W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 01:11 AM EDT

PDB ID	:	7SRV
Title	:	Metal dependent activation of Plasmodium falciparum M17 aminopeptidase (inactive form), spacegroup P22121
Authors	:	Webb, C.T.; McGowan, S.
Deposited on	:	2021-11-08
Resolution	:	2.03 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.03 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.
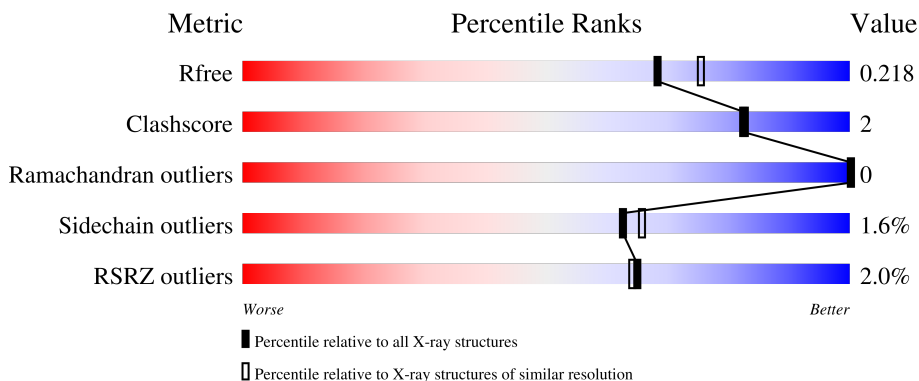
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 <=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	527	% 93% 6% •
1	B	527	4% 91% 7% •
1	C	527	2% 93% 6% •
1	D	527	2% 87% 9% •
1	E	527	% 90% 7% •

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Mol	Chain	Length	Quality of chain
1	F	527	

2%

88%

7% 5%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 25540 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total 3964	C 2546	N 638	O 759	S 21	0	3	0
1	B	518	Total 3898	C 2506	N 630	O 743	S 19	0	4	0
1	C	524	Total 4021	C 2579	N 654	O 769	S 19	0	3	0
1	D	506	Total 3867	C 2488	N 623	O 736	S 20	0	2	0
1	E	513	Total 3944	C 2533	N 641	O 751	S 19	0	2	0
1	F	502	Total 3820	C 2456	N 610	O 736	S 18	0	2	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	conflict	UNP Q8IL11
A	515	GLN	ASN	conflict	UNP Q8IL11
A	546	GLN	ASN	conflict	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11
A	607	HIS	-	expression tag	UNP Q8IL11
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	conflict	UNP Q8IL11
B	515	GLN	ASN	conflict	UNP Q8IL11
B	546	GLN	ASN	conflict	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	conflict	UNP Q8IL11
C	515	GLN	ASN	conflict	UNP Q8IL11
C	546	GLN	ASN	conflict	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	conflict	UNP Q8IL11
D	515	GLN	ASN	conflict	UNP Q8IL11
D	546	GLN	ASN	conflict	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	conflict	UNP Q8IL11
E	515	GLN	ASN	conflict	UNP Q8IL11
E	546	GLN	ASN	conflict	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	conflict	UNP Q8IL11
F	515	GLN	ASN	conflict	UNP Q8IL11
F	546	GLN	ASN	conflict	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11

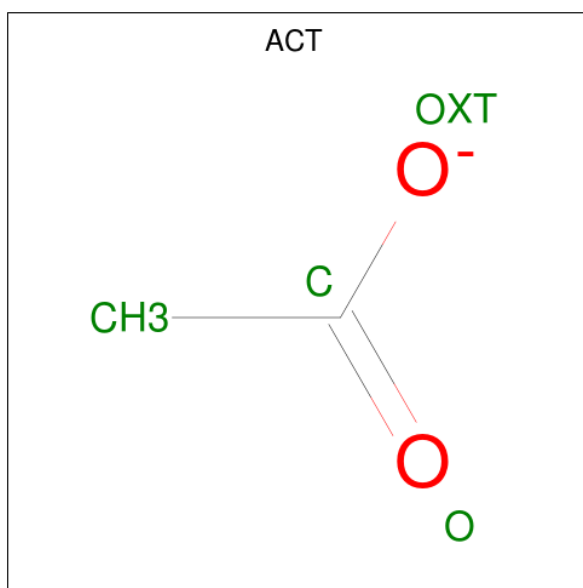- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).
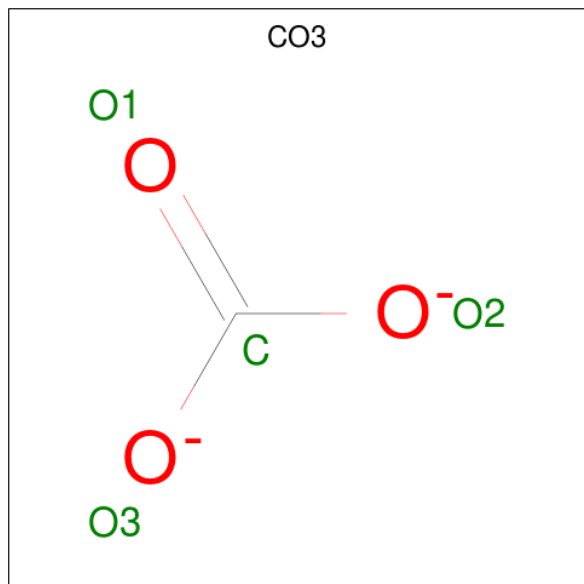
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 1	O 3	0	0
3	B	1	Total 4	C 1	O 3	0	0
3	C	1	Total 4	C 1	O 3	0	0
3	D	1	Total 4	C 1	O 3	0	0
3	E	1	Total 4	C 1	O 3	0	0
3	F	1	Total 4	C 1	O 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	F	1	Total 4	C 2	O 2	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total Ca 1 1		0	0
5	E	3	Total Ca 3 3		0	0
5	F	1	Total Ca 1 1		0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
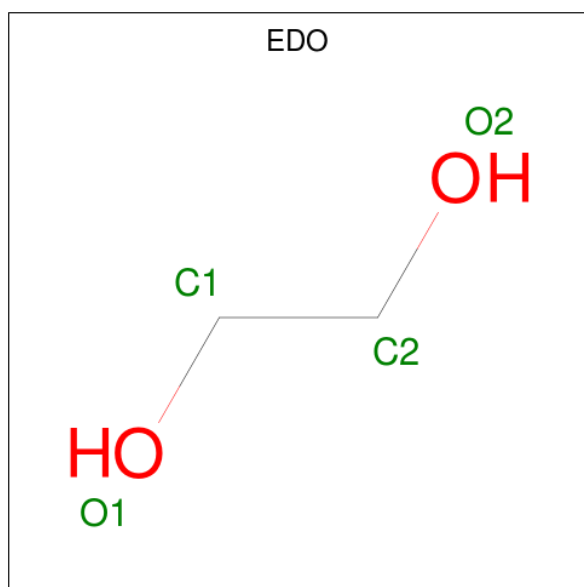
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P ═ O O1

P

O⁻

O4
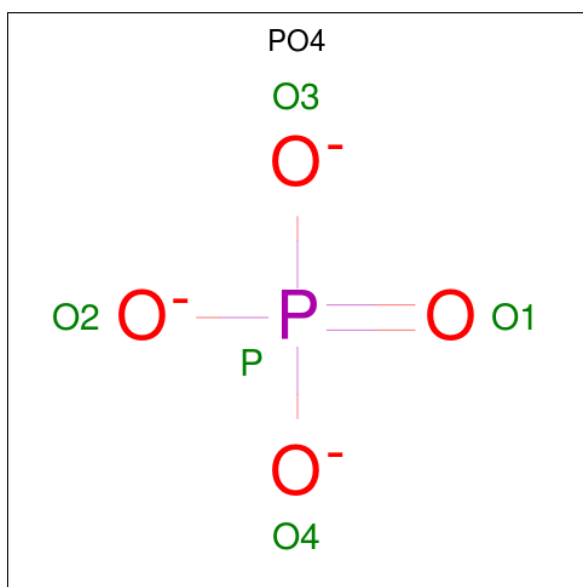
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 5	O 4	P 1	0	0
7	F	1	Total 5	O 4	P 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO   OH

O1   O2
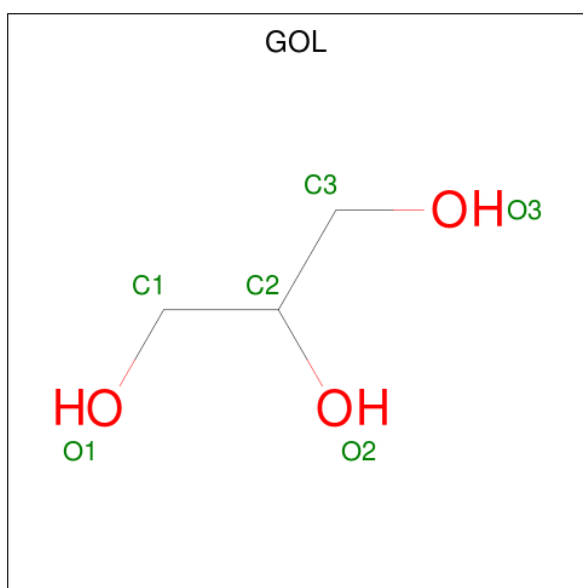
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total 6	C 3	O 3	0	0

- Molecule 9 is water.

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	343	Total 343	O 343	0	0
9	B	236	Total 236	O 236	0	0
9	C	370	Total 370	O 370	0	0
9	D	312	Total 312	O 312	0	0
9	E	387	Total 387	O 387	0	0
9	F	258	Total 258	O 258	0	0

3 Residue-property plots ⓘ

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.

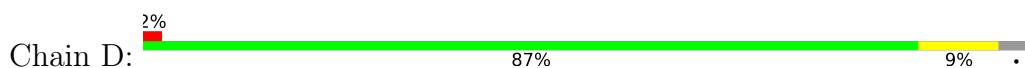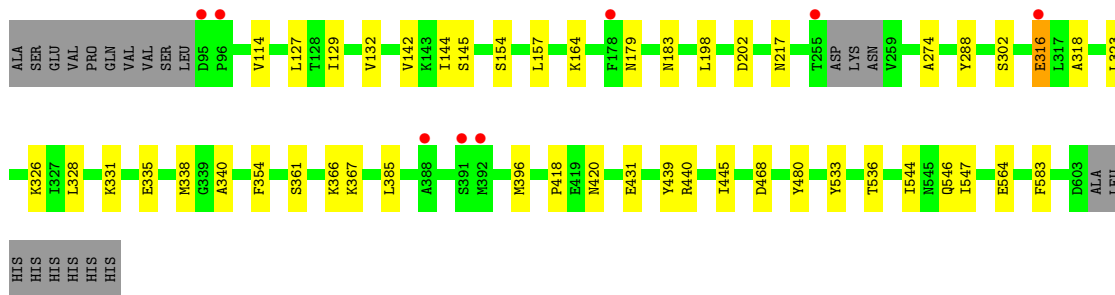- Molecule 1: M17 leucyl aminopeptidase

Chain A:
%
93%   6% •

ALA S86 S98 V114 Y115 V132 P135 G136 V142 F175 V187 S194 R205 A274 Y288 S302 N322 L328 A340 F354 D364 L385 G390 N420 V421 Y439 I445 I481 V482 D483 Y533 T536 W571

D603 A604 LEU HIS HIS HIS HIS HIS HIS

- Molecule 1: M17 leucyl aminopeptidase

Chain B:
4%
91%   7% •

ALA S86 E87 V88 P89 Q90 V91 V92 S93 L94 I117 G120 V132 P135 G136 G140 P141 V142 S146 E155 E160 N161 M162 F175 Y176 D180 S184 V185 A186 S194 V195 A196 D197 L198 R236 E240 N273 T276 E282 K283 Y288

S302 L328 Y350 F354 K367 F378 P389 M392 K417 V421 S435 Y439 K475 Q515 Y533 T536 I544 V551 E564 Q567 D603 ALA LEU HIS HIS HIS HIS HIS HIS

- Molecule 1: M17 leucyl aminopeptidase

Chain C:
2%
93%   6% •

ALA S86 E87 V88 P89 Q90 V91 V92 S93 L94 D95 E102 T105 V114 N134 K137 S154 E155 K173 E200 R236 E240 A274 Y288 S302 V308 L328 E332 A340 F354 K362 G363 D364 L385 P389 GLY S391 M392 I393

N420 Y439 I445 L487 Y533 T536 Q546 I547 H607 H608 H609 H610 HIS

- Molecule 1: M17 leucyl aminopeptidase

Chain D:
2%
87%   9% •

ALA SER GLU VAL PRO GLN VAL VAL SER LEU D95 P96 V114 L127 T128 I129 V132 V142 K143 I144 S145 S154 L157 K164 F178 N179 N183 L198 D202 N217 T255 ASP LYS ASN V259 A274 Y288 S302 E316 L317 A318 L323

K326 I327 L328 K331 E335 M338 G339 A340 F354 S361 K366 K367 L385 A388 S391 M392 M396 P418 E419 N420 E431 Y439 R440 I445 D468 Y480 Y533 T536 I544 N545 Q546 I547 E564 F583 D603 ALA LEU

HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain E:

ALA SER GLU V88 P89 Q90 V91 VAL SER L94 D95 V114 Y115 D116 I117 K118 N122 V132 P135 V142 N149 Q152 E160 S194 D216 K232 S254 K257 ASN VAL ASN MET E262 A274 E279 Y288 S302 L328 E332 S348

F354 D364 K367 G375 A387 ALA PRO GLY S391 M392 L395 M396 M400 N420 V429 C430 E431 K436 N437 S438 Y439 K475 Y480 I544 S548 E564 H609 HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain F:

ALA SER GLU VAL PRO GLN VAL VAL SER LEU ASP P96 E102 V114 T128 V132 G136 LYS E138 V142 V153 S154 E155 F156 L157 M177 F178 V187 M213 L214 H215 D216 N217 L222 R236 E240 S254 T255 D256 LYS ASN VAL ASN MET E262

A274 D275 Y288 S302 L328 S348 F354 G363 G375 L385 K386 A387 P389 ALA G390 S391 M392 M396 K397 F398 V429 C430 E431 Y439 R440 K451 K475 D483 E564 D603 A604 LEU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.54Å 172.67Å 179.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.03 49.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.19-2.03) 100.0 (49.19-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.189 , 0.219 0.188 , 0.218	Depositor DCC
R_{free} test set	11547 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25540	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, CA, ZN, CO3, ACT, PO4, 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	0.25	0/4048	0.44	0/5497
1	B	0.25	0/3982	0.45	0/5417
1	C	0.29	1/4109 (0.0%)	0.49	2/5577 (0.0%)
1	D	0.26	0/3949	0.48	2/5358 (0.0%)
1	E	0.25	0/4028	0.46	0/5462
1	F	0.27	1/3900 (0.0%)	0.53	5/5296 (0.1%)
All	All	0.26	2/24016 (0.0%)	0.47	9/32607 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	187	VAL	CB-CG1	-5.98	1.40	1.52
1	C	155	GLU	CD-OE1	5.10	1.31	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	397	LYS	CB-CG-CD	12.00	142.81	111.60
1	F	397	LYS	CD-CE-NZ	8.21	130.58	111.70
1	F	187	VAL	CG1-CB-CG2	8.07	123.82	110.90
1	C	155	GLU	OE1-CD-OE2	-7.50	114.31	123.30
1	D	316	GLU	CB-CA-C	-7.05	96.31	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3964	0	3861	13	0
1	B	3898	0	3737	22	0
1	C	4021	0	3910	17	0
1	D	3867	0	3784	24	0
1	E	3944	0	3846	22	0
1	F	3820	0	3682	21	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	8	0	6	0	0
4	D	8	0	6	0	0
4	E	4	0	3	1	0
4	F	4	0	3	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	4	0	0	0	0
5	D	1	0	0	0	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
6	A	4	0	6	0	0
6	C	12	0	18	1	0
6	D	4	0	6	0	0
6	F	4	0	6	0	0
7	B	5	0	0	1	0
7	F	5	0	0	0	0
8	E	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	343	0	0	4	0
9	B	236	0	0	5	0
9	C	370	0	0	1	0
9	D	312	0	0	2	0
9	E	387	0	0	5	0
9	F	258	0	0	6	0
All	All	25540	0	22888	115	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 2.

The worst 5 of 115 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:D:440:ARG:NH1	1:E:431:GLU:OE2	2.19	0.70
1:D:366:LYS:HG3	1:D:420:ASN:HB3	1.75	0.69
1:E:90:GLN:NE2	1:E:95:ASP:O	2.26	0.68
1:A:205:ARG:NE	9:A:1106:HOH:O	2.28	0.67
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.78	0.66

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	519/527 (98%)	506 (98%)	13 (2%)	0	100	100
1	B	518/527 (98%)	504 (97%)	14 (3%)	0	100	100
1	C	522/527 (99%)	509 (98%)	13 (2%)	0	100	100
1	D	504/527 (96%)	492 (98%)	12 (2%)	0	100	100
1	E	507/527 (96%)	493 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	496/527 (94%)	484 (98%)	12 (2%)	0	100	100
All	All	3066/3162 (97%)	2988 (98%)	78 (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	420/454 (92%)	413 (98%)	7 (2%)	60	63
1	B	402/454 (88%)	398 (99%)	4 (1%)	76	80
1	C	428/454 (94%)	422 (99%)	6 (1%)	67	70
1	D	409/454 (90%)	402 (98%)	7 (2%)	60	63
1	E	419/454 (92%)	412 (98%)	7 (2%)	60	63
1	F	399/454 (88%)	389 (98%)	10 (2%)	47	48
All	All	2477/2724 (91%)	2436 (98%)	41 (2%)	62	63

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	436	LYS
1	F	302	SER
1	E	437	ASN
1	F	154[B]	SER
1	F	397	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	GLN
1	B	272	ASN
1	D	161	ASN

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Mol	Chain	Res	Type
1	D	568	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
4	ACT	E	1003	-	3,3,3	1.27	0	3,3,3	1.37	0
4	ACT	D	1003	-	3,3,3	1.27	0	3,3,3	1.38	0
3	CO3	A	1002	-	2,3,3	0.40	0	2,3,3	0.15	0
6	EDO	F	1005	-	3,3,3	0.46	0	2,2,2	0.32	0
7	PO4	B	1004	-	4,4,4	0.94	0	6,6,6	0.47	0
6	EDO	A	1005	-	3,3,3	0.46	0	2,2,2	0.34	0
4	ACT	B	1003	-	3,3,3	1.32	0	3,3,3	1.51	0
4	ACT	C	1011	-	3,3,3	1.26	0	3,3,3	1.37	0
6	EDO	C	1008	-	3,3,3	0.46	0	2,2,2	0.33	0
4	ACT	A	1003	-	3,3,3	1.27	0	3,3,3	1.38	0
7	PO4	F	1003	-	4,4,4	0.93	0	6,6,6	0.41	0
3	CO3	E	1002	-	2,3,3	0.41	0	2,3,3	0.21	0
3	CO3	F	1002	-	2,3,3	0.41	0	2,3,3	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
6	EDO	C	1010	-	3,3,3	0.44	0	2,2,2	0.40	0
3	CO3	B	1002	-	2,3,3	0.40	0	2,3,3	0.20	0
4	ACT	C	1003	-	3,3,3	1.28	0	3,3,3	1.53	0
4	ACT	D	1006	-	3,3,3	1.31	0	3,3,3	1.52	0
6	EDO	C	1009	-	3,3,3	0.46	0	2,2,2	0.35	0
8	GOL	E	1007	-	5,5,5	0.93	0	5,5,5	0.97	0
4	ACT	F	1006	-	3,3,3	1.30	0	3,3,3	1.35	0
3	CO3	C	1002	-	2,3,3	0.39	0	2,3,3	0.12	0
3	CO3	D	1002	-	2,3,3	0.41	0	2,3,3	0.23	0
6	EDO	D	1005	-	3,3,3	0.45	0	2,2,2	0.36	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
6	EDO	F	1005	-	-	0/1/1/1	-
6	EDO	A	1005	-	-	0/1/1/1	-
6	EDO	C	1009	-	-	1/1/1/1	-
6	EDO	C	1008	-	-	0/1/1/1	-
8	GOL	E	1007	-	-	1/4/4/4	-
6	EDO	C	1010	-	-	0/1/1/1	-
6	EDO	D	1005	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	1007	GOL	O1-C1-C2-C3
6	C	1009	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1003	ACT	1	0
7	B	1004	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1010	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	519/527 (98%)	-0.11	4 (0%)	86	85	26, 35, 56, 80	6 (1%)
1	B	518/527 (98%)	0.02	19 (3%)	41	41	27, 41, 69, 83	9 (1%)
1	C	524/527 (99%)	-0.23	11 (2%)	63	63	24, 33, 58, 80	11 (2%)
1	D	506/527 (96%)	-0.29	8 (1%)	72	71	25, 36, 55, 87	11 (2%)
1	E	513/527 (97%)	-0.30	7 (1%)	75	74	25, 34, 54, 70	12 (2%)
1	F	502/527 (95%)	-0.13	12 (2%)	59	58	27, 40, 68, 88	10 (1%)
All	All	3082/3162 (97%)	-0.17	61 (1%)	65	64	24, 36, 63, 88	59 (1%)

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	VAL	4.9
1	E	91	VAL	4.2
1	C	88	VAL	4.1
1	B	94	LEU	4.1
1	C	93	SER	4.1

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	B	1006	1/1	0.70	0.20	83,83,83,83	0
5	CA	C	1005	1/1	0.73	0.07	84,84,84,84	0
5	CA	E	1006	1/1	0.75	0.20	79,79,79,79	0
6	EDO	C	1009	4/4	0.75	0.19	40,54,57,59	0
8	GOL	E	1007	6/6	0.75	0.21	43,49,63,66	0
5	CA	C	1006	1/1	0.77	0.13	60,60,60,60	0
5	CA	C	1007	1/1	0.86	0.11	75,75,75,75	0
6	EDO	A	1005	4/4	0.86	0.14	51,54,58,60	0
6	EDO	C	1008	4/4	0.87	0.09	48,51,56,61	0
4	ACT	D	1006	4/4	0.88	0.12	43,50,53,54	0
6	EDO	D	1005	4/4	0.89	0.13	47,48,52,53	0
4	ACT	C	1011	4/4	0.91	0.17	34,45,46,49	0
6	EDO	C	1010	4/4	0.93	0.12	41,43,51,53	0
4	ACT	F	1006	4/4	0.94	0.14	35,35,39,43	0
4	ACT	D	1003	4/4	0.94	0.17	35,37,39,43	0
6	EDO	F	1005	4/4	0.94	0.07	46,50,53,54	0
4	ACT	E	1003	4/4	0.94	0.13	31,40,42,45	0
3	CO3	E	1002	4/4	0.95	0.12	28,31,40,44	0
3	CO3	F	1002	4/4	0.95	0.12	28,32,37,47	0
4	ACT	B	1003	4/4	0.95	0.11	30,34,34,38	0
3	CO3	C	1002	4/4	0.95	0.14	25,28,34,42	0
3	CO3	D	1002	4/4	0.95	0.11	29,31,36,41	0
3	CO3	A	1002	4/4	0.96	0.13	26,29,33,45	0
3	CO3	B	1002	4/4	0.96	0.12	29,32,33,38	0
2	ZN	F	1007	1/1	0.97	0.08	33,33,33,33	1
4	ACT	A	1003	4/4	0.97	0.13	32,36,38,42	0
2	ZN	C	1012	1/1	0.97	0.11	31,31,31,31	1
5	CA	E	1005	1/1	0.97	0.08	48,48,48,48	0
4	ACT	C	1003	4/4	0.97	0.10	31,32,33,37	0
2	ZN	D	1007	1/1	0.97	0.07	37,37,37,37	1
2	ZN	A	1006	1/1	0.98	0.10	34,34,34,34	1
2	ZN	E	1008	1/1	0.98	0.14	34,34,34,34	1
7	PO4	B	1004	5/5	0.98	0.15	34,39,44,50	0
7	PO4	F	1003	5/5	0.98	0.21	48,51,52,57	0
2	ZN	D	1001	1/1	0.98	0.08	33,33,33,33	1
2	ZN	B	1007	1/1	0.99	0.05	39,39,39,39	1
2	ZN	E	1001	1/1	0.99	0.12	32,32,32,32	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	1001	1/1	0.99	0.10	29,29,29,29	1
5	CA	D	1004	1/1	0.99	0.04	34,34,34,34	0
2	ZN	F	1001	1/1	0.99	0.10	30,30,30,30	1
5	CA	B	1005	1/1	0.99	0.06	36,36,36,36	0
5	CA	F	1004	1/1	0.99	0.09	36,36,36,36	0
2	ZN	B	1001	1/1	0.99	0.06	34,34,34,34	1
5	CA	A	1004	1/1	1.00	0.08	33,33,33,33	0
5	CA	C	1004	1/1	1.00	0.05	33,33,33,33	0
2	ZN	C	1001	1/1	1.00	0.03	44,44,44,44	0
5	CA	E	1004	1/1	1.00	0.06	33,33,33,33	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.
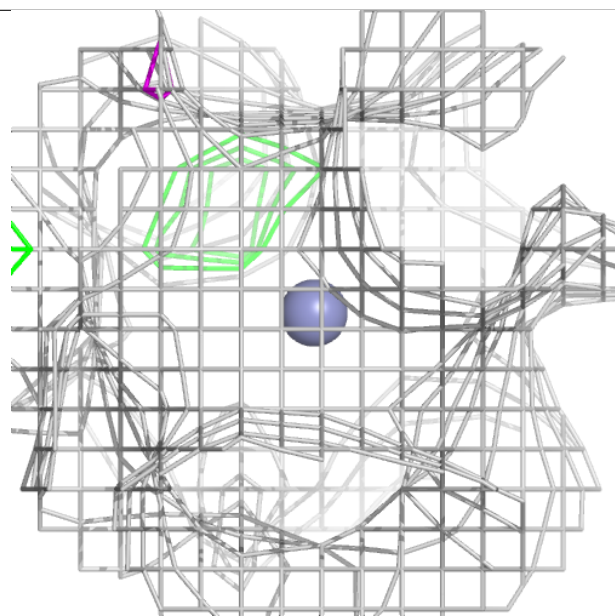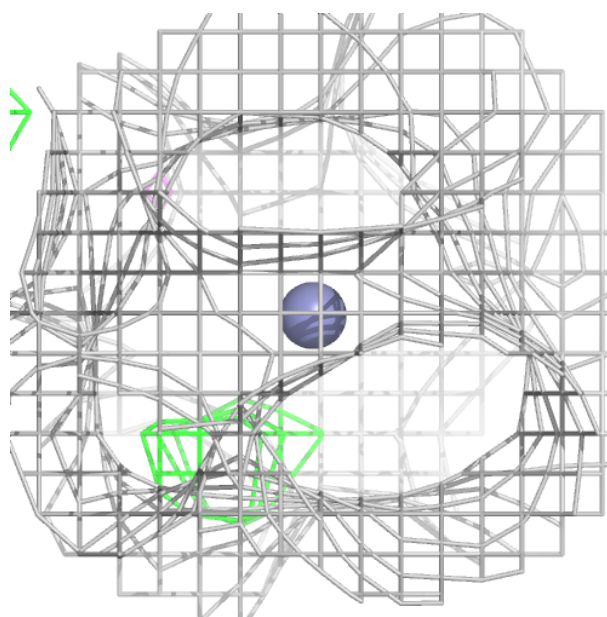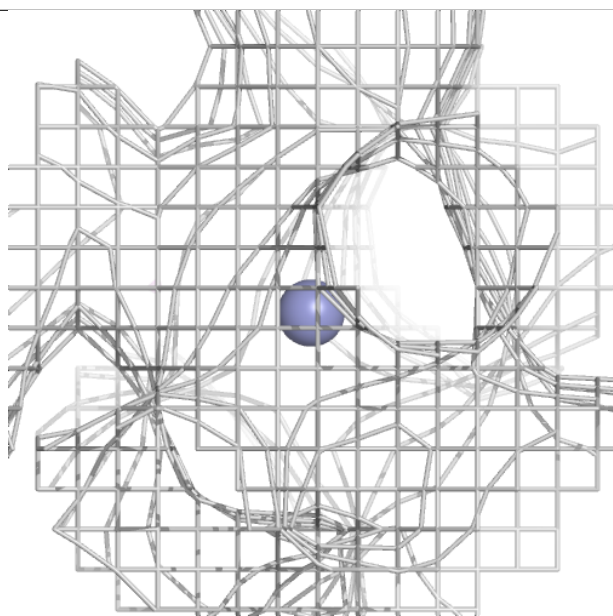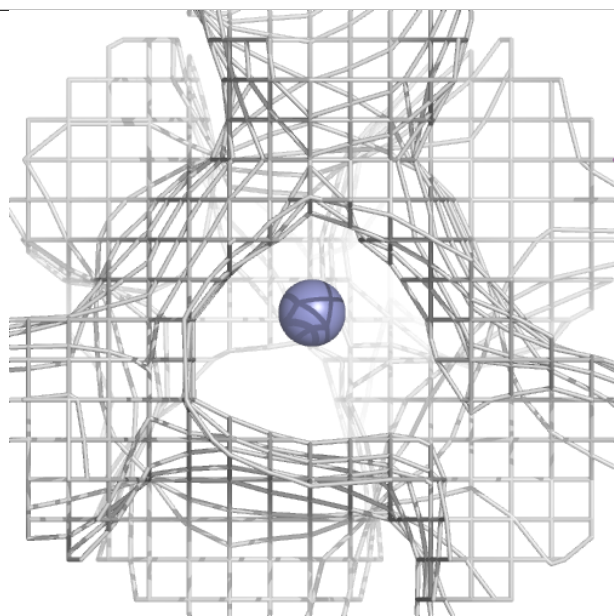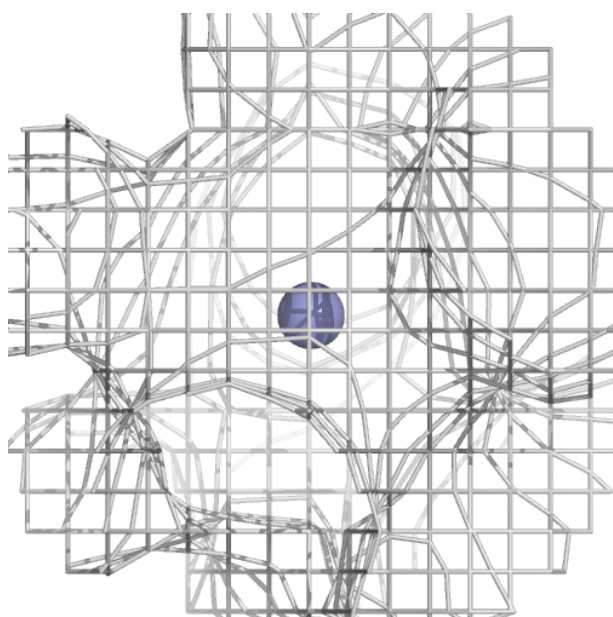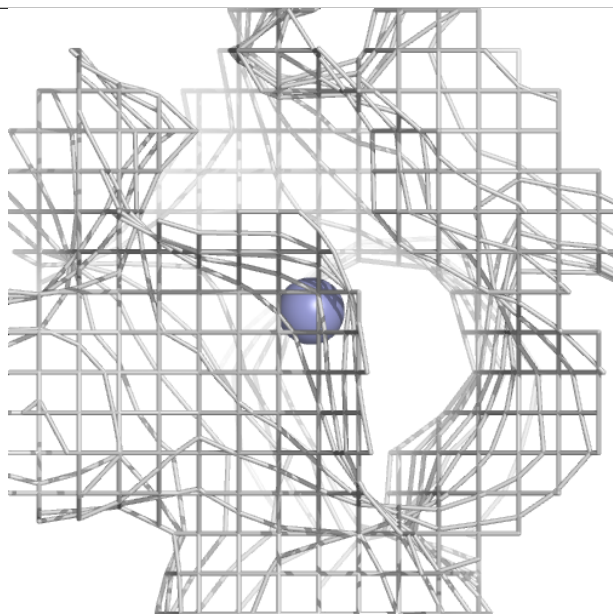
Electron density around ZN F 1007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
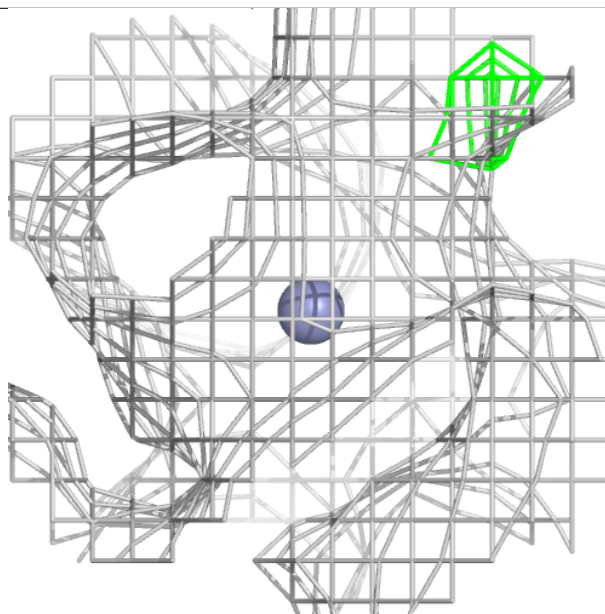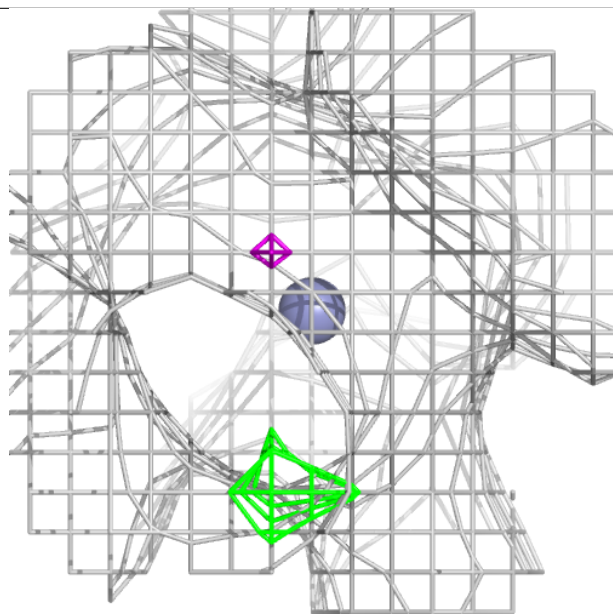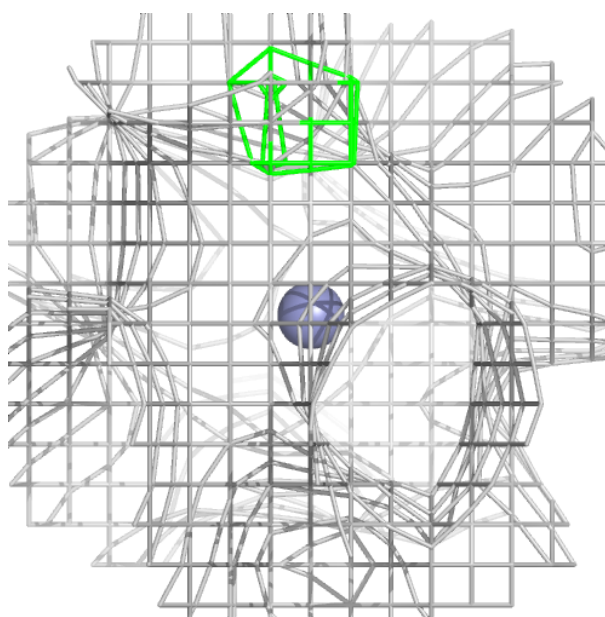
Electron density around ZN C 1012:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
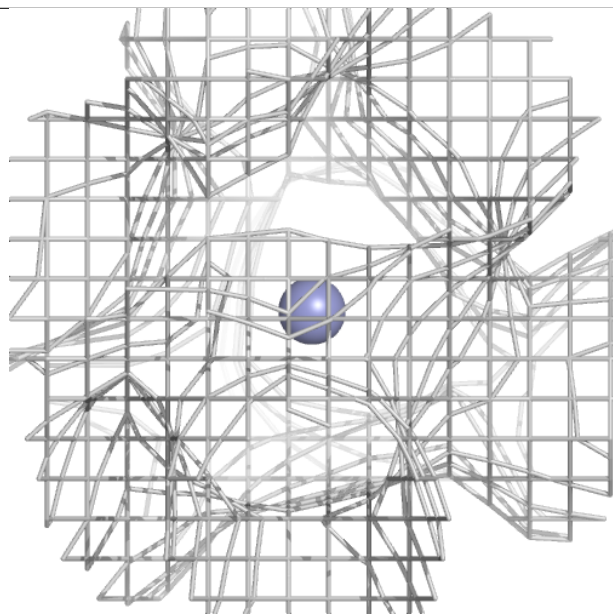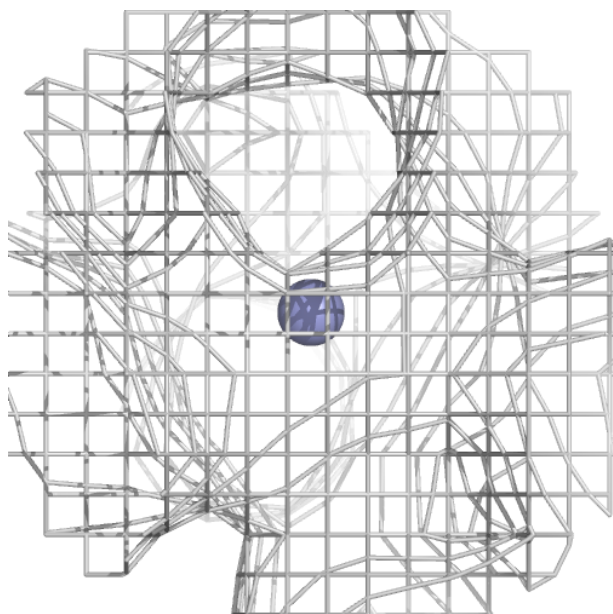and green (positive)
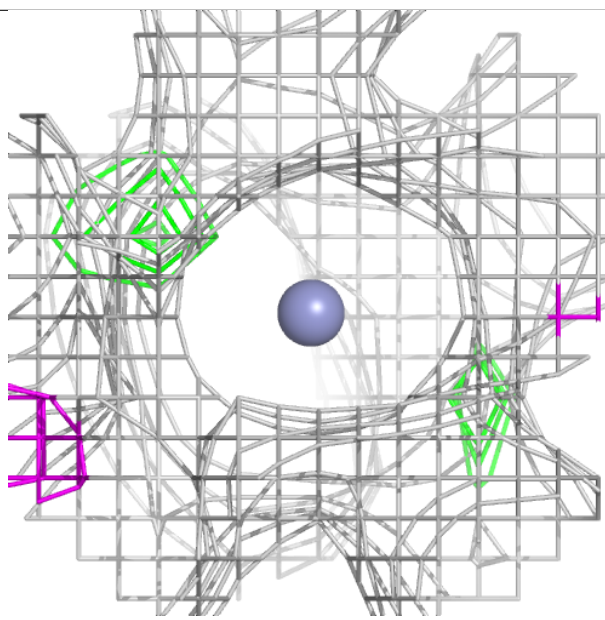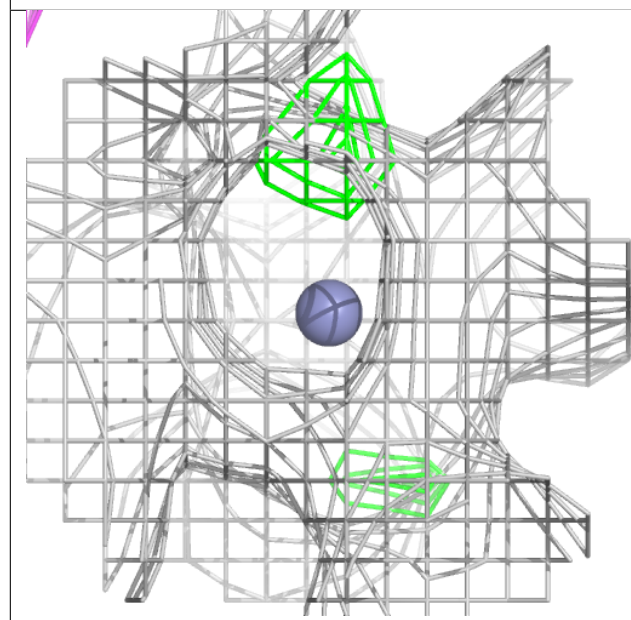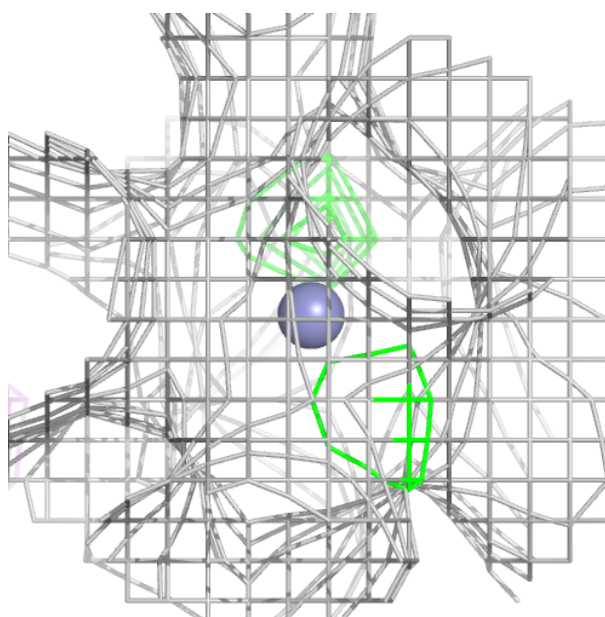
Electron density around ZN D 1007:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
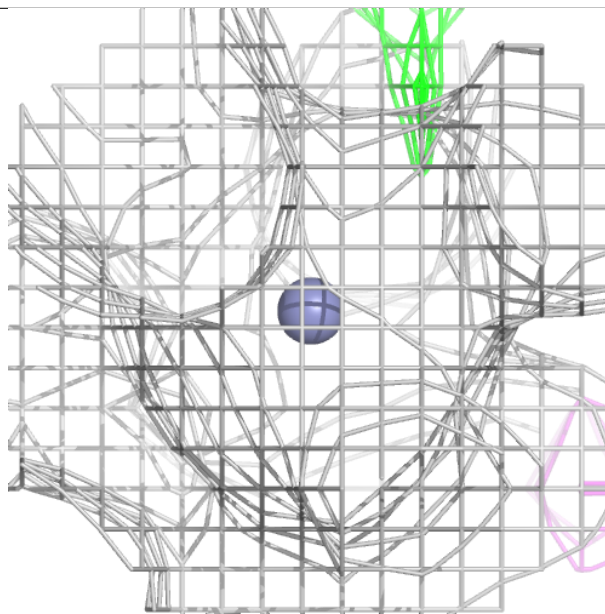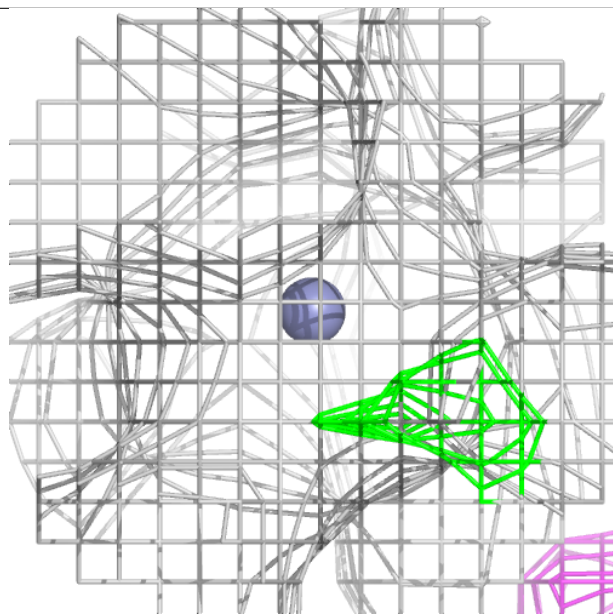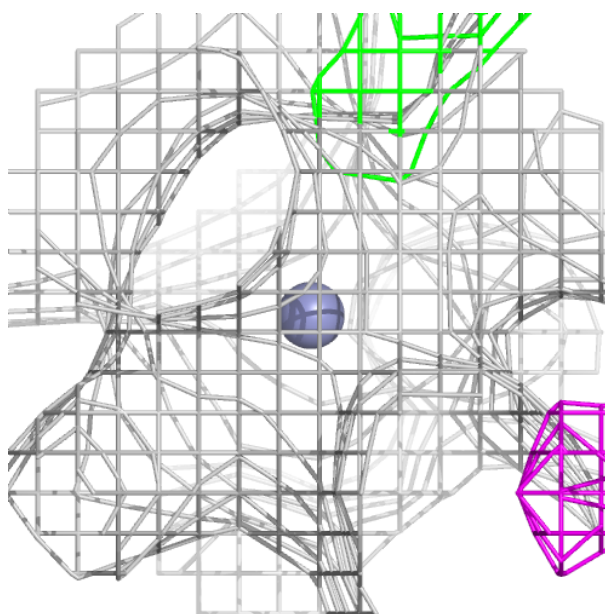
Electron density around ZN A 1006:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
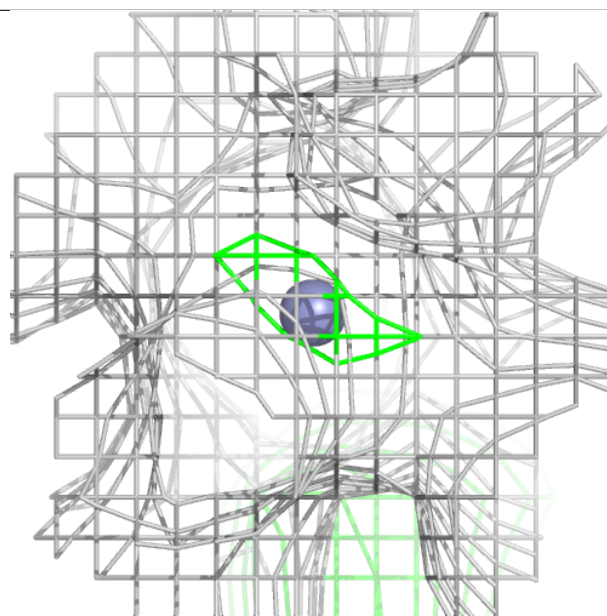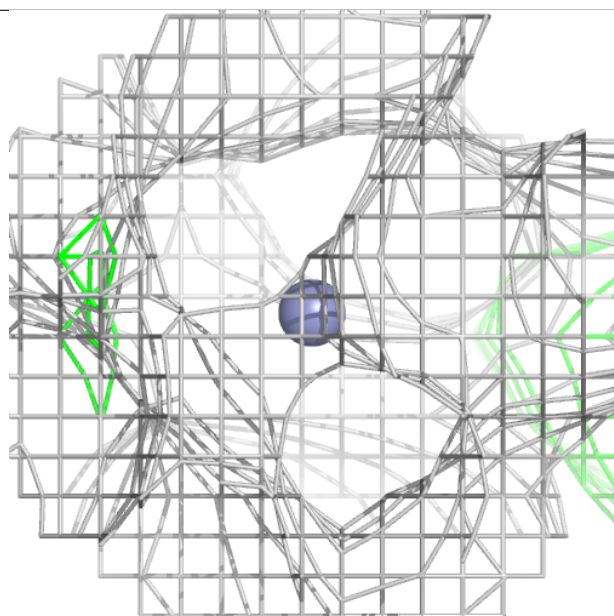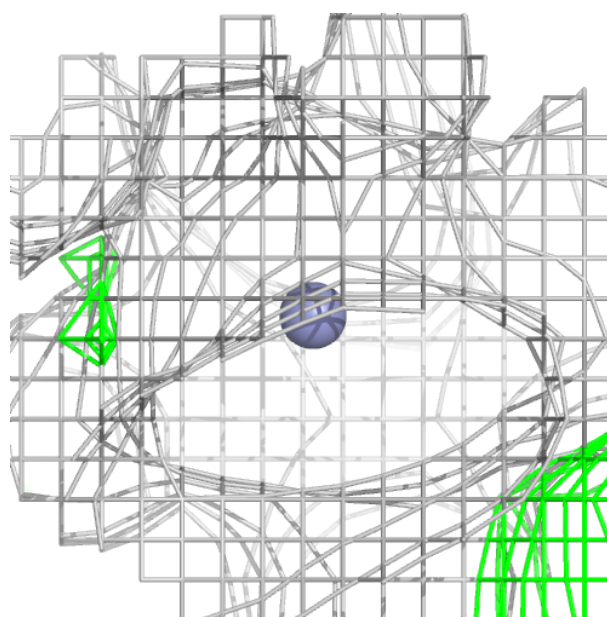
Electron density around ZN E 1008:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
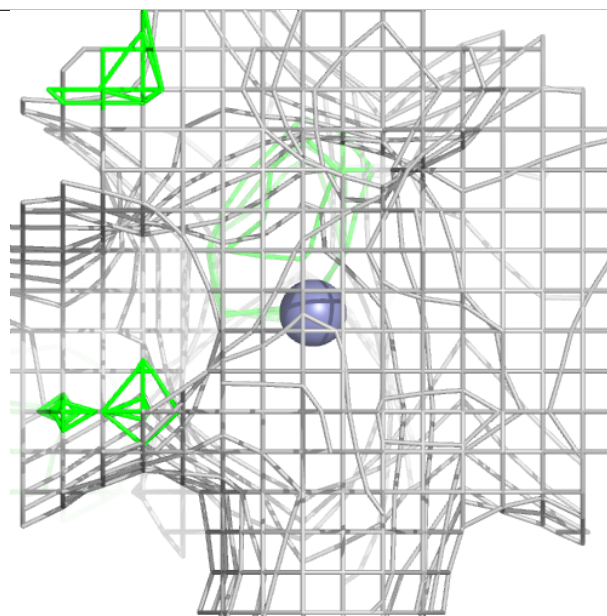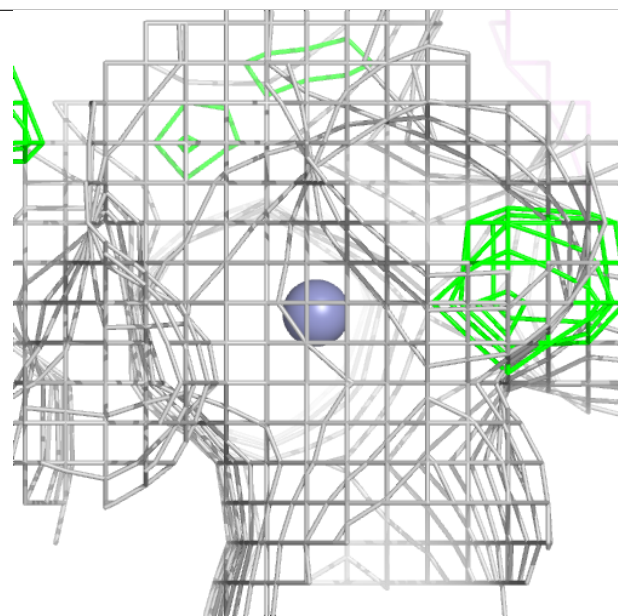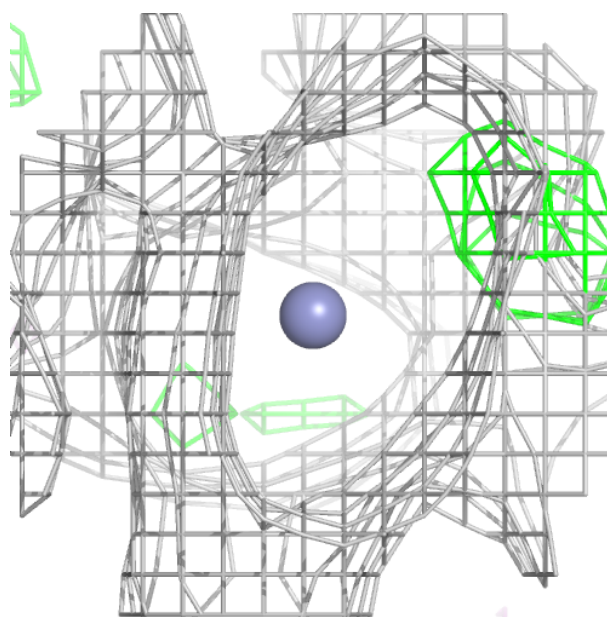
Electron density around ZN D 1001:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
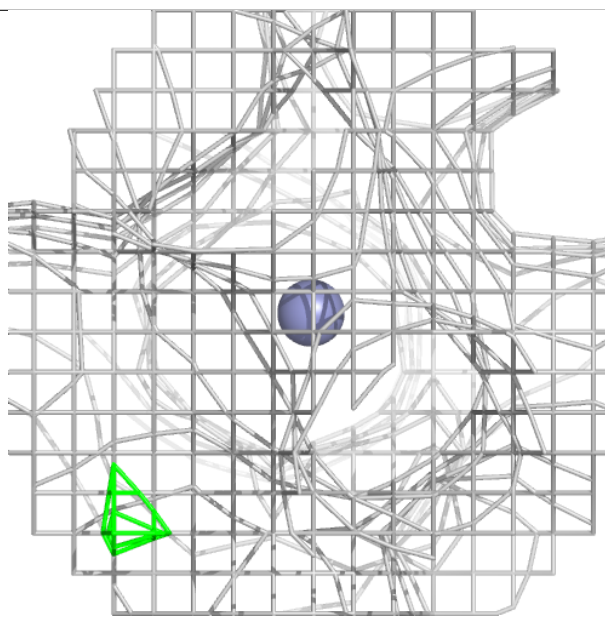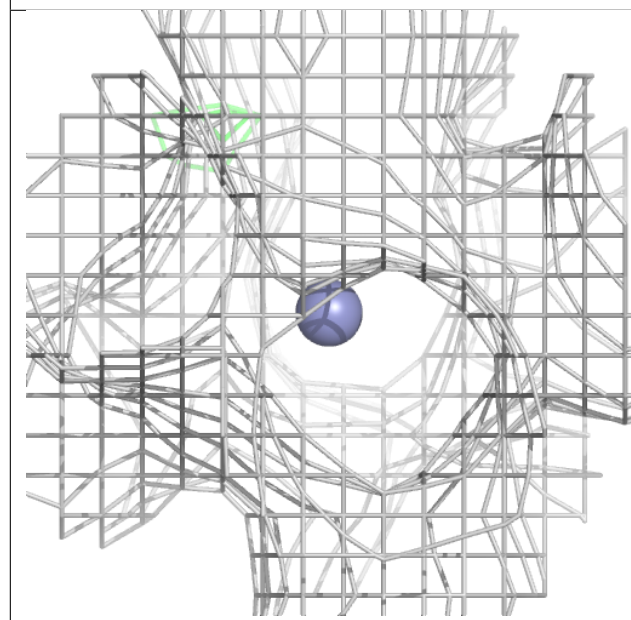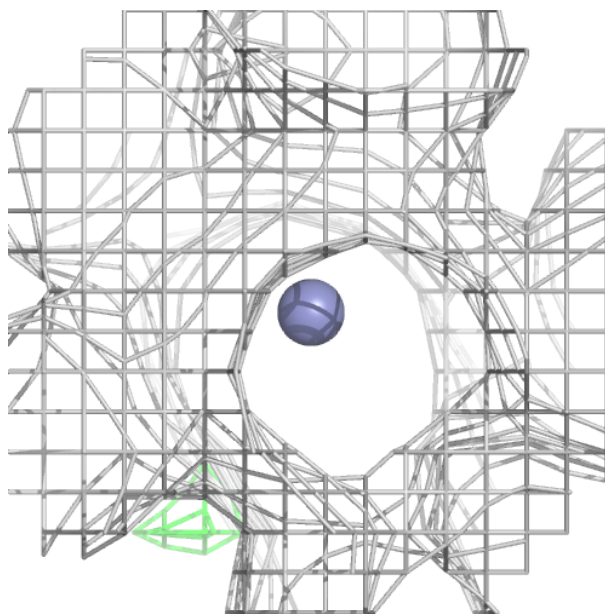
Electron density around ZN B 1007:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
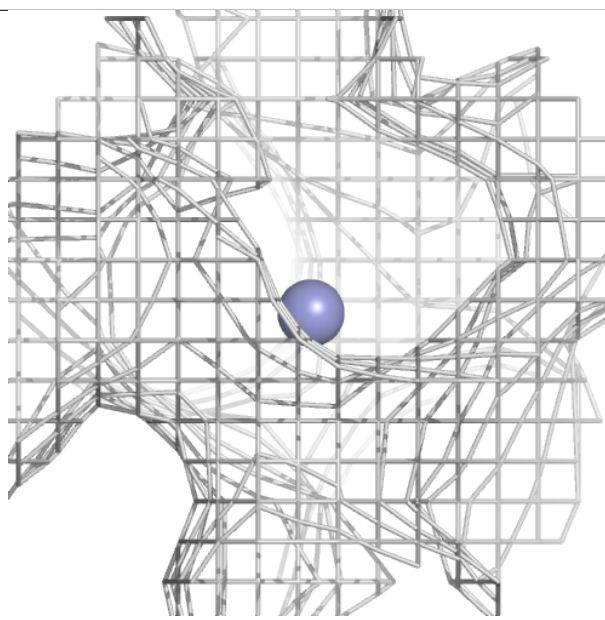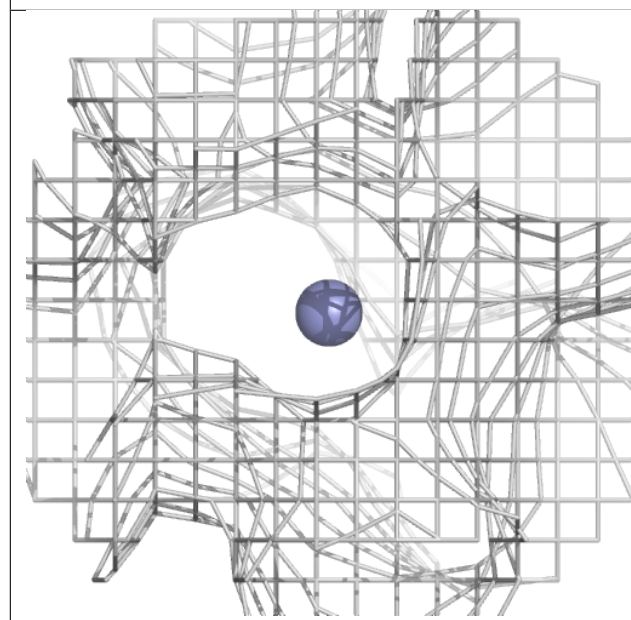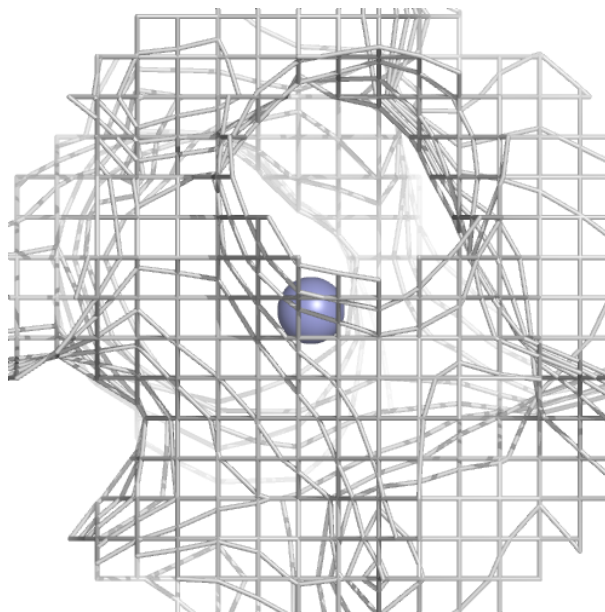and green (positive)
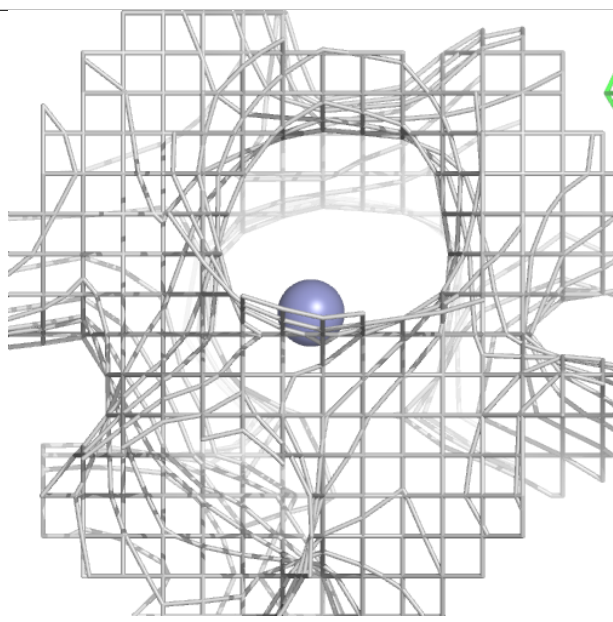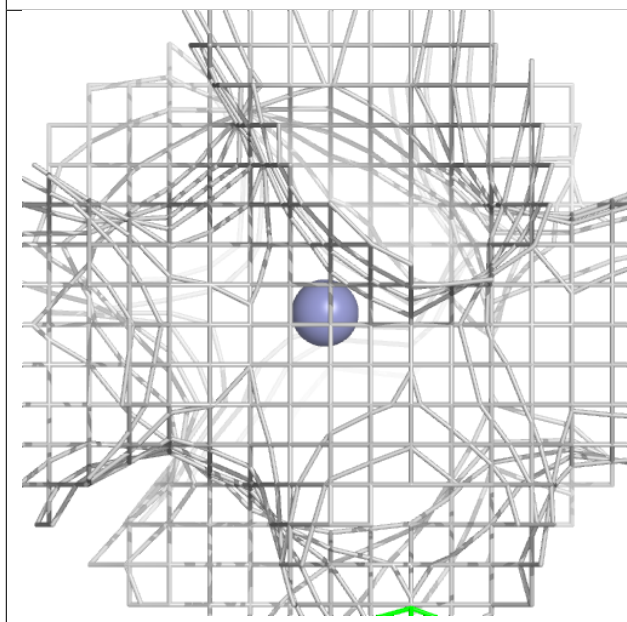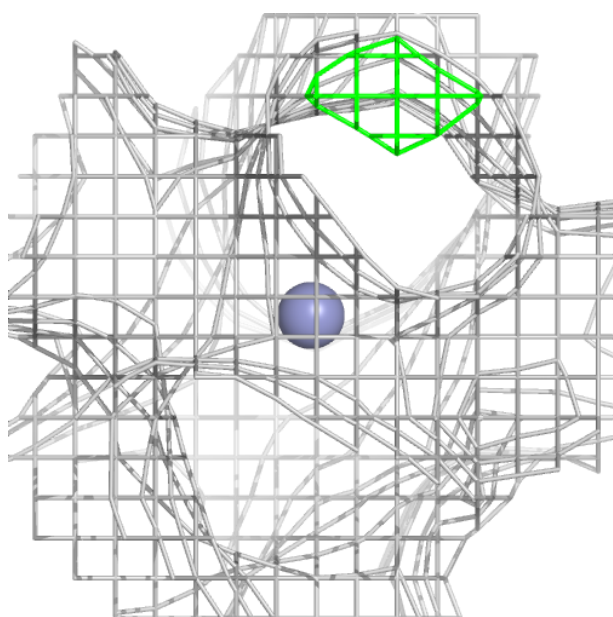
Electron density around ZN E 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
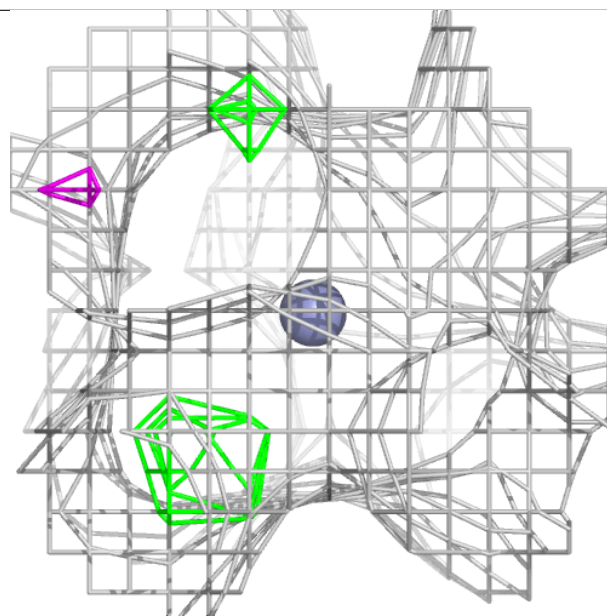
Electron density around ZN A 1001:

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

Electron density around ZN F 1001:

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

Electron density around ZN B 1001:
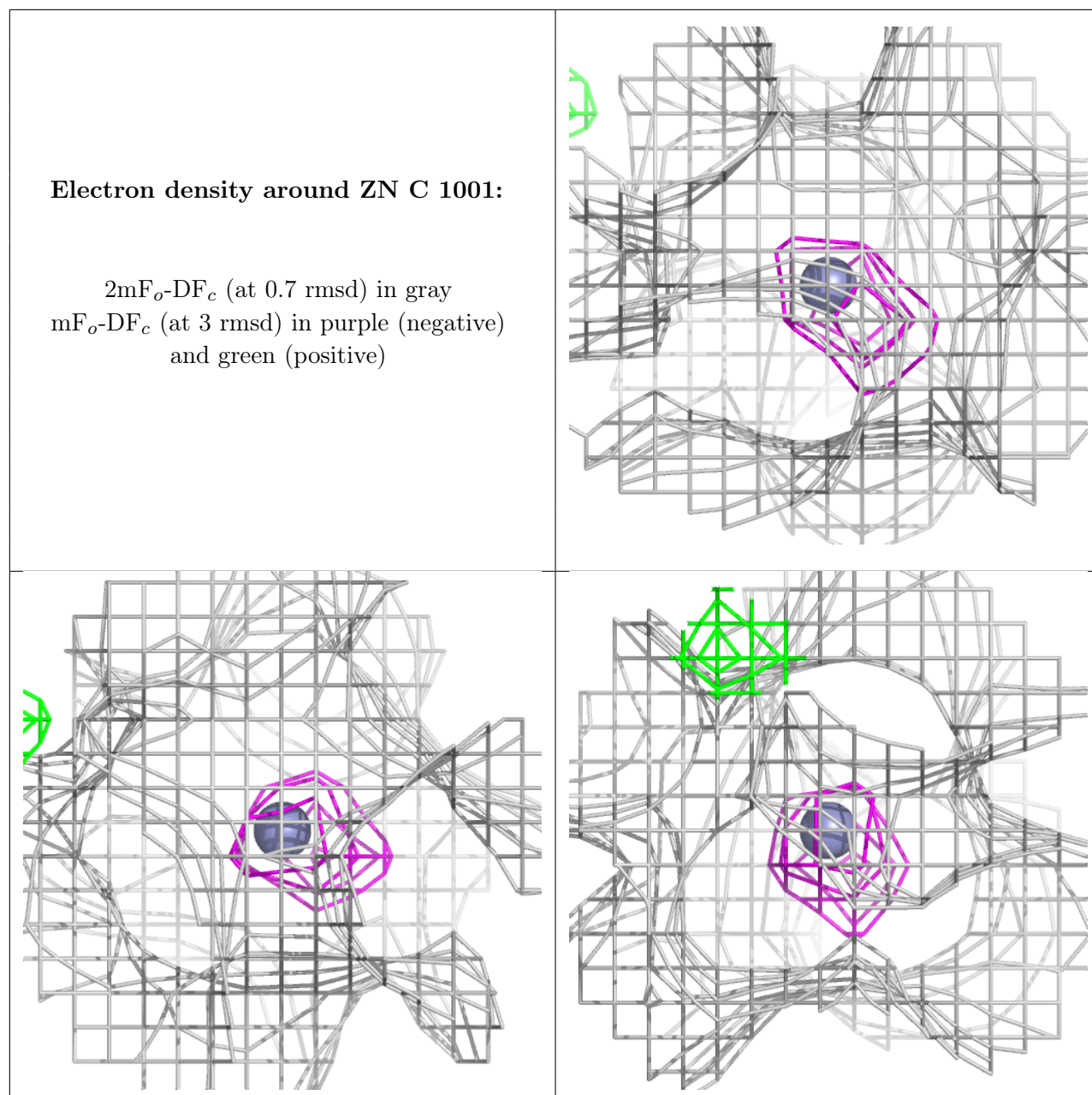
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ZN C 1001:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.