



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:20 PM UTC

PDB ID : 8XV7 / pdb_00008xv7
Title : Crystal structure of TTD-PHD domain of UHRF1 in complex with hStella peptide (residues 75-121)
Authors : Du, X.; Gan, Q.; Xu, J.; Liu, J.
Deposited on : 2024-01-14
Resolution : 2.25 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

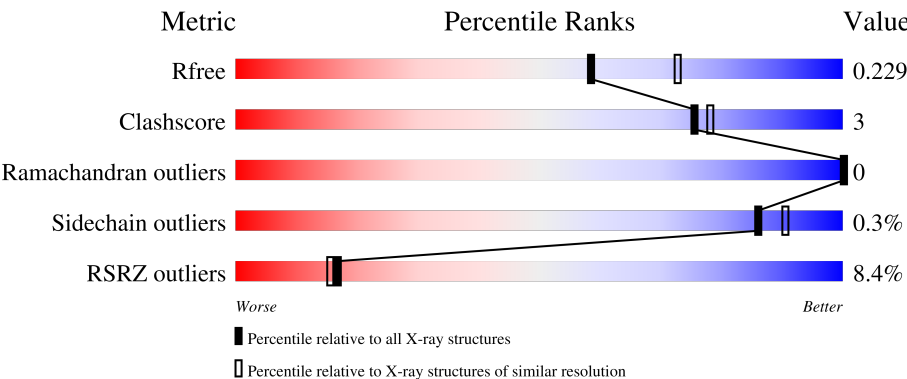
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	229	4% 93% 6%
1	C	229	14% 93% 6%
1	E	229	9% 90% 6%
1	G	229	3% 92% 5%
2	B	47	9% 66% 6% 26%

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Mol	Chain	Length	Quality of chain
2	D	47	4%47%6%47%
2	F	47	13%64%9%28%
2	H	47	6%47%. .49%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8594 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 E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1829	1132	330	348	19			
1	C	227	Total	C	N	O	S	0	0	0
			1829	1132	330	348	19			
1	E	221	Total	C	N	O	S	0	0	0
			1786	1105	324	339	18			
1	G	218	Total	C	N	O	S	0	0	0
			1769	1094	318	338	19			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	GLY	-	expression tag	UNP Q96T88
A	130	PRO	-	expression tag	UNP Q96T88
A	131	LEU	-	expression tag	UNP Q96T88
A	132	GLY	-	expression tag	UNP Q96T88
A	133	SER	-	expression tag	UNP Q96T88
A	?	-	SER	deletion	UNP Q96T88
A	?	-	ARG	deletion	UNP Q96T88
A	?	-	ASP	deletion	UNP Q96T88
A	?	-	GLU	deletion	UNP Q96T88
A	?	-	PRO	deletion	UNP Q96T88
A	?	-	CYS	deletion	UNP Q96T88
A	?	-	SER	deletion	UNP Q96T88
A	?	-	SER	deletion	UNP Q96T88
A	?	-	THR	deletion	UNP Q96T88
C	129	GLY	-	expression tag	UNP Q96T88
C	130	PRO	-	expression tag	UNP Q96T88
C	131	LEU	-	expression tag	UNP Q96T88
C	132	GLY	-	expression tag	UNP Q96T88
C	133	SER	-	expression tag	UNP Q96T88
C	?	-	SER	deletion	UNP Q96T88
C	?	-	ARG	deletion	UNP Q96T88

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP Q96T88
C	?	-	GLU	deletion	UNP Q96T88
C	?	-	PRO	deletion	UNP Q96T88
C	?	-	CYS	deletion	UNP Q96T88
C	?	-	SER	deletion	UNP Q96T88
C	?	-	SER	deletion	UNP Q96T88
C	?	-	THR	deletion	UNP Q96T88
E	129	GLY	-	expression tag	UNP Q96T88
E	130	PRO	-	expression tag	UNP Q96T88
E	131	LEU	-	expression tag	UNP Q96T88
E	132	GLY	-	expression tag	UNP Q96T88
E	133	SER	-	expression tag	UNP Q96T88
E	?	-	SER	deletion	UNP Q96T88
E	?	-	ARG	deletion	UNP Q96T88
E	?	-	ASP	deletion	UNP Q96T88
E	?	-	GLU	deletion	UNP Q96T88
E	?	-	PRO	deletion	UNP Q96T88
E	?	-	CYS	deletion	UNP Q96T88
E	?	-	SER	deletion	UNP Q96T88
E	?	-	SER	deletion	UNP Q96T88
E	?	-	THR	deletion	UNP Q96T88
G	129	GLY	-	expression tag	UNP Q96T88
G	130	PRO	-	expression tag	UNP Q96T88
G	131	LEU	-	expression tag	UNP Q96T88
G	132	GLY	-	expression tag	UNP Q96T88
G	133	SER	-	expression tag	UNP Q96T88
G	?	-	SER	deletion	UNP Q96T88
G	?	-	ARG	deletion	UNP Q96T88
G	?	-	ASP	deletion	UNP Q96T88
G	?	-	GLU	deletion	UNP Q96T88
G	?	-	PRO	deletion	UNP Q96T88
G	?	-	CYS	deletion	UNP Q96T88
G	?	-	SER	deletion	UNP Q96T88
G	?	-	SER	deletion	UNP Q96T88
G	?	-	THR	deletion	UNP Q96T88

- Molecule 2 is a protein called Developmental pluripotency-associated protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	35	Total	C	N	O	S	0	0	0
			298	187	61	48	2			
2	D	25	Total	C	N	O	S	0	0	0
			204	128	42	32	2			

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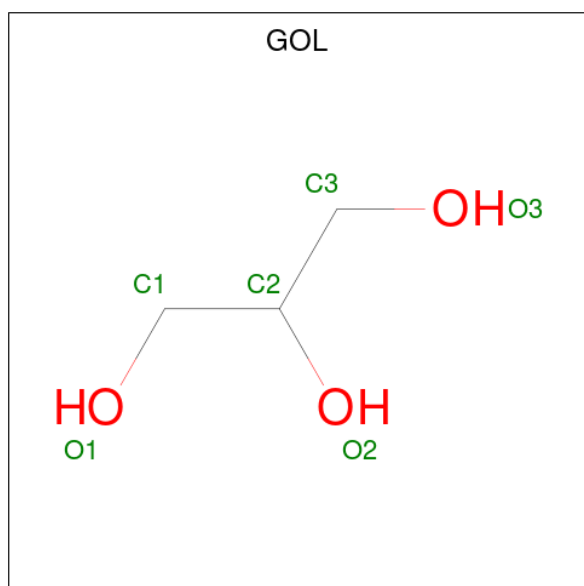
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	34	Total	C	N	O	S	0	0	0
			289	181	58	48	2			
2	H	24	Total	C	N	O	S	0	0	0
			190	120	38	30	2			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		
3	C	3	Total	Zn	0	0
			3	3		
3	E	3	Total	Zn	0	0
			3	3		
3	F	1	Total	Zn	0	0
			1	1		
3	G	4	Total	Zn	0	0
			4	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



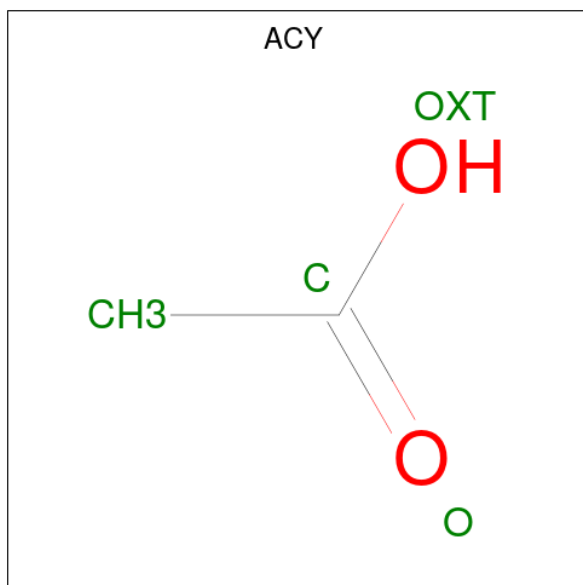
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	129	Total	O	0	0
			129	129		
6	B	15	Total	O	0	0
			15	15		
6	C	48	Total	O	0	0
			48	48		
6	D	3	Total	O	0	0
			3	3		
6	E	75	Total	O	0	0
			75	75		
6	F	8	Total	O	0	0
			8	8		
6	G	79	Total	O	0	0
			79	79		

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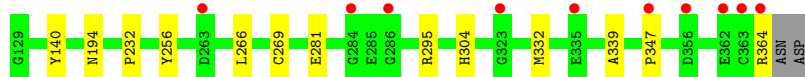
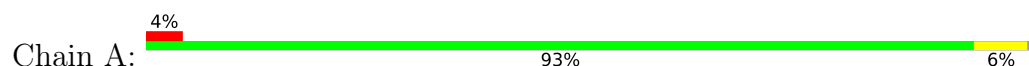
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	13	Total 13	O 13	0	0

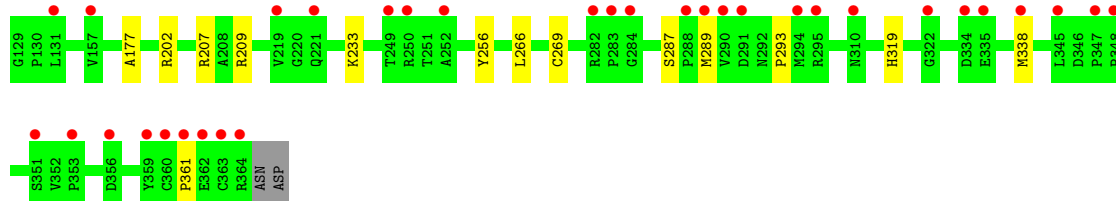
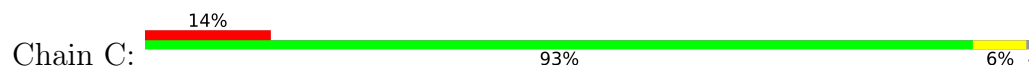
3 Residue-property plots [i](#)

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: E3 ubiquitin-protein ligase UHRF1



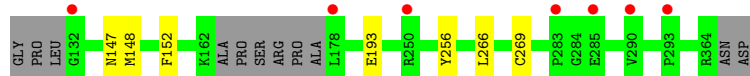
- Molecule 1: E3 ubiquitin-protein ligase UHRF1



- Molecule 1: E3 ubiquitin-protein ligase UHRF1

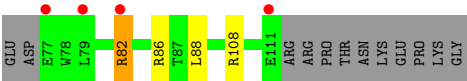


- Molecule 1: E3 ubiquitin-protein ligase UHRF1

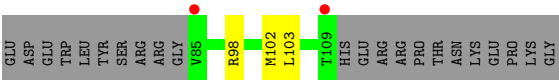


- Molecule 2: Developmental pluripotency-associated protein 3

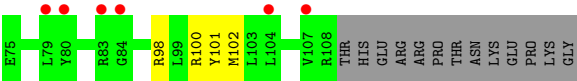




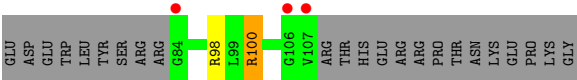
● Molecule 2: Developmental pluripotency-associated protein 3



● Molecule 2: Developmental pluripotency-associated protein 3



● Molecule 2: Developmental pluripotency-associated protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	153.55Å 153.55Å 61.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.25 30.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.25) 99.9 (30.00-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.193 , 0.226 0.199 , 0.229	Depositor DCC
R_{free} test set	3682 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.026 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8594	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: ZN, ACY, 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	0.52	0/1870	0.83	0/2532
1	C	0.49	0/1870	0.80	0/2532
1	E	0.52	0/1823	0.81	0/2463
1	G	0.50	0/1806	0.81	0/2441
2	B	0.49	0/302	0.81	0/402
2	D	0.52	0/204	0.88	0/270
2	F	0.49	0/292	0.80	0/388
2	H	0.51	0/190	0.81	0/251
All	All	0.51	0/8357	0.81	0/11279

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
1	C	0	1
2	B	0	1
2	F	0	2
2	H	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	364	ARG	Sidechain
2	B	82	ARG	Sidechain
1	C	202	ARG	Sidechain
2	F	100	ARG	Sidechain
2	F	98	ARG	Sidechain
2	H	100	ARG	Sidechain
2	H	98	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	1829	0	1745	22	0
1	C	1829	0	1745	10	0
1	E	1786	0	1702	11	0
1	G	1769	0	1681	8	0
2	B	298	0	313	6	0
2	D	204	0	230	2	0
2	F	289	0	303	2	0
2	H	190	0	213	1	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
3	G	4	0	0	0	0
4	A	12	0	16	4	0
5	A	4	0	3	0	0
6	A	129	0	0	2	0
6	B	15	0	0	0	0
6	C	48	0	0	1	0
6	D	3	0	0	0	0
6	E	75	0	0	0	0
6	F	8	0	0	0	0
6	G	79	0	0	1	0
6	H	13	0	0	0	0
All	All	8594	0	7951	48	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 (48) 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:G:193:GLU:OE2	6:G:501:HOH:O	1.67	1.08
1:A:332:MET:HE1	1:A:339:ALA:CB	1.99	0.91
1:A:332:MET:HE1	1:A:339:ALA:HB2	1.62	0.80
1:A:281:GLU:O	6:A:501:HOH:O	1.98	0.80
1:C:289:MET:HE3	1:C:293:PRO:HA	1.65	0.78
2:F:102:MET:HA	2:F:102:MET:HE2	1.71	0.71
2:D:98:ARG:HG3	2:D:102:MET:HE3	1.78	0.65
1:E:177:ALA:O	1:E:178:LEU:HG	1.97	0.64
1:G:148:MET:HE1	2:H:100:ARG:HG3	1.81	0.63
1:A:332:MET:HE1	1:A:339:ALA:HB1	1.77	0.62
1:C:319:HIS:ND1	1:C:338:MET:HE2	2.14	0.62
1:A:140:TYR:CD1	4:A:404:GOL:H32	2.35	0.61
1:A:194:ASN:HD21	2:B:108:ARG:HH11	1.48	0.61
1:A:332:MET:HE3	2:B:88:LEU:N	2.15	0.60
1:A:332:MET:HE3	2:B:88:LEU:CA	2.32	0.59
2:B:82:ARG:HH12	2:B:86:ARG:HA	1.69	0.58
1:A:140:TYR:CE1	4:A:404:GOL:H32	2.39	0.57
1:A:347:PRO:O	6:A:502:HOH:O	2.17	0.57
1:A:304:HIS:NE2	1:E:183:ILE:HD12	2.21	0.56
1:A:304:HIS:CD2	1:E:183:ILE:HD12	2.42	0.55
1:E:233:LYS:HA	1:E:272:ILE:HD11	1.88	0.54
1:G:266:LEU:HB3	1:G:269:CYS:SG	2.48	0.53
1:A:304:HIS:CE1	1:E:183:ILE:HD12	2.45	0.52
1:A:266:LEU:HB3	1:A:269:CYS:SG	2.50	0.51
1:A:295:ARG:HD2	4:A:405:GOL:H31	1.93	0.51
1:E:164:PRO:HD3	1:E:179:GLU:O	2.10	0.51
1:C:177:ALA:HA	2:F:101:TYR:CD2	2.46	0.50
1:G:148:MET:HE3	1:G:152:PHE:CE2	2.45	0.50
1:E:266:LEU:HB3	1:E:269:CYS:SG	2.53	0.49
1:A:332:MET:CE	1:A:339:ALA:CB	2.83	0.48
1:E:148:MET:HE1	1:E:237:PHE:CD2	2.49	0.47
1:A:332:MET:HE3	2:B:88:LEU:HB2	1.96	0.47
1:C:266:LEU:HB3	1:C:269:CYS:SG	2.54	0.47
1:C:361:PRO:HA	6:C:535:HOH:O	2.14	0.46
1:A:332:MET:CE	2:B:88:LEU:HB2	2.46	0.45
1:C:207:ARG:HG2	1:C:289:MET:HE1	1.99	0.43
1:C:256:TYR:HA	1:C:269:CYS:O	2.19	0.43
1:A:256:TYR:HA	1:A:269:CYS:O	2.19	0.42
1:C:233:LYS:H	1:G:147:ASN:HD21	1.66	0.42
1:G:256:TYR:HA	1:G:269:CYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:TYR:HA	1:E:269:CYS:O	2.19	0.42
1:A:140:TYR:CE1	4:A:404:GOL:C3	3.03	0.41
1:G:148:MET:HE3	1:G:152:PHE:HE2	1.85	0.41
1:A:304:HIS:CD2	1:E:183:ILE:CD1	3.04	0.41
1:C:209:ARG:NH1	1:C:287:SER:O	2.53	0.41
2:D:103:LEU:HD21	1:G:193:GLU:HG2	2.03	0.41
1:C:319:HIS:HD1	1:C:338:MET:HE2	1.82	0.40
1:A:232:PRO:HD2	1:E:147:ASN:CG	2.47	0.40

There are no symmetry-related clashes.

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	225/229 (98%)	220 (98%)	5 (2%)	0	100	100
1	C	225/229 (98%)	220 (98%)	5 (2%)	0	100	100
1	E	215/229 (94%)	210 (98%)	5 (2%)	0	100	100
1	G	214/229 (93%)	209 (98%)	5 (2%)	0	100	100
2	B	33/47 (70%)	33 (100%)	0	0	100	100
2	D	23/47 (49%)	23 (100%)	0	0	100	100
2	F	32/47 (68%)	31 (97%)	1 (3%)	0	100	100
2	H	22/47 (47%)	22 (100%)	0	0	100	100
All	All	989/1104 (90%)	968 (98%)	21 (2%)	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	203/205 (99%)	203 (100%)	0	100	100
1	C	203/205 (99%)	203 (100%)	0	100	100
1	E	197/205 (96%)	194 (98%)	3 (2%)	57	68
1	G	197/205 (96%)	197 (100%)	0	100	100
2	B	31/42 (74%)	31 (100%)	0	100	100
2	D	22/42 (52%)	22 (100%)	0	100	100
2	F	30/42 (71%)	30 (100%)	0	100	100
2	H	20/42 (48%)	20 (100%)	0	100	100
All	All	903/988 (91%)	900 (100%)	3 (0%)	86	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	178	LEU
1	E	292	ASN
1	E	311	ARG

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	194	ASN
1	A	267	ASN
2	B	110	HIS
1	C	267	ASN
1	C	292	ASN
1	E	194	ASN
1	E	267	ASN
1	G	147	ASN
1	G	194	ASN
1	G	267	ASN
1	G	330	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 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 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	GOL	A	404	-	5,5,5	0.11	0	5,5,5	0.29	0
5	ACY	A	406	-	3,3,3	1.19	0	3,3,3	0.66	0
4	GOL	A	405	-	5,5,5	0.17	0	5,5,5	0.50	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	A	404	-	-	2/4/4/4	-
4	GOL	A	405	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

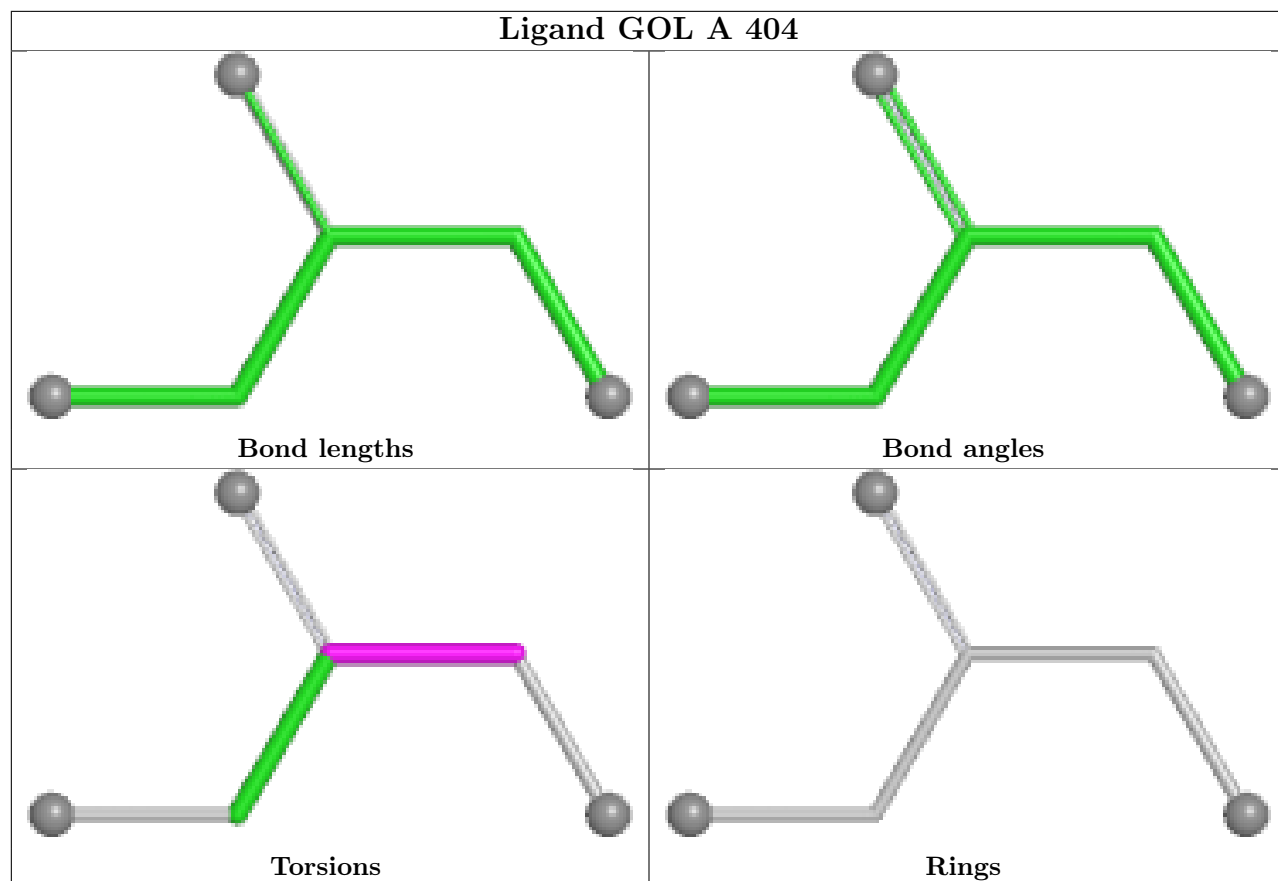
Mol	Chain	Res	Type	Atoms
4	A	404	GOL	O1-C1-C2-C3
4	A	405	GOL	O1-C1-C2-C3
4	A	404	GOL	O1-C1-C2-O2
4	A	405	GOL	O1-C1-C2-O2

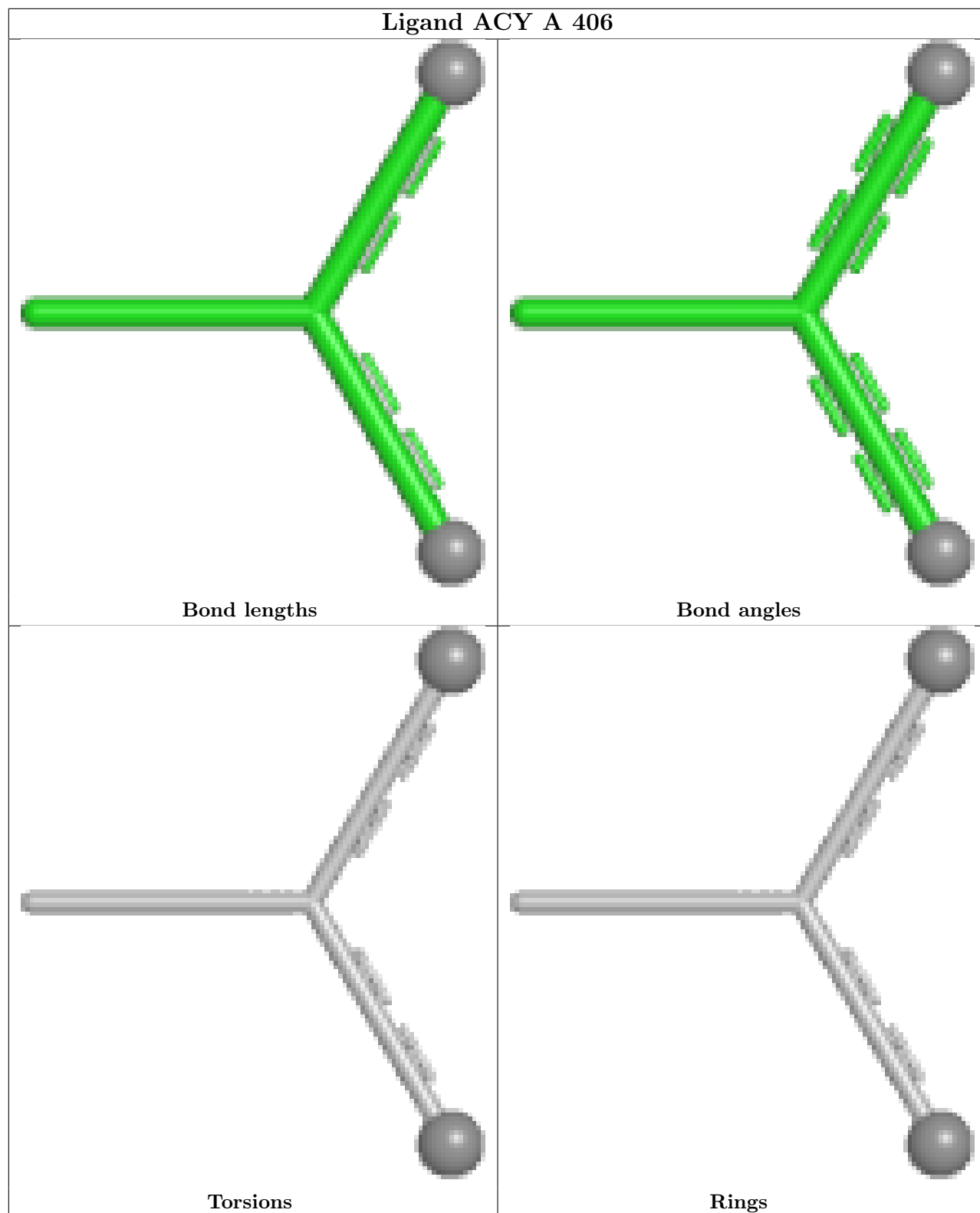
There are no ring outliers.

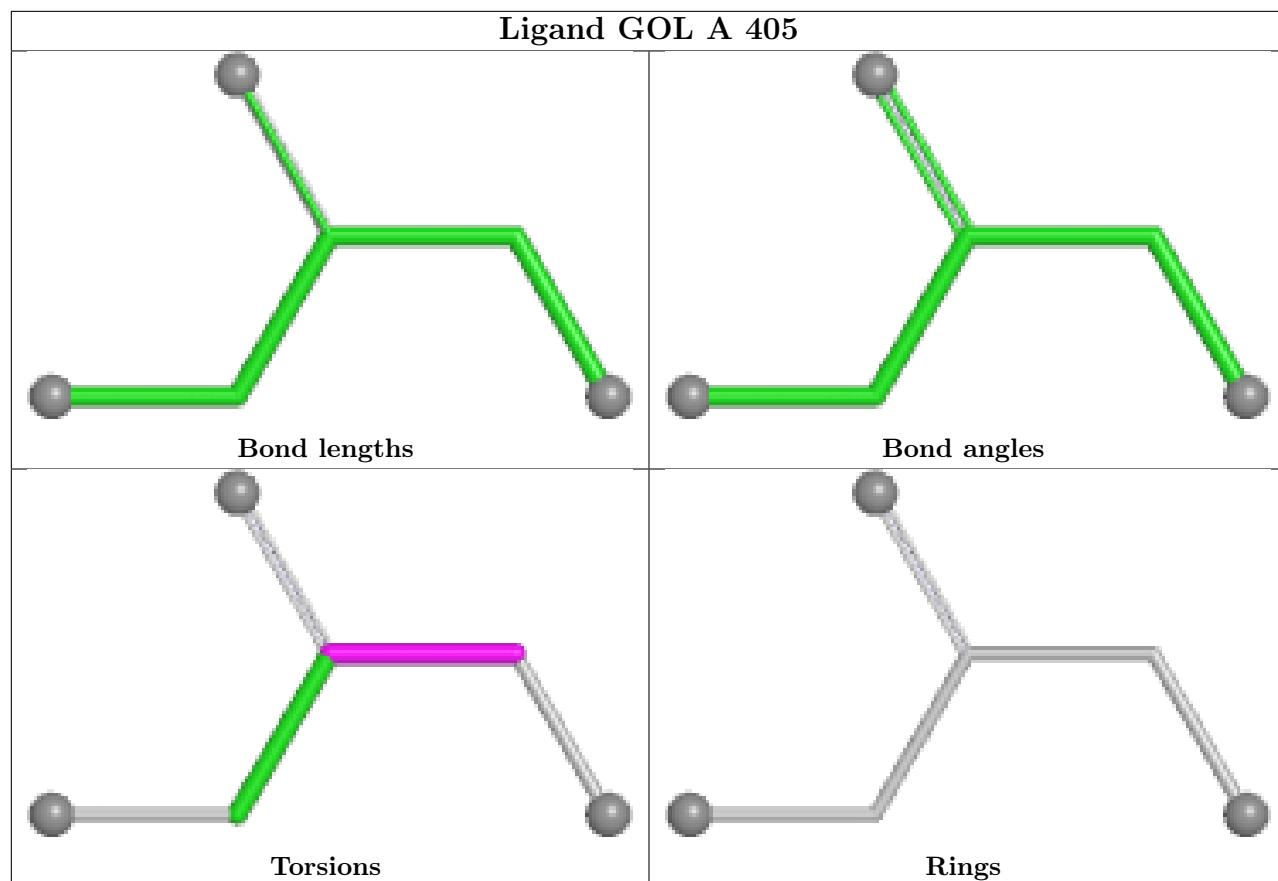
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	GOL	3	0
4	A	405	GOL	1	0

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	227/229 (99%)	0.06	10 (4%) 39 38	21, 37, 73, 99	0
1	C	227/229 (99%)	0.91	33 (14%) 6 5	28, 53, 105, 131	0
1	E	221/229 (96%)	0.50	20 (9%) 15 14	23, 45, 93, 115	0
1	G	218/229 (95%)	0.06	7 (3%) 50 50	22, 39, 80, 112	0
2	B	35/47 (74%)	0.40	4 (11%) 10 9	25, 37, 90, 114	0
2	D	25/47 (53%)	0.30	2 (8%) 18 16	30, 44, 59, 81	0
2	F	34/47 (72%)	0.90	6 (17%) 4 3	29, 47, 97, 116	0
2	H	24/47 (51%)	0.25	3 (12%) 8 7	25, 33, 84, 99	0
All	All	1011/1104 (91%)	0.40	85 (8%) 17 15	21, 44, 92, 131	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	178	LEU	6.9
1	C	290	VAL	5.8
2	H	84	GLY	5.2
1	E	286	GLY	5.1
1	E	163	ALA	4.8
1	E	164	PRO	4.8
2	H	107	VAL	4.8
1	C	364	ARG	4.4
1	E	177	ALA	4.4
2	B	82	ARG	3.9
2	F	107	VAL	3.6
1	E	247	ARG	3.5
1	E	165	SER	3.5
1	C	361	PRO	3.4
1	G	178	LEU	3.4
2	F	84	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	109	THR	3.4
1	G	290	VAL	3.3
1	E	292	ASN	3.3
1	E	166	ARG	3.2
1	E	364	ARG	3.2
1	A	364	ARG	3.2
1	C	345	LEU	3.1
1	C	282	ARG	3.1
1	E	284	GLY	3.0
1	E	294	MET	3.0
2	F	80	TYR	3.0
1	C	359	TYR	3.0
1	C	284	GLY	3.0
1	C	294	MET	2.9
1	C	348	PRO	2.9
2	B	79	LEU	2.9
1	G	285	GLU	2.8
1	E	250	ARG	2.8
1	G	293	PRO	2.8
1	C	295	ARG	2.8
1	C	219	VAL	2.7
1	E	285	GLU	2.7
2	F	83	ARG	2.7
1	E	252	ALA	2.6
1	C	131	LEU	2.6
1	C	322	GLY	2.6
1	C	347	PRO	2.6
1	A	263	ASP	2.6
1	C	353	PRO	2.6
1	E	348	PRO	2.6
1	E	311	ARG	2.5
1	C	289	MET	2.5
1	C	288	PRO	2.5
1	G	132	GLY	2.5
2	F	79	LEU	2.5
1	C	291	ASP	2.5
1	E	303	LYS	2.5
1	C	221	GLN	2.5
1	C	363	CYS	2.5
1	C	249	THR	2.5
1	C	334	ASP	2.5
1	E	349	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	356	ASP	2.4
1	G	250	ARG	2.4
1	C	250	ARG	2.4
1	A	335	GLU	2.3
1	C	283	PRO	2.3
1	A	356	ASP	2.3
1	A	347	PRO	2.3
1	G	283	PRO	2.2
1	A	323	GLY	2.2
2	B	77	GLU	2.2
2	D	85	VAL	2.2
1	C	338	MET	2.2
1	C	335	GLU	2.2
2	B	111	GLU	2.2
2	H	106	GLY	2.2
1	C	310	ASN	2.1
1	E	251	THR	2.1
1	A	363	CYS	2.1
1	C	360	CYS	2.1
1	A	362	GLU	2.1
2	F	104	LEU	2.1
1	C	157	VAL	2.1
1	A	284	GLY	2.1
1	A	286	GLY	2.1
1	C	252	ALA	2.0
1	C	362	GLU	2.0
1	C	351	SER	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,

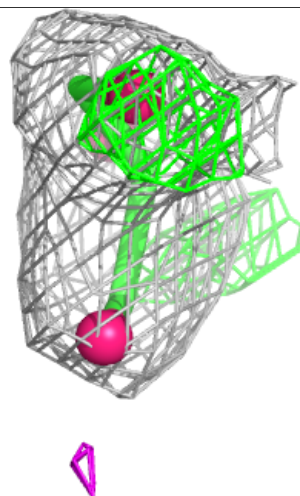
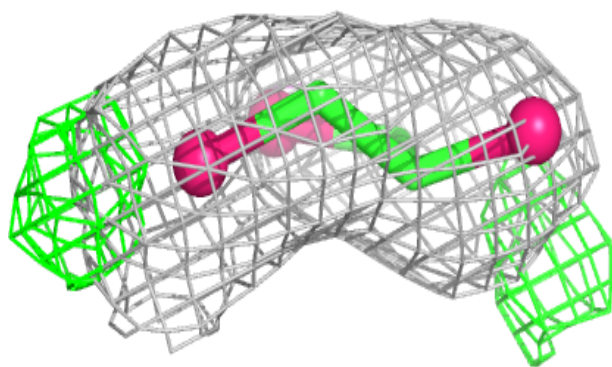
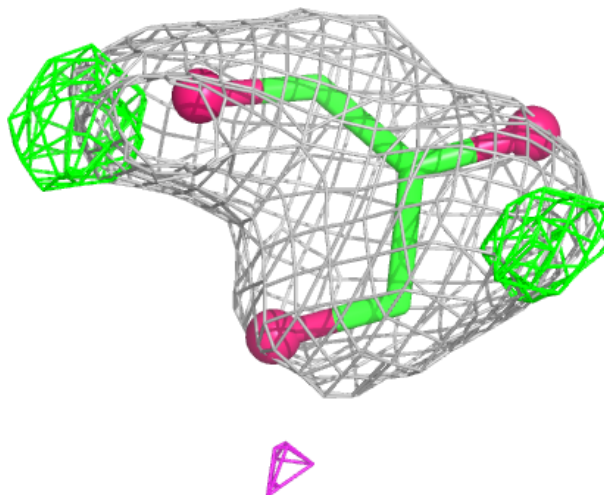
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	405	6/6	0.79	0.23	55,61,65,71	0
5	ACY	A	406	4/4	0.83	0.20	44,52,53,54	0
4	GOL	A	404	6/6	0.88	0.13	48,51,57,66	0
3	ZN	F	201	1/1	0.89	0.11	103,103,103,103	0
3	ZN	G	401	1/1	0.90	0.12	108,108,108,108	0
3	ZN	C	403	1/1	0.97	0.06	80,80,80,80	0
3	ZN	A	402	1/1	0.97	0.04	51,51,51,51	0
3	ZN	A	403	1/1	0.97	0.05	58,58,58,58	0
3	ZN	E	403	1/1	0.98	0.03	53,53,53,53	0
3	ZN	C	402	1/1	0.98	0.07	45,45,45,45	0
3	ZN	C	401	1/1	0.98	0.04	42,42,42,42	0
3	ZN	G	402	1/1	0.99	0.01	33,33,33,33	0
3	ZN	A	401	1/1	0.99	0.02	35,35,35,35	0
3	ZN	E	401	1/1	0.99	0.03	41,41,41,41	0
3	ZN	E	402	1/1	0.99	0.03	51,51,51,51	0
3	ZN	G	404	1/1	1.00	0.01	25,25,25,25	0
3	ZN	G	403	1/1	1.00	0.01	27,27,27,27	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.

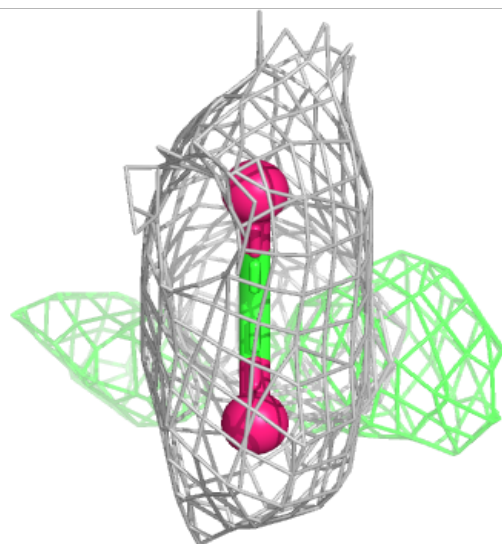
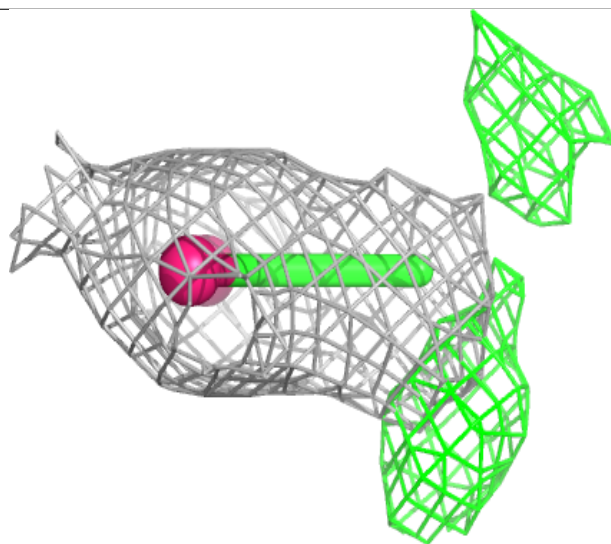
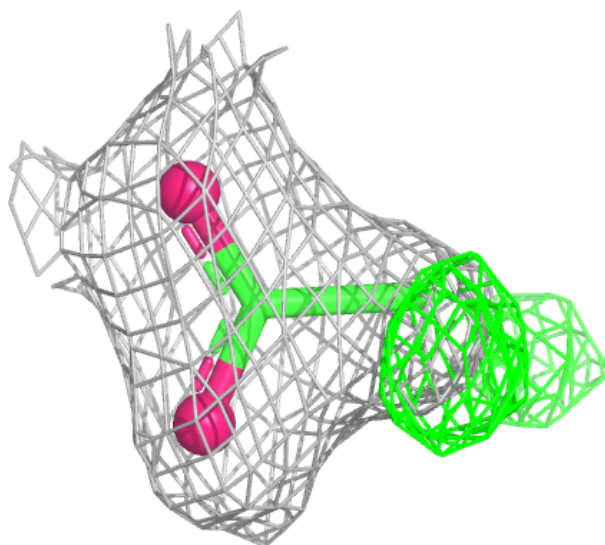
Electron density around GOL A 405:

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



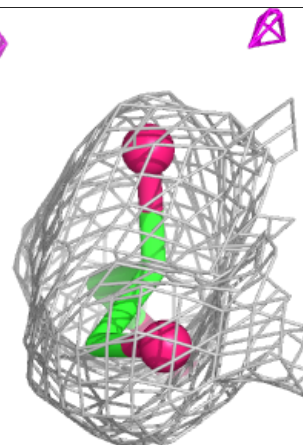
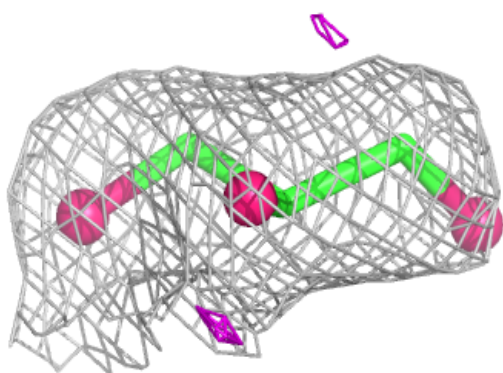
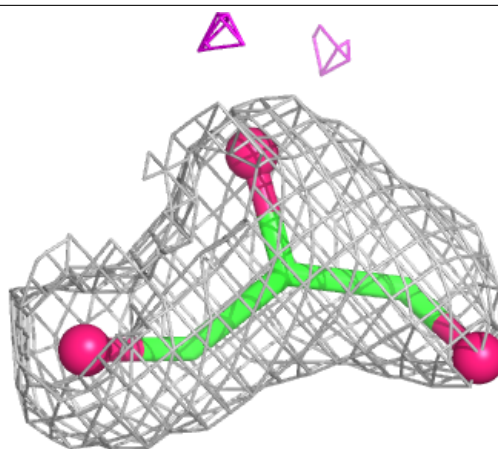
Electron density around ACY A 406:

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and green (positive)



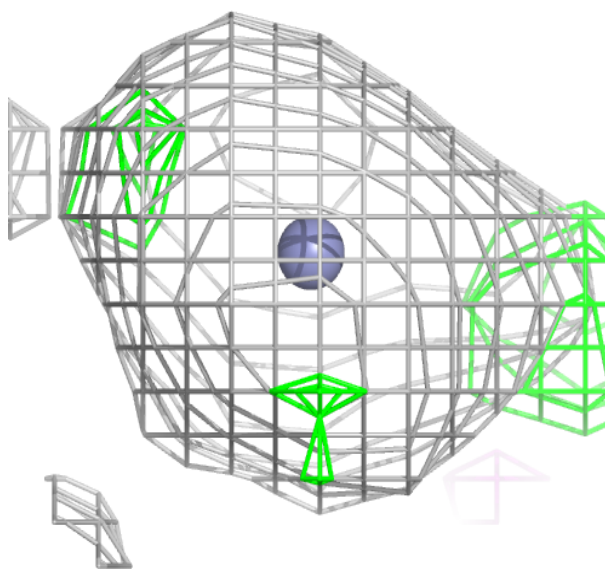
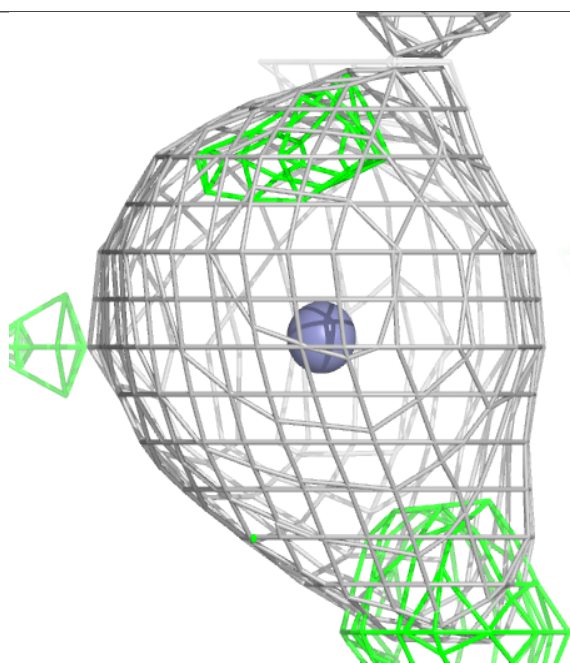
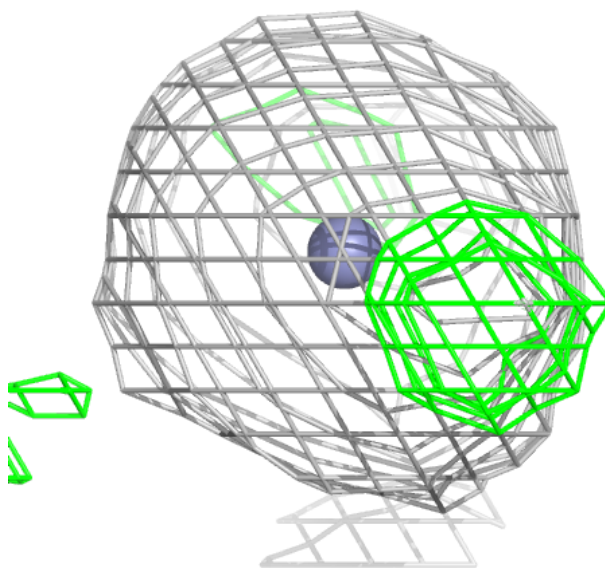
Electron density around GOL A 404:

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



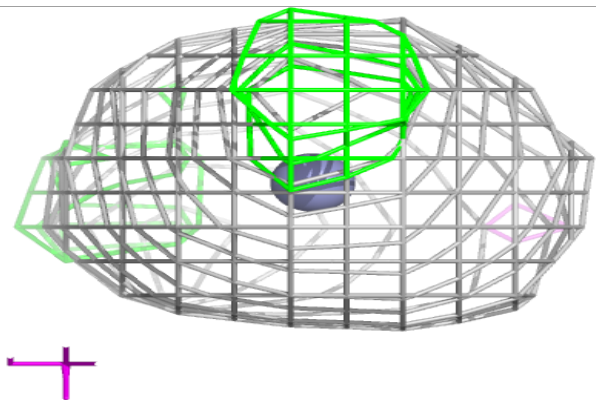
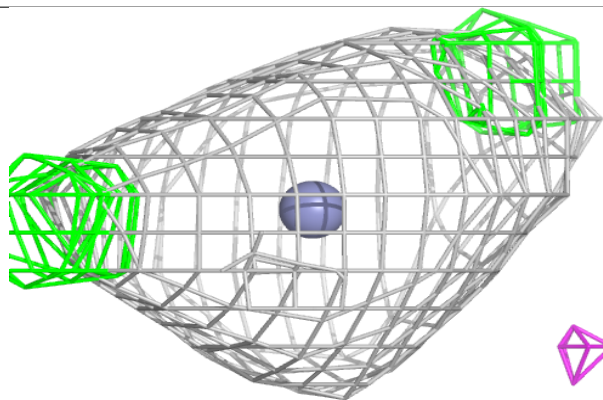
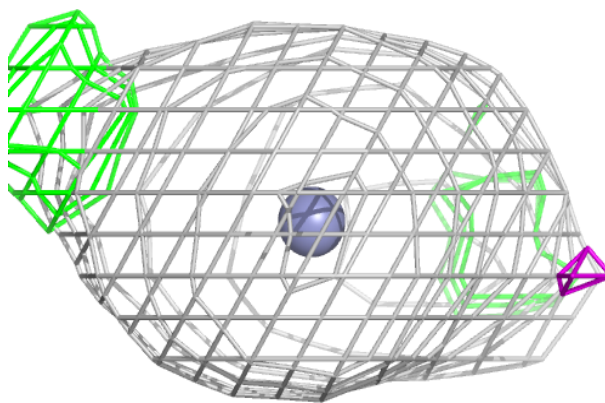
Electron density around ZN F 201:

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



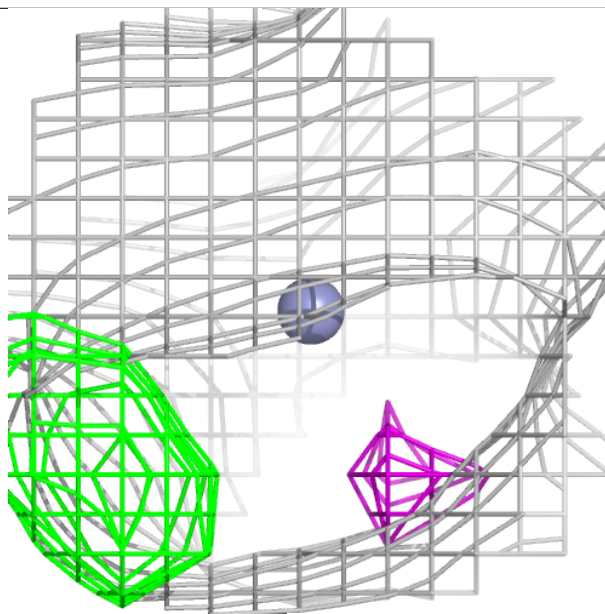
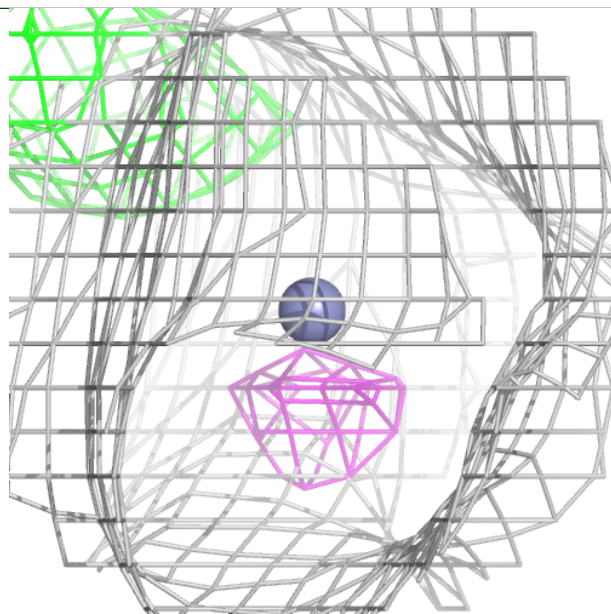
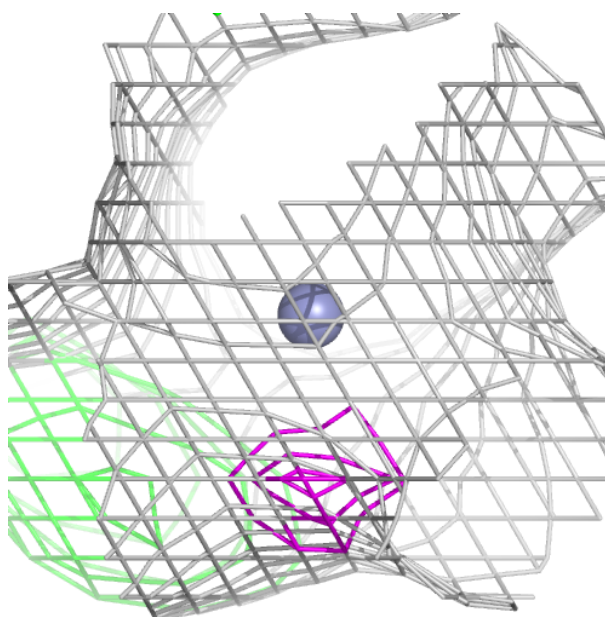
Electron density around ZN G 401:

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



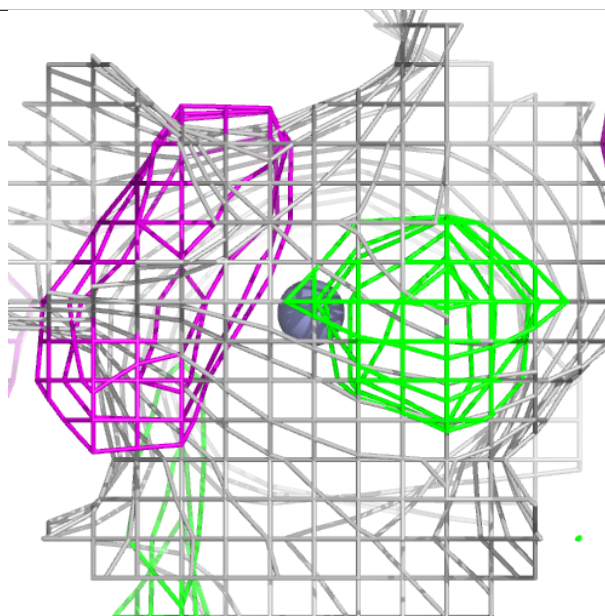
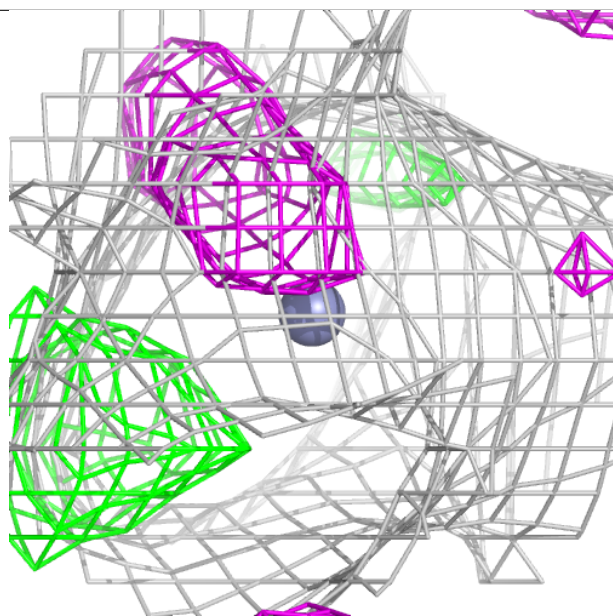
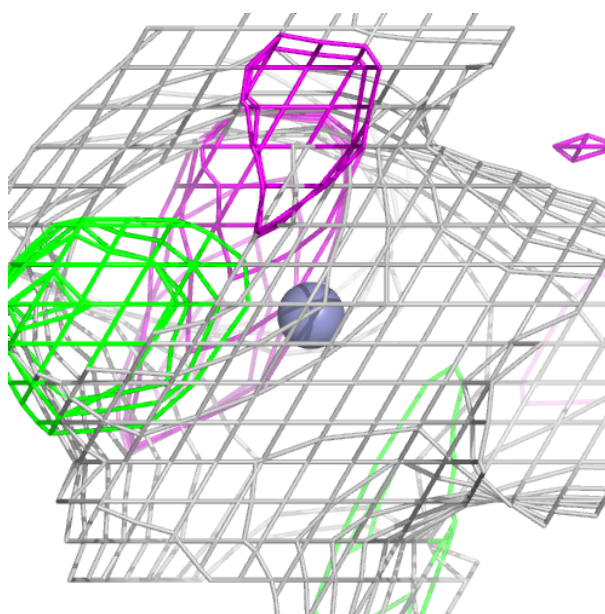
Electron density around ZN C 403:

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and green (positive)



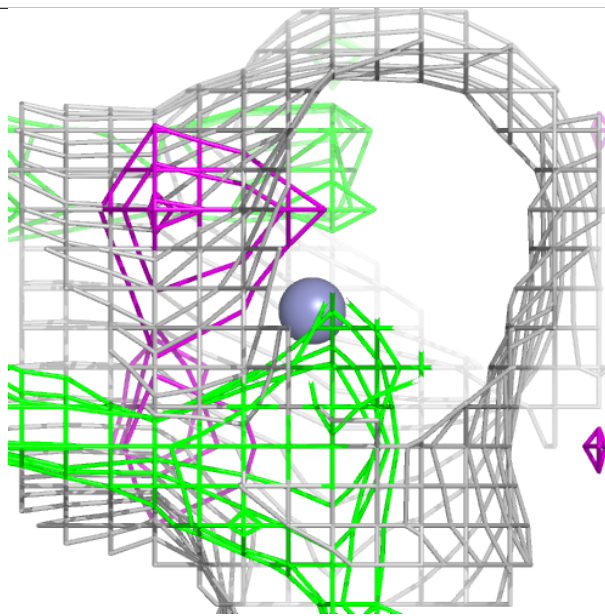
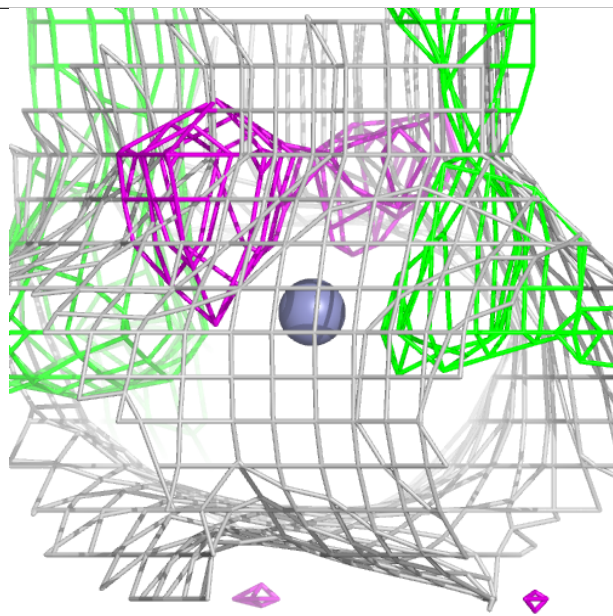
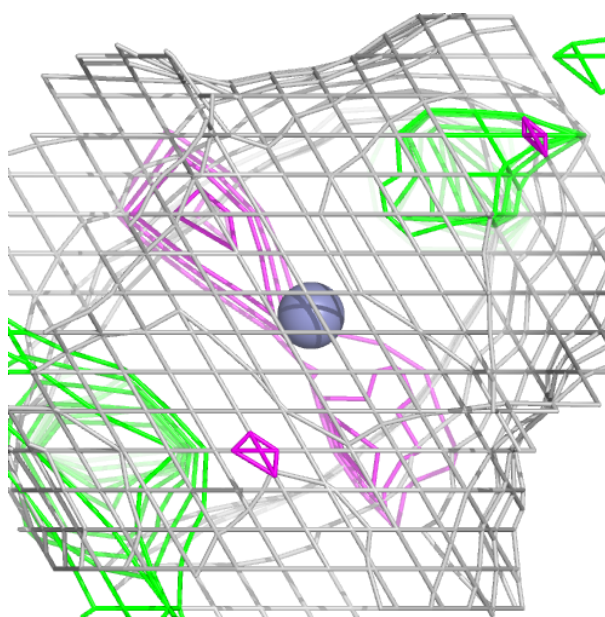
Electron density around ZN A 402:

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and green (positive)



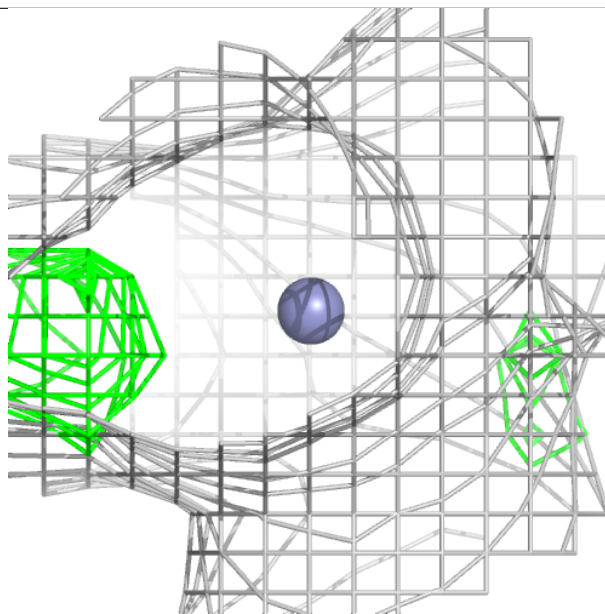
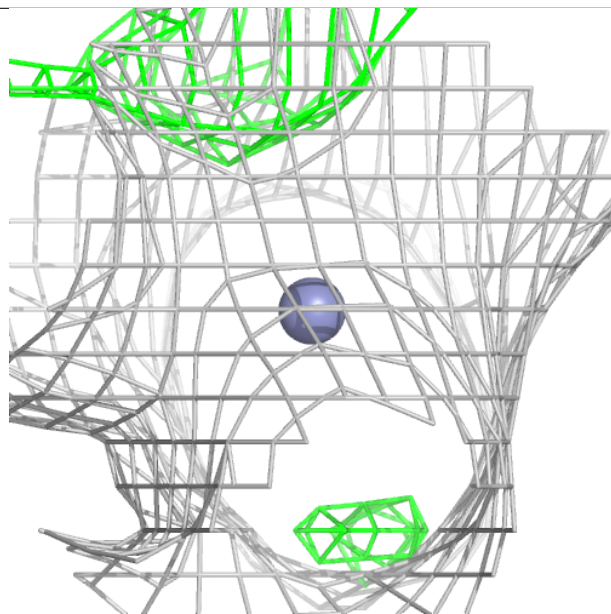
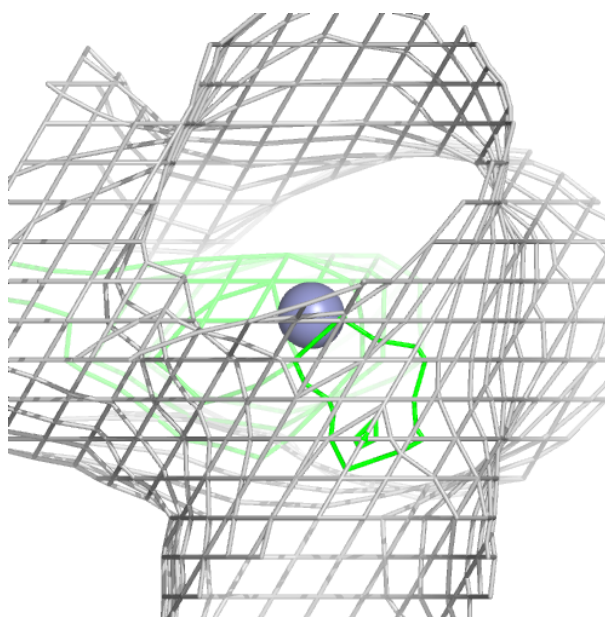
Electron density around ZN A 403:

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



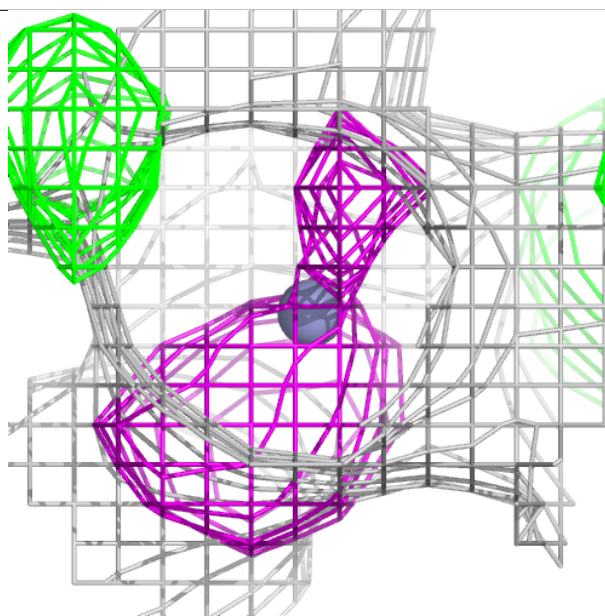
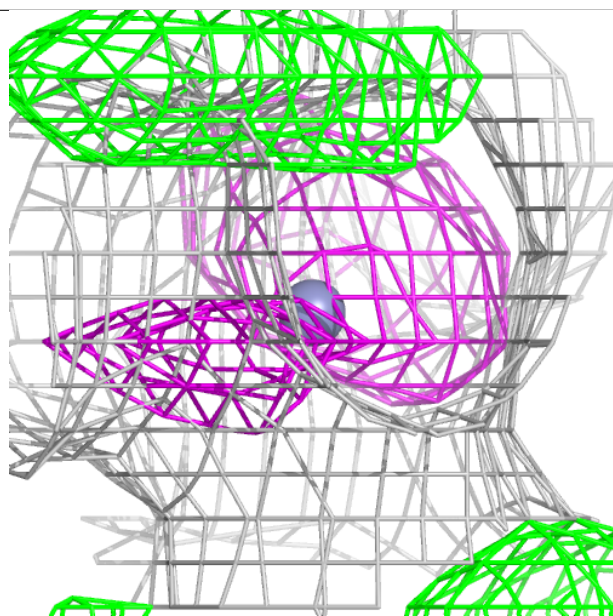
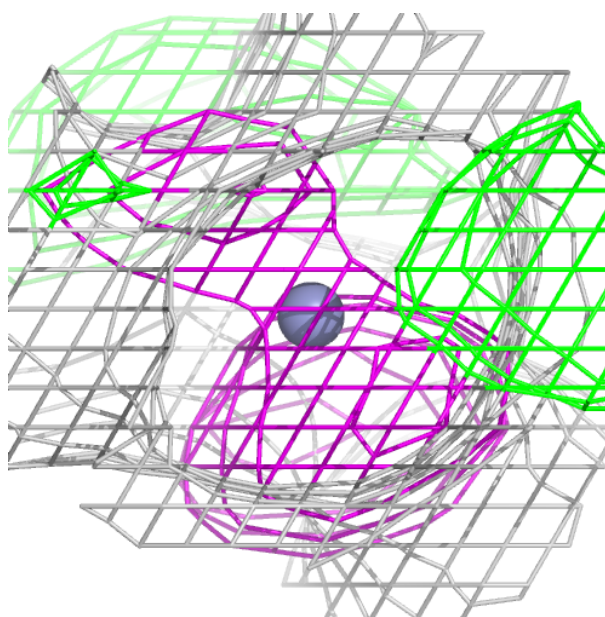
Electron density around ZN E 403:

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and green (positive)



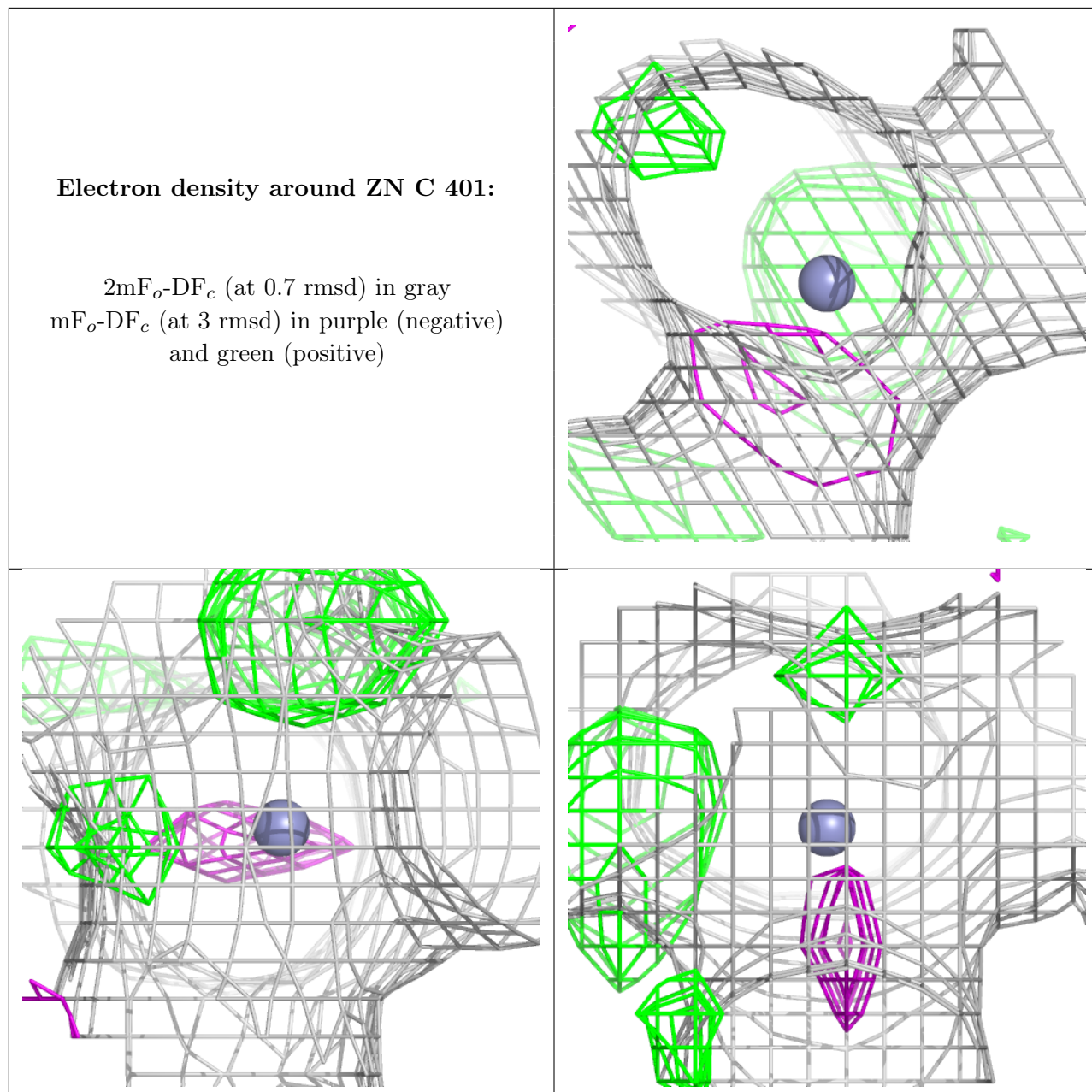
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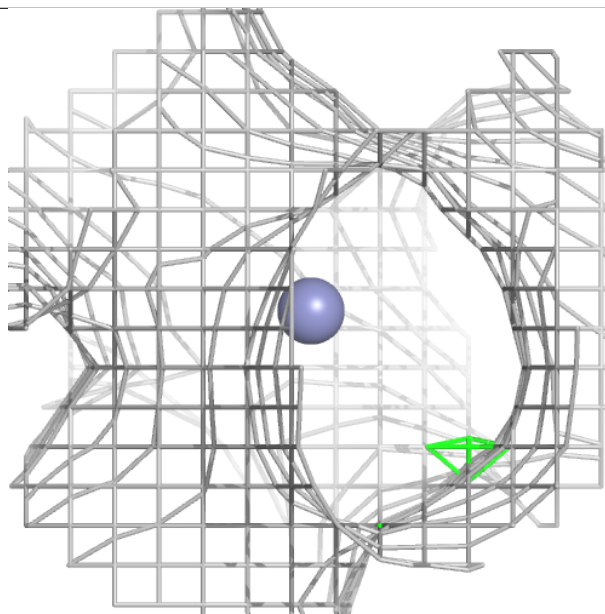
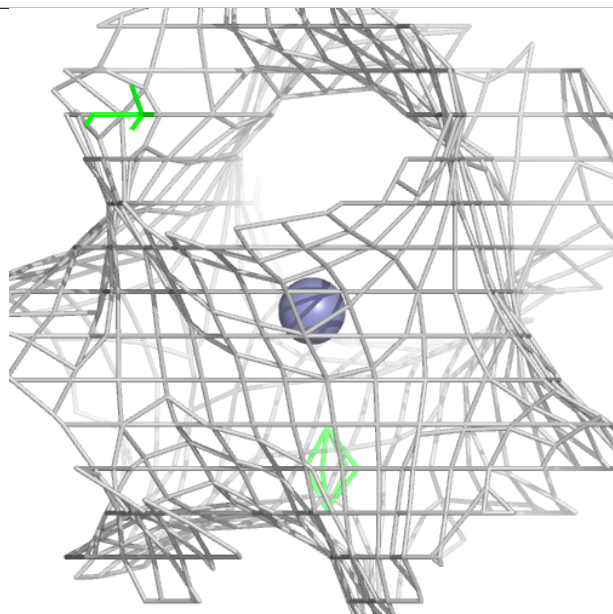
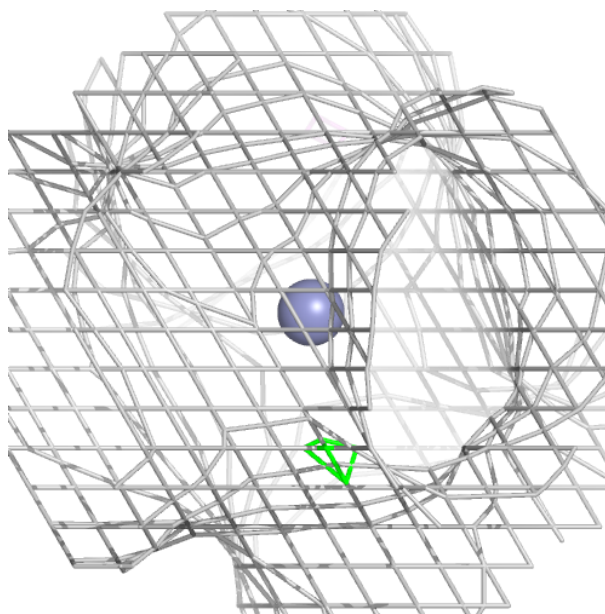
Electron density around ZN C 401:

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



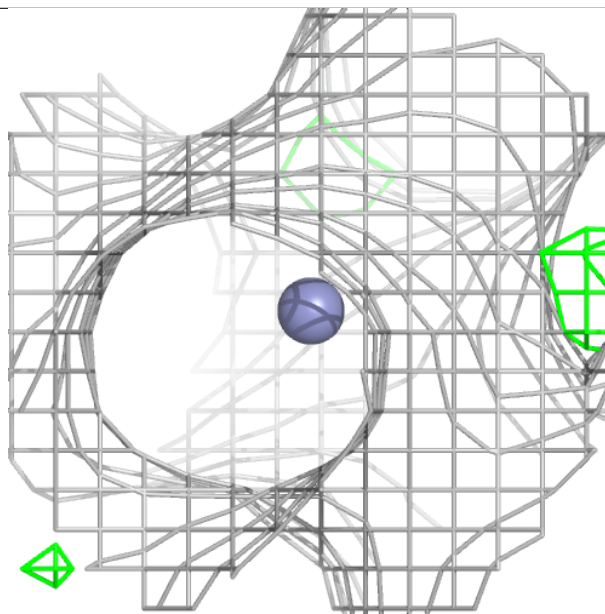
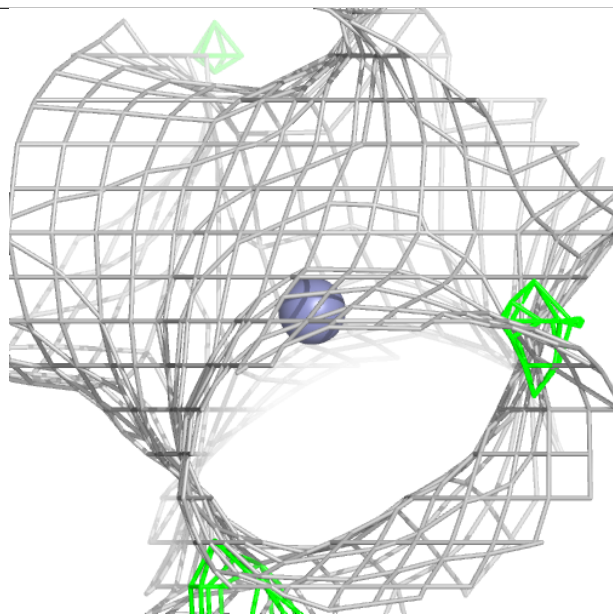
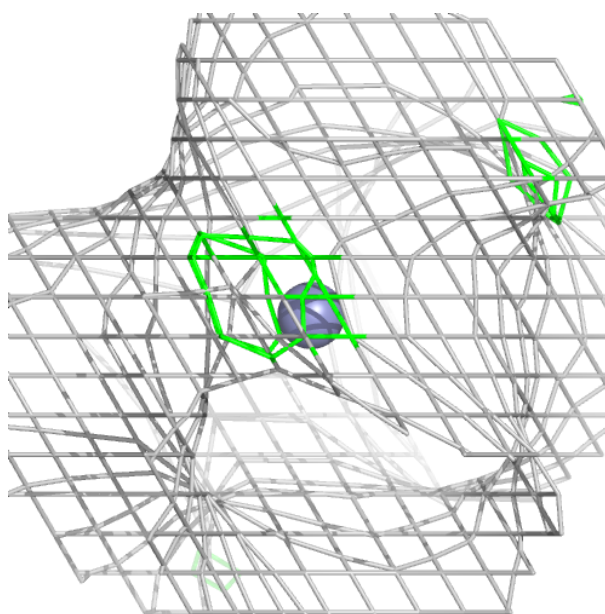
Electron density around ZN G 402:

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



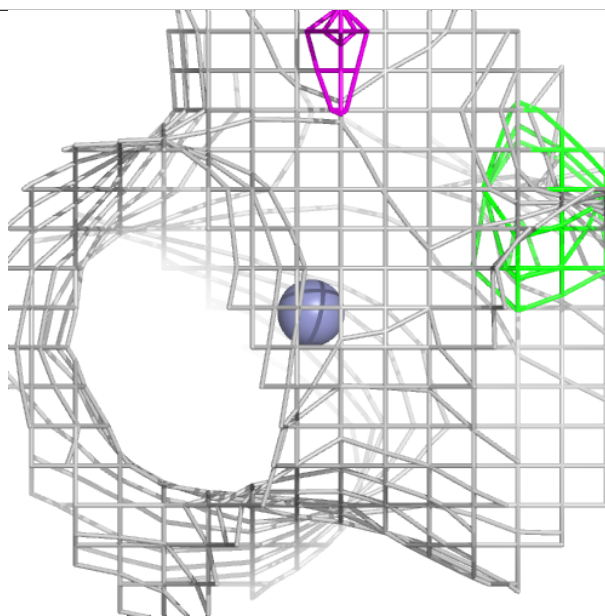
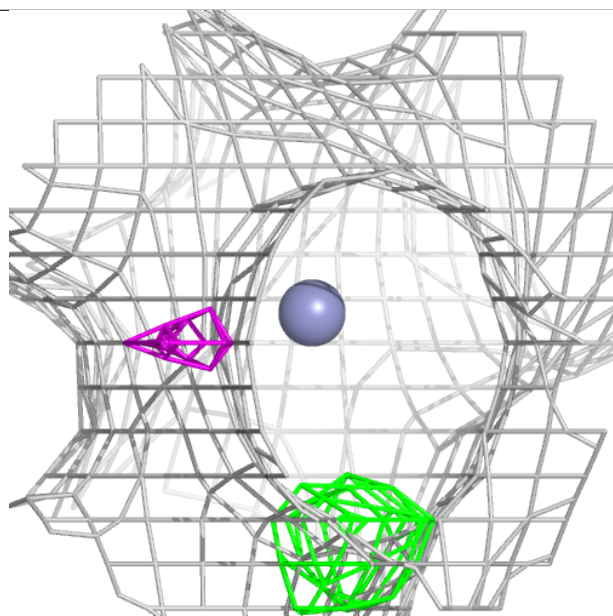
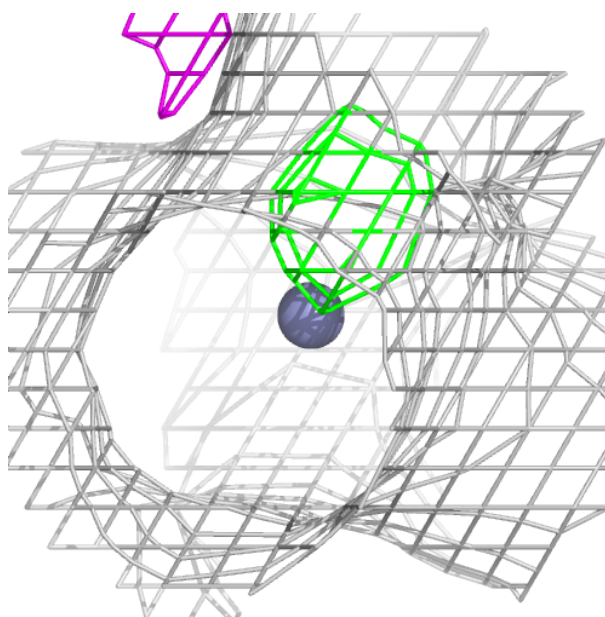
Electron density around ZN A 401:

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



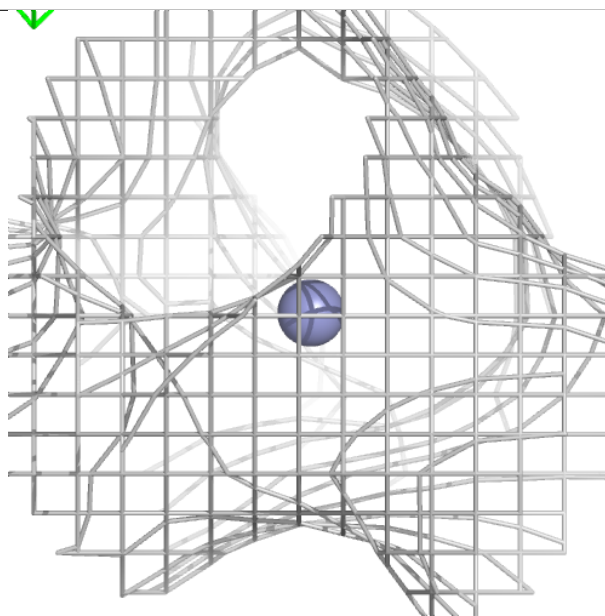
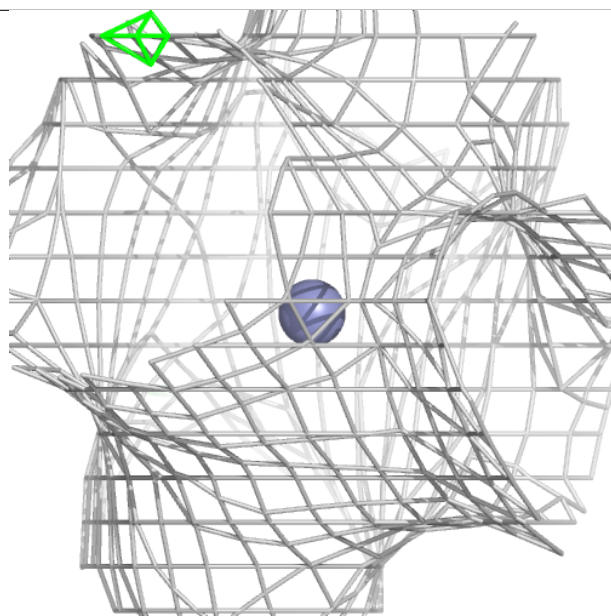
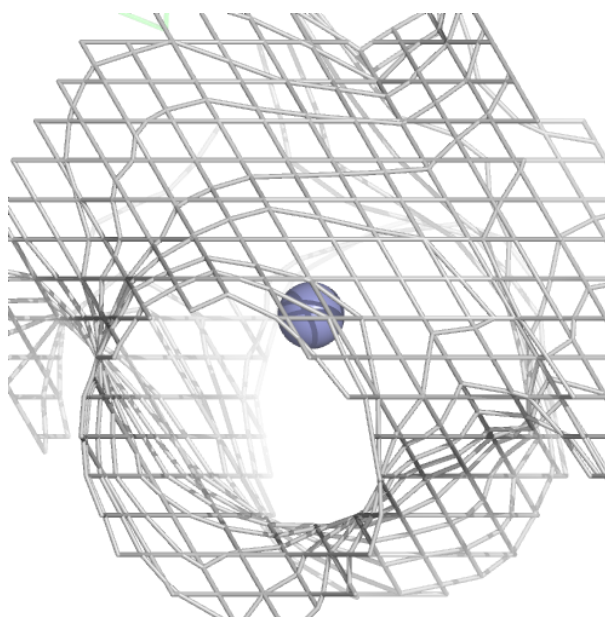
Electron density around ZN E 401:

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



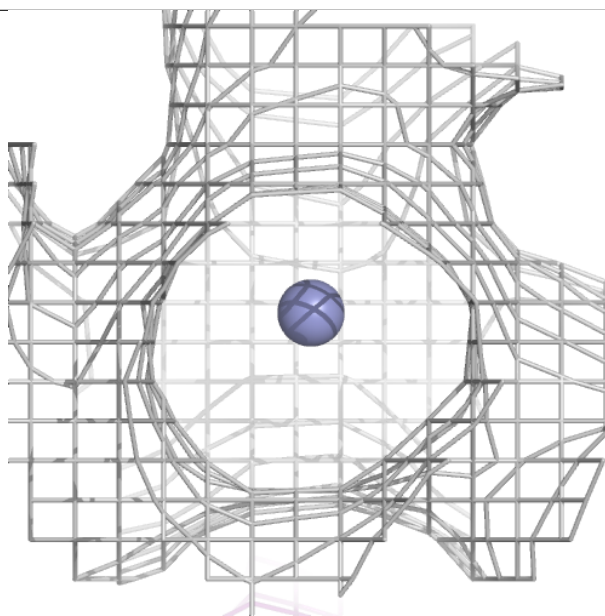
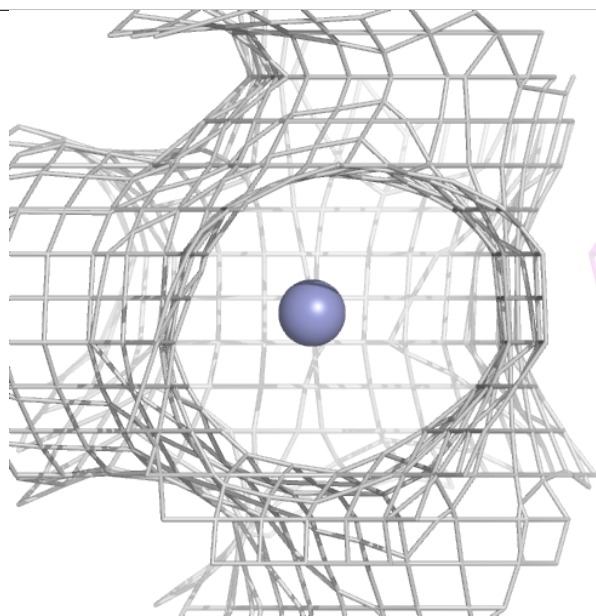
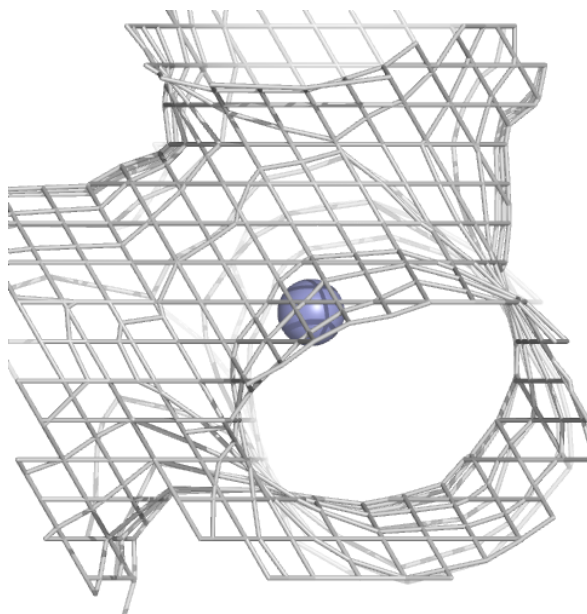
Electron density around ZN E 402:

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



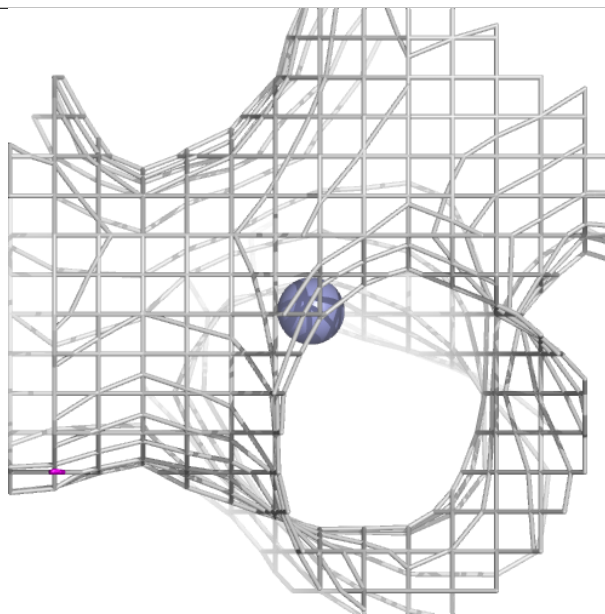
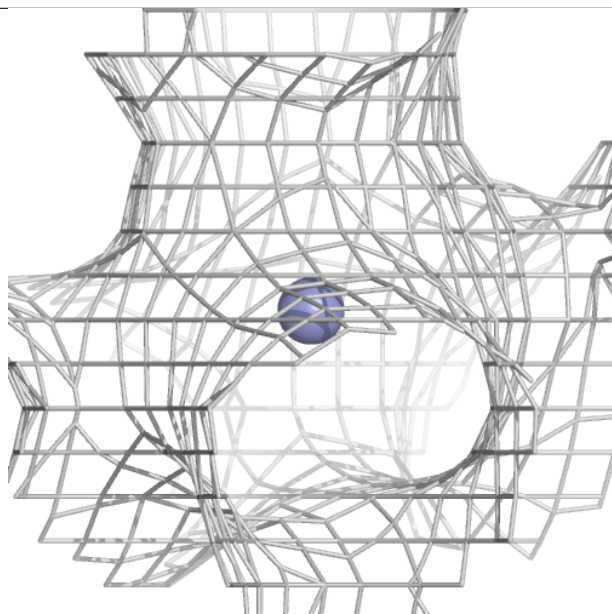
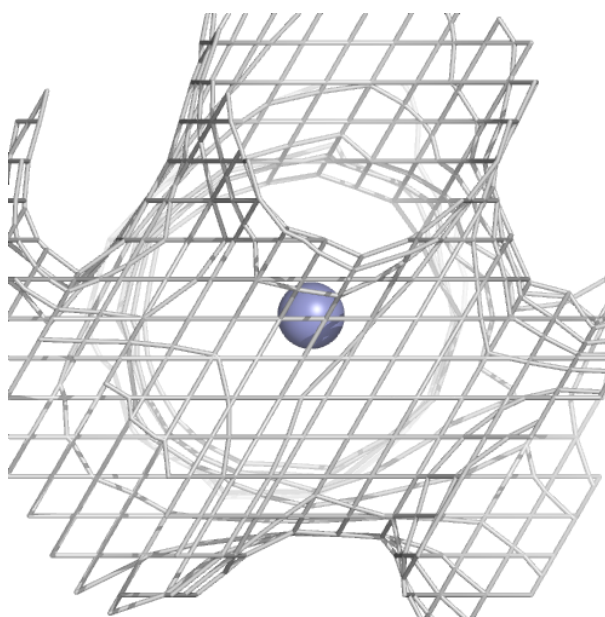
Electron density around ZN G 404:

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



Electron density around ZN G 403:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.