



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 7, 2025 – 10:21 am BST

PDB ID : 9QDI / pdb\_00009qdi  
Title : Crystal structure of BF3526 peptidase from Bacteroides fragilis in complex with a peptide  
Authors : Martinez Gascuena, A.; Marquez-Monino, M.A.; Manzanares-Gomez, A.; Aguillo-Urarte, M.; Trastoy, B.  
Deposited on : 2025-03-06  
Resolution : 1.94 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

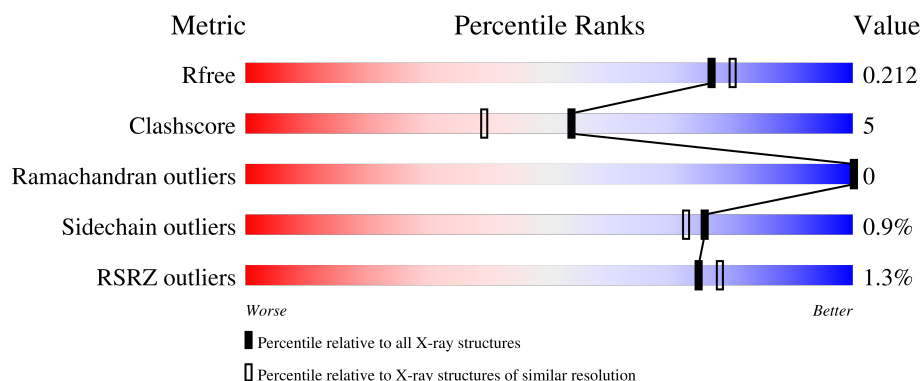
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



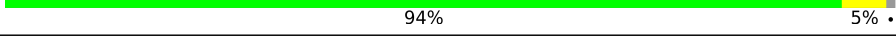
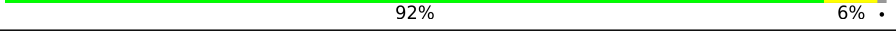
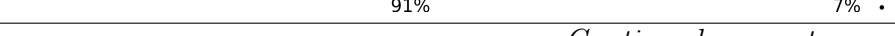
The reported resolution of this entry is 1.94 Å.

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))
$R_{free}$	164625	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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  $\geq 3$ , 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	409	
1	B	409	
1	C	409	
1	D	409	
1	E	409	

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Mol	Chain	Length	Quality of chain
1	F	409	<div><div>%</div><div><div></div><div>91%</div><div>7%</div><div></div></div><div></div></div>
1	G	409	<div><div>%</div><div><div></div><div>89%</div><div>9%</div><div></div></div><div></div></div>
1	H	409	<div><div>5%</div><div><div></div><div>75%</div><div>23%</div><div></div></div><div></div></div>
2	I	4	<div><div><div></div><div>50%</div><div>25%</div><div></div></div><div>25%</div></div>
2	J	4	<div><div><div></div><div>50%</div><div></div></div><div>100%</div></div>
2	K	4	<div><div>25%</div><div><div></div><div>25%</div><div>75%</div></div><div></div></div>
2	L	4	<div><div>25%</div><div><div></div><div>25%</div><div>50%</div><div></div></div><div>25%</div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 43108 atoms, of which 15771 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 Lipoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	402	Total	C	H	N	O	S	0	1	0
			3266	2058	53	537	607	11			
1	B	402	Total	C	H	N	O	S	0	1	0
			3261	2059	47	536	608	11			
1	C	406	Total	C	H	N	O	S	0	1	0
			6331	2077	3086	541	615	12			
1	D	403	Total	C	H	N	O	S	0	1	0
			6314	2066	3089	537	611	11			
1	E	403	Total	C	H	N	O	S	0	1	0
			6321	2063	3100	538	608	12			
1	F	402	Total	C	H	N	O	S	0	1	0
			6302	2059	3088	536	608	11			
1	G	401	Total	C	H	N	O	S	0	1	0
			6290	2054	3085	535	605	11			
1	H	401	Total	C	H	N	O	S	0	1	0
			3252	2054	47	535	605	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP Q5L9L3
B	18	GLY	-	expression tag	UNP Q5L9L3
C	18	GLY	-	expression tag	UNP Q5L9L3
D	18	GLY	-	expression tag	UNP Q5L9L3
E	18	GLY	-	expression tag	UNP Q5L9L3
F	18	GLY	-	expression tag	UNP Q5L9L3
G	18	GLY	-	expression tag	UNP Q5L9L3
H	18	GLY	-	expression tag	UNP Q5L9L3

- Molecule 2 is a protein called Synthetic peptide SER-THR-PRO-PRO.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	3	Total	C	H	N	O	0	0	0
			25	13	4	3	5			
2	J	4	Total	C	N	O		0	0	0
			28	17	4	7				
2	K	4	Total	C	H	N	O	0	0	0
			32	17	4	4	7			
2	L	3	Total	C	H	N	O	0	0	0
			25	13	4	3	5			

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		
3	G	1	Total	K	0	0
			1	1		
3	H	1	Total	K	0	0
			1	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

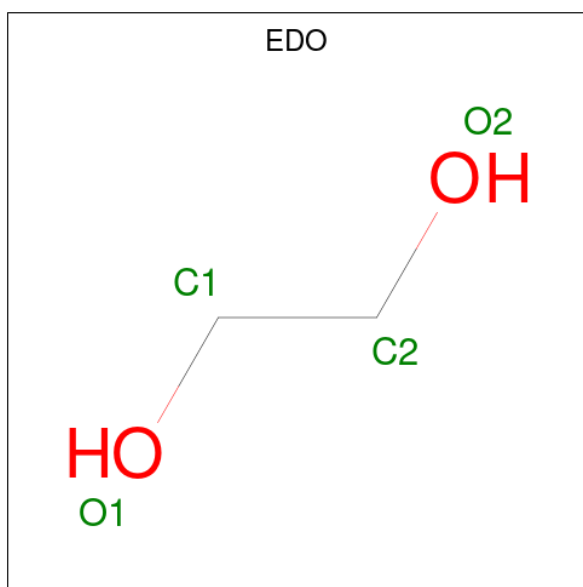
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	E	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	2	Total 2	Zn 2	0	0
4	G	2	Total 2	Zn 2	0	0
4	H	2	Total 2	Zn 2	0	0

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



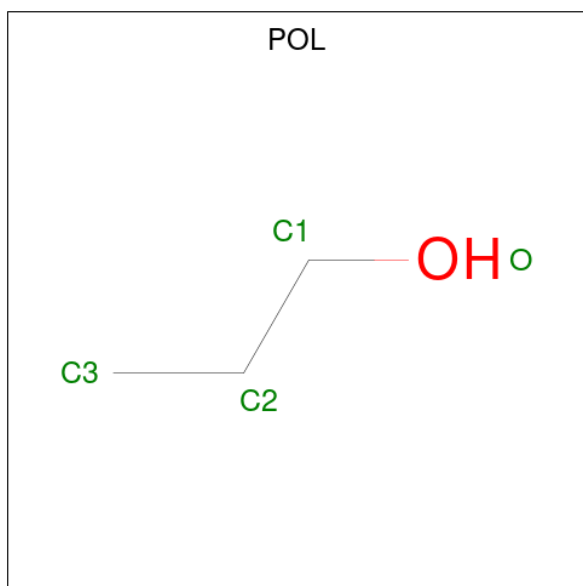
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 10	C 2	H 6	O 2	0	0
5	A	1	Total 10	C 2	H 6	O 2	0	0
5	B	1	Total 10	C 2	H 6	O 2	0	0
5	C	1	Total 10	C 2	H 6	O 2	0	0
5	C	1	Total 10	C 2	H 6	O 2	0	0
5	D	1	Total 10	C 2	H 6	O 2	0	0
5	D	1	Total 10	C 2	H 6	O 2	0	0
5	D	1	Total 10	C 2	H 6	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	F	1	Total	C	H	O	0	0
			10	2	6	2		
5	F	1	Total	C	H	O	0	0
			10	2	6	2		
5	G	1	Total	C	H	O	0	0
			10	2	6	2		
5	G	1	Total	C	H	O	0	0
			10	2	6	2		
5	H	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is N-PROPANOL (CCD ID: POL) (formula:  $C_3H_8O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			12	3	8	1		
6	C	1	Total	C	H	O	0	0
			12	3	8	1		
6	E	1	Total	C	H	O	0	0
			12	3	8	1		
6	F	1	Total	C	H	O	0	0
			12	3	8	1		

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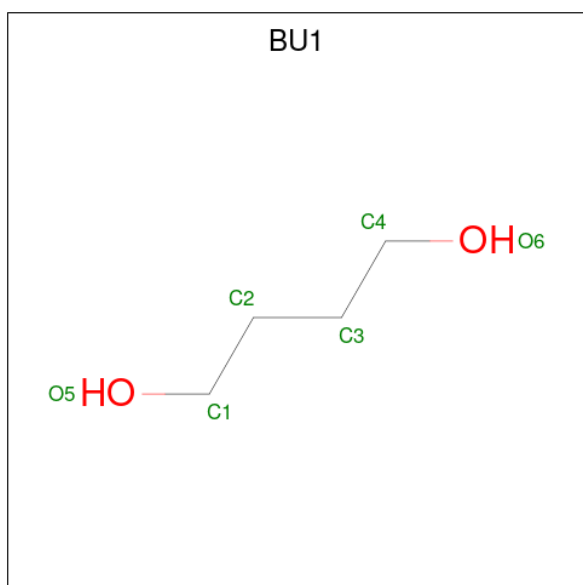
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	H	O	0	0
			12	3	8	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



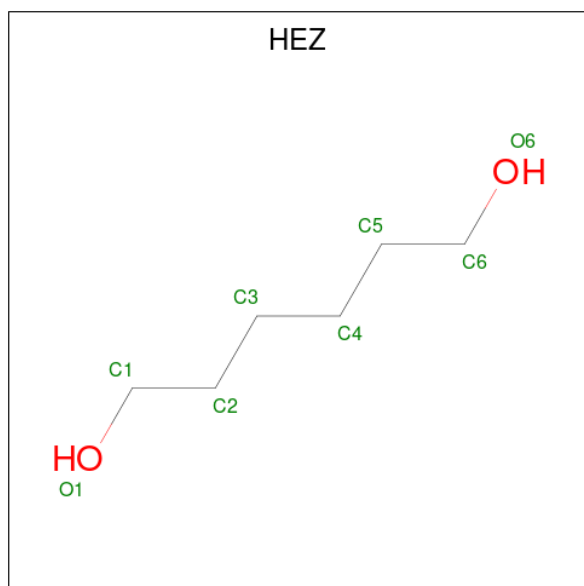
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 8 is 1,4-BUTANEDIOL (CCD ID: BU1) (formula:  $C_4H_{10}O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 9 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	G	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	210	Total	O	0	0
			210	210		
10	B	214	Total	O	0	0
			214	214		
10	C	233	Total	O	0	0
			233	233		
10	D	176	Total	O	0	0
			176	176		
10	E	192	Total	O	0	0
			192	192		
10	F	184	Total	O	0	0
			184	184		
10	G	103	Total	O	0	0
			103	103		
10	H	57	Total	O	0	0
			57	57		

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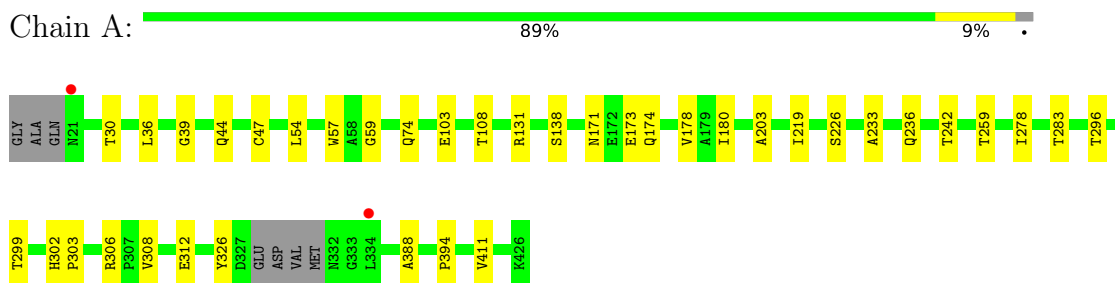
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	I	1	Total	O	0	0
			1	1		
10	L	2	Total	O	0	0
			2	2		

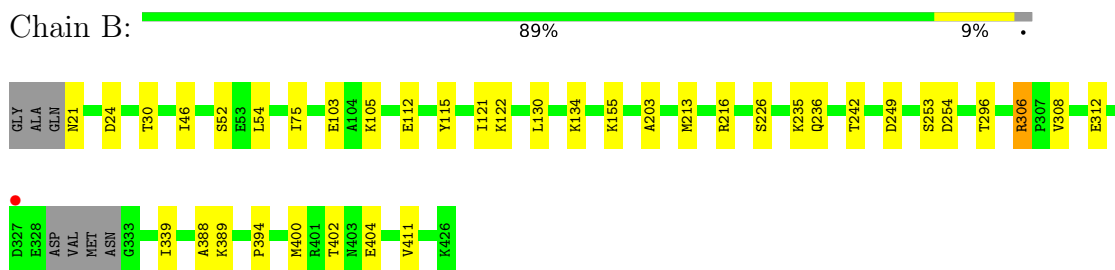
### 3 Residue-property plots [i](#)

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.

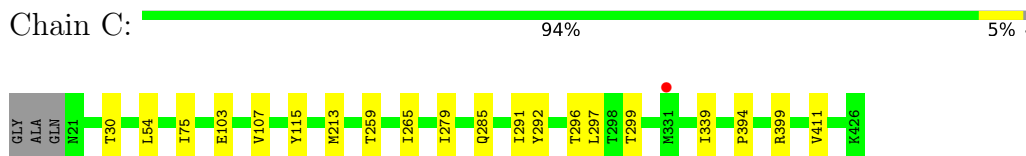
#### • Molecule 1: Lipoprotein



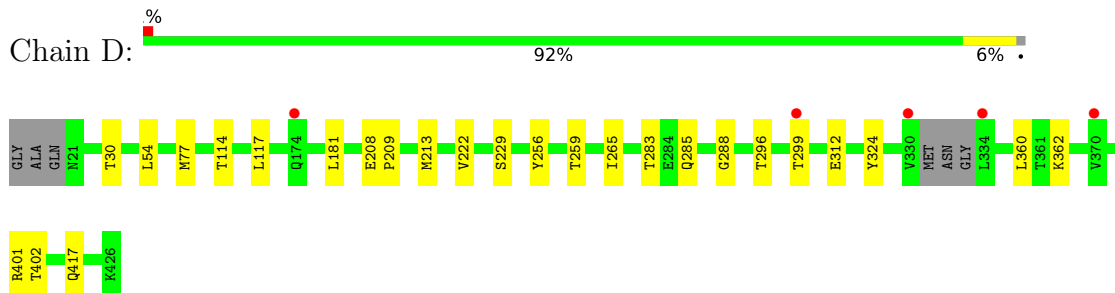
#### • Molecule 1: Lipoprotein



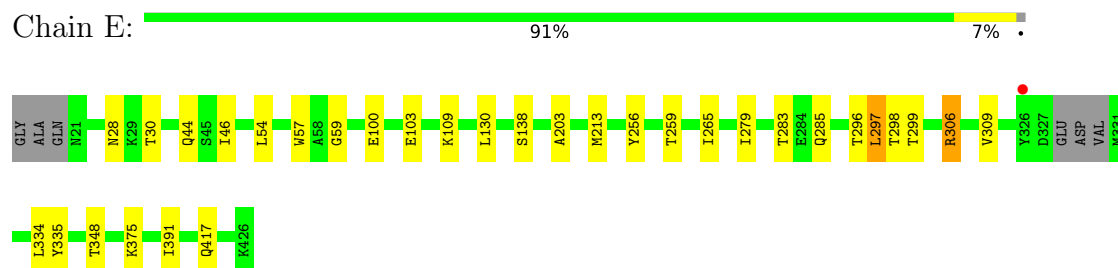
#### • Molecule 1: Lipoprotein



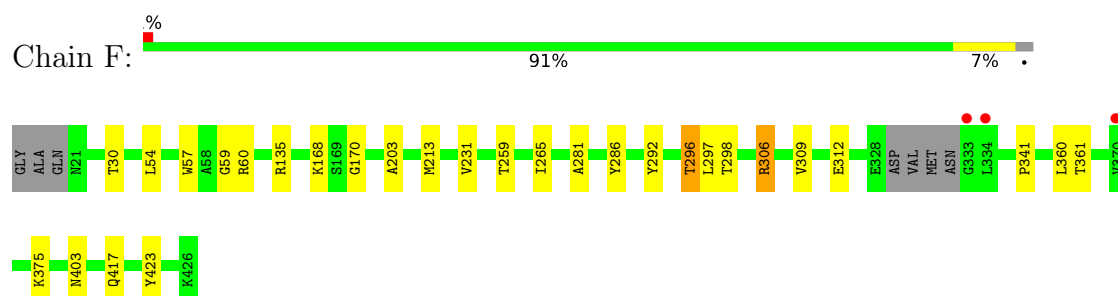
#### • Molecule 1: Lipoprotein



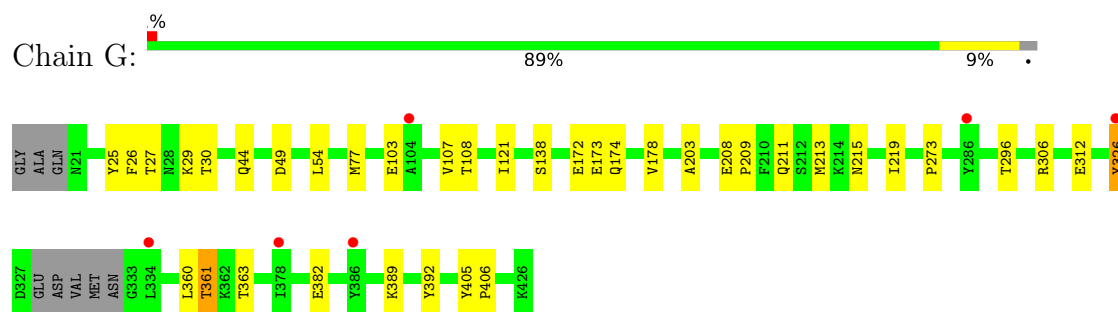
- Molecule 1: Lipoprotein



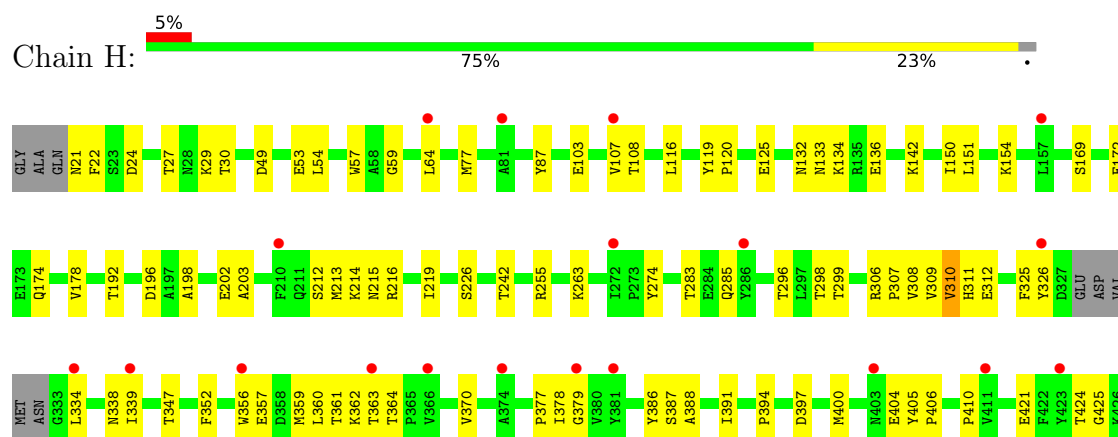
- Molecule 1: Lipoprotein



- Molecule 1: Lipoprotein



- Molecule 1: Lipoprotein



- Molecule 2: Synthetic peptide SER-THR-PRO-PRO







- Molecule 2: Synthetic peptide SER-THR-PRO-PRO



- Molecule 2: Synthetic peptide SER-THR-PRO-PRO



- Molecule 2: Synthetic peptide SER-THR-PRO-PRO



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.29Å 99.44Å 103.39Å 74.16° 88.13° 82.44°	Depositor
Resolution (Å)	29.64 – 1.94 29.64 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.64-1.94) 97.0 (29.64-1.94)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.93Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.171 , 0.213 0.171 , 0.212	Depositor DCC
$R_{free}$ test set	13912 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	43108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, BU1, POL, PEG, EDO, K, HEZ

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	0.57	0/3304	0.62	0/4487
1	B	0.55	1/3305 (0.0%)	0.62	0/4488
1	C	0.50	0/3337	0.59	0/4533
1	D	0.46	0/3316	0.58	0/4504
1	E	0.46	0/3312	0.61	0/4497
1	F	0.47	0/3305	0.59	0/4488
1	G	0.39	0/3296	0.53	0/4476
1	H	0.36	0/3296	0.48	0/4476
2	I	0.69	0/21	0.40	0/25
2	J	0.65	0/29	0.76	0/39
2	K	0.53	0/29	0.67	0/39
2	L	0.48	0/21	0.43	0/25
All	All	0.48	1/26571 (0.0%)	0.58	0/36077

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	B	0	1
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	400	MET	SD-CE	-6.53	1.63	1.79

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	ARG	Sidechain
1	C	399	ARG	Sidechain
1	E	306	ARG	Sidechain
1	F	306	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	3213	53	3106	26	0
1	B	3214	47	3106	32	0
1	C	3245	3086	3135	14	0
1	D	3225	3089	3116	20	0
1	E	3221	3100	3115	25	0
1	F	3214	3088	3106	22	0
1	G	3205	3085	3100	28	0
1	H	3205	47	3100	79	0
2	I	21	4	21	0	0
2	J	28	0	28	6	0
2	K	28	4	28	3	0
2	L	21	4	21	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
5	A	8	12	11	0	0
5	B	4	6	5	0	0
5	C	8	12	11	0	0
5	D	12	18	18	0	0
5	E	8	12	11	0	0
5	F	8	12	11	3	0
5	G	8	12	11	0	0
5	H	4	6	5	0	0
6	A	4	8	8	0	0
6	C	4	8	8	2	0
6	E	4	8	8	3	0
6	F	4	8	8	3	0
6	G	4	8	8	0	0
7	D	7	10	10	3	0
8	E	6	10	10	0	0
9	G	8	14	14	1	0
10	A	210	0	0	1	0
10	B	214	0	0	1	0
10	C	233	0	0	1	0
10	D	176	0	0	2	0
10	E	192	0	0	1	0
10	F	184	0	0	0	0
10	G	103	0	0	0	0
10	H	57	0	0	6	0
10	I	1	0	0	0	0
10	L	2	0	0	0	0
All	All	27337	15771	25139	246	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.

The worst 5 of 246 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:285:GLN:O	1:C:299:THR:HG21	1.66	0.95
1:E:259:THR:HG21	1:E:265:ILE:HD11	1.49	0.92
1:F:292:TYR:H	6:F:505:POL:H31	1.35	0.92
1:D:259:THR:HG21	1:D:265:ILE:HD11	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:THR:HG21	1:C:265:ILE:HD11	1.55	0.86

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	399/409 (98%)	389 (98%)	10 (2%)	0	100	100
1	B	399/409 (98%)	393 (98%)	6 (2%)	0	100	100
1	C	405/409 (99%)	396 (98%)	9 (2%)	0	100	100
1	D	400/409 (98%)	390 (98%)	10 (2%)	0	100	100
1	E	400/409 (98%)	392 (98%)	8 (2%)	0	100	100
1	F	399/409 (98%)	393 (98%)	6 (2%)	0	100	100
1	G	398/409 (97%)	383 (96%)	15 (4%)	0	100	100
1	H	398/409 (97%)	376 (94%)	22 (6%)	0	100	100
2	J	2/4 (50%)	2 (100%)	0	0	100	100
2	K	2/4 (50%)	2 (100%)	0	0	100	100
All	All	3202/3280 (98%)	3116 (97%)	86 (3%)	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	345/349 (99%)	343 (99%)	2 (1%)	84	83
1	B	345/349 (99%)	344 (100%)	1 (0%)	91	91
1	C	349/349 (100%)	347 (99%)	2 (1%)	84	83
1	D	347/349 (99%)	345 (99%)	2 (1%)	84	83
1	E	346/349 (99%)	344 (99%)	2 (1%)	84	83
1	F	345/349 (99%)	343 (99%)	2 (1%)	84	83
1	G	344/349 (99%)	339 (98%)	5 (2%)	60	52
1	H	344/349 (99%)	338 (98%)	6 (2%)	56	45
2	I	3/4 (75%)	2 (67%)	1 (33%)	0	0
2	J	4/4 (100%)	3 (75%)	1 (25%)	0	0
2	K	4/4 (100%)	3 (75%)	1 (25%)	0	0
2	L	3/4 (75%)	3 (100%)	0	100	100
All	All	2779/2808 (99%)	2754 (99%)	25 (1%)	75	72

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	326	TYR
1	H	212	SER
2	K	1	SER
1	H	24	ASP
1	H	296	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	241	HIS
1	G	276	HIS
1	H	417	GLN
1	G	215	ASN
1	G	285	GLN

### 5.3.3 RNA ⓘ

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 47 ligands modelled in this entry, 24 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	EDO	A	506	-	3,3,3	0.34	0	2,2,2	0.20	0
8	BU1	E	507	-	5,5,5	0.25	0	4,4,4	0.42	0
6	POL	F	505	-	3,3,3	0.39	0	2,2,2	0.33	0
5	EDO	C	504	3	3,3,3	0.21	0	2,2,2	0.23	0
5	EDO	A	504	3	3,3,3	0.36	0	2,2,2	0.21	0
5	EDO	D	506	-	3,3,3	0.40	0	2,2,2	0.07	0
5	EDO	C	505	-	3,3,3	0.36	0	2,2,2	0.30	0
5	EDO	D	505	-	3,3,3	0.30	0	2,2,2	0.11	0
9	HEZ	G	501	-	7,7,7	0.27	0	6,6,6	0.20	0
6	POL	A	505	-	3,3,3	0.37	0	2,2,2	0.24	0
6	POL	G	507	-	3,3,3	0.41	0	2,2,2	0.22	0
7	PEG	D	507	-	6,6,6	0.34	0	5,5,5	0.49	0
5	EDO	E	505	-	3,3,3	0.57	0	2,2,2	0.23	0
6	POL	E	506	-	3,3,3	0.33	0	2,2,2	0.32	0
6	POL	C	506	-	3,3,3	0.56	0	2,2,2	0.20	0
5	EDO	G	505	3	3,3,3	0.30	0	2,2,2	1.21	0
5	EDO	H	504	3	3,3,3	0.24	0	2,2,2	0.44	0
5	EDO	B	504	3	3,3,3	0.23	0	2,2,2	0.21	0
5	EDO	G	506	-	3,3,3	0.32	0	2,2,2	0.15	0
5	EDO	D	504	3	3,3,3	0.36	0	2,2,2	0.57	0
5	EDO	F	506	-	3,3,3	0.26	0	2,2,2	0.34	0
5	EDO	F	504	3	3,3,3	0.24	0	2,2,2	0.79	0
5	EDO	E	504	3	3,3,3	0.19	0	2,2,2	0.15	0



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	506	-	-	0/1/1/1	-
8	BU1	E	507	-	-	1/3/3/3	-
6	POL	F	505	-	-	1/1/1/1	-
5	EDO	C	504	3	-	0/1/1/1	-
5	EDO	A	504	3	-	1/1/1/1	-
5	EDO	D	506	-	-	0/1/1/1	-
5	EDO	C	505	-	-	0/1/1/1	-
5	EDO	D	505	-	-	1/1/1/1	-
9	HEZ	G	501	-	-	2/5/5/5	-
6	POL	A	505	-	-	1/1/1/1	-
6	POL	G	507	-	-	1/1/1/1	-
7	PEG	D	507	-	-	2/4/4/4	-
5	EDO	E	505	-	-	1/1/1/1	-
6	POL	E	506	-	-	0/1/1/1	-
6	POL	C	506	-	-	0/1/1/1	-
5	EDO	G	505	3	-	1/1/1/1	-
5	EDO	H	504	3	-	1/1/1/1	-
5	EDO	B	504	3	-	1/1/1/1	-
5	EDO	G	506	-	-	0/1/1/1	-
5	EDO	D	504	3	-	0/1/1/1	-
5	EDO	F	506	-	-	1/1/1/1	-
5	EDO	F	504	3	-	1/1/1/1	-
5	EDO	E	504	3	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	507	PEG	O1-C1-C2-O2
5	B	504	EDO	O1-C1-C2-O2
9	G	501	HEZ	C3-C4-C5-C6
5	D	505	EDO	O1-C1-C2-O2
5	E	504	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	505	POL	3	0
9	G	501	HEZ	1	0
7	D	507	PEG	3	0
6	E	506	POL	3	0
6	C	506	POL	2	0
5	F	506	EDO	1	0
5	F	504	EDO	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	402/409 (98%)	-0.18	2 (0%) 87 90	22, 32, 54, 79	1 (0%)
1	B	402/409 (98%)	-0.11	1 (0%) 92 94	23, 34, 55, 77	1 (0%)
1	C	406/409 (99%)	-0.34	1 (0%) 92 94	18, 37, 57, 85	1 (0%)
1	D	403/409 (98%)	-0.11	5 (1%) 76 79	24, 41, 61, 101	1 (0%)
1	E	403/409 (98%)	-0.23	1 (0%) 92 94	21, 39, 64, 85	1 (0%)
1	F	402/409 (98%)	-0.22	3 (0%) 84 88	22, 40, 60, 83	1 (0%)
1	G	401/409 (98%)	0.24	6 (1%) 71 76	32, 52, 74, 92	1 (0%)
1	H	401/409 (98%)	0.68	19 (4%) 37 41	29, 54, 74, 92	1 (0%)
2	I	3/4 (75%)	1.21	0 100 100	40, 40, 42, 47	0
2	J	4/4 (100%)	1.89	2 (50%) 0 0	45, 53, 53, 56	0
2	K	4/4 (100%)	1.53	1 (25%) 2 2	38, 38, 46, 49	2 (50%)
2	L	3/4 (75%)	1.70	1 (33%) 1 1	48, 48, 49, 52	0
All	All	3234/3288 (98%)	-0.03	42 (1%) 74 78	18, 41, 68, 101	10 (0%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	330	VAL	5.3
2	K	2	THR	3.7
1	G	326	TYR	3.5
1	D	334	LEU	3.4
1	F	334	LEU	3.1

### 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	BU1	E	507	6/6	0.65	0.15	57,68,78,82	0
9	HEZ	G	501	8/8	0.75	0.15	56,68,76,77	0
7	PEG	D	507	7/7	0.80	0.16	33,50,62,62	0
5	EDO	E	504	4/4	0.81	0.13	20,20,20,20	0
5	EDO	D	505	4/4	0.81	0.19	50,60,72,75	0
6	POL	G	507	4/4	0.82	0.16	42,55,60,68	0
5	EDO	E	505	4/4	0.83	0.16	35,54,62,68	0
5	EDO	G	506	4/4	0.83	0.09	59,71,79,79	0
5	EDO	A	506	4/4	0.83	0.17	42,59,70,71	0
5	EDO	H	504	4/4	0.85	0.11	62,75,82,82	0
5	EDO	F	504	4/4	0.88	0.13	40,50,60,64	0
6	POL	A	505	4/4	0.89	0.18	34,44,55,55	0
6	POL	F	505	4/4	0.91	0.11	24,45,56,61	0
5	EDO	D	506	4/4	0.92	0.15	33,48,52,58	0
5	EDO	C	504	4/4	0.92	0.09	37,45,51,51	0
5	EDO	F	506	4/4	0.92	0.09	43,52,57,59	0
5	EDO	G	505	4/4	0.92	0.09	48,58,62,74	0
6	POL	C	506	4/4	0.93	0.12	26,41,49,59	0
5	EDO	B	504	4/4	0.93	0.08	39,47,53,53	0
5	EDO	A	504	4/4	0.93	0.09	34,42,51,51	0
6	POL	E	506	4/4	0.94	0.10	34,41,49,49	0
5	EDO	D	504	4/4	0.95	0.07	35,42,47,50	0
3	K	H	501	1/1	0.96	0.05	51,51,51,51	0
4	ZN	E	502	1/1	0.96	0.14	73,73,73,73	0
4	ZN	G	504	1/1	0.97	0.05	48,48,48,48	0
4	ZN	H	503	1/1	0.97	0.05	51,51,51,51	0
5	EDO	C	505	4/4	0.97	0.13	34,44,57,57	0
4	ZN	C	502	1/1	0.98	0.09	59,59,59,59	0
3	K	G	502	1/1	0.98	0.03	42,42,42,42	0
4	ZN	F	502	1/1	0.98	0.09	62,62,62,62	0
4	ZN	F	503	1/1	0.98	0.03	34,34,34,34	0
3	K	E	501	1/1	0.98	0.03	28,28,28,28	0

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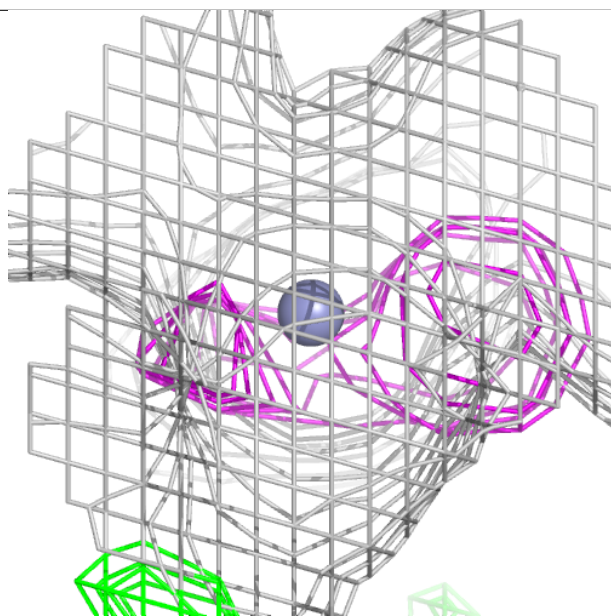
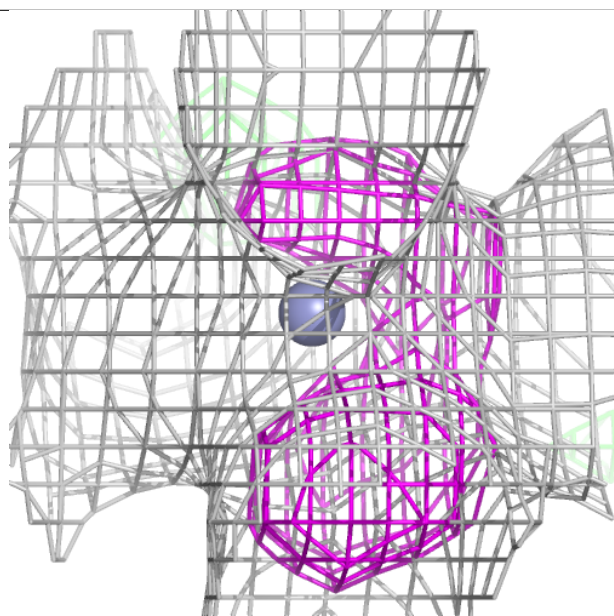
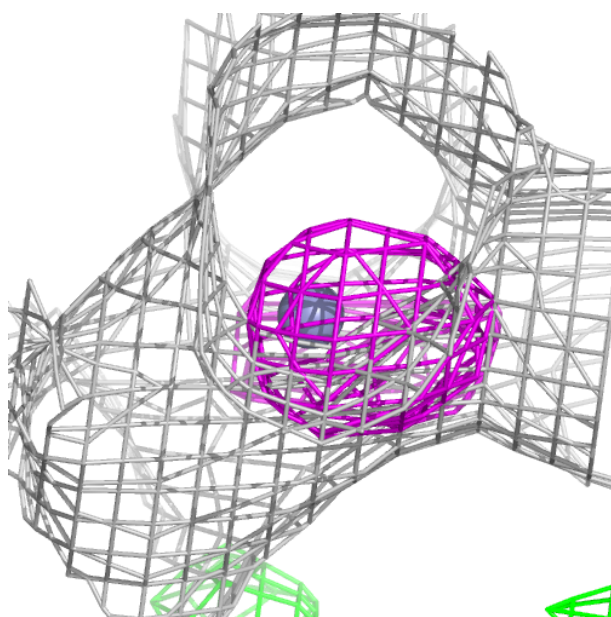
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	H	502	1/1	0.98	0.08	56,56,56,56	0
3	K	C	501	1/1	0.99	0.02	28,28,28,28	0
4	ZN	A	502	1/1	0.99	0.04	37,37,37,37	0
4	ZN	B	502	1/1	0.99	0.03	37,37,37,37	0
4	ZN	B	503	1/1	0.99	0.03	30,30,30,30	0
3	K	D	501	1/1	0.99	0.02	27,27,27,27	0
4	ZN	C	503	1/1	0.99	0.02	29,29,29,29	0
4	ZN	D	502	1/1	0.99	0.09	59,59,59,59	0
4	ZN	D	503	1/1	0.99	0.02	33,33,33,33	0
3	K	A	501	1/1	0.99	0.02	26,26,26,26	0
4	ZN	E	503	1/1	0.99	0.02	35,35,35,35	0
3	K	F	501	1/1	0.99	0.02	28,28,28,28	0
3	K	B	501	1/1	0.99	0.03	31,31,31,31	0
4	ZN	G	503	1/1	0.99	0.03	48,48,48,48	0
4	ZN	A	503	1/1	1.00	0.01	29,29,29,29	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.

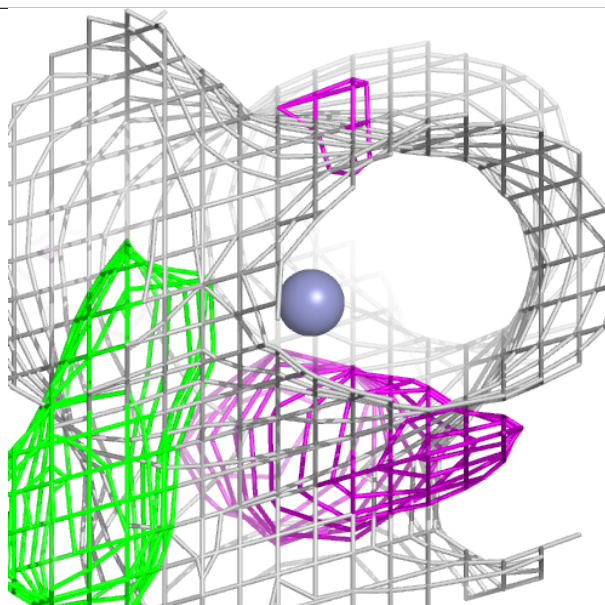
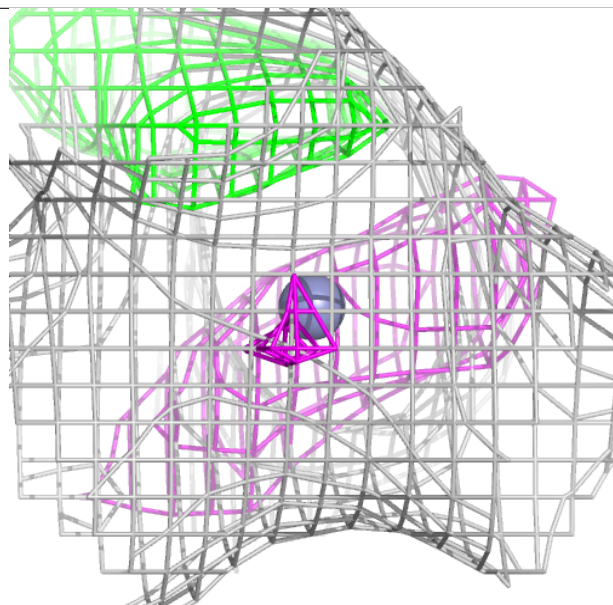
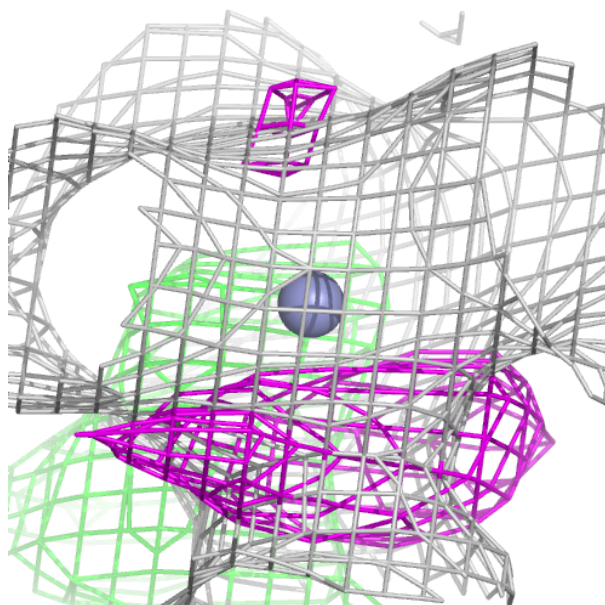
**Electron density around ZN E 502:**

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



**Electron density around ZN G 504:**

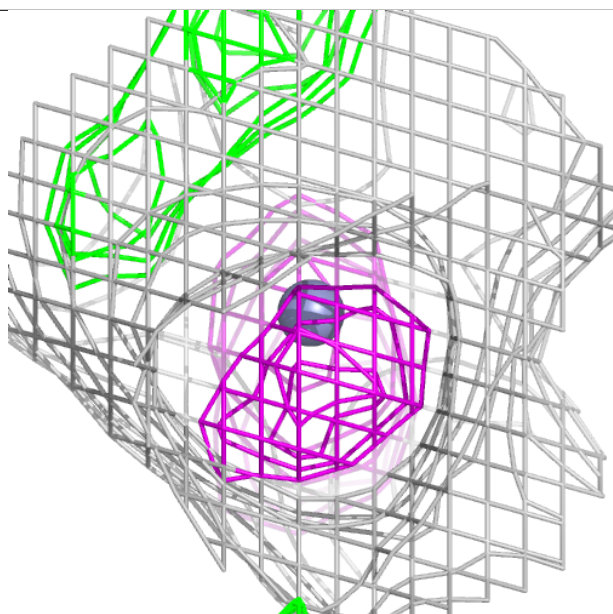
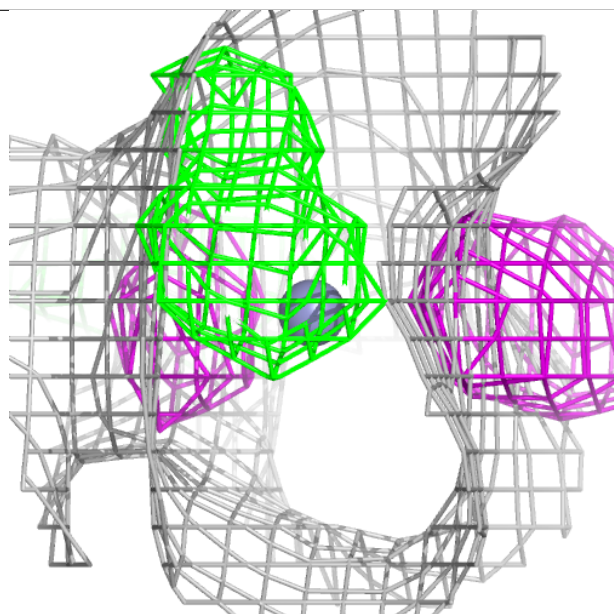
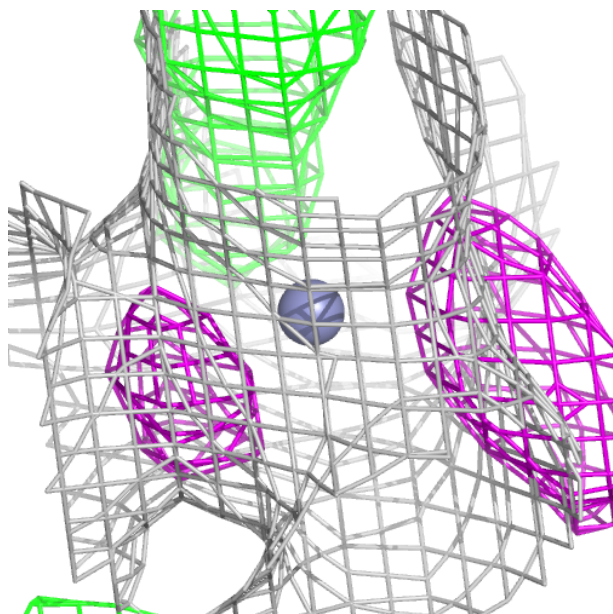
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and green (positive)





**Electron density around ZN H 503:**

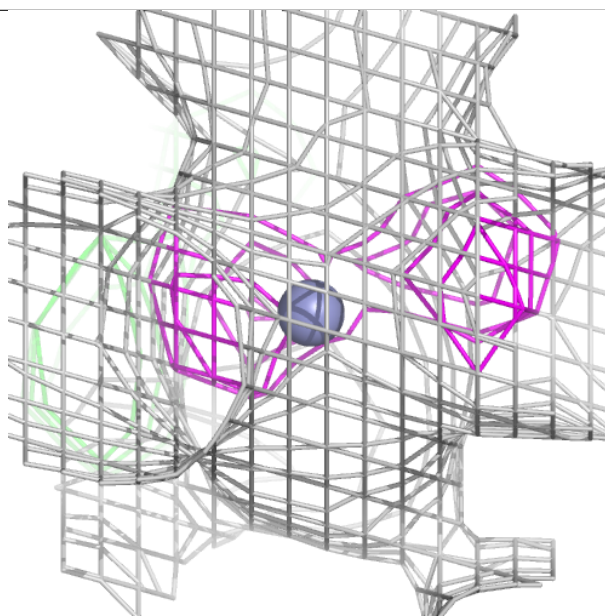
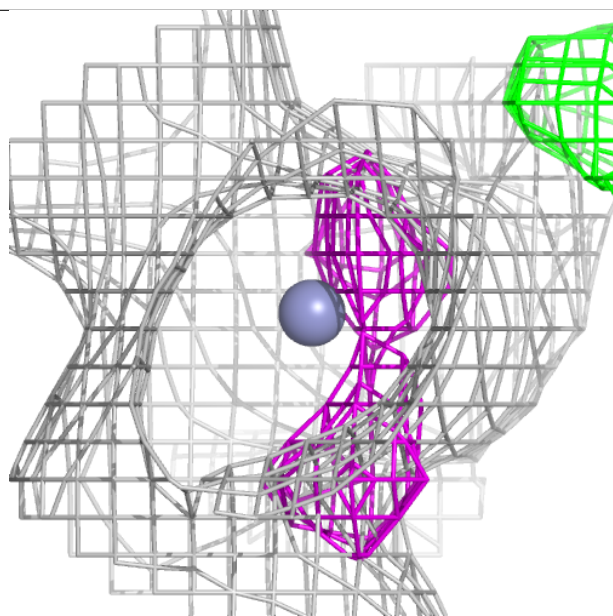
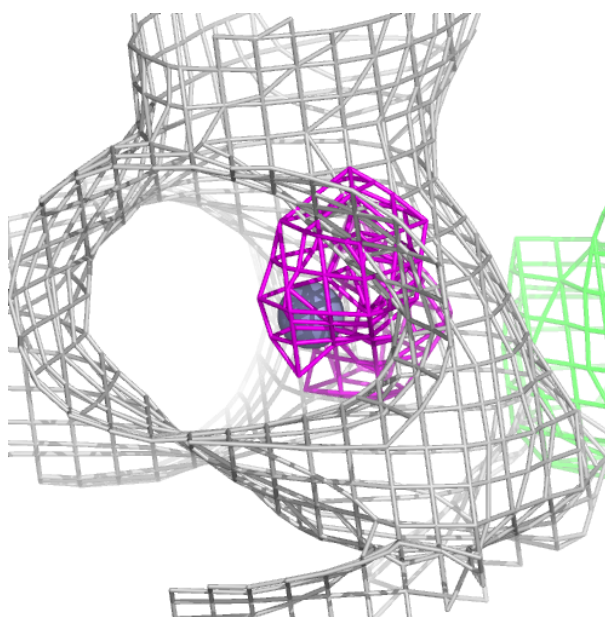
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and green (positive)





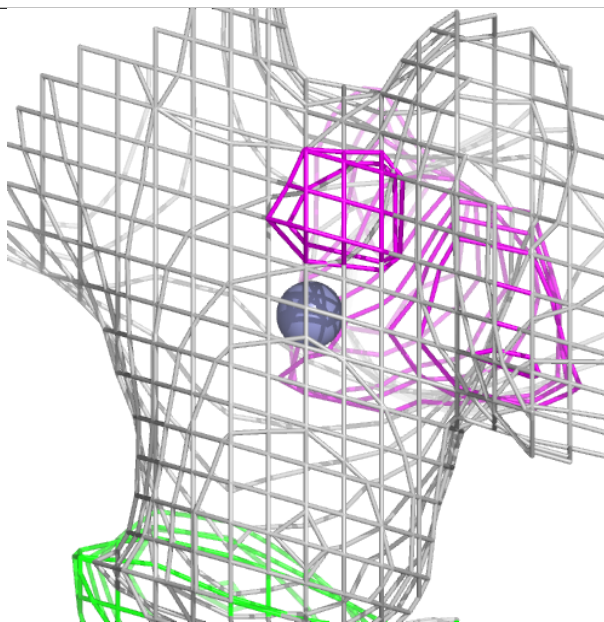
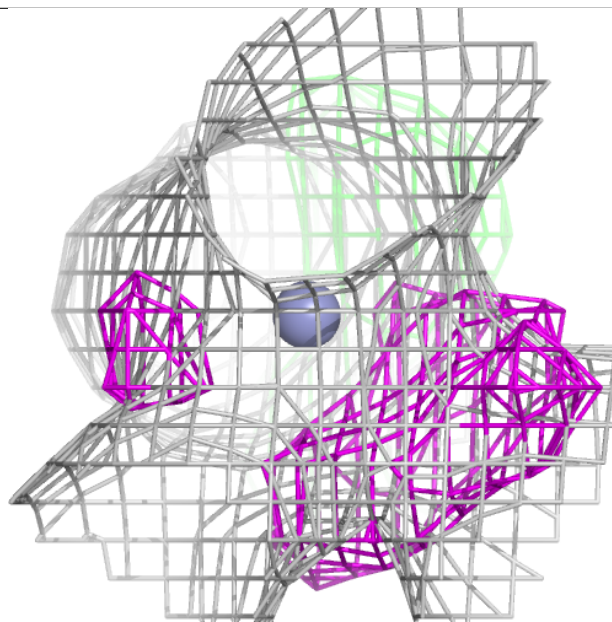
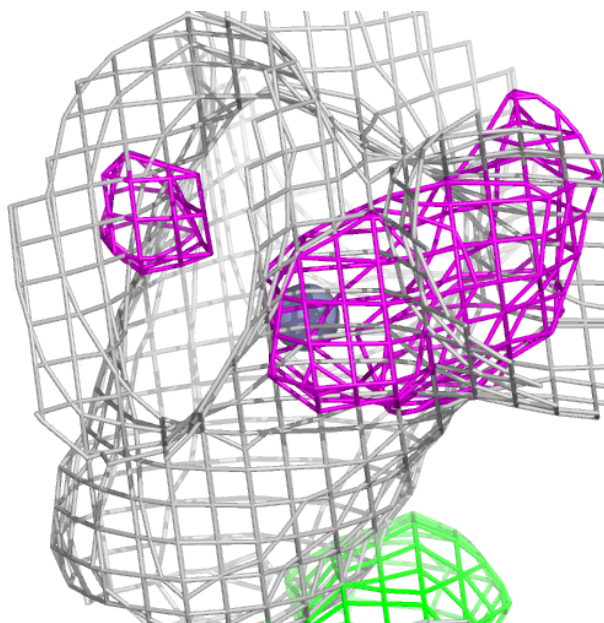
**Electron density around ZN C 502:**

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and green (positive)



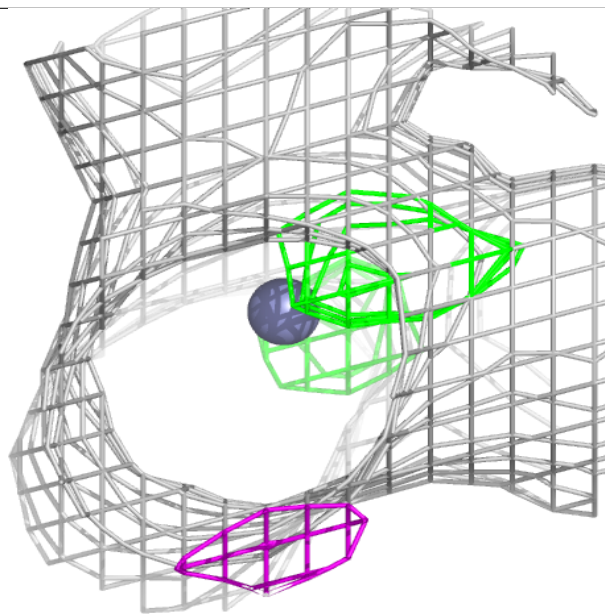
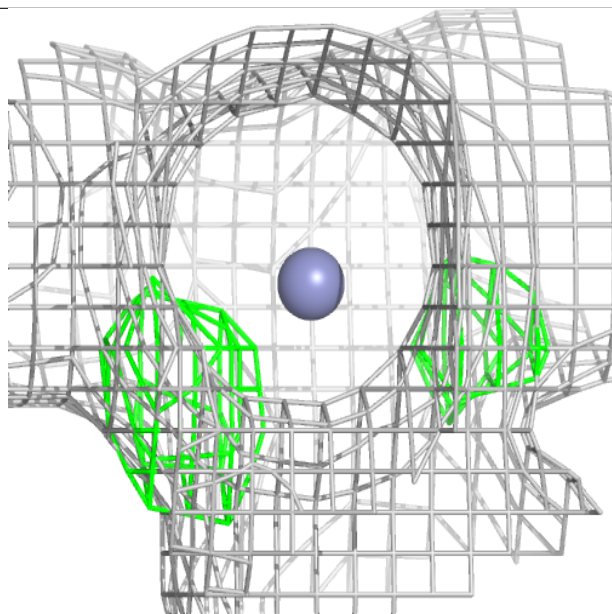
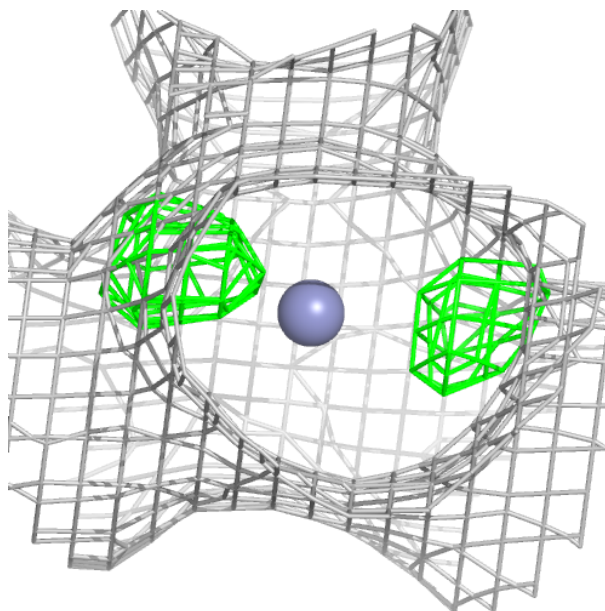
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and green (positive)



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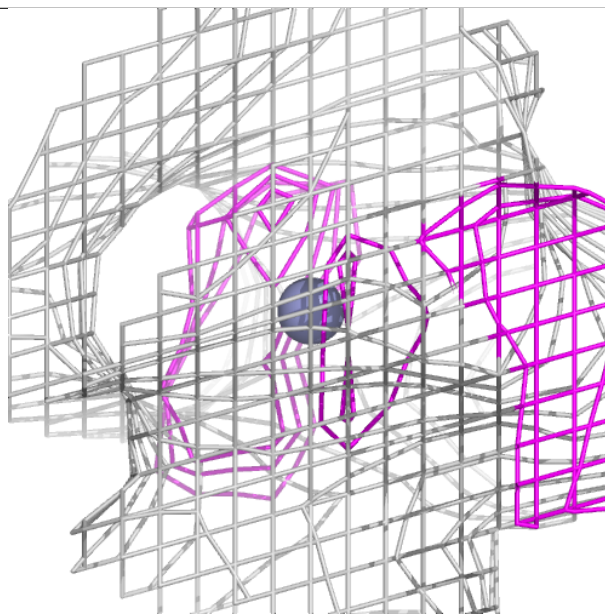
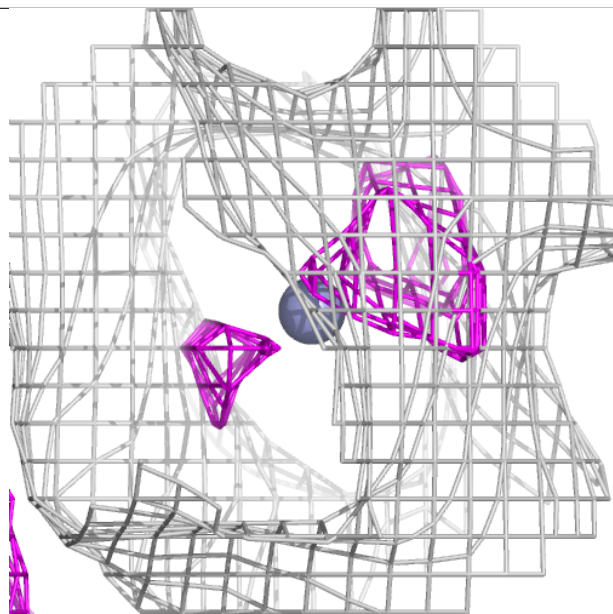
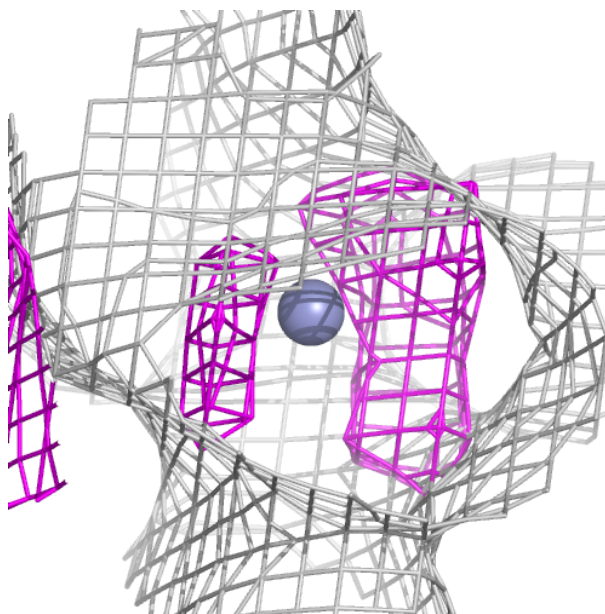
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





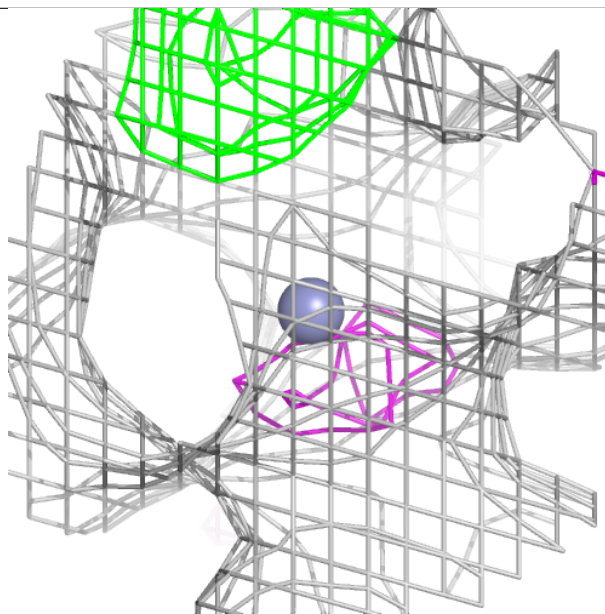
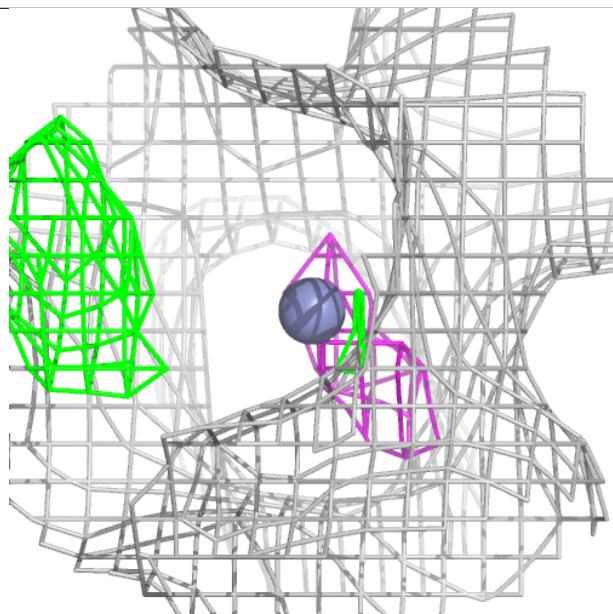
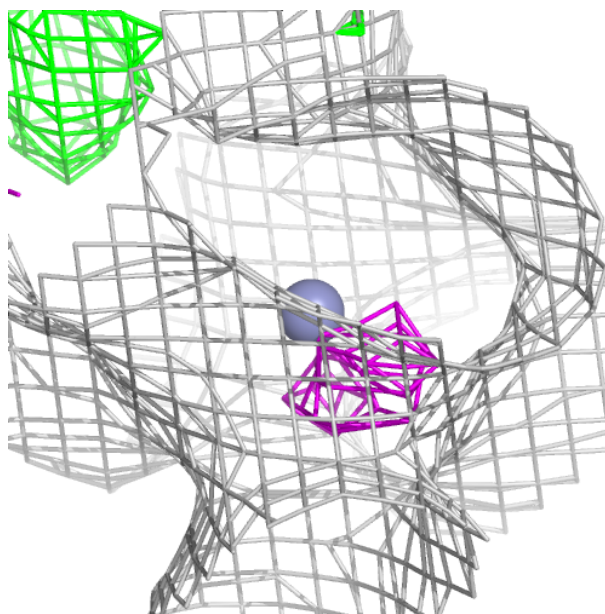
**Electron density around ZN H 502:**

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



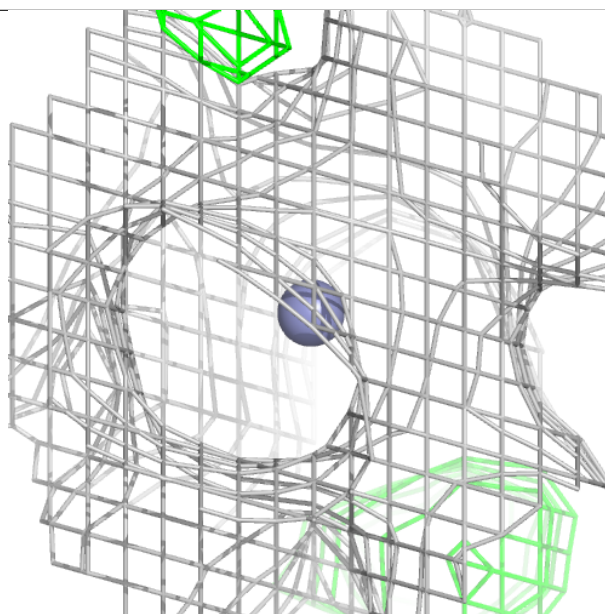
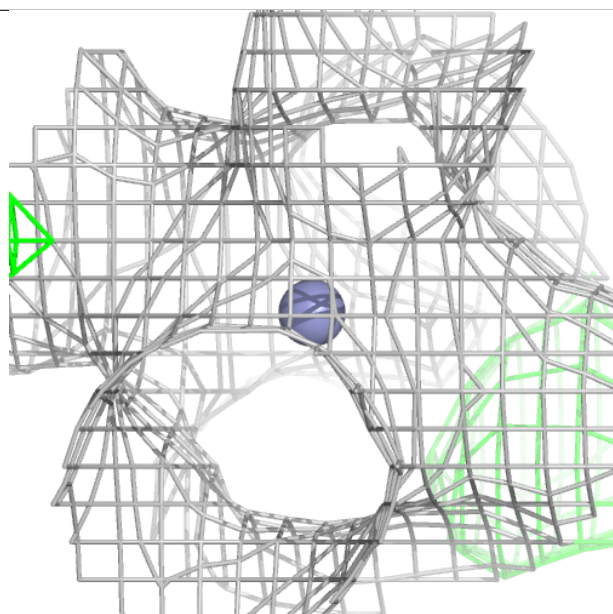
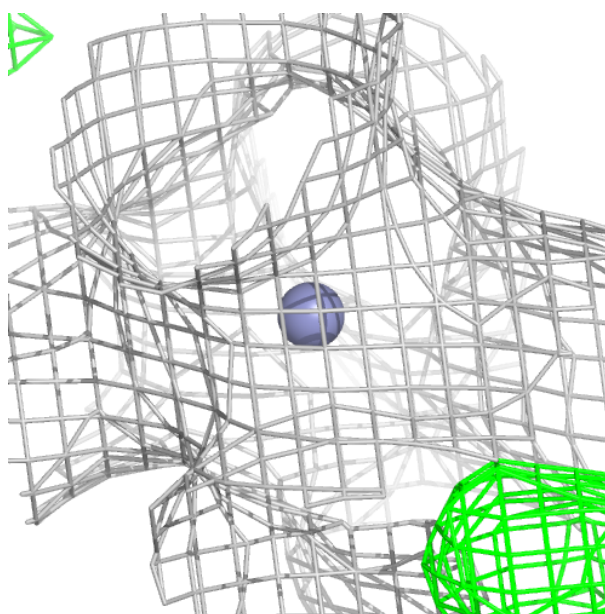
**Electron density around ZN A 502:**

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



**Electron density around ZN B 502:**

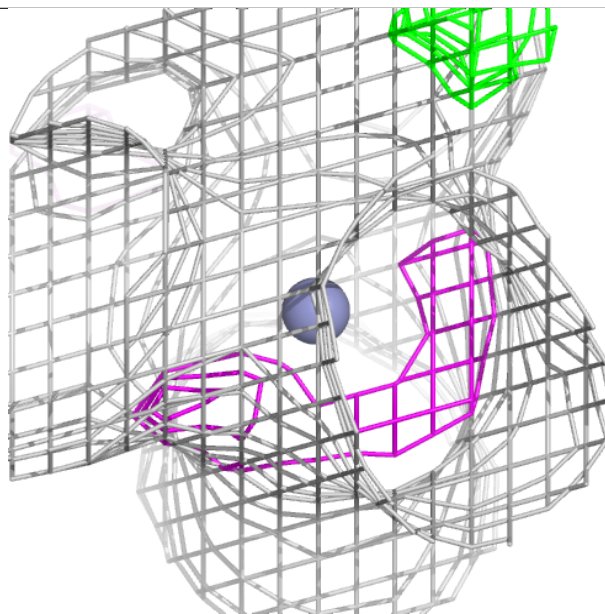
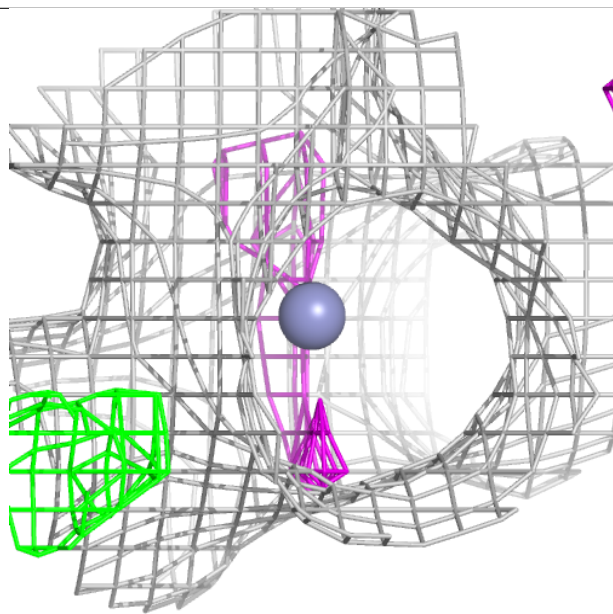
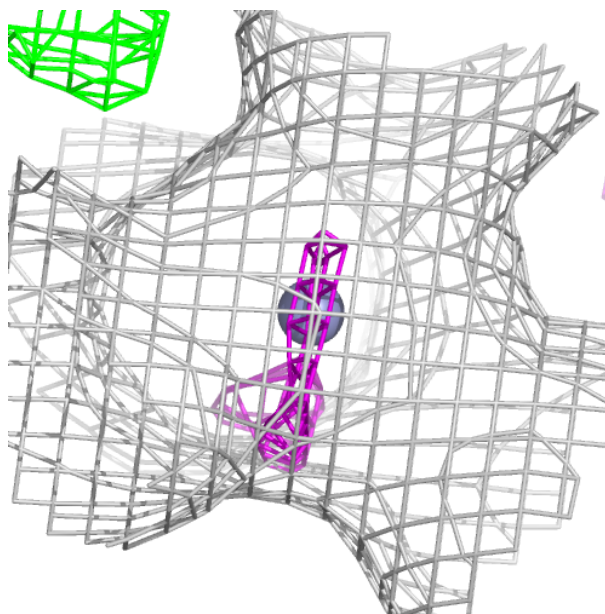
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





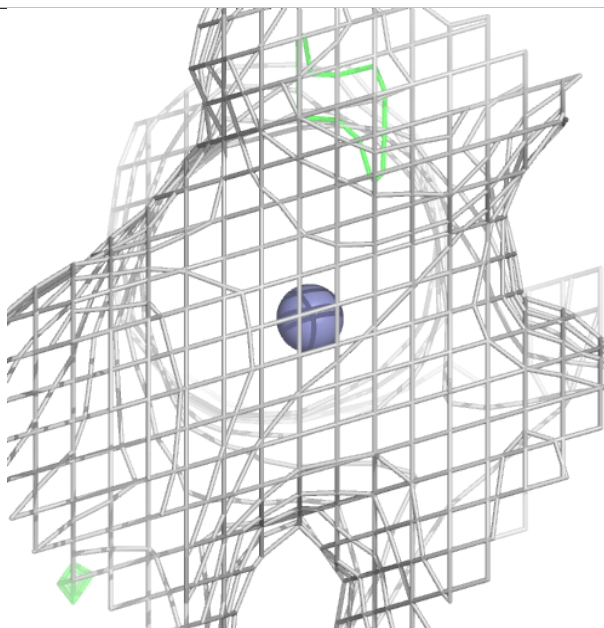
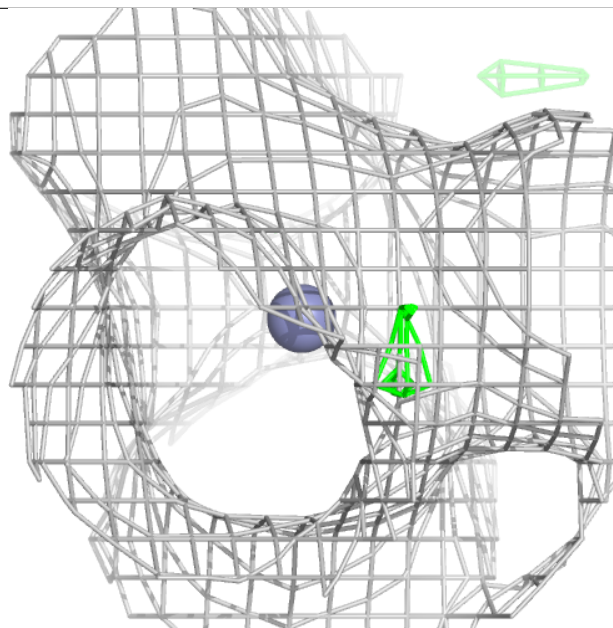
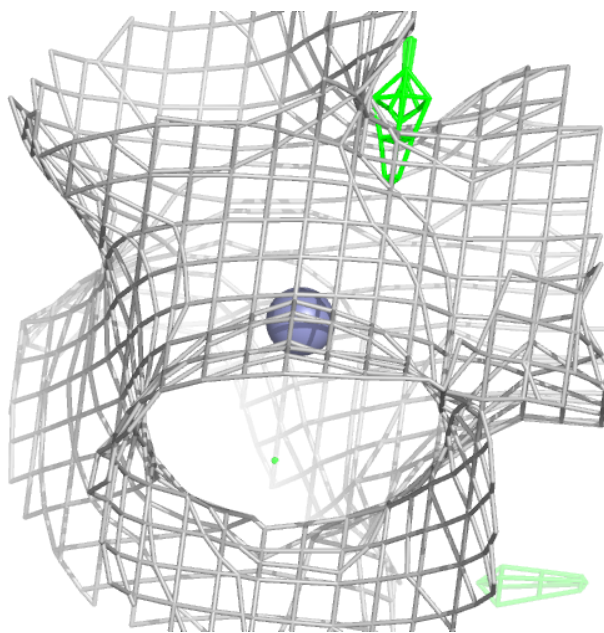
**Electron density around ZN B 503:**

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



**Electron density around ZN C 503:**

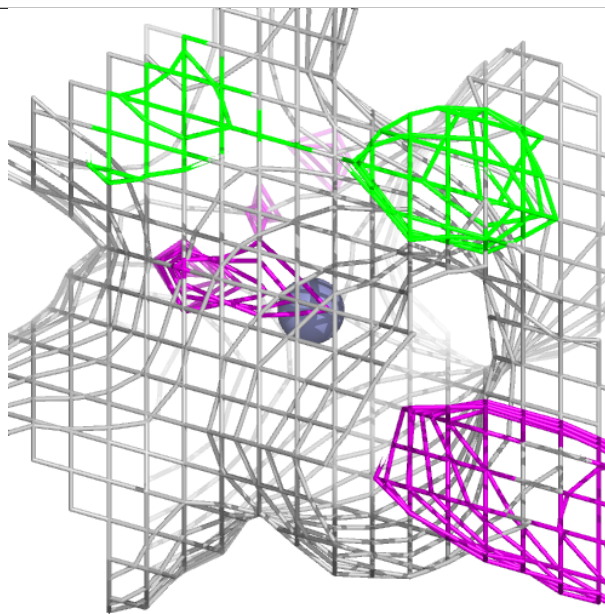
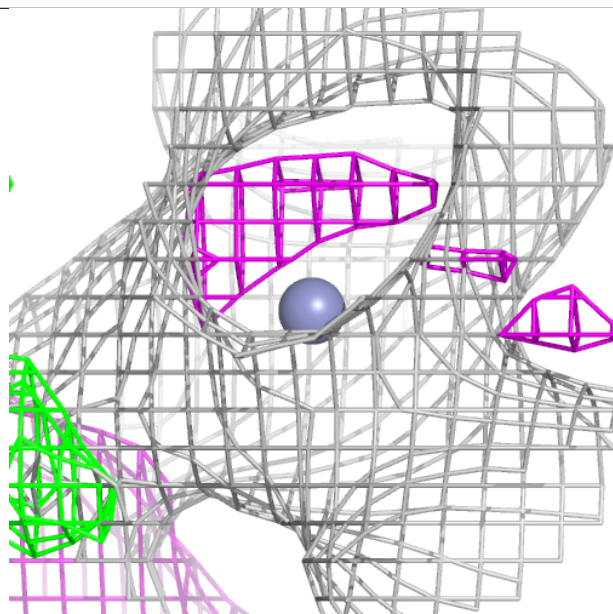
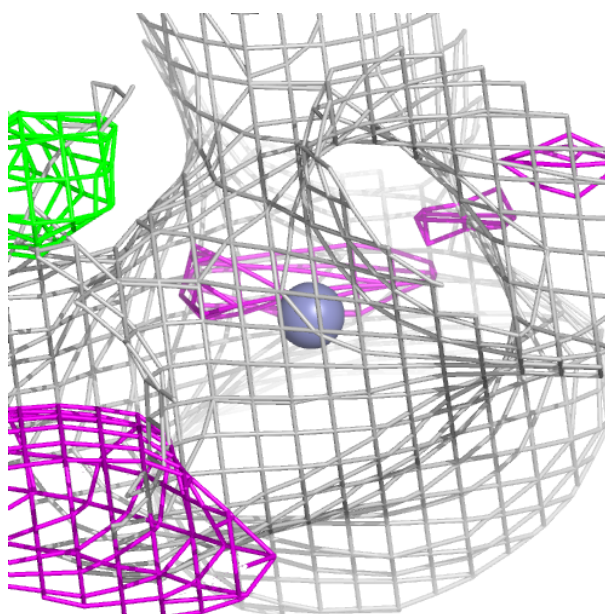
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





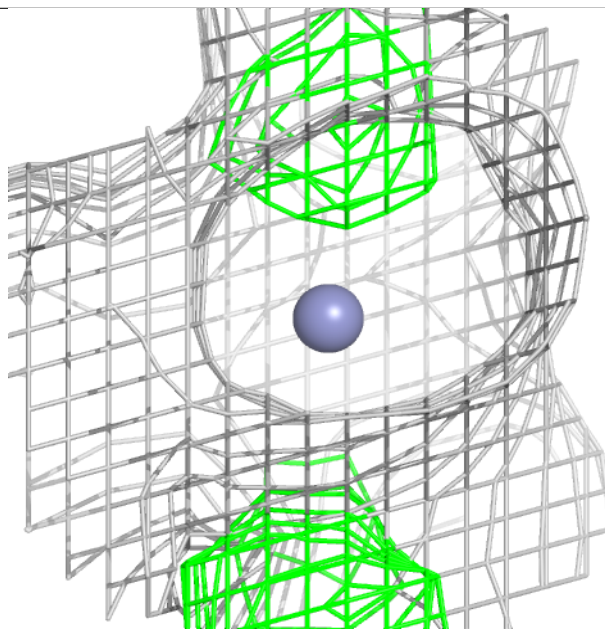
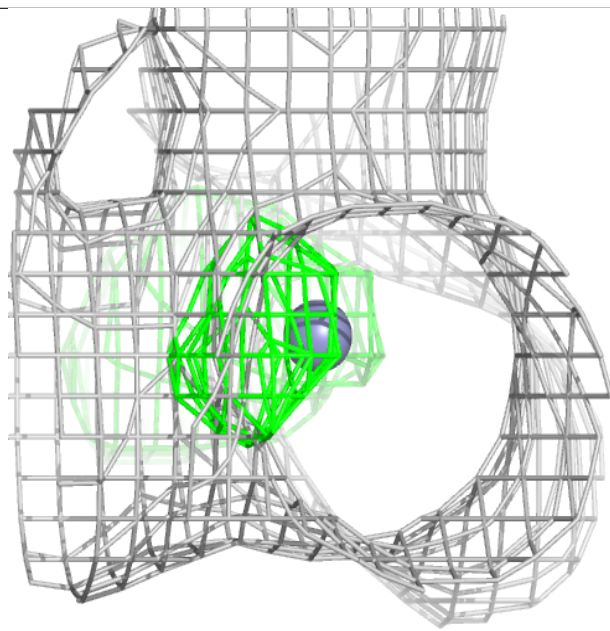
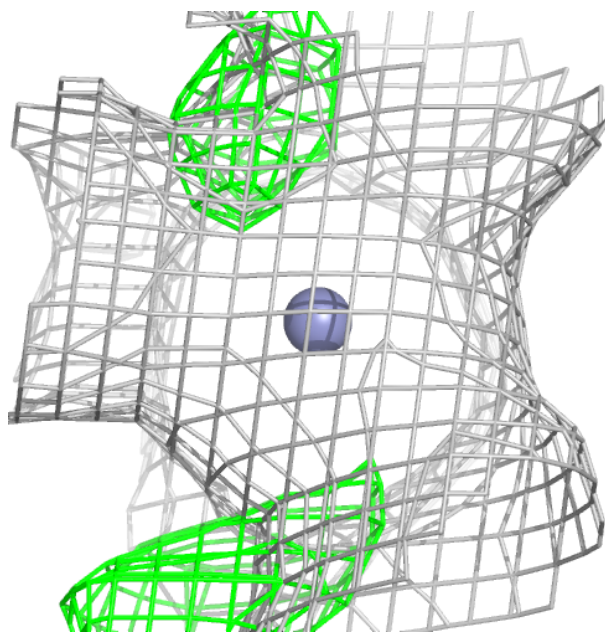
**Electron density around ZN D 502:**

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



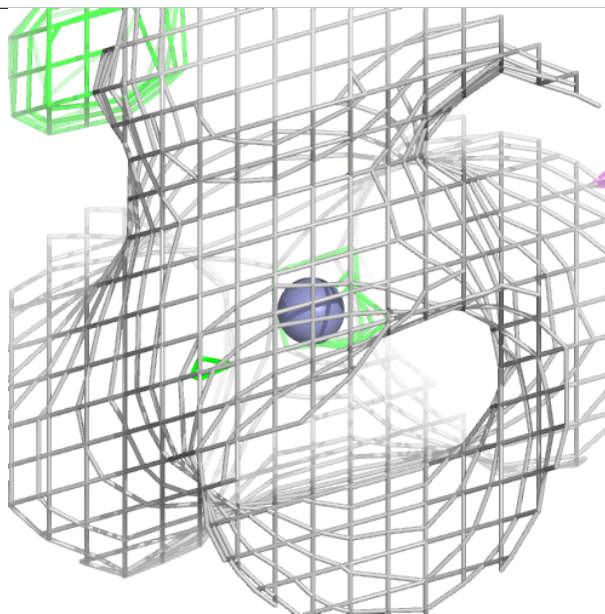
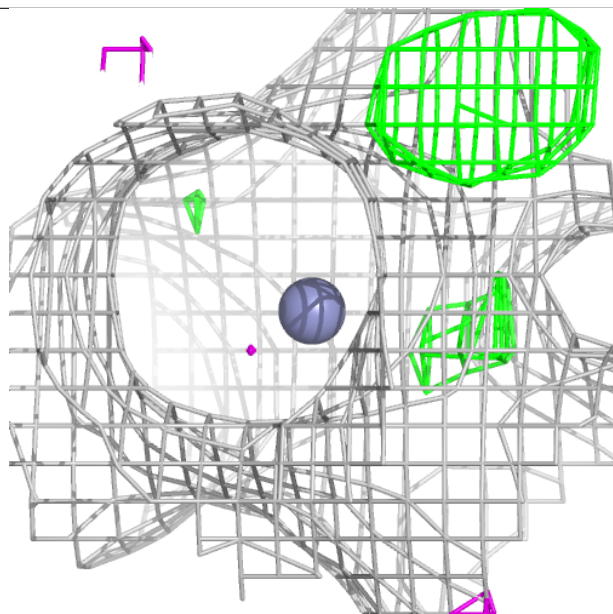
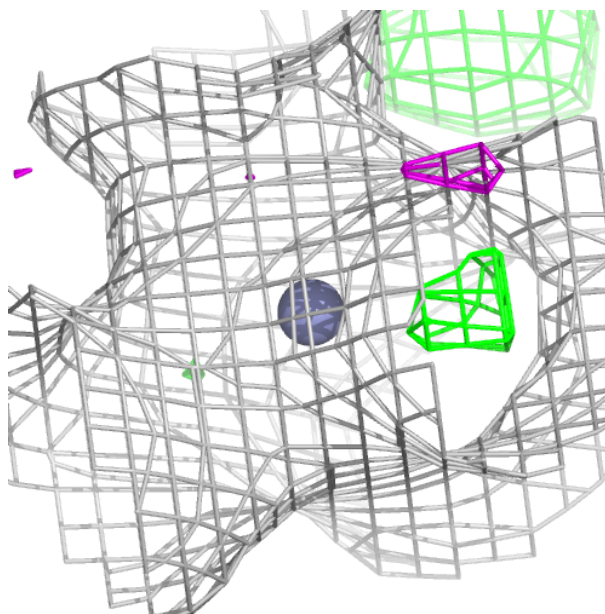
**Electron density around ZN D 503:**

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



**Electron density around ZN E 503:**

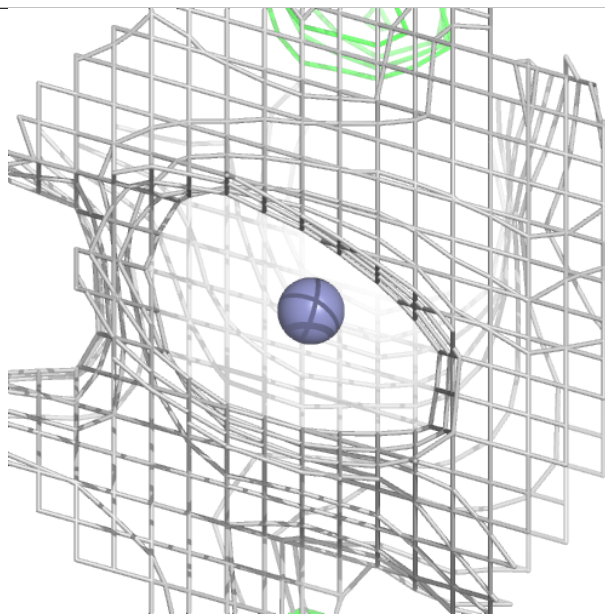
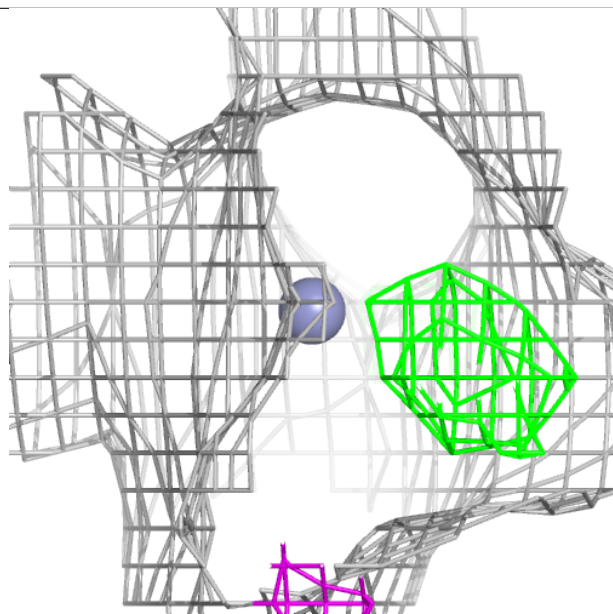
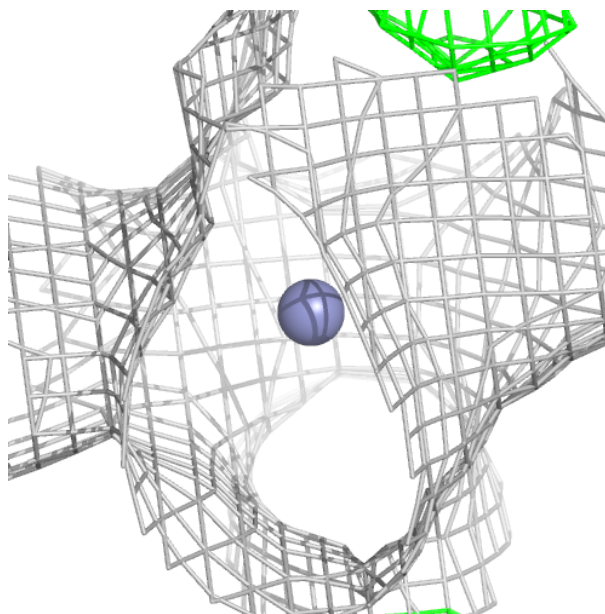
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





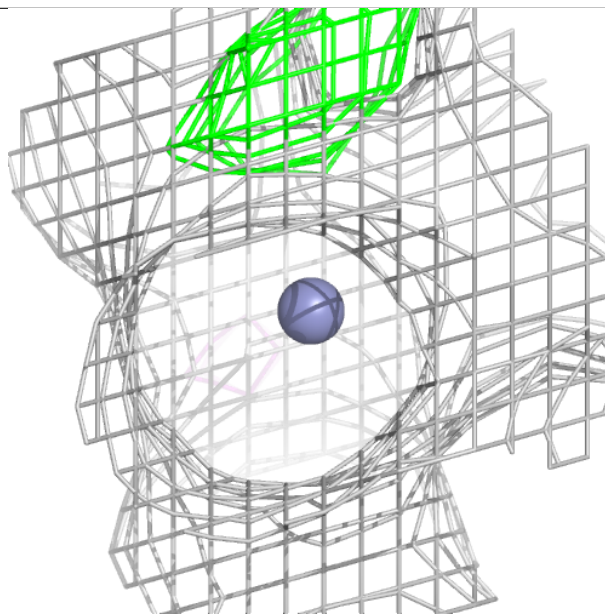
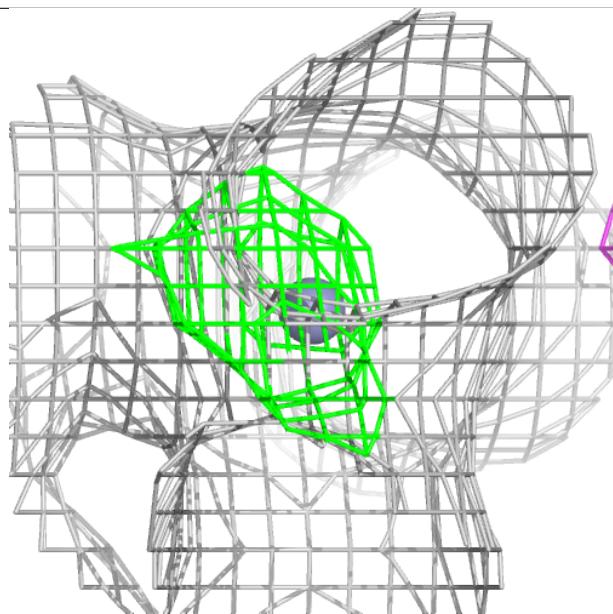
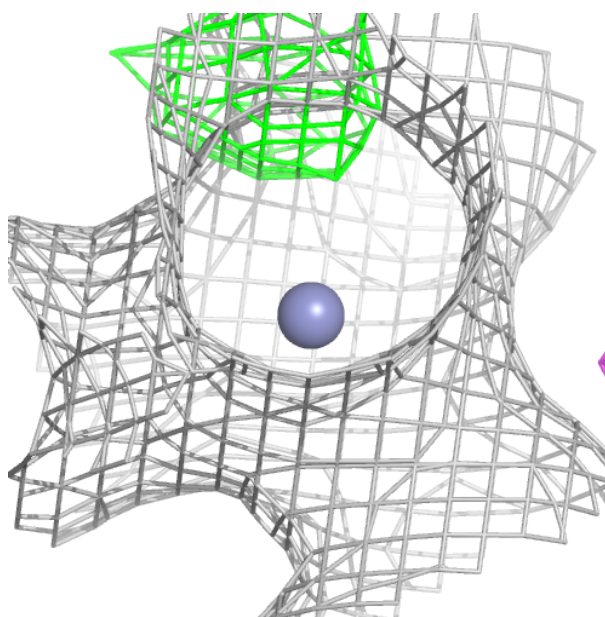
**Electron density around ZN G 503:**

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



**Electron density around ZN A 503:**

$2mF_o-DF_c$  (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.