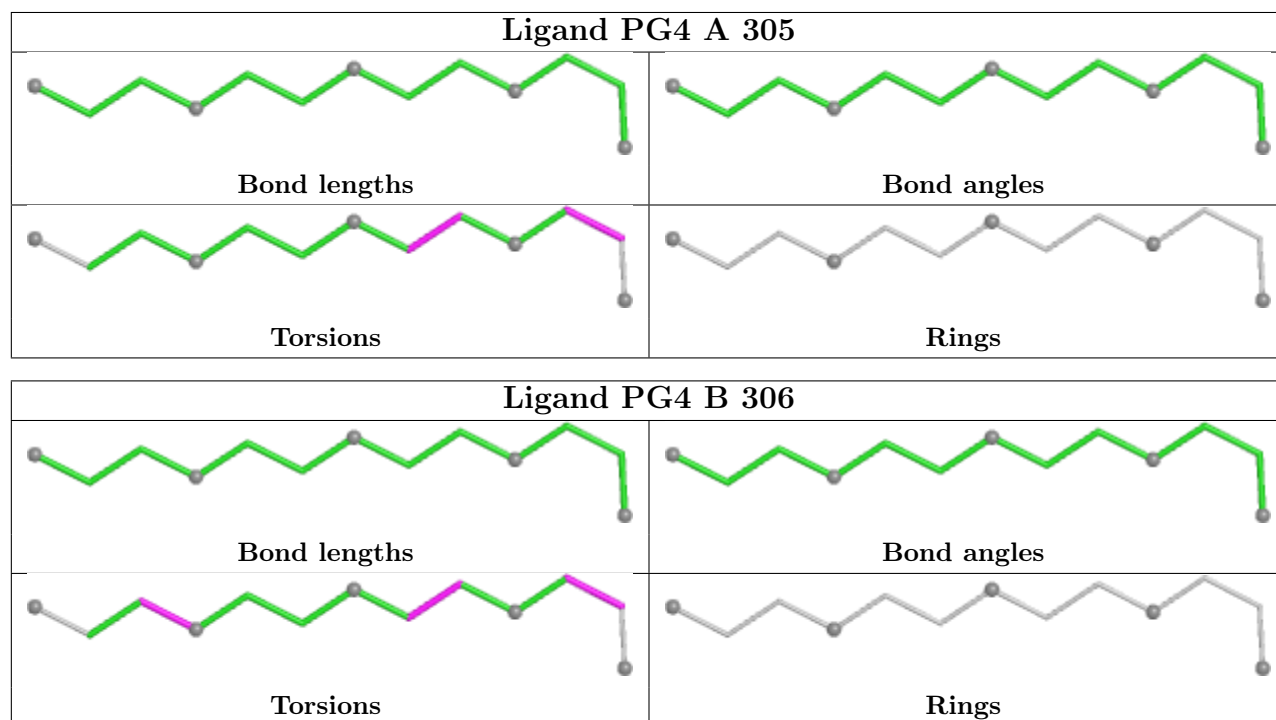
All (10) torsion outliers are listed below:

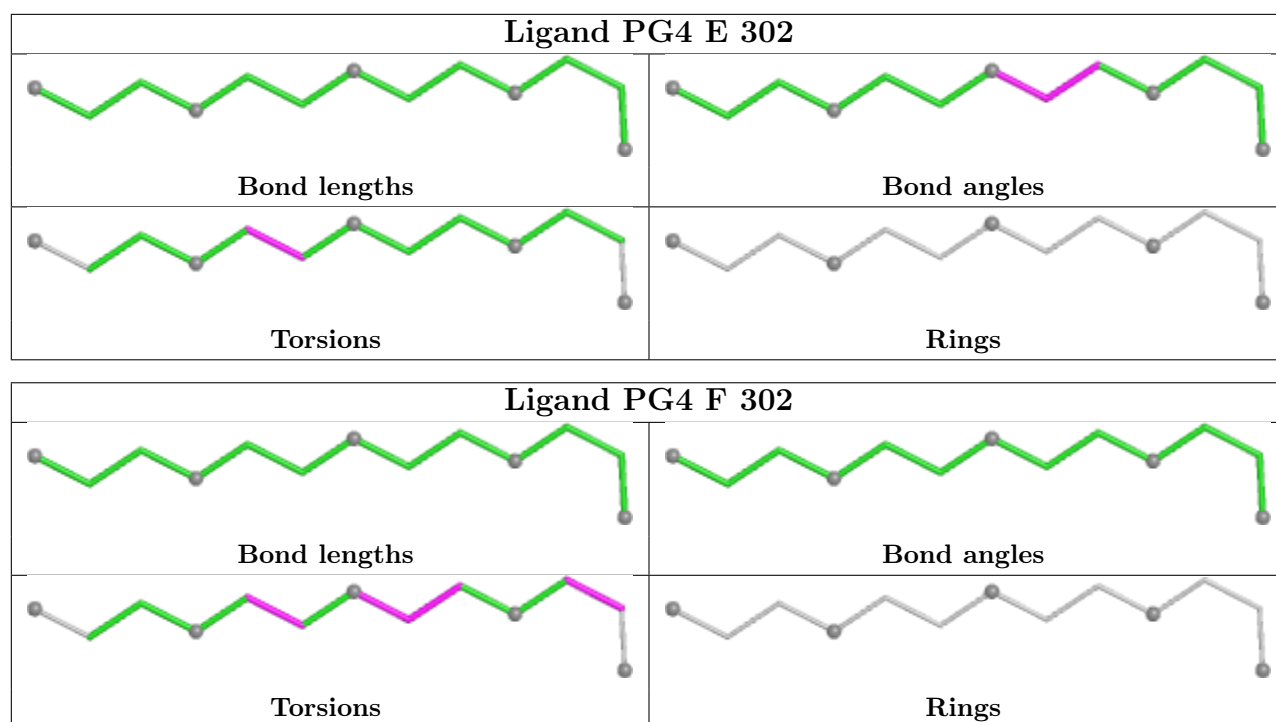
Mol	Chain	Res	Type	Atoms
4	A	305	PG4	O1-C1-C2-O2
4	F	302	PG4	O2-C3-C4-O3
4	A	305	PG4	O2-C3-C4-O3
4	B	306	PG4	O2-C3-C4-O3
4	E	302	PG4	O3-C5-C6-O4
4	F	302	PG4	O3-C5-C6-O4
4	F	302	PG4	O1-C1-C2-O2
4	B	306	PG4	C8-C7-O4-C6
4	B	306	PG4	O1-C1-C2-O2
4	F	302	PG4	C3-C4-O3-C5

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	222/243 (91%)	0.08	5 (2%) 61 60	23, 33, 59, 83	0
1	B	222/243 (91%)	0.24	10 (4%) 38 37	23, 36, 61, 80	0
1	C	222/243 (91%)	1.27	42 (18%) 3 3	32, 54, 82, 102	0
1	D	222/243 (91%)	1.22	45 (20%) 3 2	32, 52, 85, 114	0
1	E	222/243 (91%)	0.72	16 (7%) 21 20	32, 47, 78, 105	0
1	F	222/243 (91%)	0.89	24 (10%) 11 10	31, 47, 78, 98	0
All	All	1332/1458 (91%)	0.74	142 (10%) 11 10	23, 45, 78, 114	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	237	ALA	6.9
1	C	237	ALA	6.3
1	E	237	ALA	6.1
1	A	237	ALA	5.2
1	C	167	VAL	4.8
1	D	163	ALA	4.6
1	F	26	HIS	4.5
1	F	236	ASN	4.3
1	A	236	ASN	4.0
1	C	236	ASN	3.9
1	D	146	GLY	3.8
1	D	158	VAL	3.8
1	B	35	GLY	3.7
1	E	26	HIS	3.7
1	C	169	LEU	3.6
1	D	167	VAL	3.6
1	D	212	MET	3.6
1	E	170	ALA	3.6
1	F	169	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	171	HIS	3.5
1	D	22	GLY	3.5
1	F	37	LEU	3.5
1	F	153	GLU	3.5
1	C	164	GLY	3.4
1	D	147	ARG	3.4
1	F	167	VAL	3.4
1	D	73	GLY	3.3
1	C	26	HIS	3.3
1	C	84	ILE	3.3
1	C	37	LEU	3.2
1	D	169	LEU	3.2
1	D	153	GLU	3.2
1	A	26	HIS	3.2
1	F	170	ALA	3.1
1	C	225	GLY	3.1
1	B	44	CYS	3.1
1	C	74	ALA	3.1
1	B	171	HIS	3.1
1	D	112	SER	3.1
1	D	162	ASN	3.0
1	E	167	VAL	3.0
1	C	223	ILE	3.0
1	C	217	ILE	3.0
1	D	218	GLU	3.0
1	C	75	THR	3.0
1	D	168	LYS	3.0
1	C	163	ALA	2.9
1	D	213	SER	2.9
1	B	22	GLY	2.9
1	B	26	HIS	2.9
1	D	72	ALA	2.9
1	F	30	GLY	2.9
1	C	22	GLY	2.9
1	D	219	LYS	2.9
1	C	170	ALA	2.9
1	C	117	LYS	2.8
1	C	213	SER	2.8
1	D	87	SER	2.8
1	E	236	ASN	2.8
1	E	169	LEU	2.8
1	C	155	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	75	THR	2.8
1	B	157	LYS	2.8
1	D	160	PRO	2.8
1	D	157	LYS	2.7
1	C	78	LEU	2.7
1	C	56	ASN	2.7
1	F	89	GLU	2.7
1	C	146	GLY	2.7
1	C	165	GLU	2.6
1	D	161	GLU	2.6
1	D	42	ILE	2.6
1	D	155	ILE	2.6
1	D	159	MET	2.6
1	D	156	TRP	2.6
1	F	211	GLU	2.5
1	D	77	VAL	2.5
1	E	226	GLY	2.5
1	D	148	GLU	2.5
1	C	44	CYS	2.5
1	C	72	ALA	2.5
1	F	173	ILE	2.5
1	D	149	ASN	2.5
1	E	44	CYS	2.5
1	C	160	PRO	2.5
1	D	150	PRO	2.5
1	D	152	LEU	2.5
1	F	78	LEU	2.5
1	D	145	GLU	2.4
1	D	215	GLU	2.4
1	E	37	LEU	2.4
1	D	164	GLY	2.4
1	C	214	LYS	2.4
1	D	217	ILE	2.4
1	C	222	LYS	2.4
1	F	72	ALA	2.4
1	D	36	ASP	2.4
1	A	171	HIS	2.4
1	C	162	ASN	2.3
1	D	71	ARG	2.3
1	C	161	GLU	2.3
1	C	86	VAL	2.3
1	F	22	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	208	GLU	2.3
1	E	28	GLU	2.3
1	C	79	ASN	2.3
1	A	32	GLU	2.2
1	B	153	GLU	2.2
1	F	215	GLU	2.2
1	C	229	ASN	2.2
1	C	166	GLU	2.2
1	C	144	LYS	2.2
1	D	223	ILE	2.2
1	D	143	PHE	2.2
1	C	226	GLY	2.2
1	E	225	GLY	2.2
1	F	41	TYR	2.2
1	F	172	LYS	2.2
1	F	162	ASN	2.2
1	C	215	GLU	2.1
1	E	215	GLU	2.1
1	F	165	GLU	2.1
1	B	29	HIS	2.1
1	F	171	HIS	2.1
1	C	147	ARG	2.1
1	F	44	CYS	2.1
1	B	38	LYS	2.1
1	D	154	LYS	2.1
1	E	39	ASP	2.1
1	E	218	GLU	2.1
1	E	151	ILE	2.1
1	F	29	HIS	2.1
1	B	170	ALA	2.1
1	E	82	HIS	2.1
1	D	30	GLY	2.1
1	D	74	ALA	2.1
1	C	28	GLU	2.1
1	C	153	GLU	2.1
1	D	117	LYS	2.1
1	C	224	MET	2.0
1	C	77	VAL	2.0
1	F	235	LEU	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.

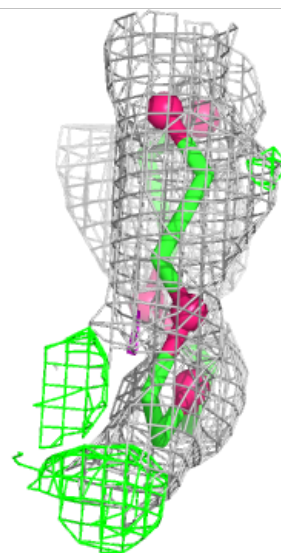
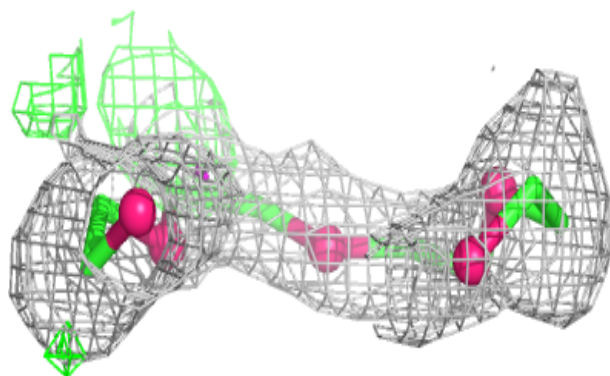
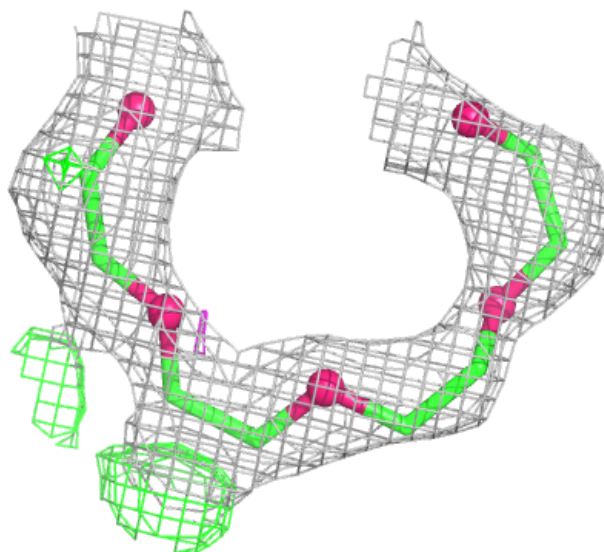
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PG4	B	306	13/13	0.76	0.19	66,72,83,90	0
3	CA	A	303	1/1	0.77	0.13	66,66,66,66	0
4	PG4	A	305	13/13	0.79	0.18	63,73,83,87	0
4	PG4	E	302	13/13	0.81	0.15	61,67,73,75	0
4	PG4	F	302	13/13	0.82	0.15	51,63,71,79	0
3	CA	D	304	1/1	0.85	0.16	73,73,73,73	0
3	CA	B	304	1/1	0.88	0.10	60,60,60,60	0
3	CA	D	303	1/1	0.89	0.08	101,101,101,101	0
3	CA	A	308	1/1	0.89	0.12	78,78,78,78	0
3	CA	B	308	1/1	0.89	0.15	78,78,78,78	0
3	CA	A	307	1/1	0.90	0.11	60,60,60,60	0
3	CA	B	305	1/1	0.94	0.14	65,65,65,65	0
3	CA	A	304	1/1	0.94	0.17	64,64,64,64	0
3	CA	D	302	1/1	0.95	0.16	53,53,53,53	0
3	CA	B	307	1/1	0.96	0.09	45,45,45,45	0
3	CA	B	303	1/1	0.97	0.09	54,54,54,54	0
3	CA	A	302	1/1	0.97	0.10	40,40,40,40	0
3	CA	B	302	1/1	0.97	0.10	39,39,39,39	0
3	CA	A	306	1/1	0.98	0.07	41,41,41,41	0
2	ZN	C	301	1/1	0.98	0.05	51,51,51,51	0
2	ZN	D	301	1/1	0.98	0.07	48,48,48,48	0
2	ZN	F	301	1/1	0.98	0.03	46,46,46,46	0
2	ZN	E	301	1/1	0.99	0.03	44,44,44,44	0
2	ZN	A	301	1/1	0.99	0.04	32,32,32,32	0
2	ZN	B	301	1/1	0.99	0.05	34,34,34,34	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.

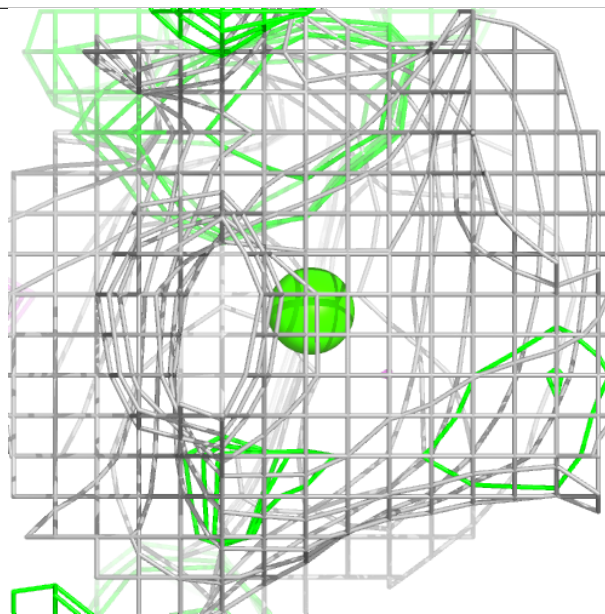
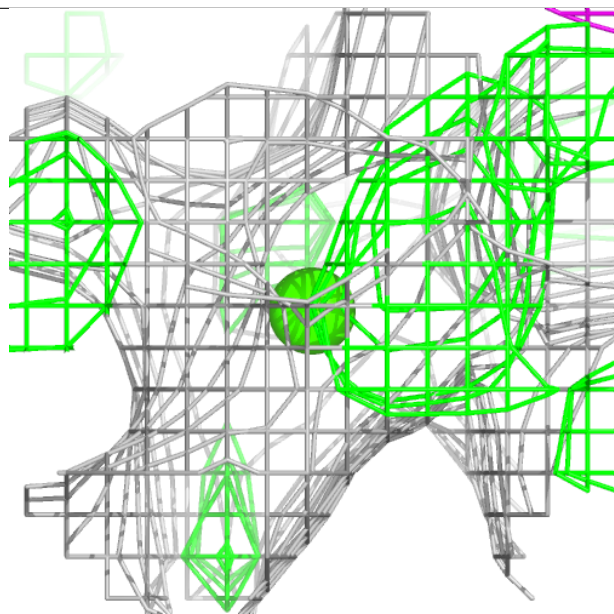
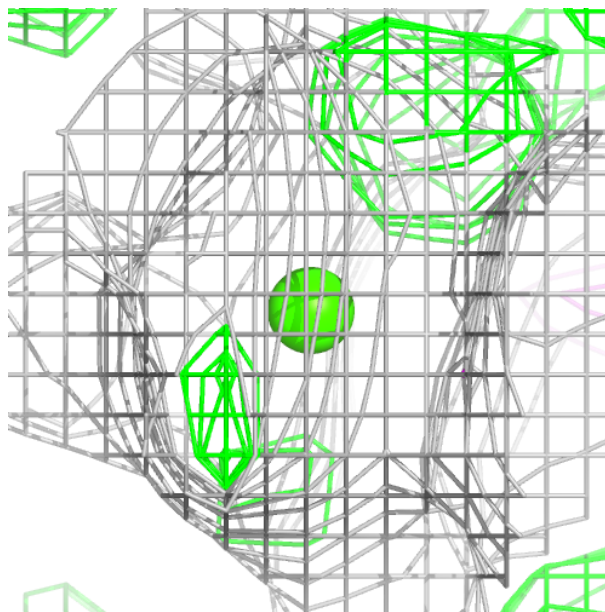
Electron density around PG4 B 306:

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



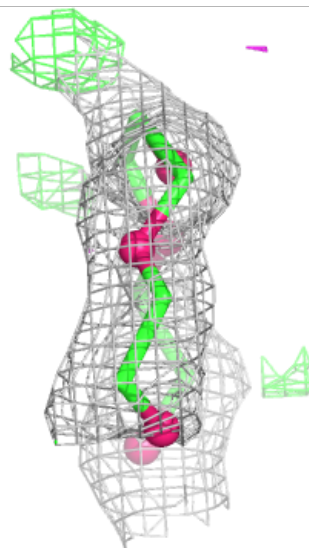
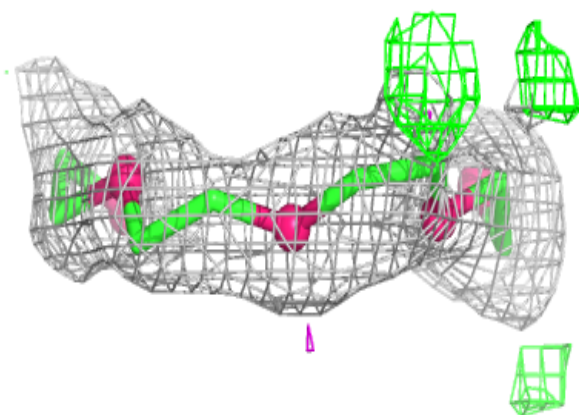
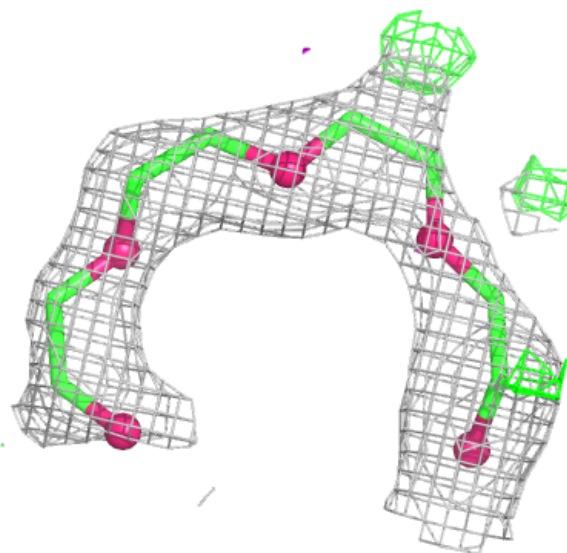
Electron density around CA A 303:

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



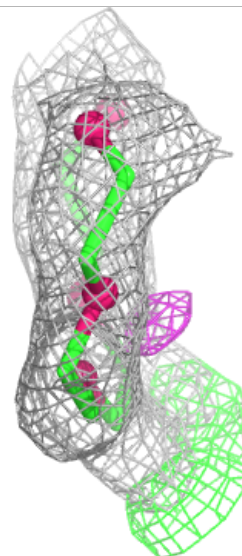
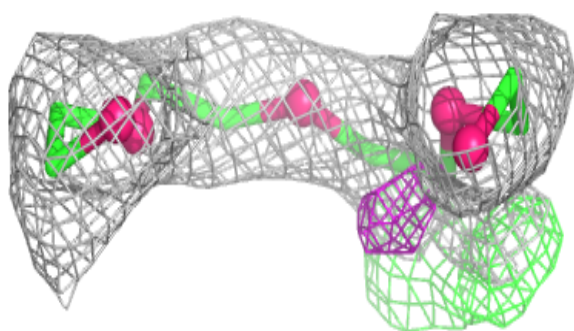
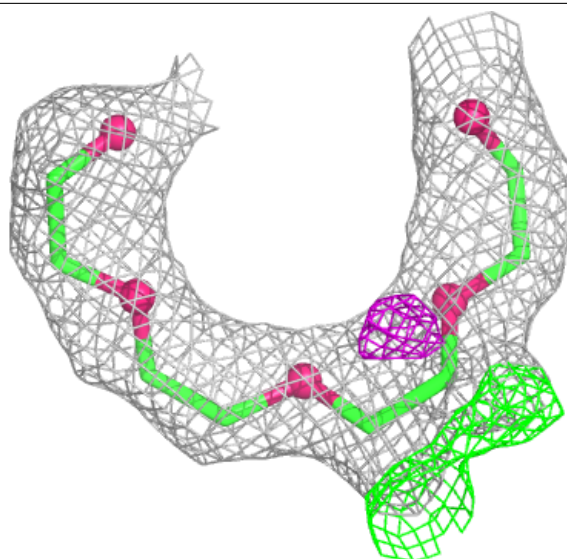
Electron density around PG4 A 305:

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



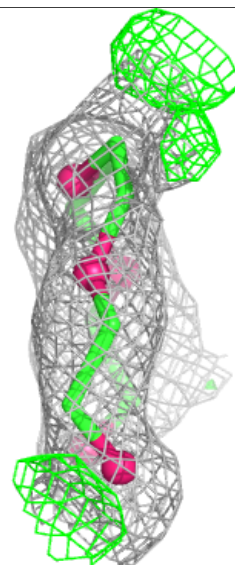
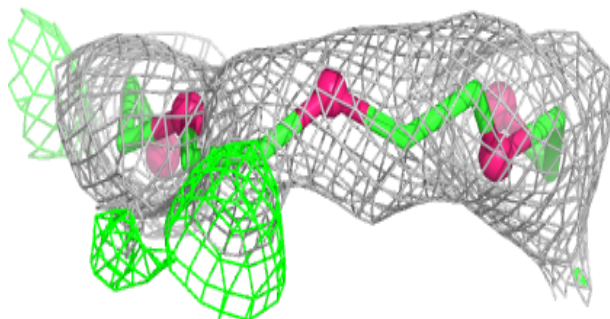
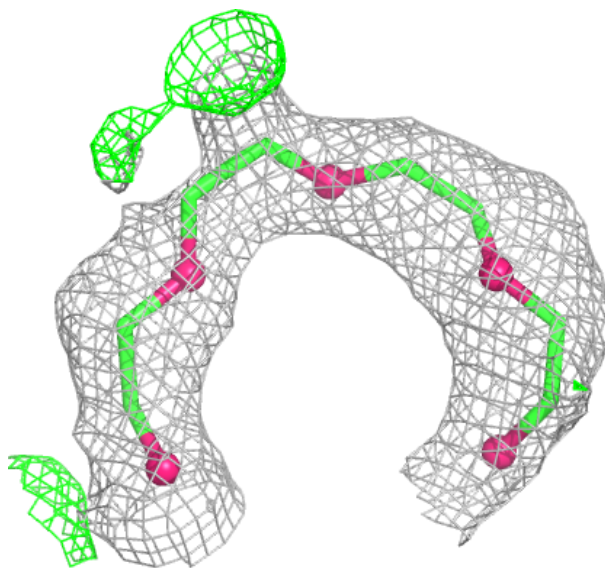
Electron density around PG4 E 302:

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



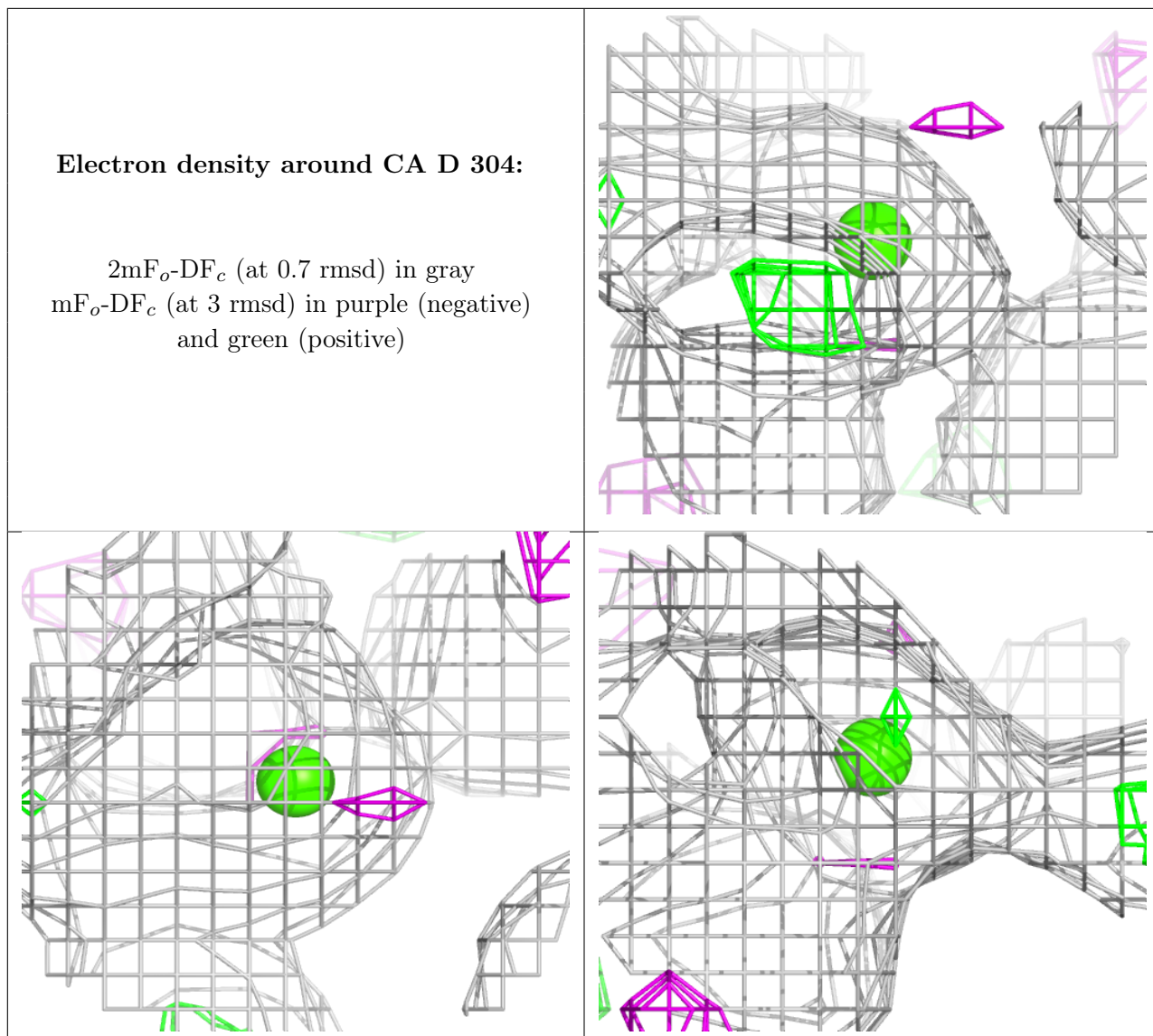
Electron density around PG4 F 302:

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



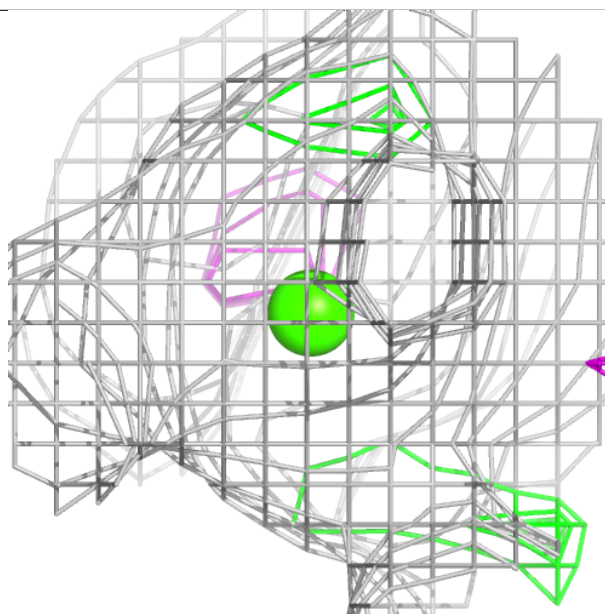
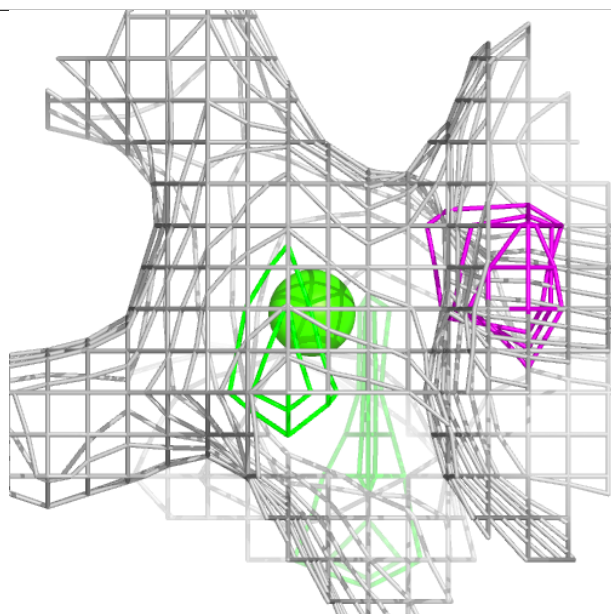
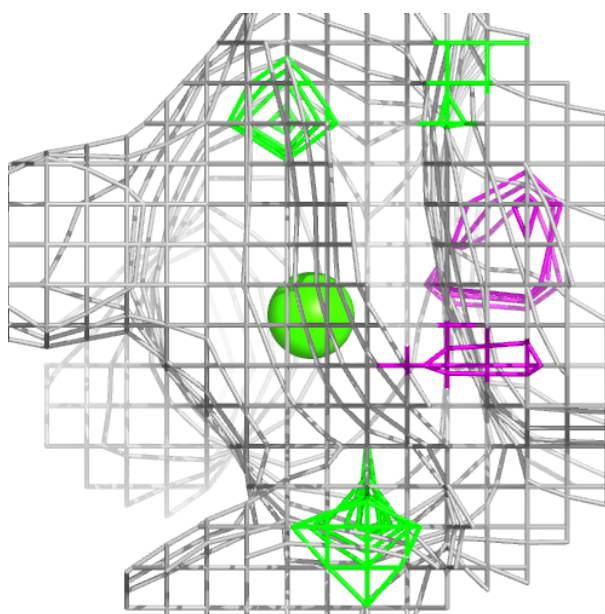
Electron density around CA D 304:

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



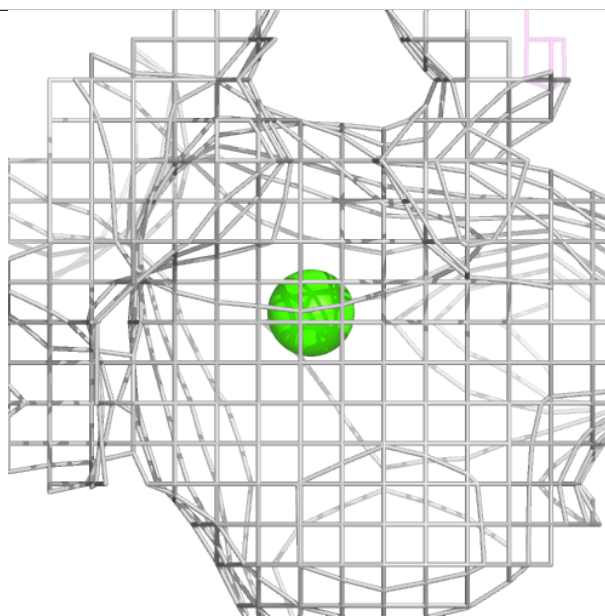
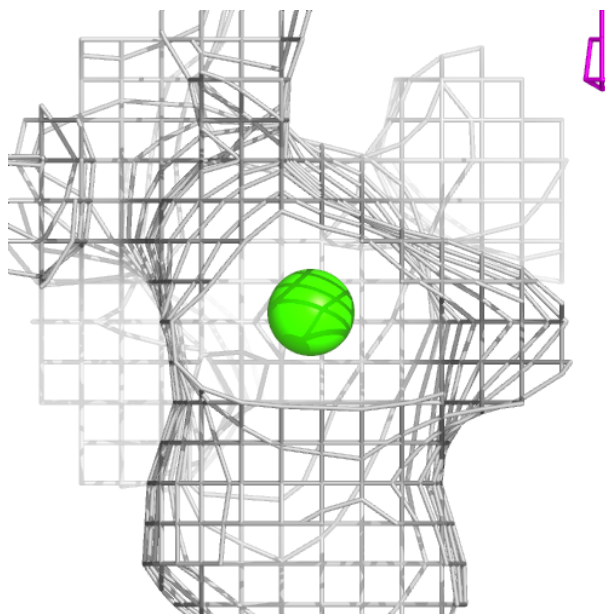
Electron density around CA B 304:

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



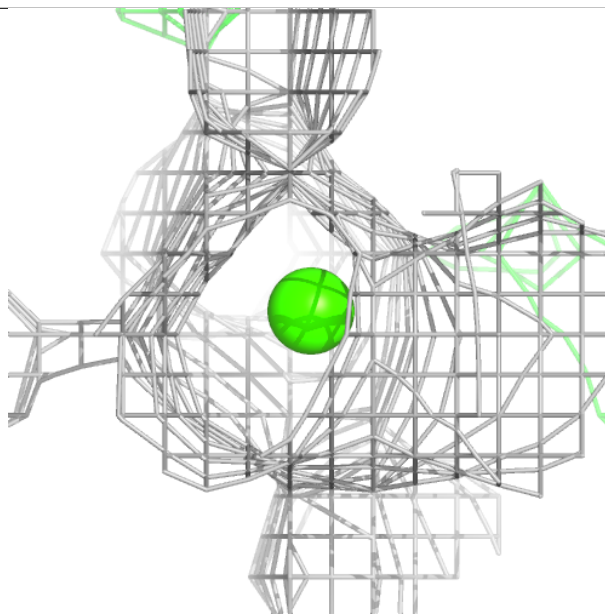
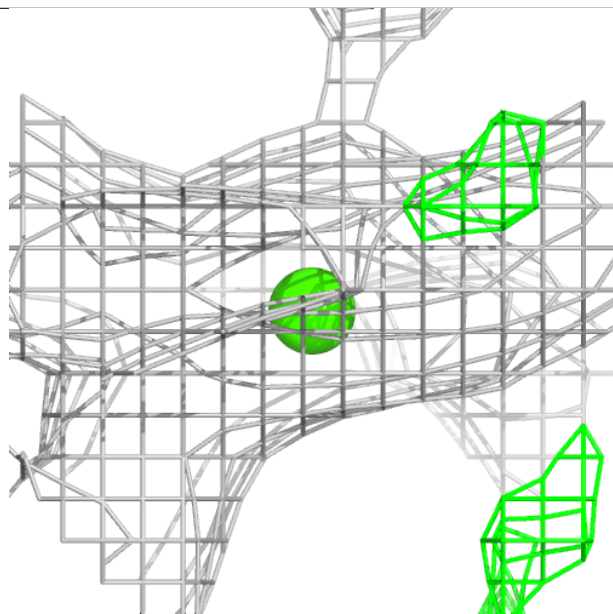
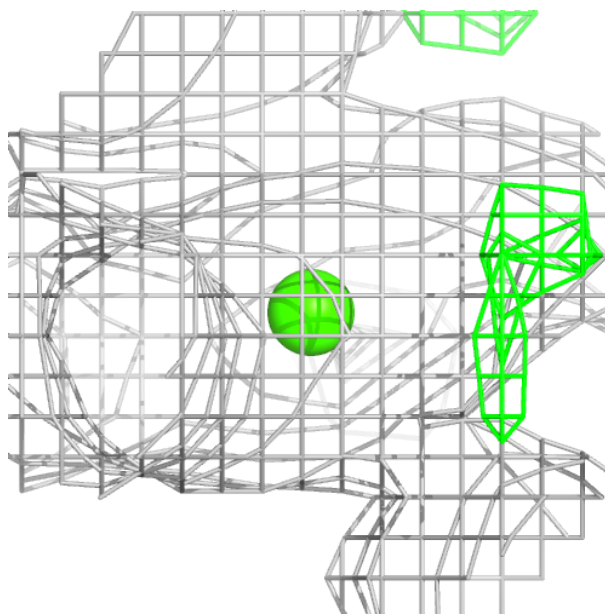
Electron density around CA D 303:

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



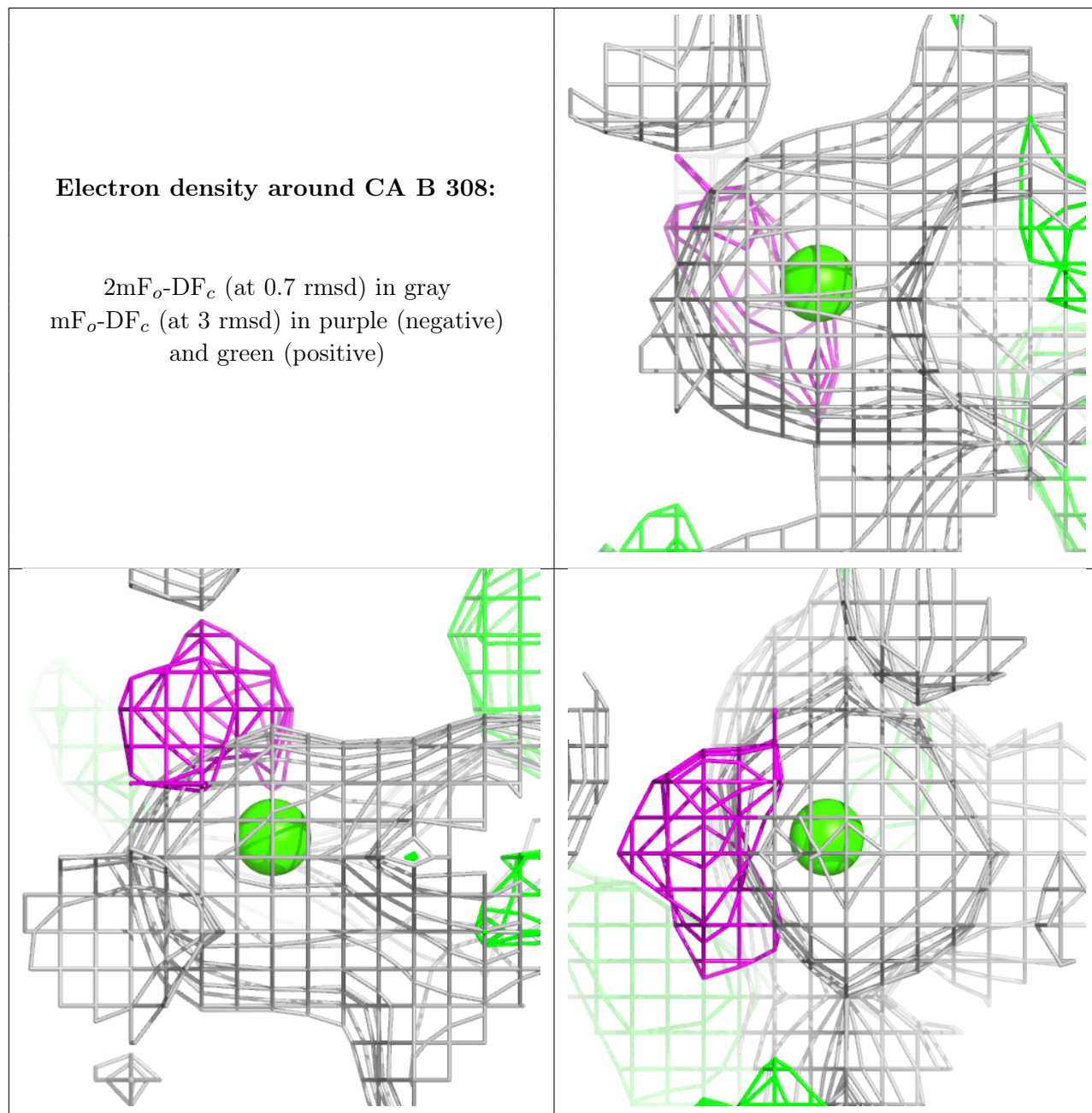
Electron density around CA A 308:

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



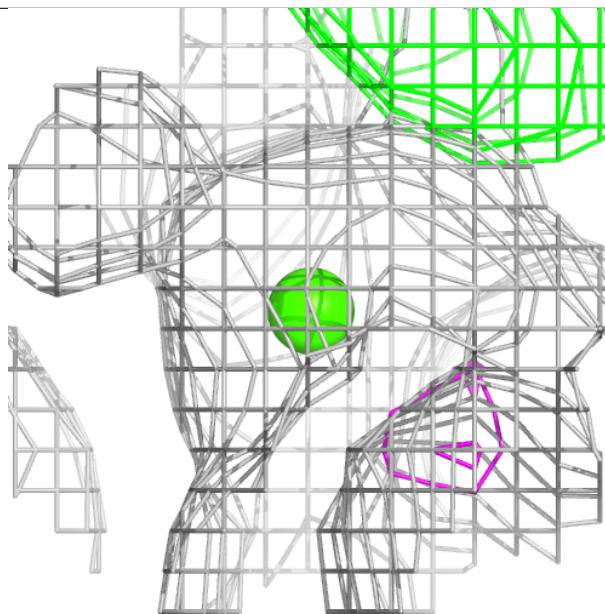
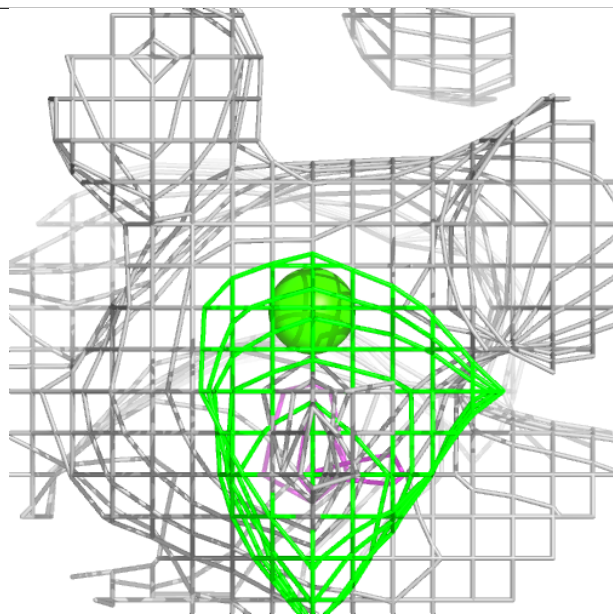
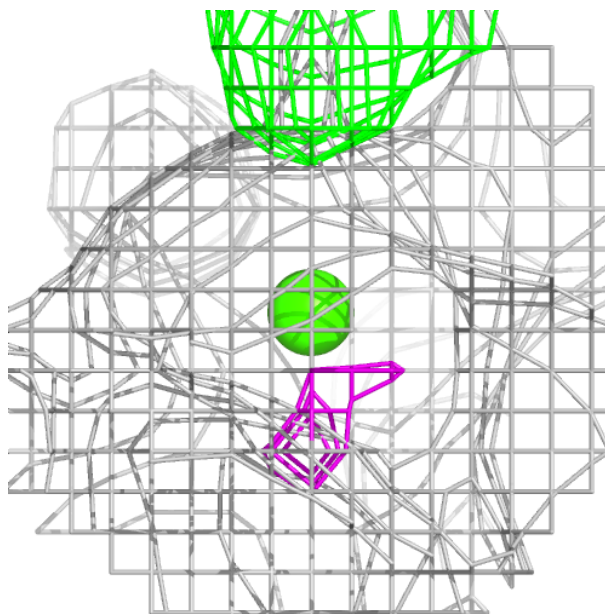
Electron density around CA B 308:

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



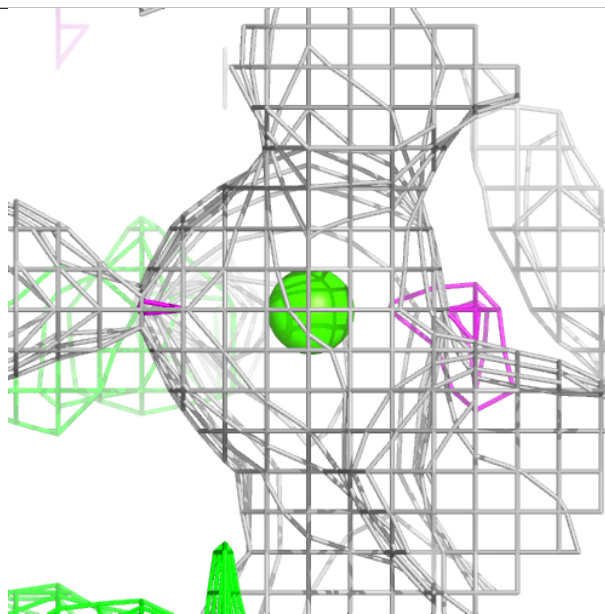
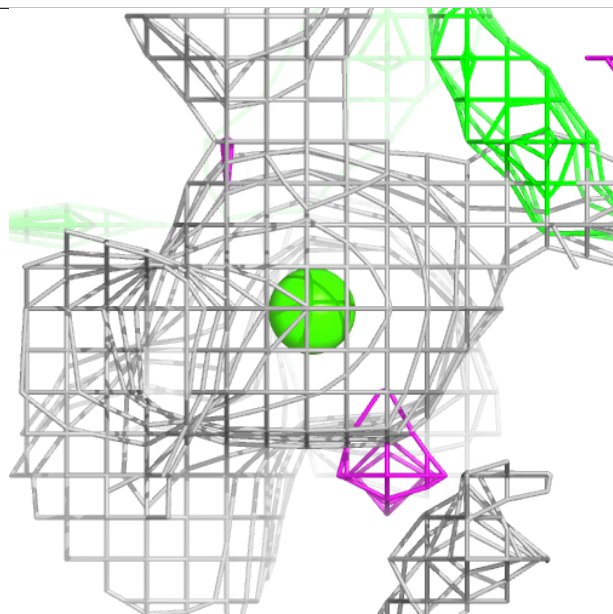
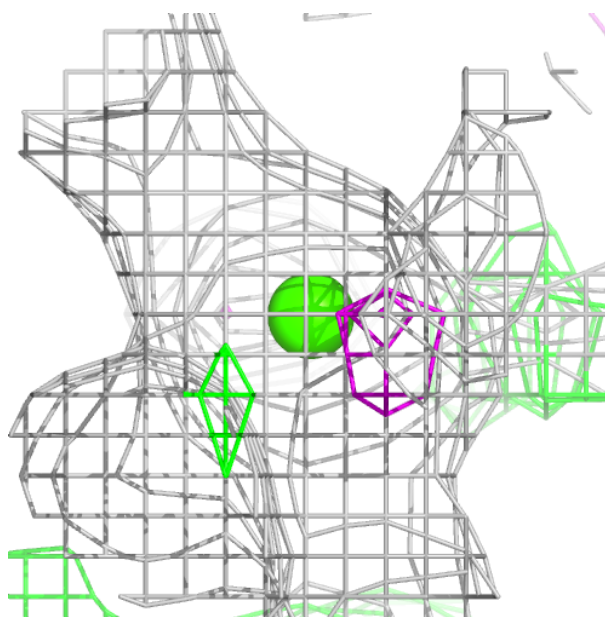
Electron density around CA A 307:

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



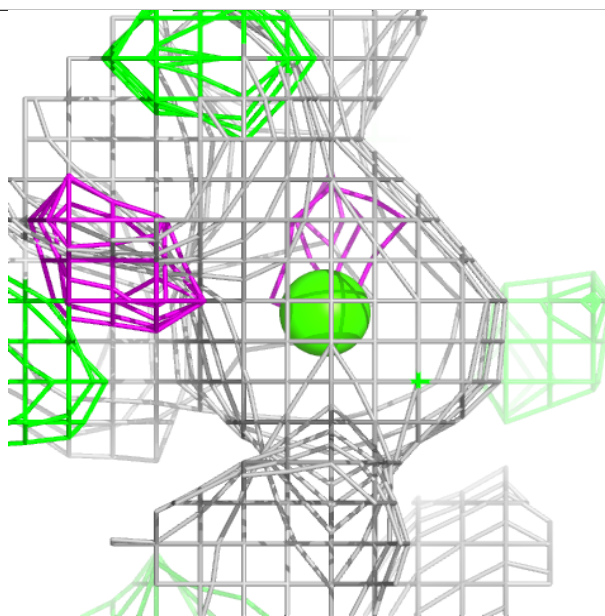
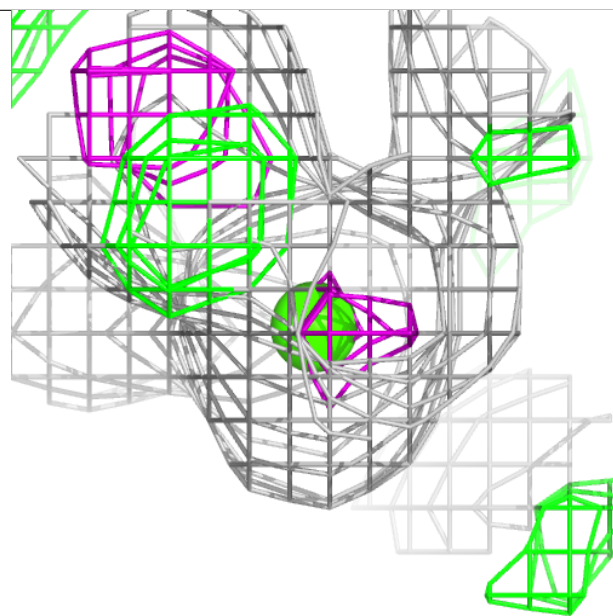
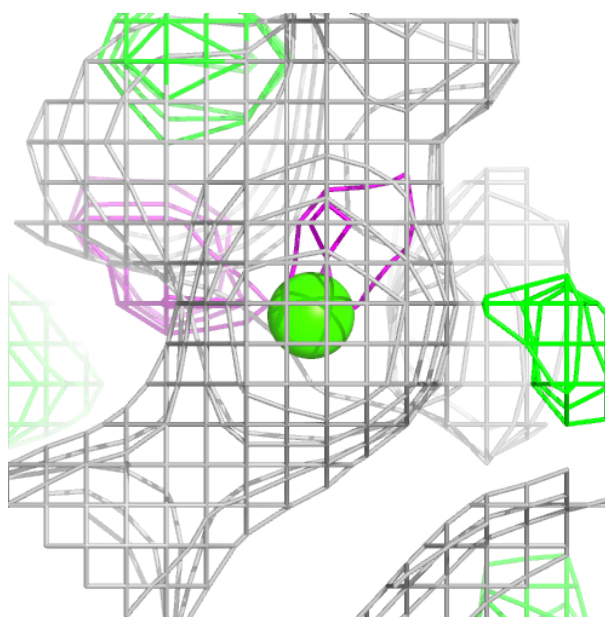
Electron density around CA B 305:

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



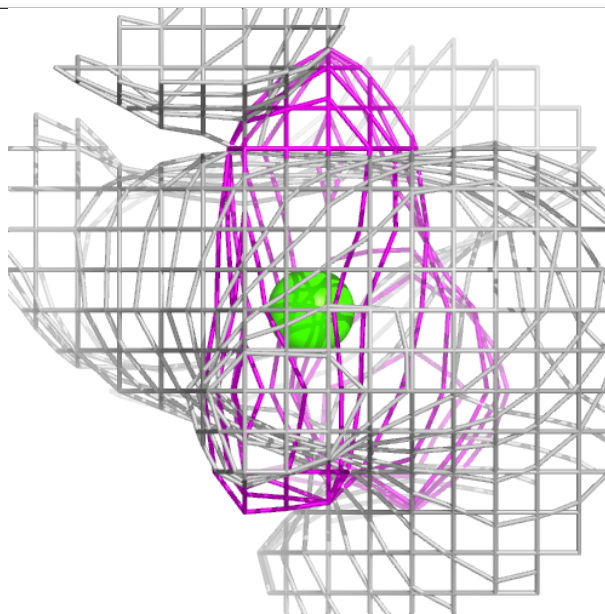
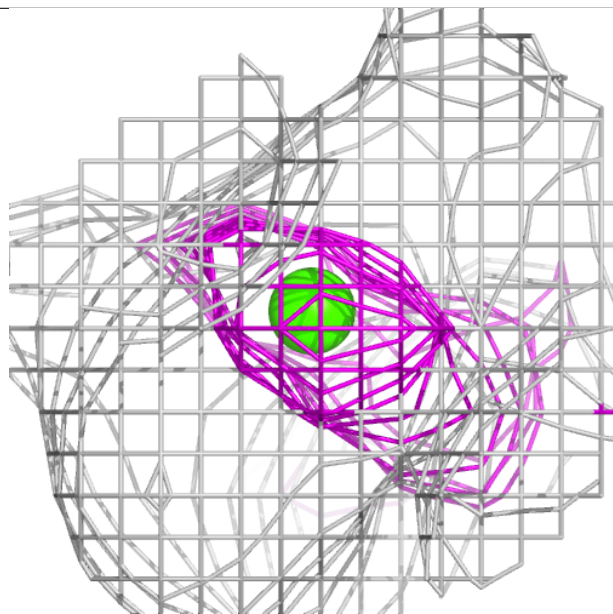
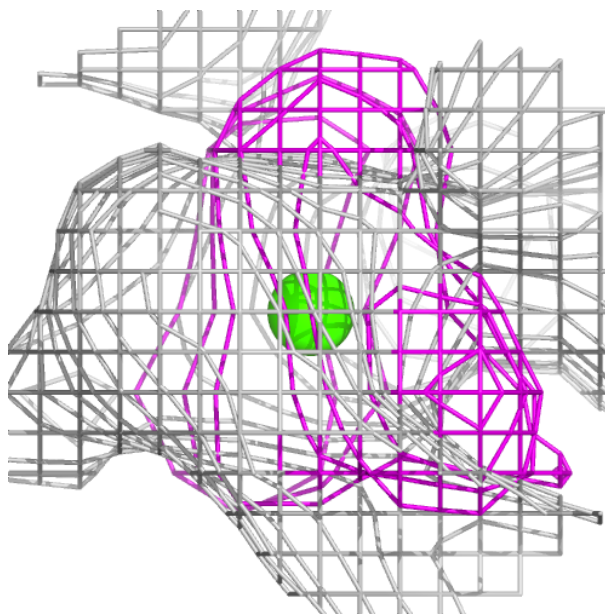
Electron density around CA A 304:

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



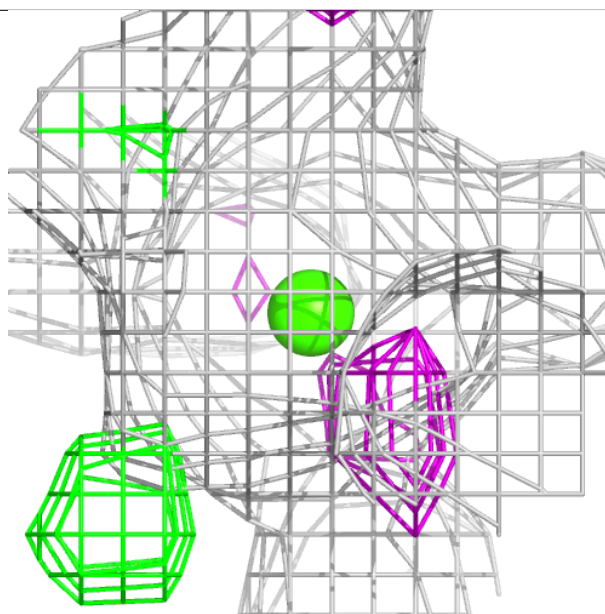
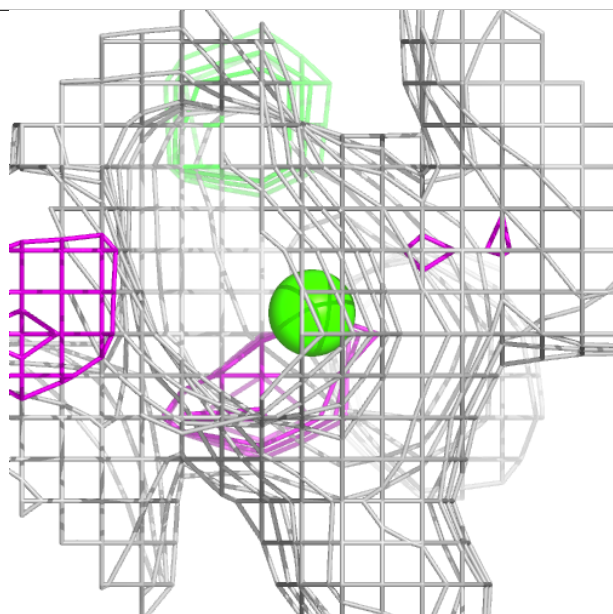
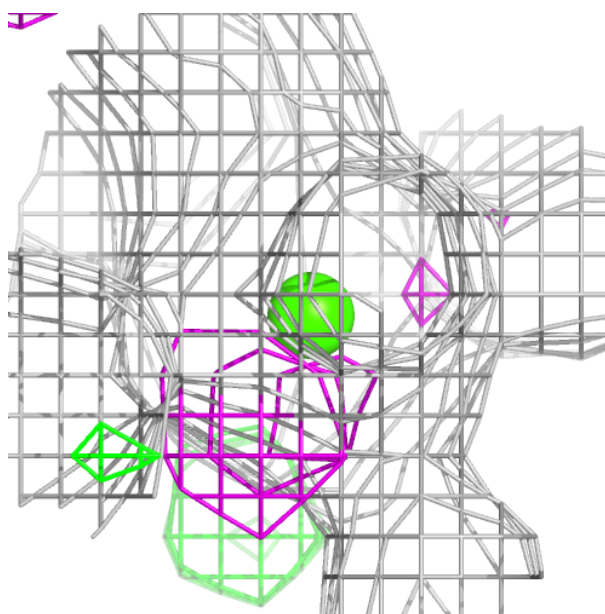
Electron density around CA D 302:

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



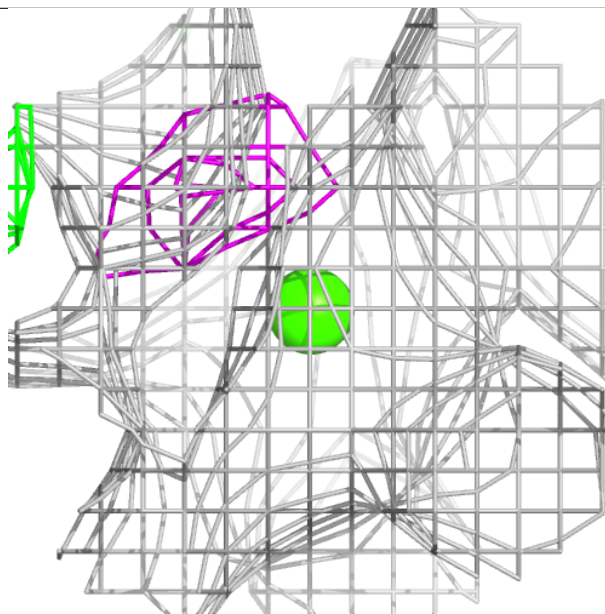
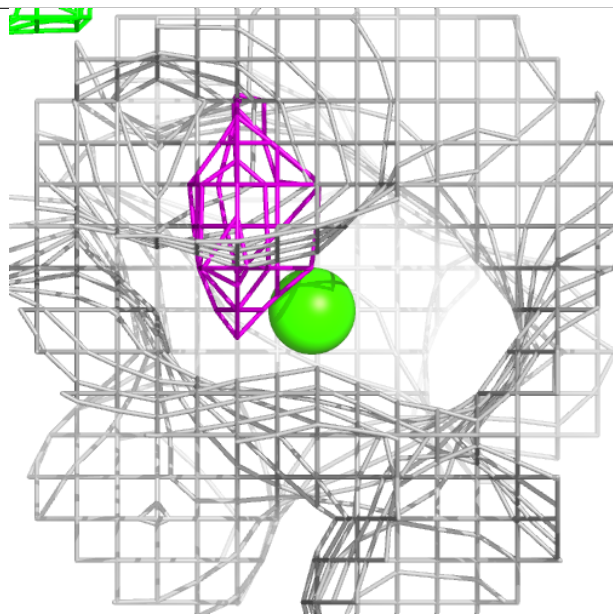
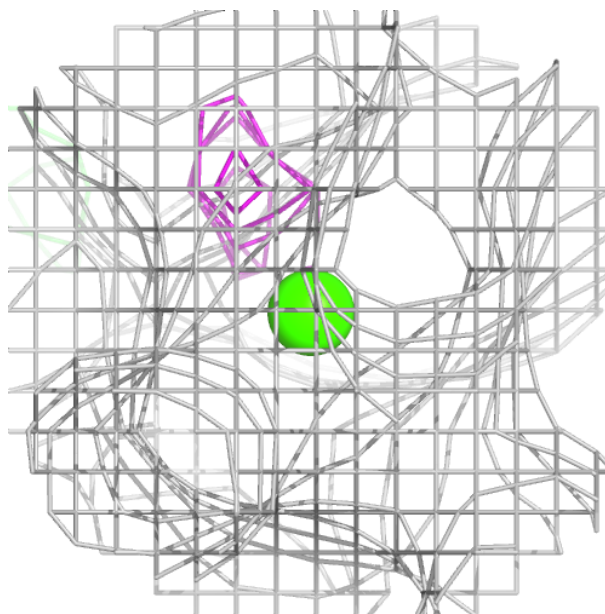
Electron density around CA B 307:

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



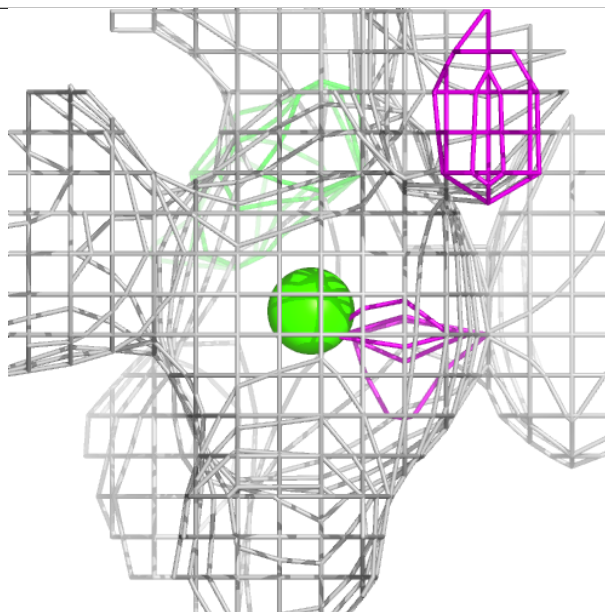
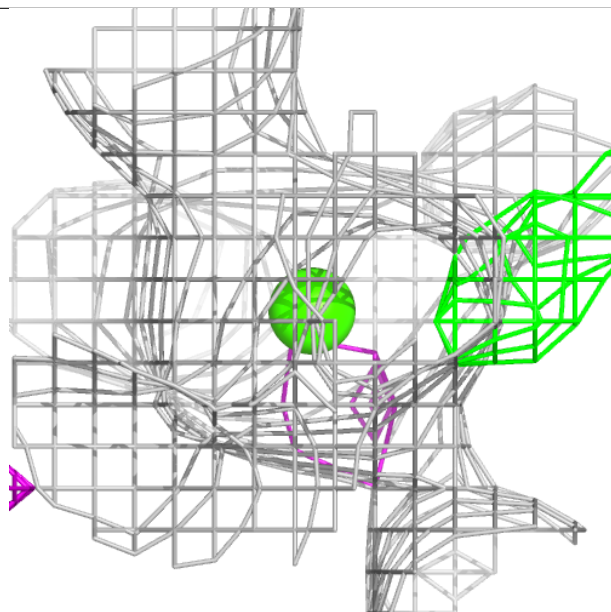
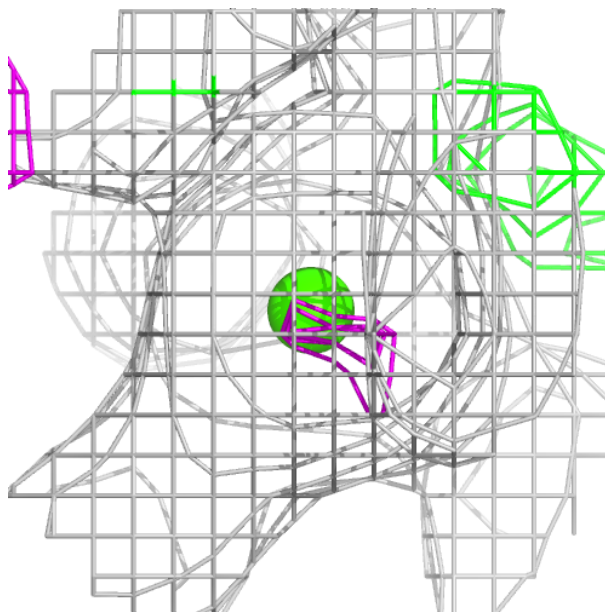
Electron density around CA B 303:

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



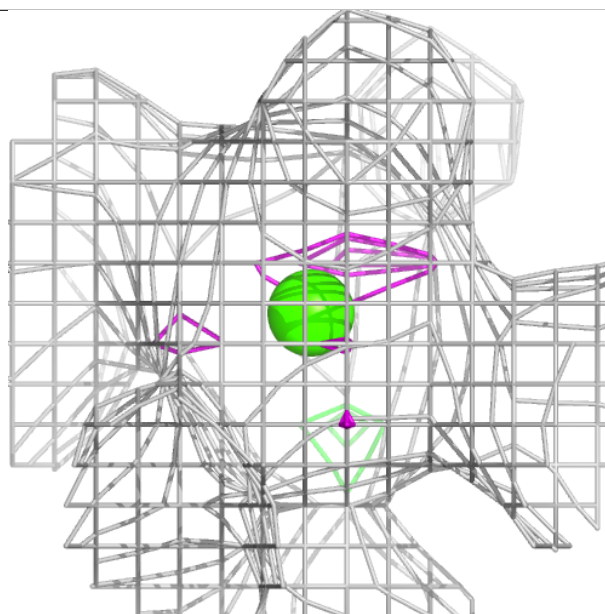
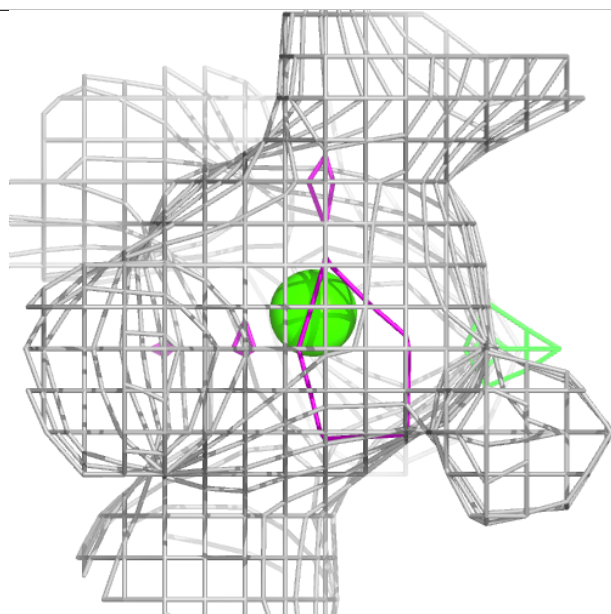
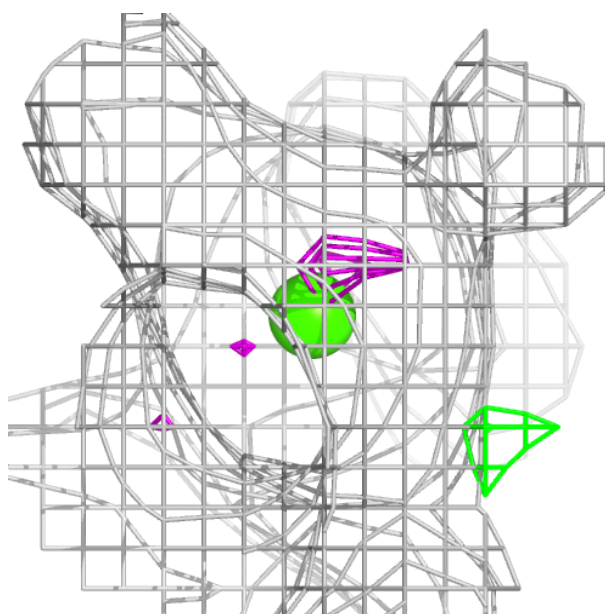
Electron density around CA A 302:

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



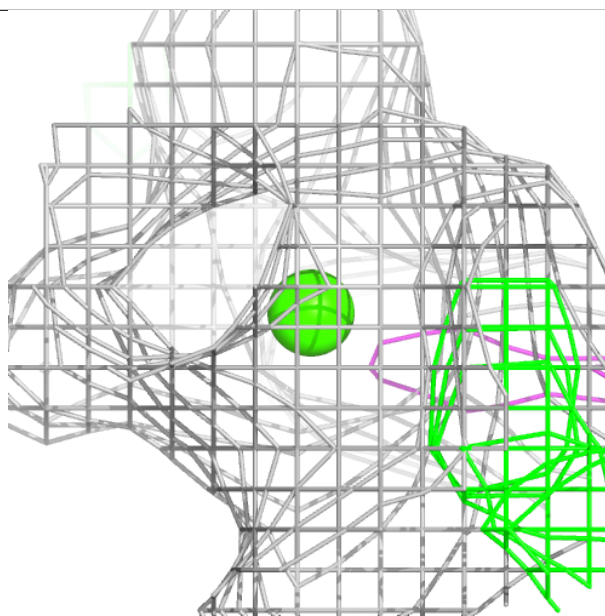
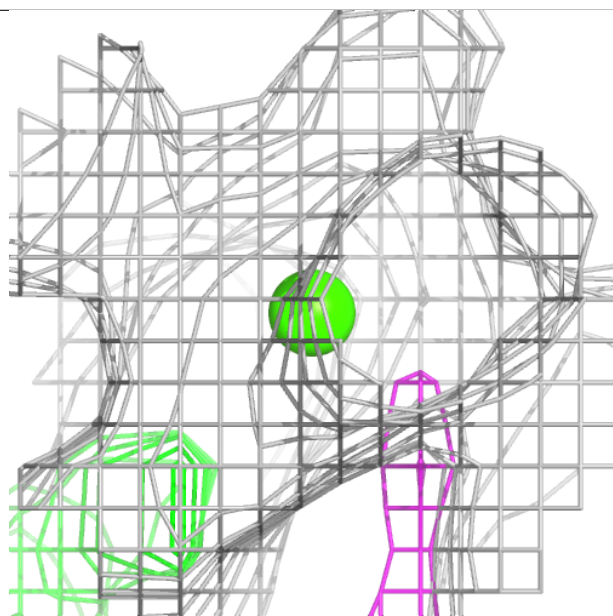
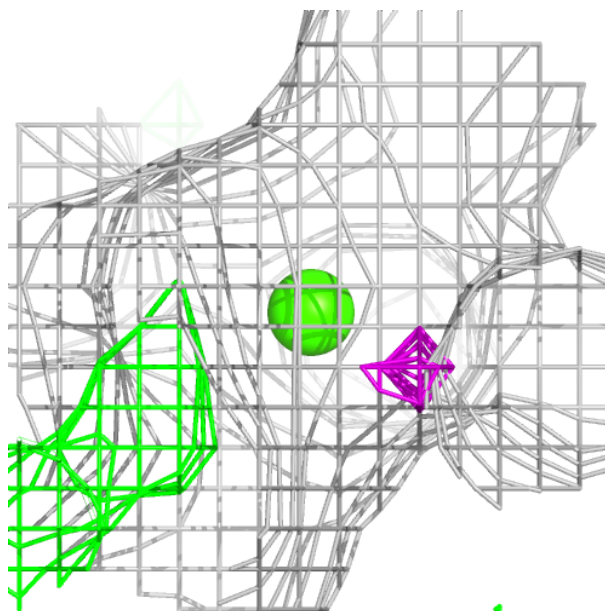
Electron density around CA B 302:

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and green (positive)



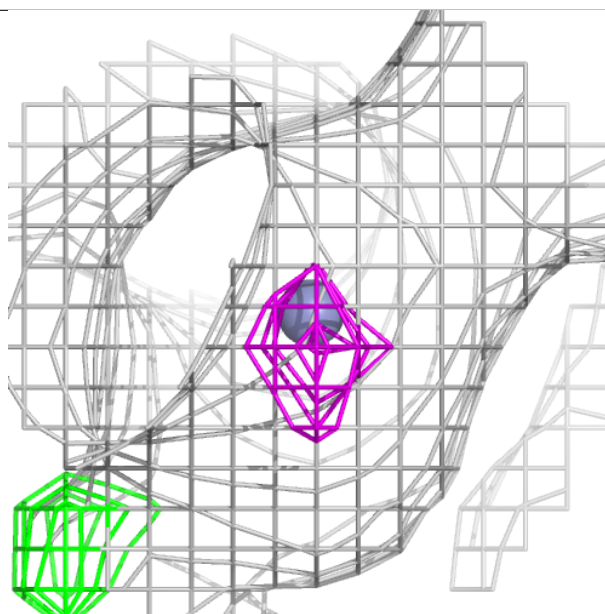
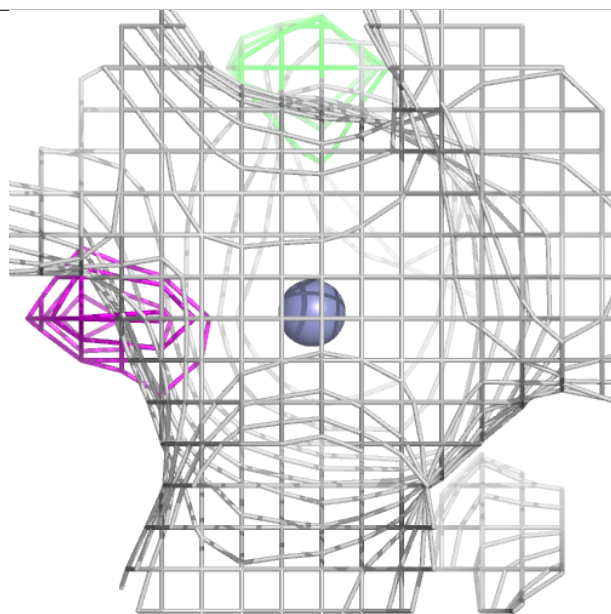
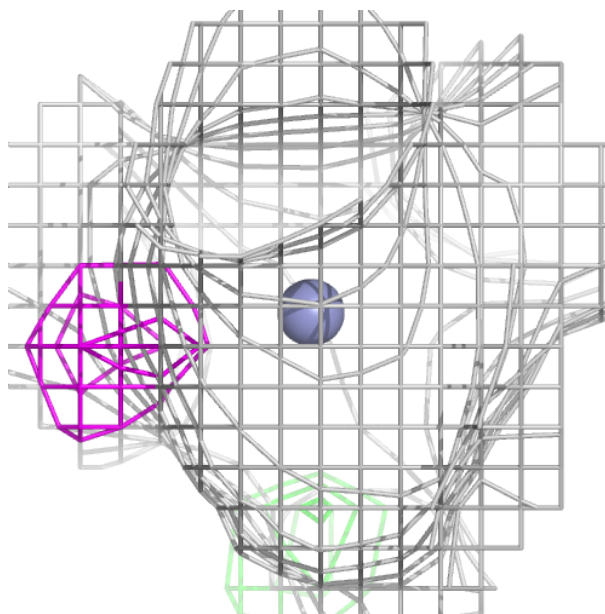
Electron density around CA A 306:

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and green (positive)



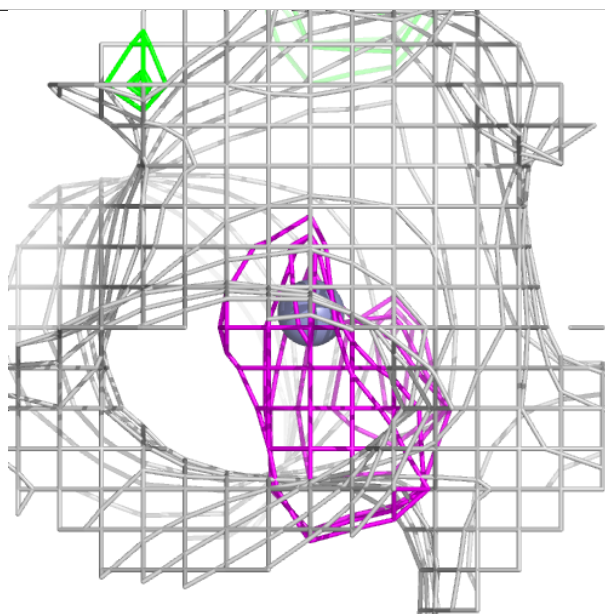
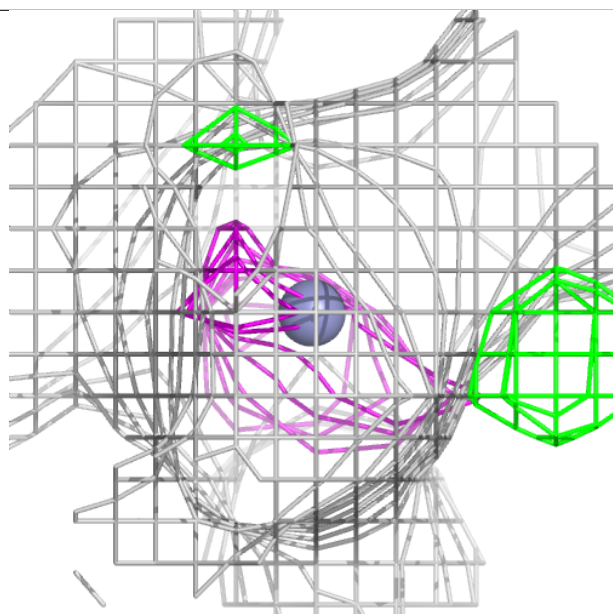
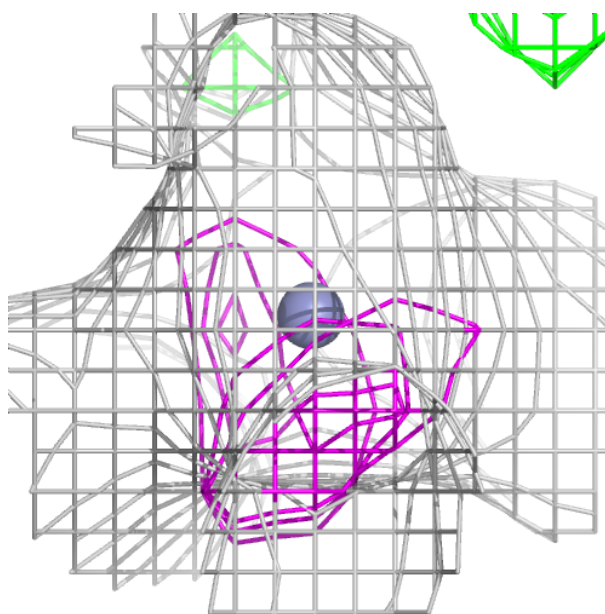
Electron density around ZN C 301:

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and green (positive)



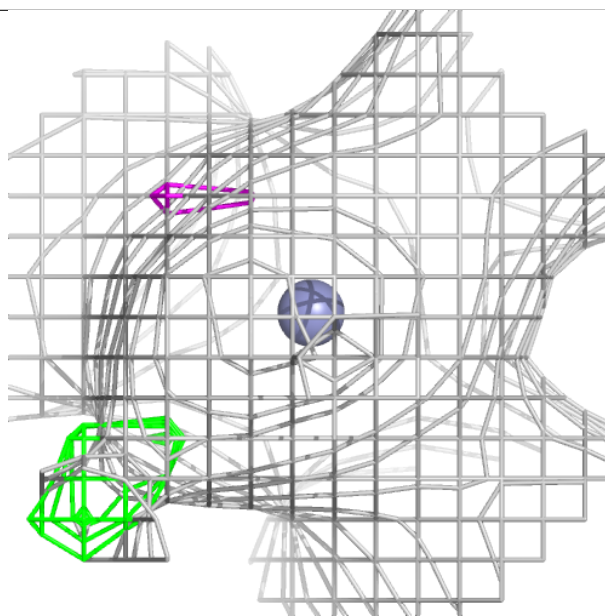
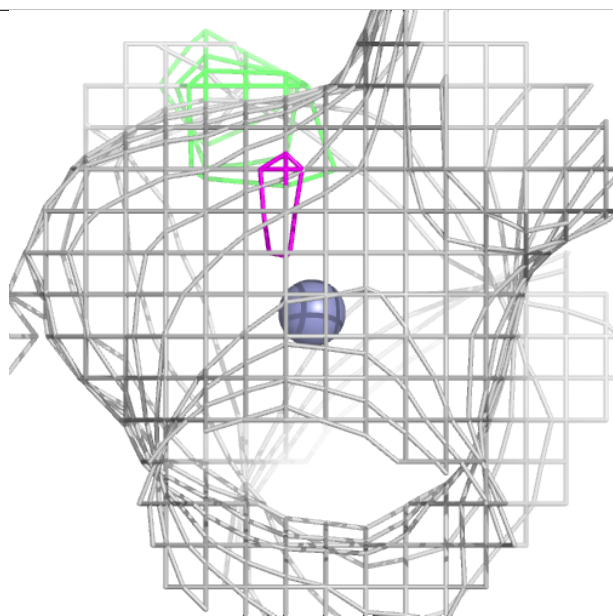
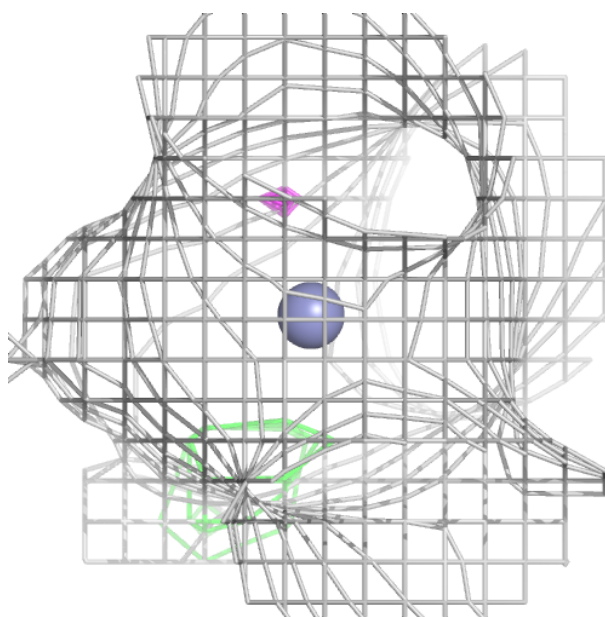
Electron density around ZN D 301:

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



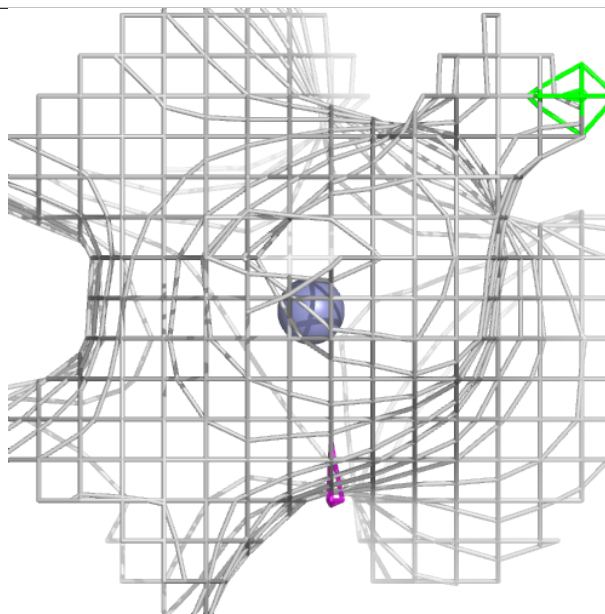
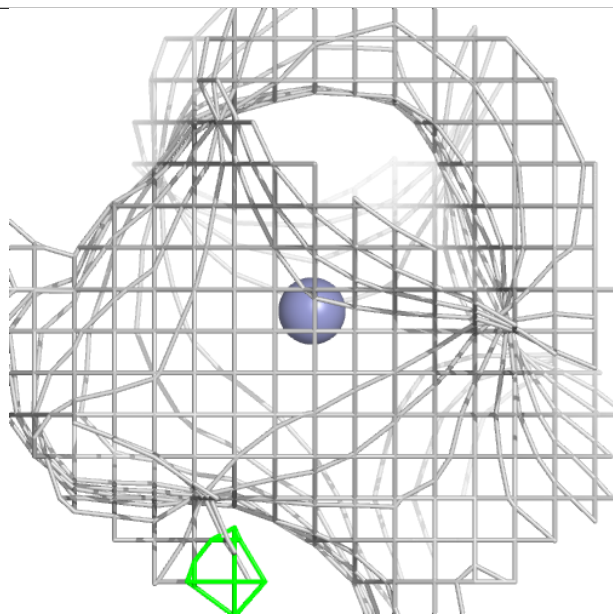
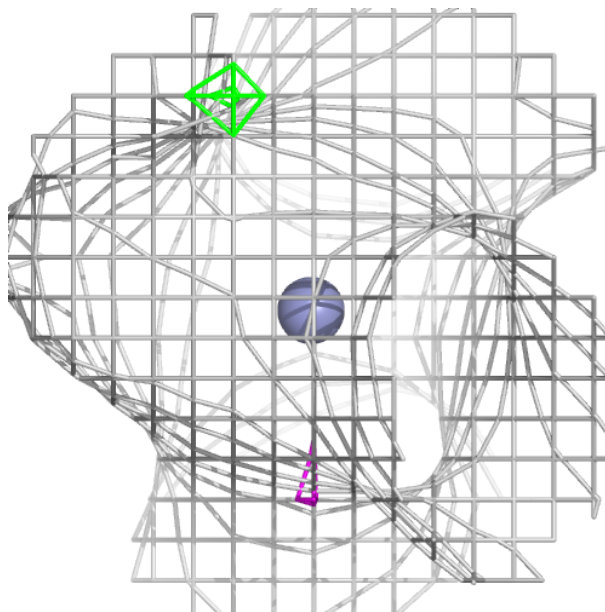
Electron density around ZN F 301:

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



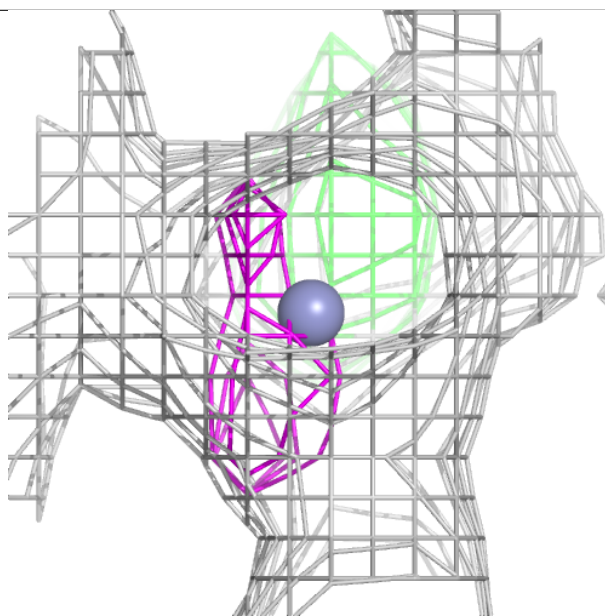
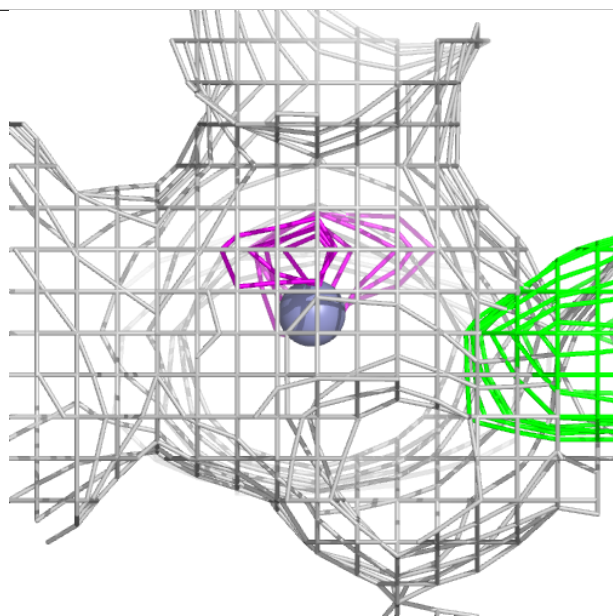
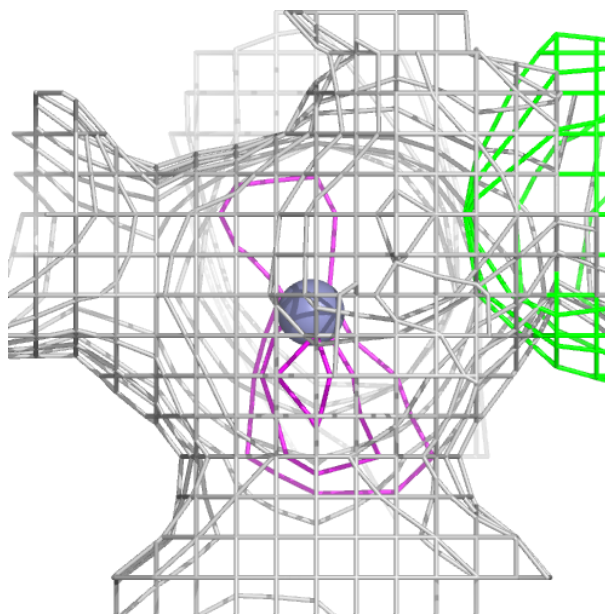
Electron density around ZN E 301:

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



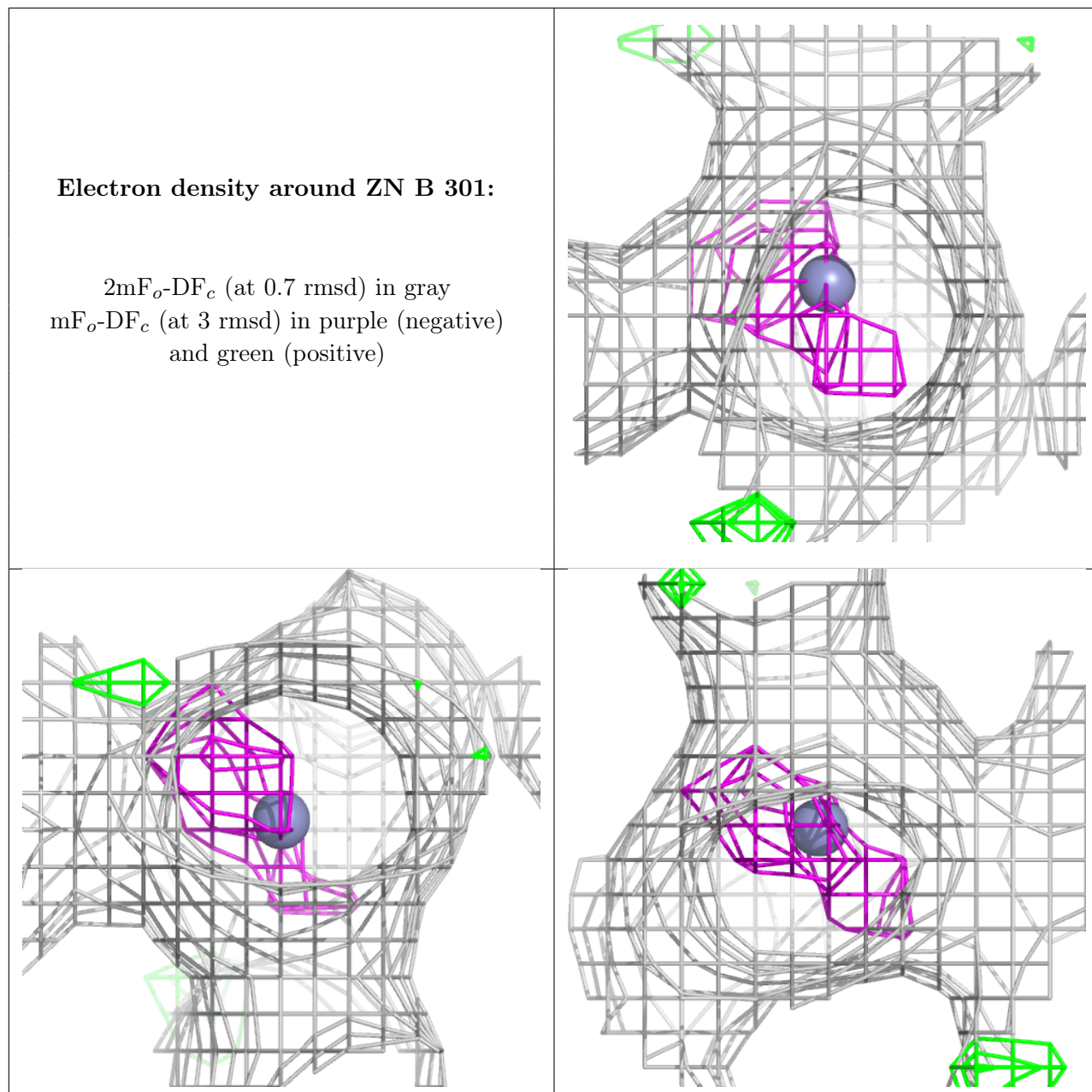
Electron density around ZN A 301:

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



Electron density around ZN B 301:

$2mF_o-DF_c$ (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.