



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2024 – 06:09 PM EDT

PDB ID : 9DR5
Title : Crystal structure of Catechol 1,2-dioxygenase from Burkholderia multivorans (Zinc bound, P1 form)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-09-25
Resolution : 1.71 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 ⓘ 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

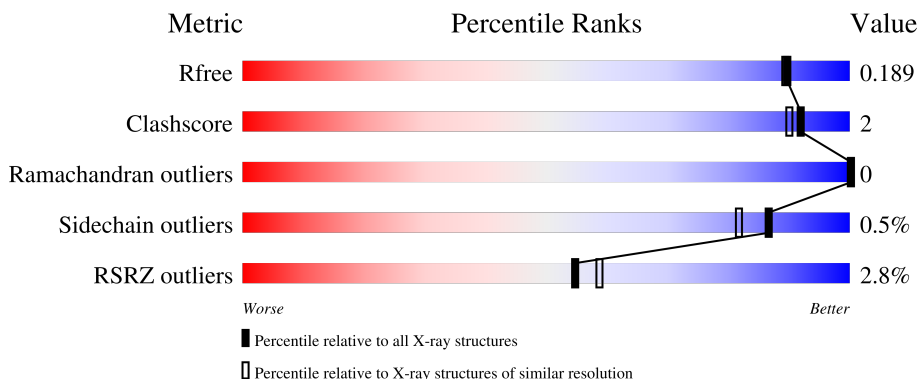
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

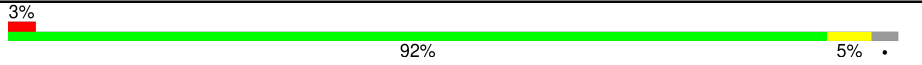
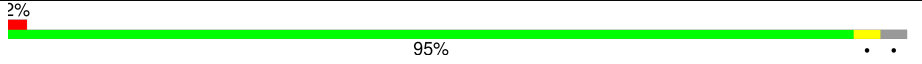
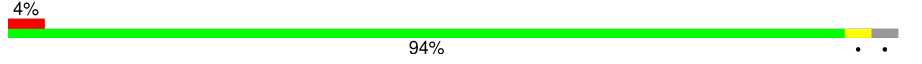

The reported resolution of this entry is 1.71 Å.

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.



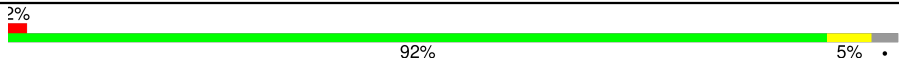
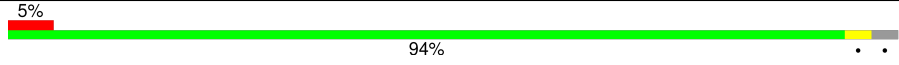
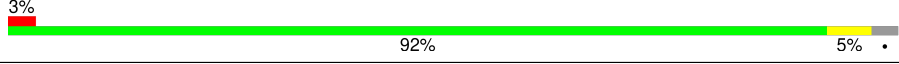
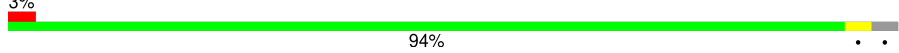
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7106 (1.74-1.70)
Clashscore	180529	7746 (1.74-1.70)
Ramachandran outliers	177936	7654 (1.74-1.70)
Sidechain outliers	177891	7654 (1.74-1.70)
RSRZ outliers	164620	7104 (1.74-1.70)

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	319	 3% 92% 5%
1	B	319	 2% 95%
1	C	319	 4% 94%
1	D	319	 2% 92% 5%

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Mol	Chain	Length	Quality of chain
1	E	319	 2% 92% 5% •
1	F	319	 5% 94% • •
1	G	319	 3% 92% 5% •
1	H	319	 3% 94% • •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22348 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 Catechol 1,2-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	Total 2401	C 1507	N 427	O 462	S 5	0	7	0
1	B	310	Total 2402	C 1508	N 429	O 460	S 5	0	8	0
1	C	310	Total 2408	C 1513	N 429	O 460	S 6	0	9	0
1	D	310	Total 2395	C 1504	N 427	O 459	S 5	0	7	0
1	E	308	Total 2383	C 1501	N 422	O 455	S 5	0	8	0
1	F	310	Total 2417	C 1519	N 432	O 461	S 5	0	10	0
1	G	310	Total 2457	C 1541	N 439	O 472	S 5	0	16	0
1	H	309	Total 2399	C 1509	N 425	O 460	S 5	0	9	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A0A0H3KXJ8
A	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
A	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
A	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
A	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
A	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
A	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
A	0	HIS	-	expression tag	UNP A0A0H3KXJ8
B	-7	MET	-	expression tag	UNP A0A0H3KXJ8
B	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
B	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
B	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
B	-3	HIS	-	expression tag	UNP A0A0H3KXJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
B	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
B	0	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-7	MET	-	expression tag	UNP A0A0H3KXJ8
C	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
C	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
C	0	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-7	MET	-	expression tag	UNP A0A0H3KXJ8
D	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
D	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
D	0	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-7	MET	-	expression tag	UNP A0A0H3KXJ8
E	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
E	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
E	0	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-7	MET	-	expression tag	UNP A0A0H3KXJ8
F	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
F	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
F	0	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-7	MET	-	expression tag	UNP A0A0H3KXJ8
G	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
G	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-1	HIS	-	expression tag	UNP A0A0H3KXJ8

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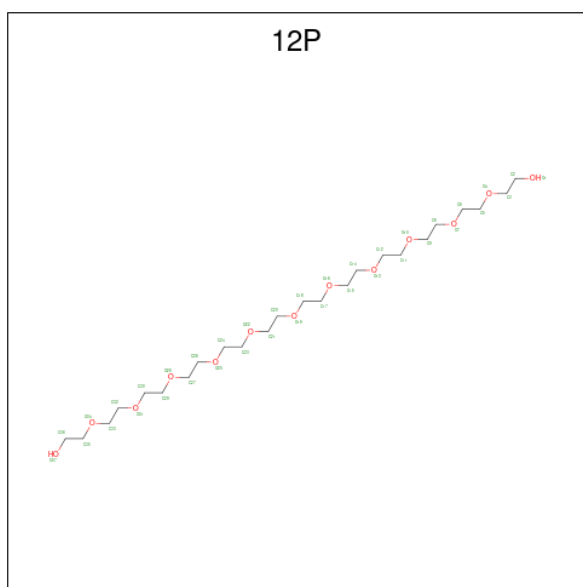
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-7	MET	-	expression tag	UNP A0A0H3KXJ8
H	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
H	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
H	0	HIS	-	expression tag	UNP A0A0H3KXJ8

- 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	1	Total Zn 1 1	0	1
2	B	1	Total Zn 1 1	0	1
2	C	1	Total Zn 1 1	0	1
2	D	1	Total Zn 1 1	0	1
2	E	1	Total Zn 1 1	0	1
2	F	1	Total Zn 1 1	0	1
2	G	1	Total Zn 1 1	0	1
2	H	1	Total Zn 1 1	0	1

- Molecule 3 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: C₂₄H₅₀O₁₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			37	24	13		
3	A	1	Total	C	O	0	0
			37	24	13		
3	C	1	Total	C	O	0	0
			37	24	13		
3	C	1	Total	C	O	0	0
			37	24	13		
3	F	1	Total	C	O	0	0
			37	24	13		
3	F	1	Total	C	O	0	0
			37	24	13		
3	G	1	Total	C	O	0	0
			37	24	13		
3	H	1	Total	C	O	0	0
			37	24	13		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



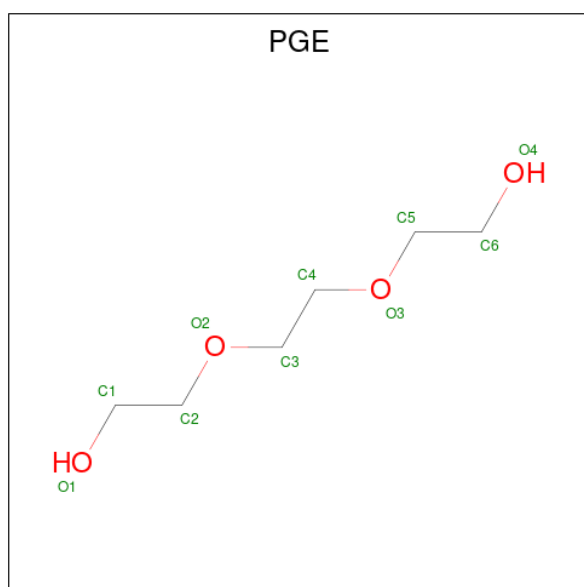
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	1
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	1
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	1
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	1
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	1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

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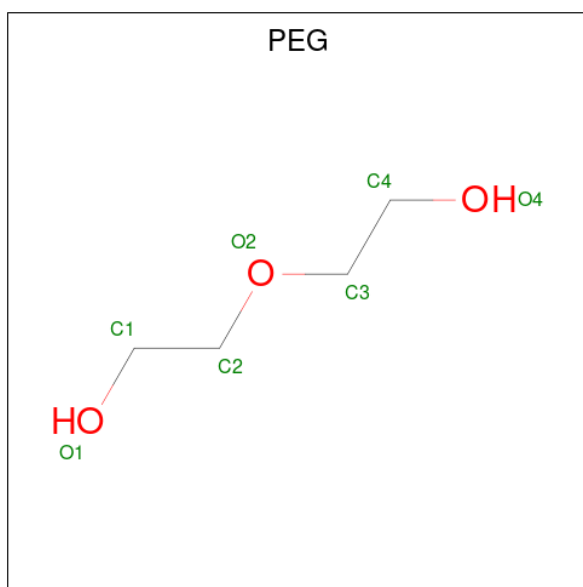
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	1

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	B	1	Total C O 10 6 4	0	0
6	C	1	Total C O 10 6 4	0	0
6	D	1	Total C O 10 6 4	0	0
6	E	1	Total C O 10 6 4	0	0
6	F	1	Total C O 10 6 4	0	0
6	G	1	Total C O 10 6 4	0	0
6	H	1	Total C O 10 6 4	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 7 4 3	0	0
7	H	1	Total C O 7 4 3	0	0

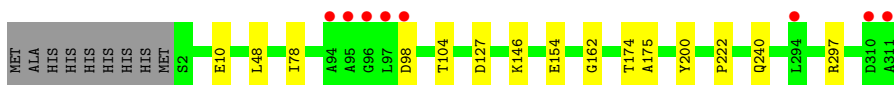
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	333	Total O 333 333	0	0
8	B	298	Total O 298 298	0	0
8	C	282	Total O 282 282	0	0
8	D	304	Total O 304 304	0	0
8	E	353	Total O 353 353	0	0
8	F	293	Total O 293 293	0	0
8	G	337	Total O 337 337	0	0
8	H	320	Total O 320 320	0	0

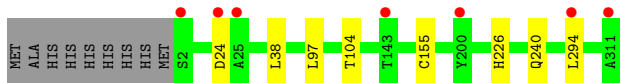
3 Residue-property plots [i](#)

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.

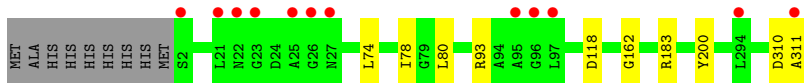
- Molecule 1: Catechol 1,2-dioxygenase



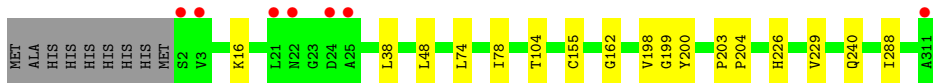
- Molecule 1: Catechol 1,2-dioxygenase



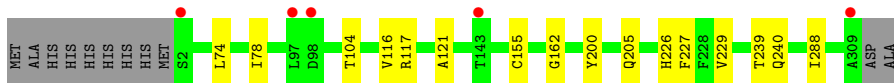
- Molecule 1: Catechol 1,2-dioxygenase



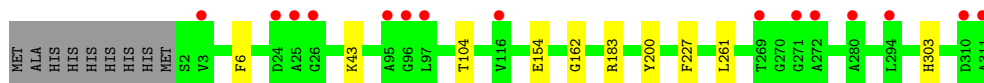
- Molecule 1: Catechol 1,2-dioxygenase



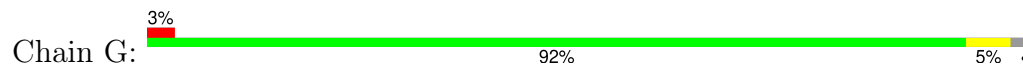
- Molecule 1: Catechol 1,2-dioxygenase



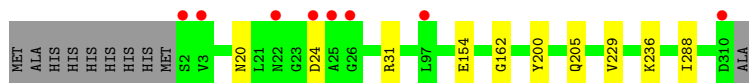
- Molecule 1: Catechol 1,2-dioxygenase



- Molecule 1: Catechol 1,2-dioxygenase



- Molecule 1: Catechol 1,2-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.97Å 86.27Å 110.16Å 106.04° 96.74° 113.15°	Depositor
Resolution (Å)	51.99 – 1.71 51.99 – 1.71	Depositor EDS
% Data completeness (in resolution range)	96.4 (51.99-1.71) 96.4 (51.99-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.71Å)	Xtrriage
Refinement program	PHENIX (1.21rc1_5156: ???)	Depositor
R, R_{free}	0.151 , 0.183 0.159 , 0.189	Depositor DCC
R_{free} test set	14081 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22348	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 12P, PEG, ZN, PGE, PG4, ACT

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	0.39	0/2458	0.63	0/3336
1	B	0.39	0/2461	0.63	0/3342
1	C	0.37	0/2474	0.63	0/3356
1	D	0.40	0/2454	0.64	0/3331
1	E	0.42	0/2445	0.65	0/3320
1	F	0.38	0/2480	0.62	0/3365
1	G	0.41	0/2523	0.65	0/3424
1	H	0.41	0/2462	0.64	0/3342
All	All	0.40	0/19757	0.64	0/26816

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2401	0	2331	9	0
1	B	2402	0	2345	4	0
1	C	2408	0	2353	8	0
1	D	2395	0	2337	9	0
1	E	2383	0	2335	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2417	0	2363	5	0
1	G	2457	0	2396	8	0
1	H	2399	0	2345	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	74	0	100	0	0
3	C	74	0	100	0	0
3	F	74	0	100	0	0
3	G	37	0	50	0	0
3	H	37	0	50	0	0
4	A	13	0	18	1	0
4	B	13	0	18	0	0
4	C	13	0	18	1	0
4	D	13	0	18	0	0
4	E	13	0	18	0	0
4	F	13	0	18	0	0
4	G	13	0	18	0	0
4	H	13	0	18	2	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
5	C	8	0	6	1	0
5	D	8	0	6	0	0
5	E	8	0	6	0	0
5	F	8	0	6	0	0
5	G	8	0	6	0	0
5	H	8	0	6	0	0
6	A	10	0	14	0	0
6	B	10	0	14	0	0
6	C	10	0	14	0	0
6	D	10	0	14	0	0
6	E	10	0	14	0	0
6	F	10	0	14	0	0
6	G	10	0	14	0	0
6	H	10	0	14	0	0
7	E	7	0	10	0	0
7	H	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	333	0	0	2	0
8	B	298	0	0	0	0
8	C	282	0	0	2	0
8	D	304	0	0	0	0
8	E	353	0	0	1	0
8	F	293	0	0	1	0
8	G	337	0	0	1	0
8	H	320	0	0	1	0
All	All	22348	0	19529	60	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 60 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:78:ILE:HD13	1:D:38:LEU:HD11	1.58	0.83
4:C:404:PG4:O5	5:C:405:ACT:H2	1.87	0.74
1:B:104:THR:HG21	1:B:240:GLN:HG2	1.80	0.62
1:F:303[B]:HIS:ND1	8:F:501:HOH:O	2.32	0.60
1:E:104:THR:HG21	1:E:240:GLN:HG2	1.84	0.59

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	315/319 (99%)	308 (98%)	7 (2%)	0	100 100
1	B	316/319 (99%)	312 (99%)	4 (1%)	0	100 100
1	C	317/319 (99%)	311 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	315/319 (99%)	309 (98%)	6 (2%)	0	100	100
1	E	314/319 (98%)	307 (98%)	7 (2%)	0	100	100
1	F	318/319 (100%)	312 (98%)	6 (2%)	0	100	100
1	G	324/319 (102%)	316 (98%)	8 (2%)	0	100	100
1	H	316/319 (99%)	310 (98%)	6 (2%)	0	100	100
All	All	2535/2552 (99%)	2485 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/246 (99%)	238 (98%)	5 (2%)	48	31
1	B	244/246 (99%)	243 (100%)	1 (0%)	89	85
1	C	245/246 (100%)	245 (100%)	0	100	100
1	D	243/246 (99%)	242 (100%)	1 (0%)	89	85
1	E	243/246 (99%)	242 (100%)	1 (0%)	89	85
1	F	246/246 (100%)	245 (100%)	1 (0%)	89	85
1	G	250/246 (102%)	250 (100%)	0	100	100
1	H	245/246 (100%)	244 (100%)	1 (0%)	89	85
All	All	1959/1968 (100%)	1949 (100%)	10 (0%)	86	82

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	205	GLN
1	F	183	ARG
1	H	205	GLN
1	A	146	LYS
1	A	297	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 50 ligands modelled in this entry, 8 are monoatomic - leaving 42 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
7	PEG	E	405	-	6,6,6	0.28	0	5,5,5	0.24	0
4	PG4	D	402	-	12,12,12	0.29	0	11,11,11	0.22	0
5	ACT	F	405	-	3,3,3	1.06	0	3,3,3	1.45	0
5	ACT	H	404	-	3,3,3	0.98	0	3,3,3	1.57	1 (33%)
5	ACT	D	403	-	3,3,3	1.03	0	3,3,3	1.57	1 (33%)
3	12P	C	403	-	36,36,36	0.30	0	35,35,35	0.38	0
5	ACT	C	405	-	3,3,3	1.21	0	3,3,3	1.06	0
6	PGE	C	407	-	9,9,9	0.33	0	8,8,8	0.49	0
6	PGE	E	406	-	9,9,9	0.39	0	8,8,8	0.54	0
6	PGE	D	405	-	9,9,9	0.36	0	8,8,8	0.57	0
6	PGE	G	406	-	9,9,9	0.36	0	8,8,8	0.57	0
4	PG4	A	404	-	12,12,12	0.33	0	11,11,11	0.29	0
5	ACT	B	404[A]	2	3,3,3	1.16	0	3,3,3	0.94	0
4	PG4	C	404	-	12,12,12	0.33	0	11,11,11	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	G	405[A]	2	3,3,3	1.32	0	3,3,3	0.77	0
4	PG4	E	402	-	12,12,12	0.35	0	11,11,11	0.27	0
4	PG4	B	402	-	12,12,12	0.32	0	11,11,11	0.15	0
5	ACT	E	404[A]	2	3,3,3	1.20	0	3,3,3	0.93	0
5	ACT	D	404[A]	2	3,3,3	1.20	0	3,3,3	0.93	0
5	ACT	H	405[A]	2	3,3,3	1.23	0	3,3,3	0.98	0
4	PG4	F	404	-	12,12,12	0.31	0	11,11,11	0.18	0
3	12P	A	403	-	36,36,36	0.30	0	35,35,35	0.33	0
5	ACT	A	405	-	3,3,3	0.98	0	3,3,3	1.61	1 (33%)
5	ACT	F	406[A]	2	3,3,3	1.16	0	3,3,3	1.15	0
3	12P	F	402	-	36,36,36	0.30	0	35,35,35	0.35	0
4	PG4	G	403	-	12,12,12	0.32	0	11,11,11	0.22	0
5	ACT	A	406[A]	2	3,3,3	1.27	0	3,3,3	0.86	0
3	12P	H	402	-	36,36,36	0.29	0	35,35,35	0.40	0
6	PGE	B	405	-	9,9,9	0.34	0	8,8,8	0.46	0
3	12P	G	402	-	36,36,36	0.29	0	35,35,35	0.43	0
5	ACT	B	403	-	3,3,3	1.00	0	3,3,3	1.53	1 (33%)
5	ACT	C	406[A]	2	3,3,3	1.30	0	3,3,3	0.93	0
4	PG4	H	403	-	12,12,12	0.34	0	11,11,11	0.27	0
6	PGE	A	407	-	9,9,9	0.33	0	8,8,8	0.49	0
3	12P	C	402	-	36,36,36	0.30	0	35,35,35	0.52	0
6	PGE	H	407	-	9,9,9	0.36	0	8,8,8	0.42	0
3	12P	F	403	-	36,36,36	0.31	0	35,35,35	0.31	0
5	ACT	E	403	-	3,3,3	1.05	0	3,3,3	1.62	1 (33%)
5	ACT	G	404	-	3,3,3	1.01	0	3,3,3	1.67	1 (33%)
3	12P	A	402	-	36,36,36	0.30	0	35,35,35	0.34	0
7	PEG	H	406	-	6,6,6	0.25	0	5,5,5	0.26	0
6	PGE	F	407	-	9,9,9	0.32	0	8,8,8	0.45	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
7	PEG	E	405	-	-	2/4/4/4	-
4	PG4	D	402	-	-	1/10/10/10	-
3	12P	C	403	-	-	16/34/34/34	-
6	PGE	C	407	-	-	2/7/7/7	-
6	PGE	E	406	-	-	2/7/7/7	-
6	PGE	D	405	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	G	406	-	-	3/7/7/7	-
4	PG4	A	404	-	-	2/10/10/10	-
4	PG4	C	404	-	-	2/10/10/10	-
4	PG4	E	402	-	-	2/10/10/10	-
4	PG4	B	402	-	-	2/10/10/10	-
4	PG4	F	404	-	-	1/10/10/10	-
3	12P	A	403	-	-	21/34/34/34	-
3	12P	F	402	-	-	17/34/34/34	-
4	PG4	G	403	-	-	1/10/10/10	-
3	12P	H	402	-	-	18/34/34/34	-
6	PGE	B	405	-	-	2/7/7/7	-
3	12P	G	402	-	-	14/34/34/34	-
4	PG4	H	403	-	-	3/10/10/10	-
6	PGE	A	407	-	-	4/7/7/7	-
3	12P	C	402	-	-	16/34/34/34	-
6	PGE	H	407	-	-	0/7/7/7	-
3	12P	F	403	-	-	18/34/34/34	-
3	12P	A	402	-	-	16/34/34/34	-
7	PEG	H	406	-	-	2/4/4/4	-
6	PGE	F	407	-	-	1/7/7/7	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	404	ACT	O-C-CH3	-2.28	113.19	122.53
5	E	403	ACT	O-C-CH3	-2.20	113.50	122.53
5	A	405	ACT	O-C-CH3	-2.17	113.61	122.53
5	H	404	ACT	O-C-CH3	-2.14	113.77	122.53
5	D	403	ACT	O-C-CH3	-2.12	113.83	122.53

There are no chirality outliers.

5 of 168 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	12P	C24-C23-O22-C21
3	C	403	12P	O19-C20-C21-O22
3	C	403	12P	O31-C32-C33-O34

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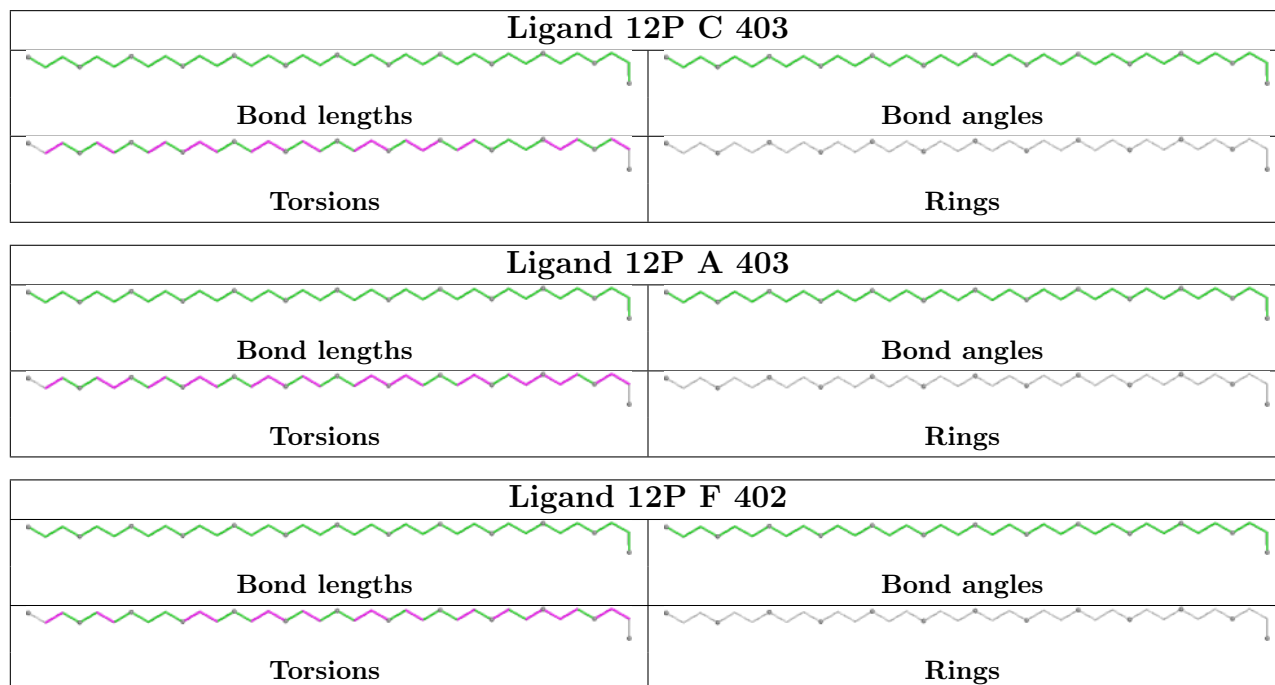
Mol	Chain	Res	Type	Atoms
3	C	403	12P	O22-C23-C24-O25
3	G	402	12P	O19-C20-C21-O22


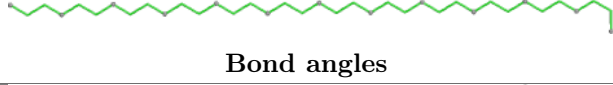
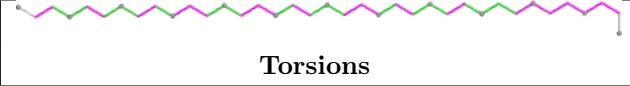


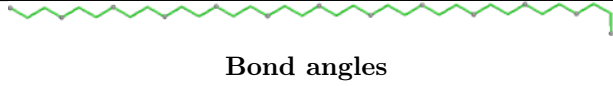
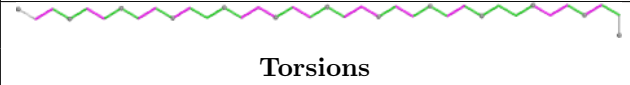


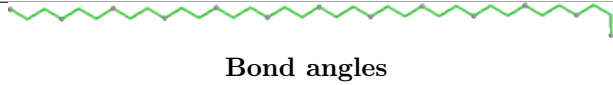


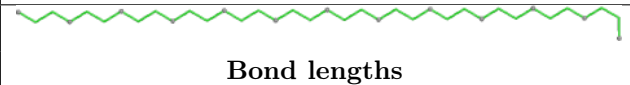
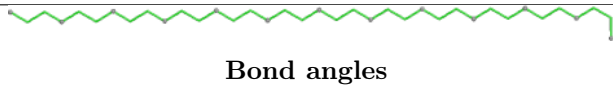






There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	405	ACT	1	0
4	A	404	PG4	1	0
4	C	404	PG4	1	0
4	H	403	PG4	2	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.



Ligand 12P H 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 12P G 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 12P C 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 12P F 403	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 12P A 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

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, 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	310/319 (97%)	-0.03	8 (2%) 57 61	10, 24, 46, 85	7 (2%)
1	B	310/319 (97%)	-0.09	7 (2%) 61 65	10, 24, 41, 75	8 (2%)
1	C	310/319 (97%)	0.03	12 (3%) 44 48	11, 25, 49, 84	9 (2%)
1	D	310/319 (97%)	-0.11	7 (2%) 61 65	9, 23, 46, 97	7 (2%)
1	E	308/319 (96%)	-0.23	5 (1%) 70 74	9, 22, 40, 89	8 (2%)
1	F	310/319 (97%)	0.18	15 (4%) 36 40	11, 26, 54, 102	10 (3%)
1	G	310/319 (97%)	-0.15	8 (2%) 57 61	10, 22, 46, 87	16 (5%)
1	H	309/319 (96%)	-0.13	8 (2%) 57 61	10, 23, 45, 130	9 (2%)
All	All	2477/2552 (97%)	-0.07	70 (2%) 55 59	9, 23, 47, 130	74 (2%)

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	172[A]	ALA	9.1
1	C	311	ALA	5.7
1	G	311	ALA	5.4
1	H	25	ALA	4.7
1	A	311	ALA	4.3

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 monosaccharides 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.

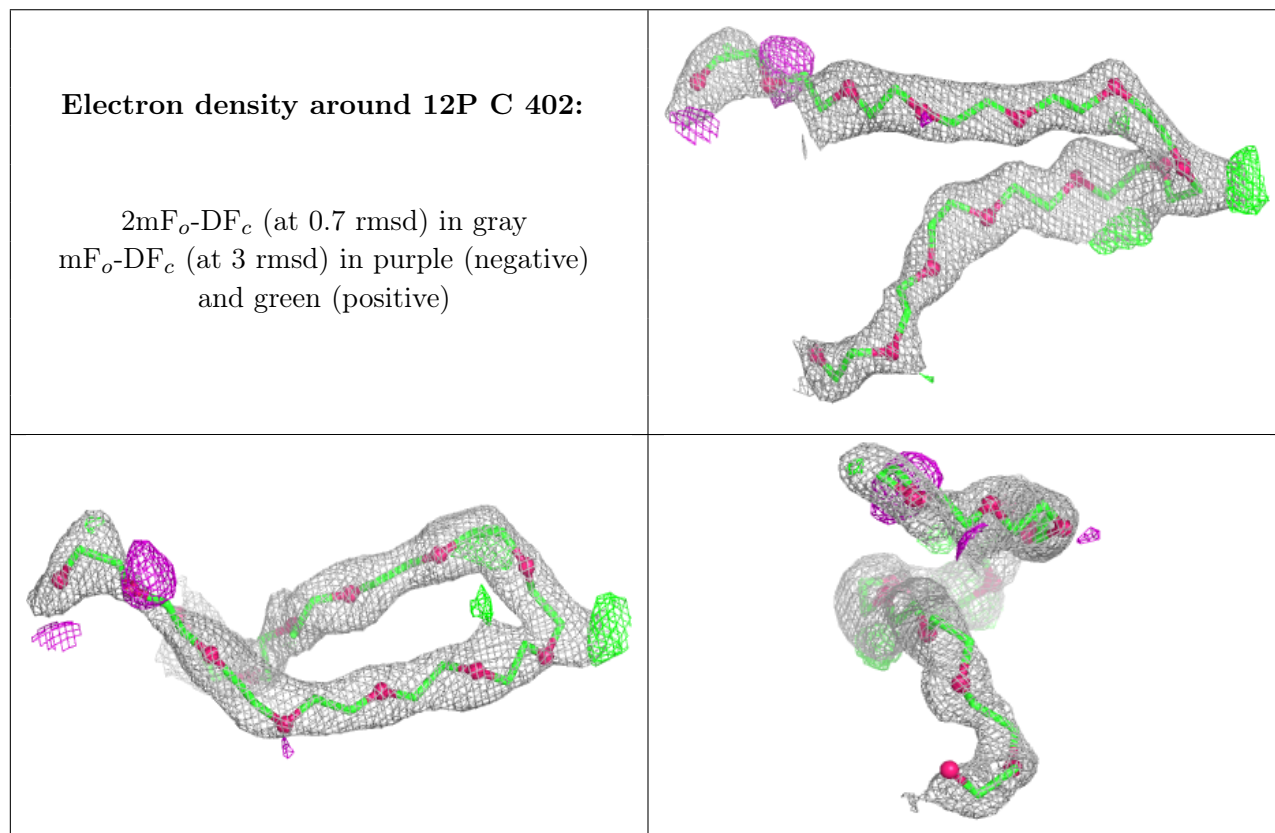
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	C	405	4/4	0.80	0.18	35,46,51,60	0
6	PGE	A	407	10/10	0.80	0.15	34,44,46,55	0
6	PGE	C	407	10/10	0.80	0.15	30,44,52,53	0
4	PG4	C	404	13/13	0.81	0.15	36,51,59,61	0
5	ACT	F	405	4/4	0.81	0.18	39,47,48,51	0
6	PGE	H	407	10/10	0.81	0.14	31,34,47,52	0
6	PGE	E	406	10/10	0.82	0.14	29,46,50,60	0
4	PG4	B	402	13/13	0.82	0.15	34,54,67,69	0
3	12P	C	402	37/37	0.83	0.14	31,51,60,65	0
5	ACT	F	406[A]	4/4	0.83	0.18	22,24,26,28	4
5	ACT	G	404	4/4	0.83	0.16	31,37,39,41	0
5	ACT	G	405[A]	4/4	0.83	0.21	16,18,20,23	4
3	12P	F	402	37/37	0.83	0.16	29,48,69,73	0
6	PGE	B	405	10/10	0.83	0.13	30,43,46,57	0
5	ACT	A	406[A]	4/4	0.83	0.15	22,23,23,24	4
5	ACT	B	403	4/4	0.83	0.17	29,33,43,44	0
6	PGE	G	406	10/10	0.83	0.15	30,40,54,57	0
3	12P	H	402	37/37	0.83	0.15	31,49,62,76	0
7	PEG	E	405	7/7	0.83	0.15	37,44,56,61	0
7	PEG	H	406	7/7	0.83	0.16	45,49,56,66	0
3	12P	F	403	37/37	0.84	0.15	34,48,63,69	0
3	12P	G	402	37/37	0.84	0.16	28,49,63,70	0
5	ACT	D	403	4/4	0.84	0.16	27,32,39,39	0
4	PG4	H	403	13/13	0.84	0.14	37,50,62,65	0
3	12P	C	403	37/37	0.84	0.15	34,48,65,76	0
4	PG4	A	404	13/13	0.85	0.15	33,53,70,71	0
3	12P	A	402	37/37	0.85	0.14	29,48,60,74	0
3	12P	A	403	37/37	0.85	0.16	34,51,62,76	0
5	ACT	H	404	4/4	0.85	0.16	29,31,42,43	0
4	PG4	F	404	13/13	0.86	0.13	37,49,58,63	0
6	PGE	F	407	10/10	0.86	0.12	29,32,42,53	0
5	ACT	A	405	4/4	0.86	0.16	31,41,47,50	0
5	ACT	B	404[A]	4/4	0.87	0.29	17,21,22,24	4
4	PG4	E	402	13/13	0.88	0.14	28,41,59,69	0
5	ACT	E	403	4/4	0.88	0.14	37,42,46,50	0
6	PGE	D	405	10/10	0.88	0.11	25,35,39,47	0
4	PG4	G	403	13/13	0.89	0.13	29,42,63,65	0

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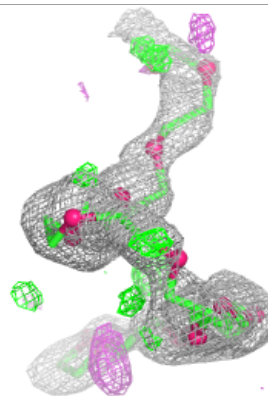
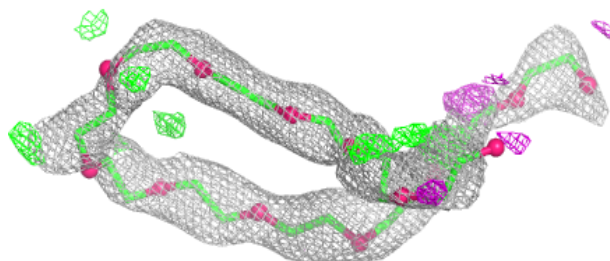
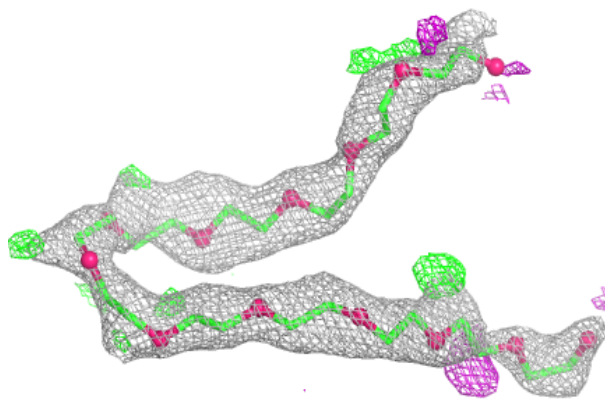
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PG4	D	402	13/13	0.89	0.12	34,41,54,57	0
5	ACT	D	404[A]	4/4	0.90	0.22	15,18,21,24	4
5	ACT	C	406[A]	4/4	0.91	0.17	21,22,22,22	4
5	ACT	H	405[A]	4/4	0.91	0.16	17,20,24,24	4
5	ACT	E	404[A]	4/4	0.91	0.14	17,19,23,23	4
2	ZN	B	401[A]	1/1	0.98	0.03	23,23,23,23	1
2	ZN	C	401[A]	1/1	0.98	0.09	29,29,29,29	1
2	ZN	F	401[A]	1/1	0.98	0.06	28,28,28,28	1
2	ZN	G	401[A]	1/1	0.99	0.06	23,23,23,23	1
2	ZN	H	401[A]	1/1	0.99	0.04	24,24,24,24	1
2	ZN	D	401[A]	1/1	0.99	0.03	23,23,23,23	1
2	ZN	A	401[A]	1/1	0.99	0.07	27,27,27,27	1
2	ZN	E	401[A]	1/1	1.00	0.10	24,24,24,24	1

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.

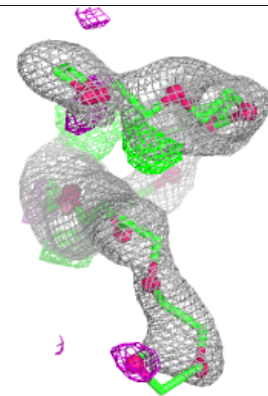
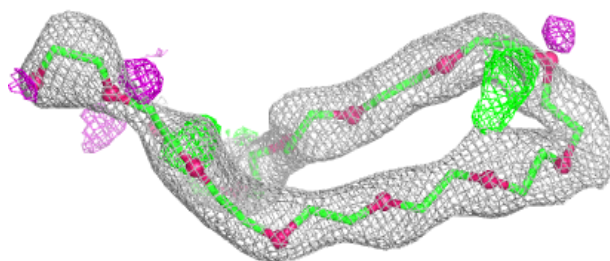
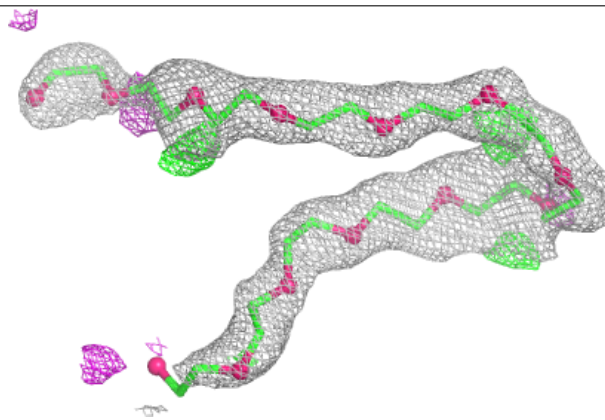


Electron density around 12P F 402:

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

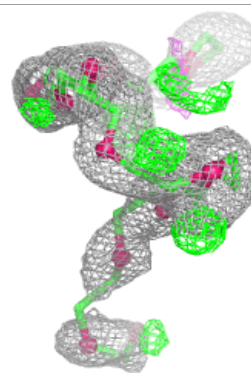
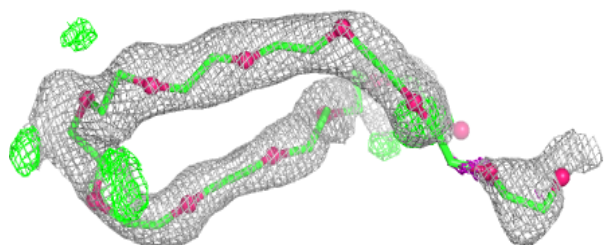
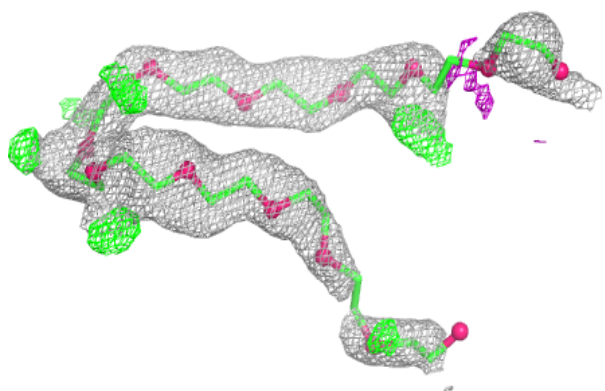
**Electron density around 12P H 402:**

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

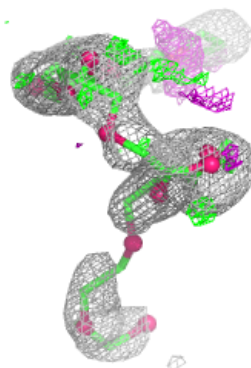
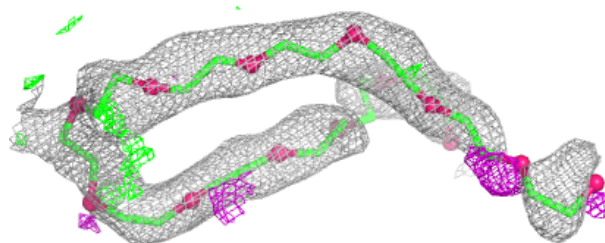
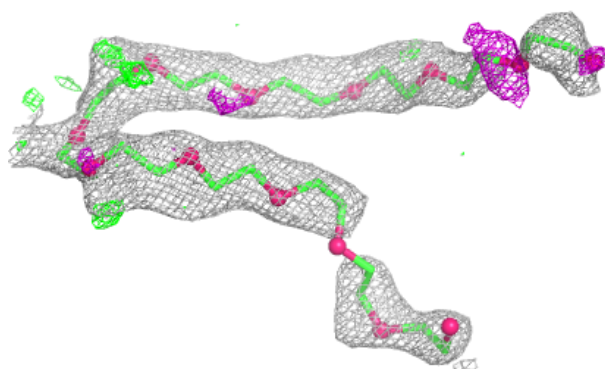


Electron density around 12P F 403:

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

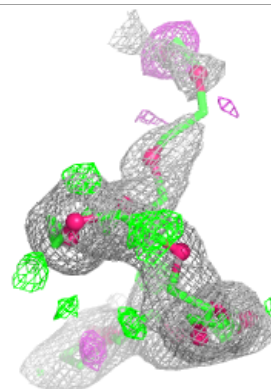
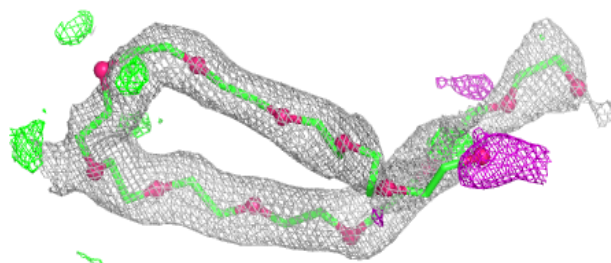
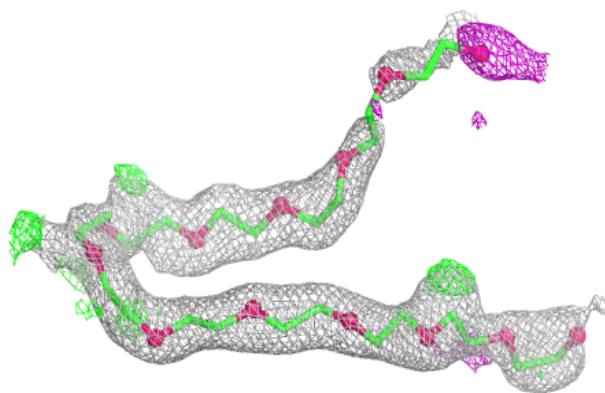
**Electron density around 12P G 402:**

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

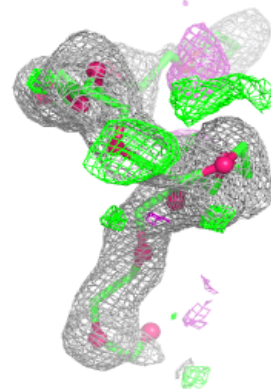
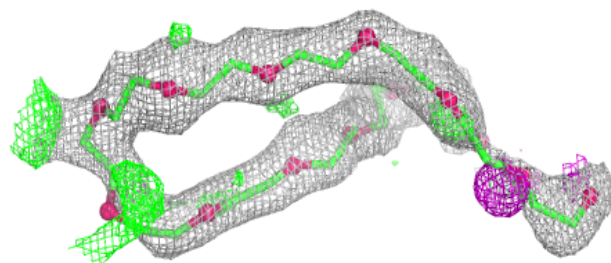
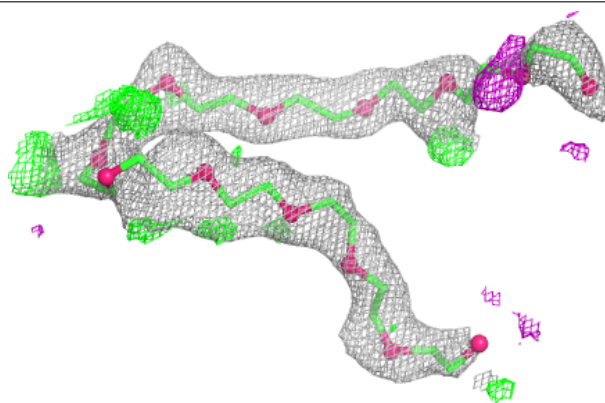


Electron density around 12P C 403:

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

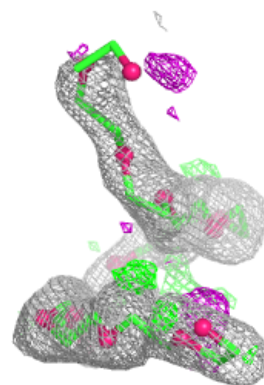
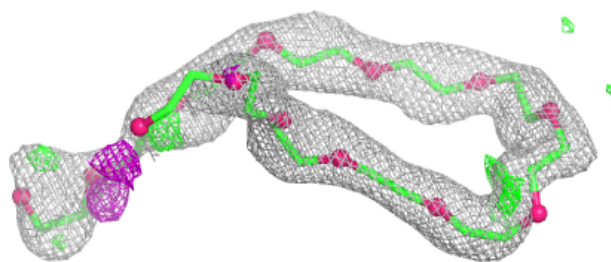
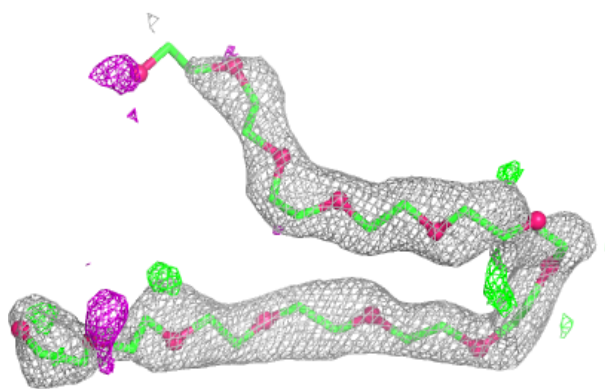
**Electron density around 12P A 402:**

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



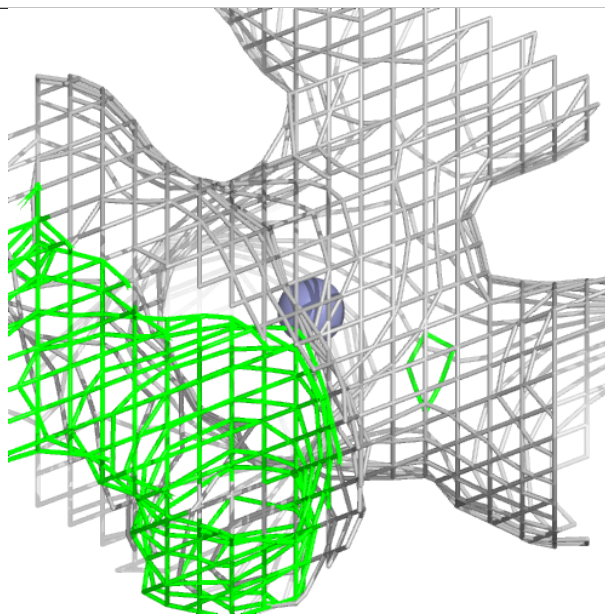
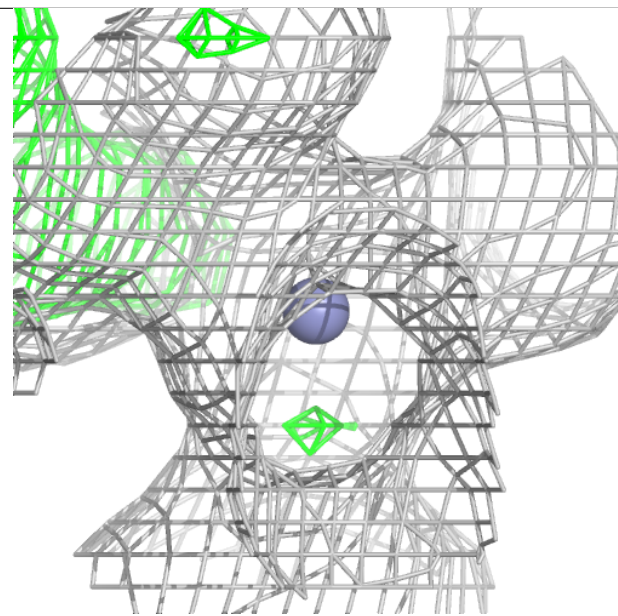
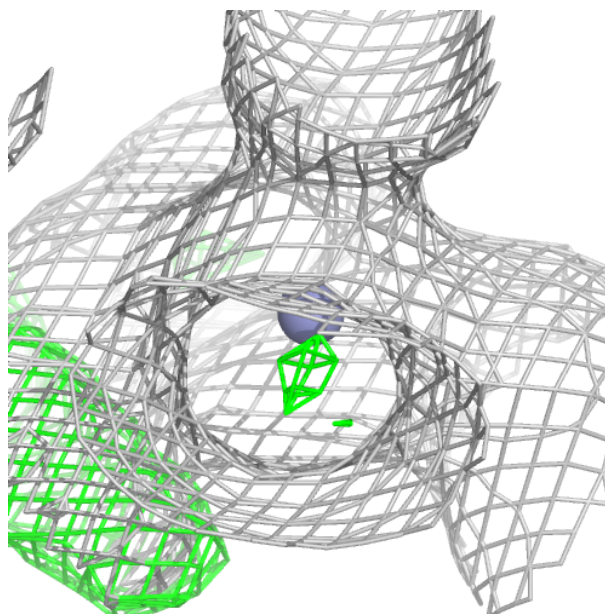
Electron density around 12P A 403:

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



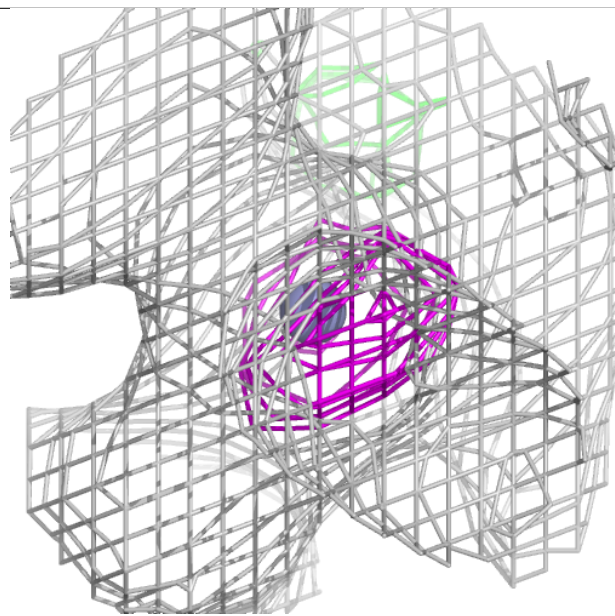
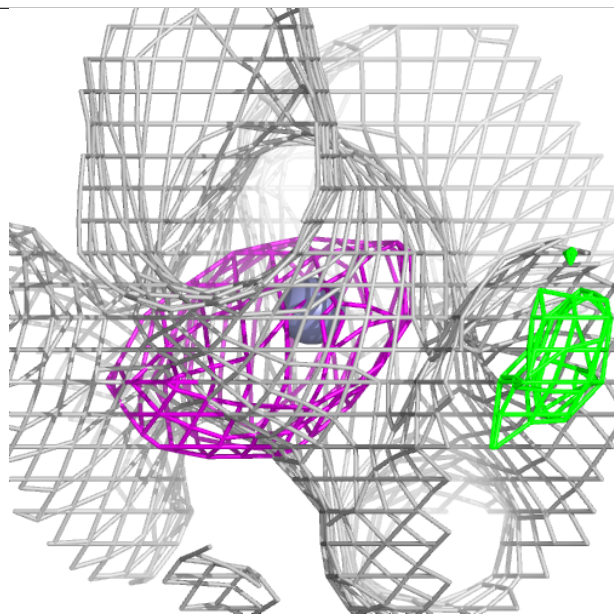
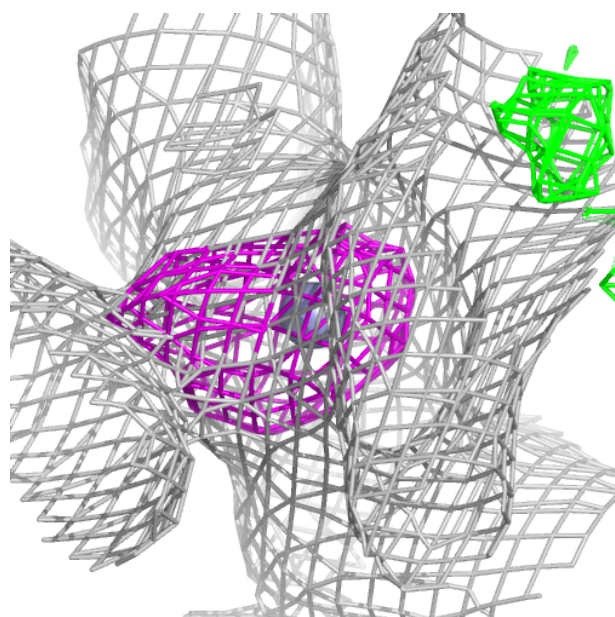
Electron density around ZN B 401 (A):

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



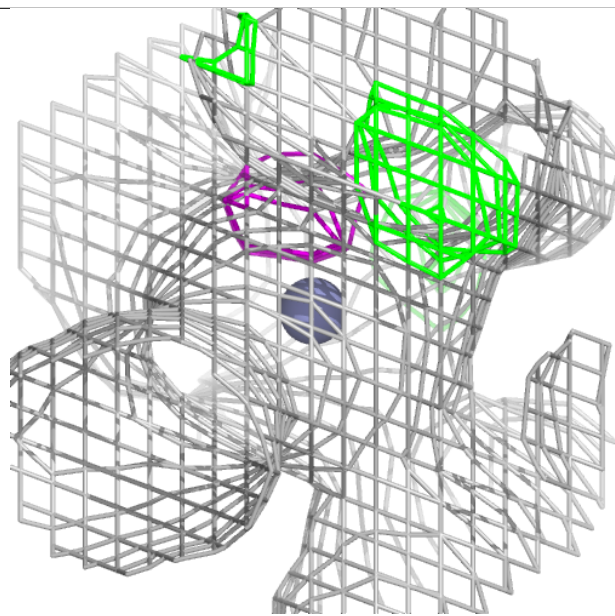
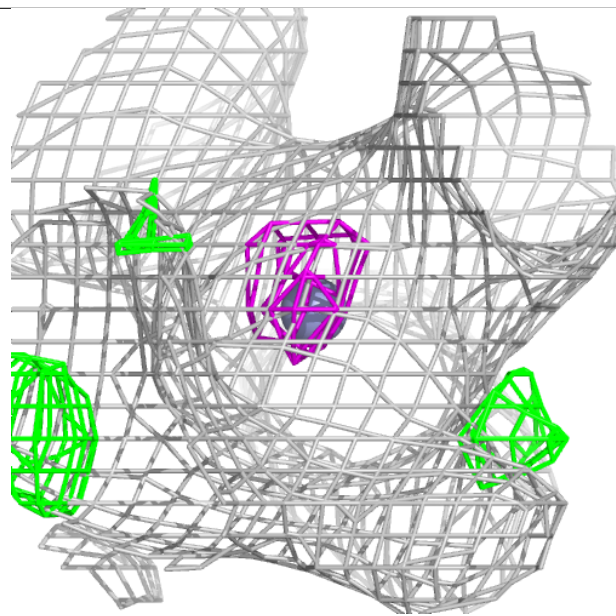
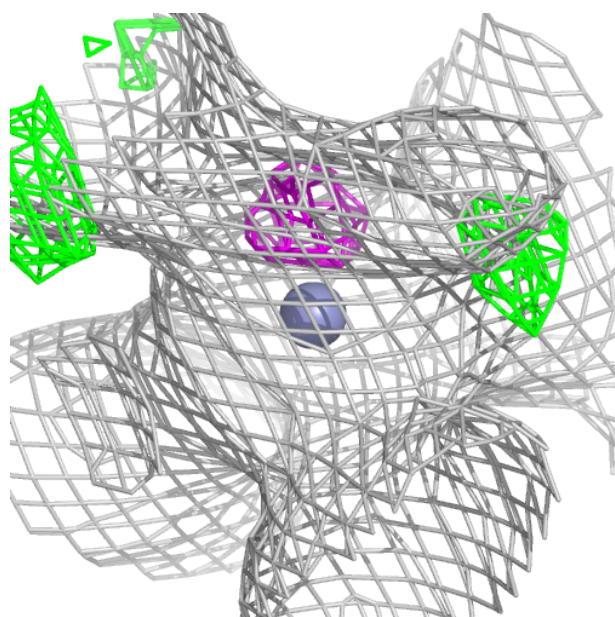
Electron density around ZN C 401 (A):

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



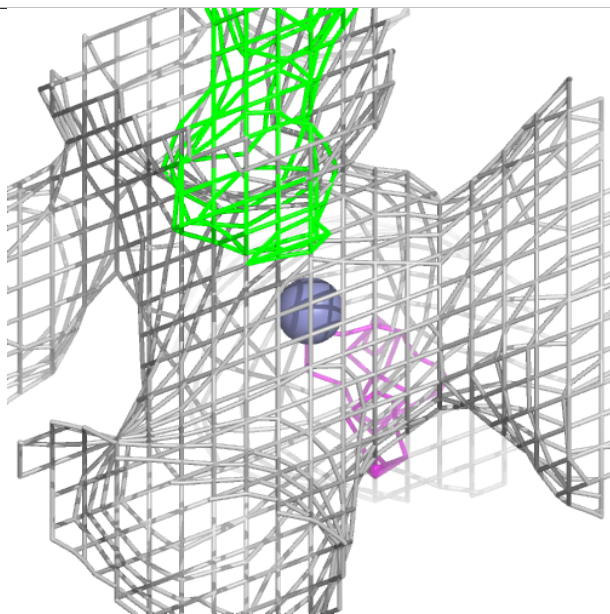
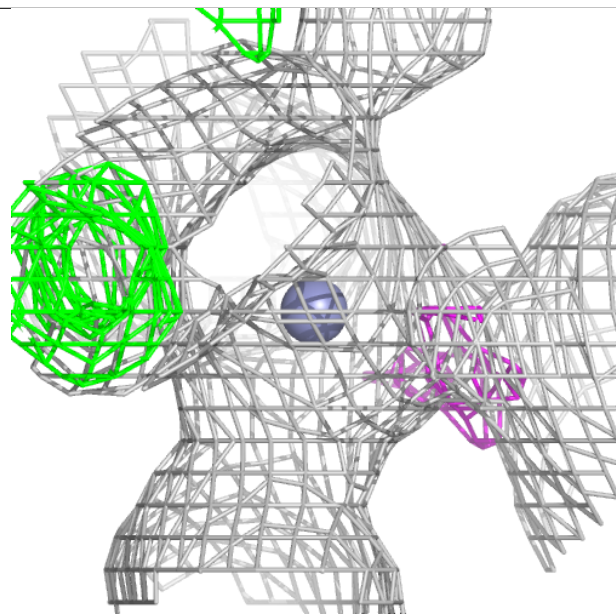
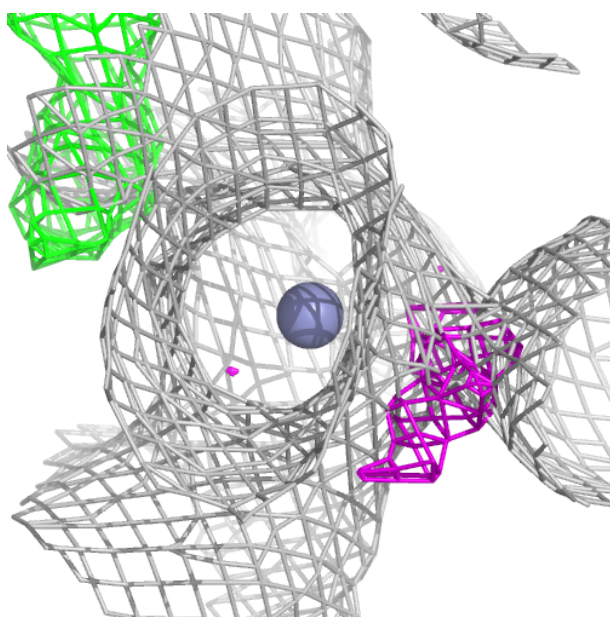
Electron density around ZN F 401 (A):

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



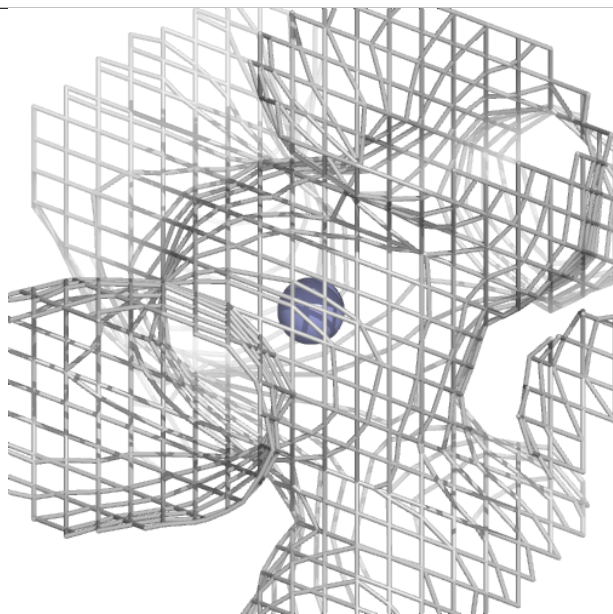
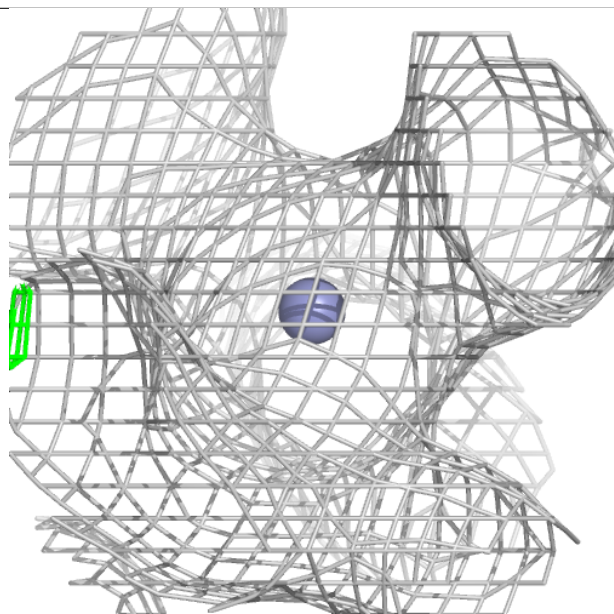
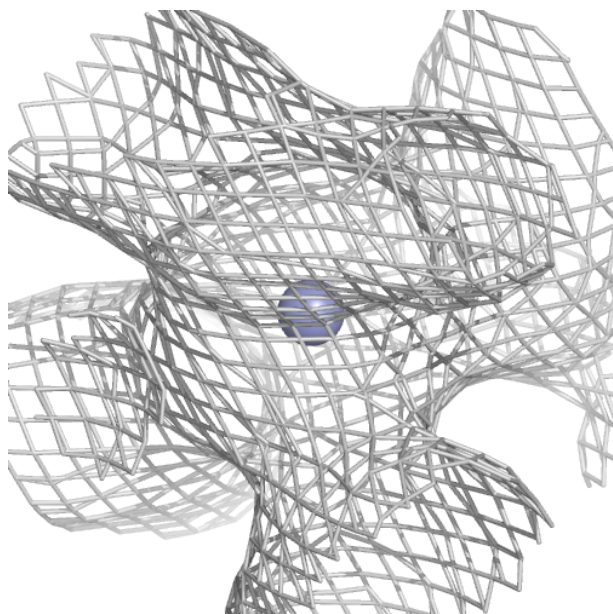
Electron density around ZN G 401 (A):

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



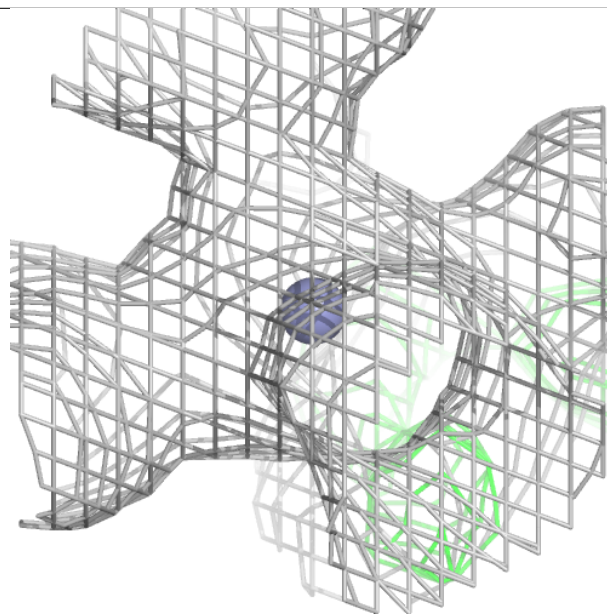
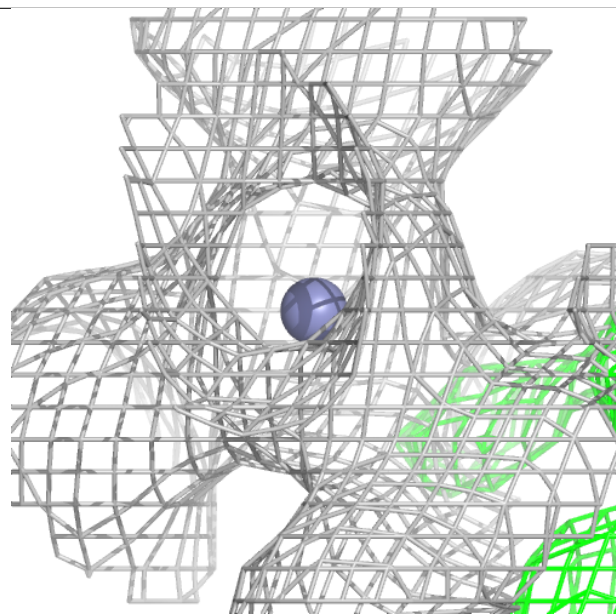
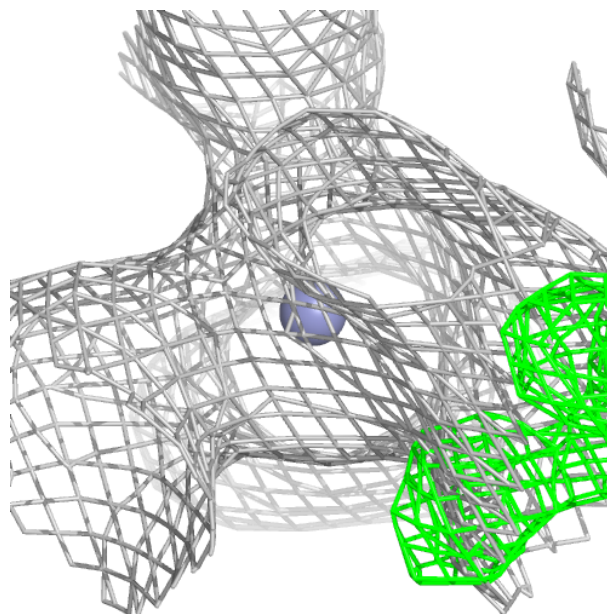
Electron density around ZN H 401 (A):

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



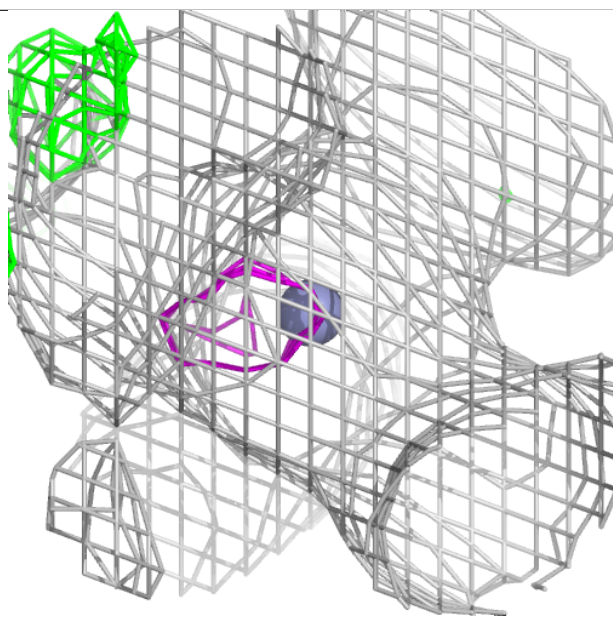
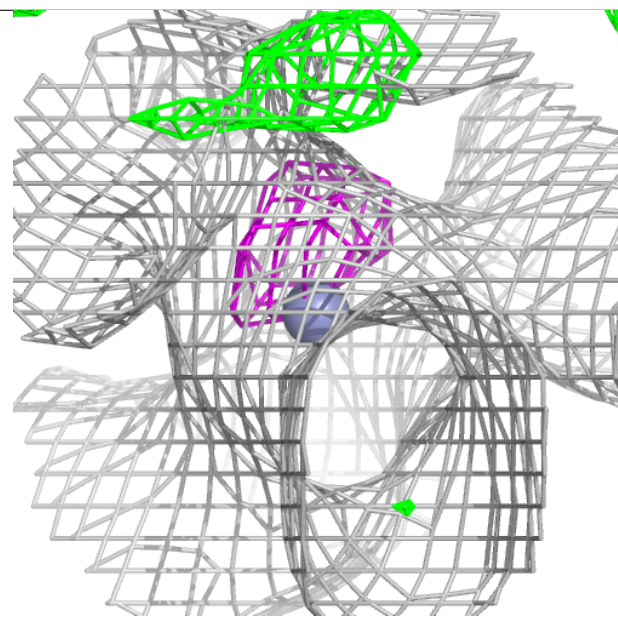
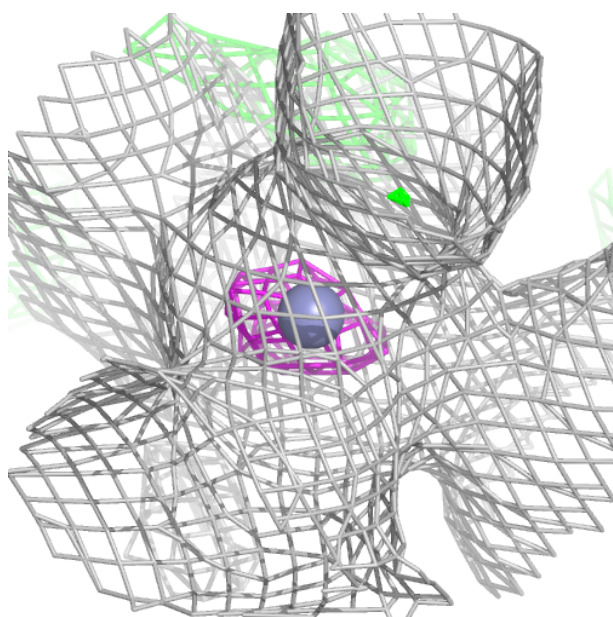
Electron density around ZN D 401 (A):

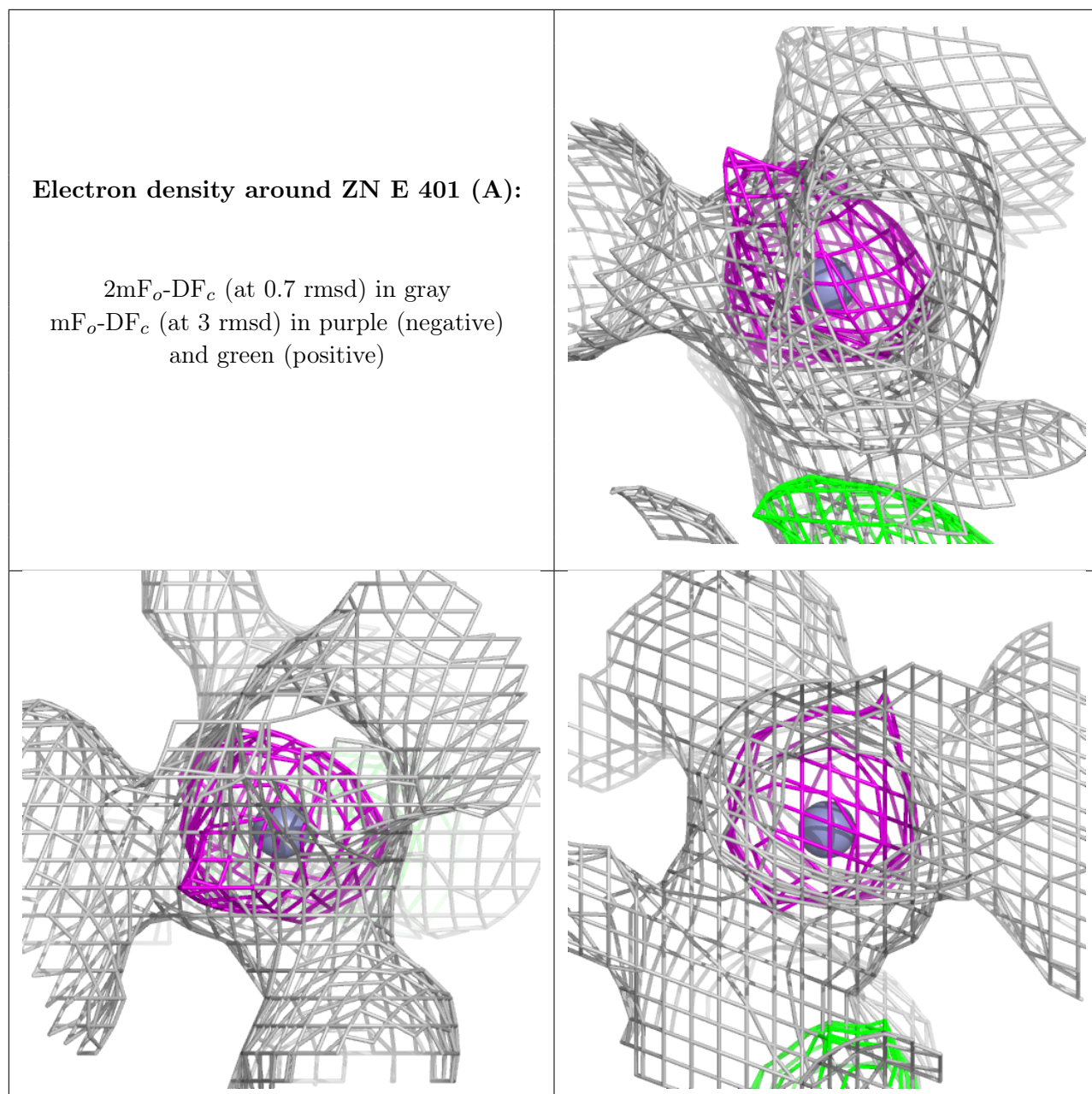
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 401 (A):

$2mF_o-DF_c$ (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.