



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 03:14 AM UTC

PDB ID : 9U4X / pdb_00009u4x
Title : Crystal Structure of Alcohol Dehydrogenase from Anoxybacillus geothermalis D9
Authors : Riem, E.A.A.; Kamarudin, N.H.A.; Ali, M.S.M.; Noor, N.D.M.
Deposited on : 2025-03-20
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

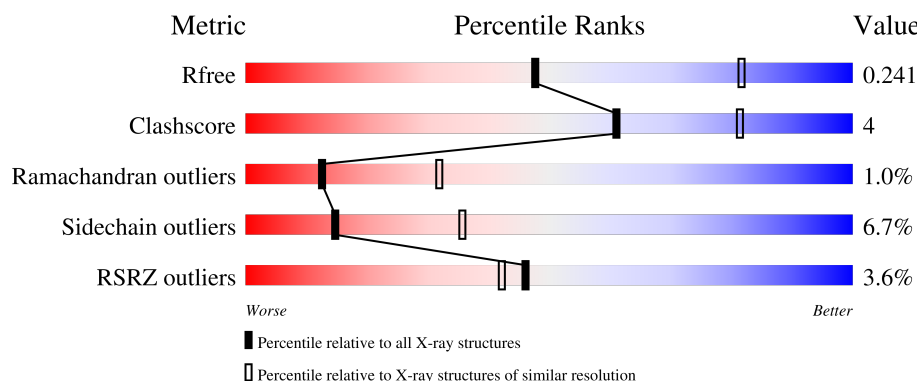
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	337	<div> <div>0%</div> <div>84% 12% ..</div> </div>
1	B	337	<div> <div>5%</div> <div>85% 12% ..</div> </div>
1	C	337	<div> <div>2%</div> <div>81% 16% .</div> </div>
1	D	337	<div> <div>3%</div> <div>83% 13% .</div> </div>
1	E	337	<div> <div>4%</div> <div>85% 12% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	337	<div><div></div><div>4%</div><div>84%</div><div>13%</div><div></div></div>
1	G	337	<div><div></div><div>5%</div><div>83%</div><div>13%</div><div></div></div>
1	H	337	<div><div></div><div>3%</div><div>85%</div><div>10%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 40614 atoms, of which 20216 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 Alcohol dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	H	N	O	S	0	0	0
			5059	1617	2527	430	471	14			
1	B	337	Total	C	H	N	O	S	0	0	0
			5059	1617	2527	430	471	14			
1	C	337	Total	C	H	N	O	S	0	0	0
			5059	1617	2527	430	471	14			
1	D	337	Total	C	H	N	O	S	0	0	0
			5059	1617	2527	430	471	14			
1	E	337	Total	C	H	N	O	S	0	0	0
			5059	1617	2527	430	471	14			
1	F	337	Total	C	H	N	O	S	0	0	0
			5059	1617	2527	430	471	14			
1	G	337	Total	C	H	N	O	S	0	0	0
			5059	1617	2527	430	471	14			
1	H	337	Total	C	H	N	O	S	0	0	0
			5059	1617	2527	430	471	14			

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

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

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

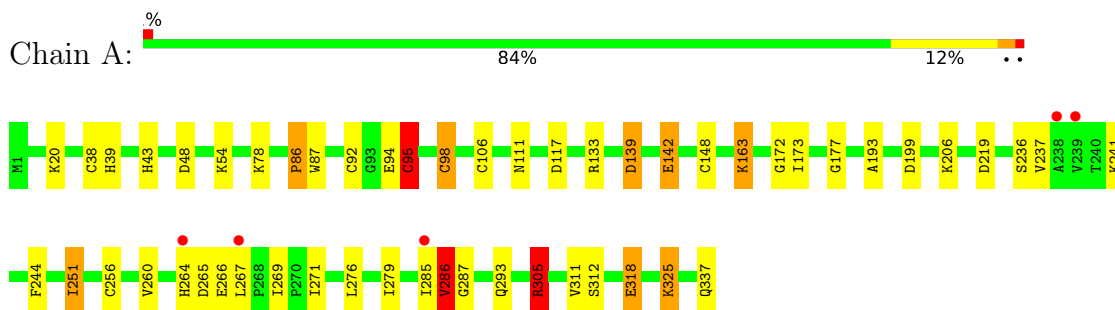
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	14	Total 14	O 14	0	0
3	C	25	Total 25	O 25	0	0
3	D	11	Total 11	O 11	0	0
3	E	14	Total 14	O 14	0	0
3	F	12	Total 12	O 12	0	0
3	G	11	Total 11	O 11	0	0
3	H	20	Total 20	O 20	0	0

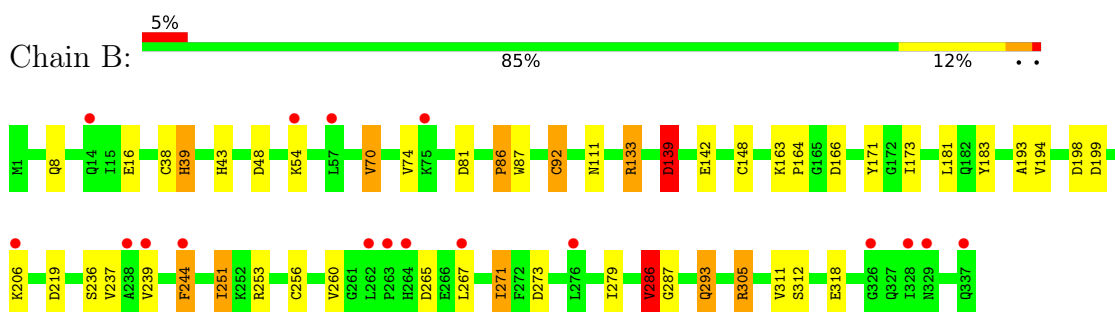
3 Residue-property plots [i](#)

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.

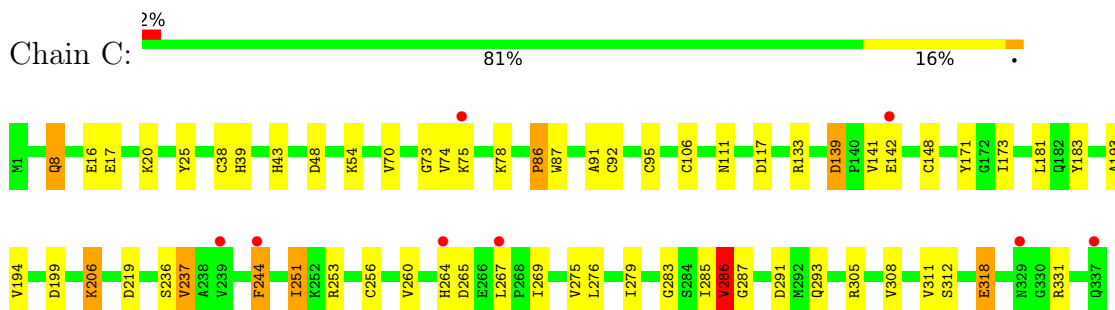
- Molecule 1: Alcohol dehydrogenase



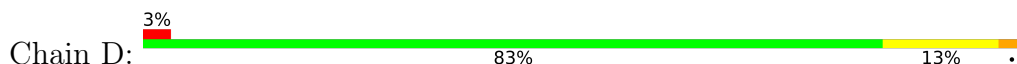
- Molecule 1: Alcohol dehydrogenase

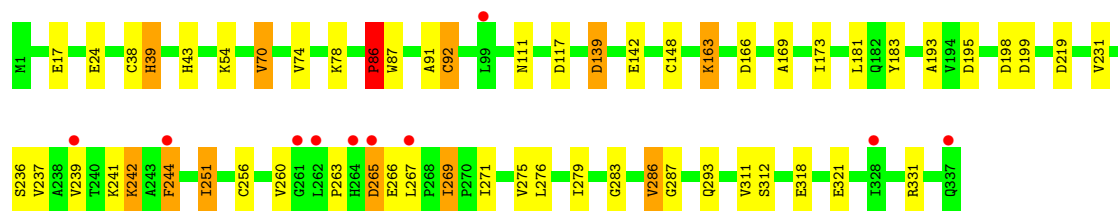


- Molecule 1: Alcohol dehydrogenase

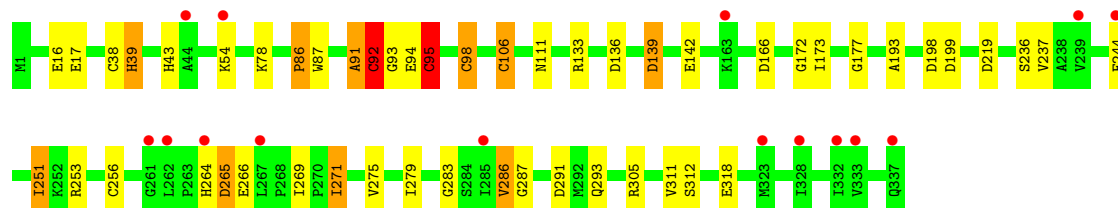
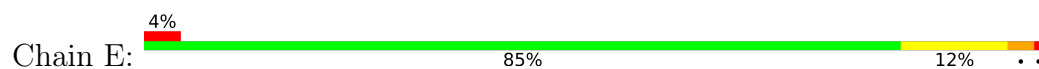


- Molecule 1: Alcohol dehydrogenase

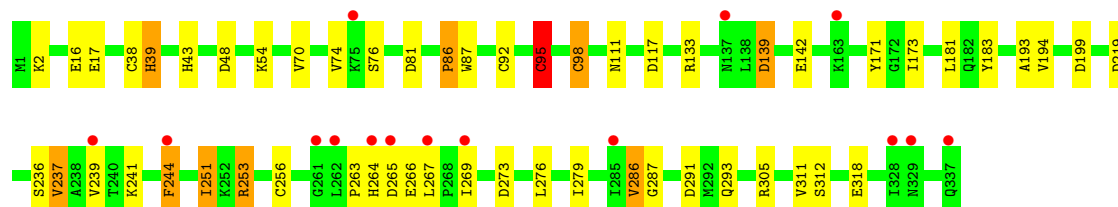
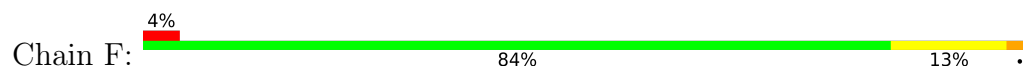




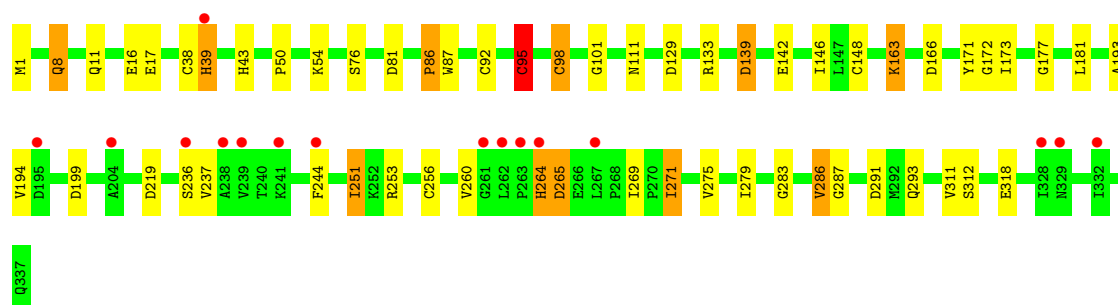
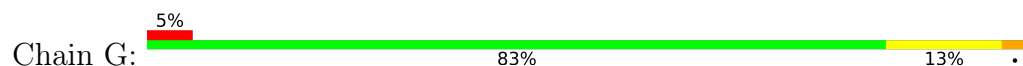
• Molecule 1: Alcohol dehydrogenase



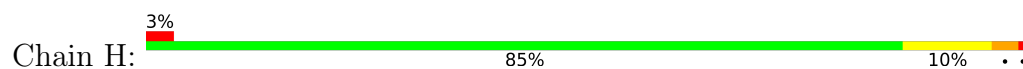
• Molecule 1: Alcohol dehydrogenase

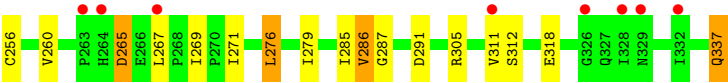


• Molecule 1: Alcohol dehydrogenase



• Molecule 1: Alcohol dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.61Å 130.77Å 134.92Å 90.00° 90.70° 90.00°	Depositor
Resolution (Å)	48.97 – 2.70 48.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.97-2.70) 99.9 (48.97-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.200 , 0.241 0.200 , 0.241	Depositor DCC
R_{free} test set	4047 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k 0.012 for -h,-l,-k 0.088 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	40614	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0167e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	0/2582	1.45	33/3505 (0.9%)
1	B	0.78	0/2582	1.37	27/3505 (0.8%)
1	C	0.82	0/2582	1.39	26/3505 (0.7%)
1	D	0.82	0/2582	1.38	25/3505 (0.7%)
1	E	0.81	0/2582	1.40	26/3505 (0.7%)
1	F	0.83	1/2582 (0.0%)	1.39	22/3505 (0.6%)
1	G	0.80	0/2582	1.38	23/3505 (0.7%)
1	H	0.83	0/2582	1.39	24/3505 (0.7%)
All	All	0.82	1/20656 (0.0%)	1.39	206/28040 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	3
1	D	0	1
1	E	0	3
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	76	SER	CA-CB	-6.59	1.43	1.53

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	HIS	CA-CB-CG	10.39	124.19	113.80
1	A	142	GLU	CB-CA-C	9.91	127.24	110.79
1	E	106	CYS	N-CA-CB	9.24	128.12	109.28
1	A	318	GLU	CB-CG-CD	9.11	128.09	112.60
1	A	325	LYS	CB-CG-CD	9.11	132.25	111.30
1	G	244	PHE	N-CA-CB	9.07	123.17	110.01
1	H	244	PHE	N-CA-CB	8.91	122.93	110.01
1	E	244	PHE	N-CA-CB	8.85	122.84	110.01
1	C	244	PHE	N-CA-CB	8.66	122.57	110.01
1	F	244	PHE	N-CA-CB	8.58	122.45	110.01
1	A	163	LYS	CB-CA-C	8.32	121.64	108.91
1	F	98	CYS	CB-CA-C	8.30	126.61	110.67
1	F	38	CYS	CB-CA-C	8.24	123.32	109.48
1	A	20	LYS	CB-CA-C	8.23	122.53	109.27
1	H	38	CYS	CB-CA-C	8.18	123.21	109.48
1	G	38	CYS	CB-CA-C	8.17	123.21	109.48
1	D	38	CYS	CB-CA-C	8.10	123.08	109.48
1	D	265	ASP	CA-CB-CG	7.99	120.59	112.60
1	E	142	GLU	CB-CA-C	-7.96	97.57	110.79
1	D	142	GLU	CB-CA-C	-7.89	97.27	110.68
1	A	305	ARG	CA-CB-CG	7.88	129.87	114.10
1	G	98	CYS	CA-CB-SG	7.81	132.37	114.40
1	H	265	ASP	CA-CB-CG	7.81	120.41	112.60
1	A	98	CYS	CA-CB-SG	7.79	132.31	114.40
1	B	38	CYS	CB-CA-C	7.75	122.51	109.48
1	B	273	ASP	CA-CB-CG	7.72	120.32	112.60
1	D	199	ASP	CA-CB-CG	7.72	120.33	112.60
1	D	293	GLN	N-CA-CB	7.69	121.42	110.12
1	E	38	CYS	CB-CA-C	7.62	122.29	109.48
1	A	38	CYS	CB-CA-C	7.58	122.22	109.48
1	C	38	CYS	CB-CA-C	7.58	122.21	109.48
1	A	293	GLN	CB-CA-C	7.55	122.74	110.88
1	C	206	LYS	CA-CB-CG	7.50	129.11	114.10
1	H	199	ASP	CA-CB-CG	7.50	120.10	112.60
1	E	293	GLN	CB-CA-C	7.48	122.62	110.88
1	E	199	ASP	CA-CB-CG	7.39	119.99	112.60
1	F	199	ASP	CA-CB-CG	7.35	119.95	112.60
1	B	139	ASP	CA-CB-CG	7.35	119.95	112.60
1	B	142	GLU	CB-CA-C	-7.33	98.22	110.68
1	B	293	GLN	CB-CA-C	7.29	122.33	110.88
1	B	199	ASP	CA-CB-CG	7.29	119.89	112.60
1	F	98	CYS	CA-CB-SG	7.23	131.04	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	98	CYS	CB-CA-C	7.19	123.93	110.63
1	D	244	PHE	N-CA-CB	7.12	120.34	110.01
1	G	199	ASP	CA-CB-CG	7.11	119.71	112.60
1	C	199	ASP	CA-CB-CG	7.11	119.71	112.60
1	F	293	GLN	CB-CA-C	7.06	121.96	110.88
1	E	98	CYS	CB-CA-C	7.01	123.59	110.63
1	A	199	ASP	CA-CB-CG	6.95	119.55	112.60
1	H	98	CYS	CB-CA-C	6.93	123.98	110.67
1	H	95	CYS	CA-CB-SG	-6.92	98.49	114.40
1	F	265	ASP	CA-CB-CG	6.88	119.48	112.60
1	F	139	ASP	CA-CB-CG	6.83	119.43	112.60
1	A	139	ASP	CA-CB-CG	6.82	119.42	112.60
1	H	106	CYS	CA-CB-SG	6.81	130.07	114.40
1	E	139	ASP	CA-CB-CG	6.80	119.40	112.60
1	C	139	ASP	CA-CB-CG	6.77	119.37	112.60
1	F	199	ASP	CB-CA-C	6.73	124.10	110.38
1	D	199	ASP	CB-CA-C	6.72	124.08	110.38
1	C	199	ASP	CB-CA-C	6.71	124.08	110.38
1	G	199	ASP	CB-CA-C	6.71	124.08	110.38
1	B	199	ASP	CB-CA-C	6.71	124.07	110.38
1	H	199	ASP	CB-CA-C	6.60	123.84	110.38
1	G	265	ASP	CA-CB-CG	6.59	119.19	112.60
1	D	318	GLU	CB-CA-C	6.56	122.01	110.85
1	E	199	ASP	CB-CA-C	6.56	123.76	110.38
1	B	244	PHE	N-CA-CB	6.51	119.45	110.01
1	C	260	VAL	N-CA-CB	-6.50	104.26	111.41
1	A	106	CYS	CB-CA-C	6.42	120.22	109.69
1	G	139	ASP	CA-CB-CG	6.41	119.01	112.60
1	H	318	GLU	CB-CA-C	6.41	121.43	110.79
1	E	265	ASP	CA-CB-CG	6.40	119.00	112.60
1	C	293	GLN	CB-CA-C	6.38	120.90	110.88
1	H	139	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	142	GLU	CG-CD-OE1	6.36	133.03	118.40
1	H	142	GLU	CB-CA-C	-6.34	100.27	110.79
1	G	129	ASP	CA-CB-CG	6.33	118.93	112.60
1	G	142	GLU	CB-CA-C	-6.28	100.37	110.79
1	B	286	VAL	CA-CB-CG1	6.27	121.05	110.40
1	B	293	GLN	N-CA-CB	-6.25	100.95	110.01
1	B	265	ASP	CA-CB-CG	6.25	118.85	112.60
1	C	293	GLN	N-CA-CB	-6.25	100.95	110.01
1	H	337	GLN	N-CA-CB	6.25	121.12	110.50
1	E	95	CYS	CA-CB-SG	-6.18	100.18	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	163	LYS	CG-CD-CE	6.14	125.42	111.30
1	F	273	ASP	CA-CB-CG	6.12	118.72	112.60
1	E	166	ASP	CA-CB-CG	6.09	118.69	112.60
1	D	139	ASP	CA-CB-CG	6.09	118.69	112.60
1	H	129	ASP	CA-CB-CG	6.09	118.69	112.60
1	D	163	LYS	CB-CG-CD	6.08	125.29	111.30
1	E	293	GLN	N-CA-CB	-6.08	101.20	110.01
1	F	117	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	293	GLN	N-CA-CB	-6.07	101.21	110.01
1	F	237	VAL	N-CA-C	-6.06	105.81	111.45
1	A	286	VAL	CB-CA-C	6.05	121.22	111.29
1	C	183	TYR	N-CA-CB	6.04	119.00	110.12
1	B	239	VAL	N-CA-CB	-6.03	105.57	112.21
1	G	293	GLN	CB-CA-C	6.02	120.33	110.88
1	H	75	LYS	CA-CB-CG	6.00	126.09	114.10
1	A	142	GLU	CG-CD-OE2	-5.99	104.63	118.40
1	A	199	ASP	CB-CA-C	5.96	122.54	110.38
1	C	286	VAL	CA-CB-CG1	5.95	120.52	110.40
1	A	117	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	286	VAL	CA-CB-CG1	5.94	120.51	110.40
1	A	78	LYS	CB-CG-CD	5.91	124.90	111.30
1	B	318	GLU	CB-CA-C	5.91	120.61	110.79
1	A	305	ARG	CB-CG-CD	5.89	124.85	111.30
1	C	8	GLN	CB-CG-CD	5.88	122.60	112.60
1	F	183	TYR	N-CA-CB	5.86	118.74	110.12
1	G	219	ASP	CA-CB-CG	5.86	118.46	112.60
1	E	17	GLU	CB-CG-CD	5.83	122.52	112.60
1	G	163	LYS	CB-CG-CD	5.81	124.67	111.30
1	A	78	LYS	CB-CA-C	5.79	121.67	109.79
1	B	260	VAL	N-CA-CB	-5.79	105.84	111.57
1	C	117	ASP	CA-CB-CG	5.77	118.37	112.60
1	E	318	GLU	CB-CA-C	5.75	120.34	110.79
1	A	265	ASP	CA-CB-CG	5.74	118.34	112.60
1	F	293	GLN	N-CA-CB	-5.73	101.71	110.01
1	G	318	GLU	CB-CA-C	5.72	120.58	110.85
1	E	219	ASP	CA-CB-CG	5.72	118.32	112.60
1	C	318	GLU	CB-CA-C	5.72	120.29	110.79
1	D	242	LYS	CB-CG-CD	5.69	124.40	111.30
1	D	166	ASP	CA-CB-CG	5.69	118.29	112.60
1	E	91	ALA	CA-C-N	5.64	132.30	121.54
1	E	91	ALA	C-N-CA	5.64	132.30	121.54
1	C	20	LYS	CB-CA-C	-5.63	100.63	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	VAL	CB-CA-C	5.62	120.51	111.29
1	H	117	ASP	CA-CB-CG	5.61	118.21	112.60
1	G	17	GLU	CB-CG-CD	5.59	122.11	112.60
1	F	244	PHE	CB-CA-C	-5.58	102.11	110.88
1	A	95	CYS	CA-CB-SG	-5.58	101.56	114.40
1	A	219	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	39	HIS	CA-CB-CG	5.57	119.37	113.80
1	E	78	LYS	CB-CA-C	5.54	121.15	109.79
1	G	293	GLN	N-CA-CB	-5.53	101.99	110.01
1	A	266	GLU	CG-CD-OE1	-5.51	105.72	118.40
1	E	92	CYS	CA-CB-SG	-5.51	101.73	114.40
1	H	219	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	219	ASP	CA-CB-CG	5.50	118.10	112.60
1	D	78	LYS	CA-CB-CG	5.50	125.09	114.10
1	G	264	HIS	CB-CA-C	5.49	120.49	110.11
1	D	195	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	163	LYS	CB-CA-C	5.46	117.26	108.91
1	G	260	VAL	N-CA-CB	-5.45	105.41	111.41
1	D	198	ASP	CA-CB-CG	5.45	118.05	112.60
1	F	39	HIS	CA-CB-CG	5.43	119.23	113.80
1	E	264	HIS	CB-CA-C	5.41	120.33	110.11
1	E	39	HIS	CA-CB-CG	5.39	119.19	113.80
1	D	117	ASP	CA-CB-CG	5.39	117.99	112.60
1	D	183	TYR	N-CA-CB	5.37	118.02	110.12
1	E	198	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	265	ASP	CA-CB-CG	5.35	117.95	112.60
1	D	219	ASP	CA-CB-CG	5.35	117.95	112.60
1	F	219	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	260	VAL	N-CA-CB	-5.34	105.54	111.41
1	G	291	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	291	ASP	CA-CB-CG	5.31	117.91	112.60
1	H	94	GLU	CA-C-N	5.30	131.66	121.54
1	H	94	GLU	C-N-CA	5.30	131.66	121.54
1	E	106	CYS	CB-CA-C	-5.29	101.62	109.60
1	A	163	LYS	CA-CB-CG	5.28	124.67	114.10
1	B	133	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	H	291	ASP	CA-CB-CG	5.26	117.86	112.60
1	F	98	CYS	N-CA-C	-5.25	105.73	111.82
1	B	81	ASP	CA-CB-CG	5.25	117.85	112.60
1	F	318	GLU	CB-CA-C	5.25	119.77	110.85
1	G	81	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	70	VAL	N-CA-CB	-5.23	103.89	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	ASP	CA-CB-CG	5.23	117.83	112.60
1	H	260	VAL	N-CA-CB	-5.21	105.68	111.41
1	B	166	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	219	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	48	ASP	CA-CB-CG	5.19	117.79	112.60
1	E	291	ASP	CA-CB-CG	5.19	117.79	112.60
1	G	166	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	266	GLU	CG-CD-OE2	5.19	130.33	118.40
1	B	133	ARG	CD-NE-CZ	5.18	131.66	124.40
1	C	181	LEU	N-CA-CB	-5.18	102.50	110.01
1	C	286	VAL	CB-CA-C	5.18	119.79	111.29
1	E	136	ASP	CA-CB-CG	5.18	117.78	112.60
1	F	48	ASP	CA-CB-CG	5.17	117.77	112.60
1	D	260	VAL	N-CA-CB	-5.16	105.74	111.41
1	F	81	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	39	HIS	CA-CB-CG	5.15	118.95	113.80
1	H	92	CYS	CA-CB-SG	-5.15	102.55	114.40
1	C	91	ALA	CA-C-N	5.09	131.27	121.54
1	C	91	ALA	C-N-CA	5.09	131.27	121.54
1	C	237	VAL	N-CA-C	-5.09	106.19	111.58
1	D	70	VAL	N-CA-CB	-5.08	104.40	111.41
1	B	183	TYR	N-CA-CB	5.08	117.58	110.12
1	G	39	HIS	CA-CB-CG	5.06	118.86	113.80
1	D	91	ALA	CA-C-N	5.05	131.19	121.54
1	D	91	ALA	C-N-CA	5.05	131.19	121.54
1	C	78	LYS	CB-CA-C	5.05	120.77	109.56
1	B	198	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	94	GLU	CA-C-N	5.04	131.17	121.54
1	A	94	GLU	C-N-CA	5.04	131.17	121.54
1	H	91	ALA	CA-C-N	5.04	131.16	121.54
1	H	91	ALA	C-N-CA	5.04	131.16	121.54
1	G	95	CYS	CA-CB-SG	-5.04	102.82	114.40
1	A	48	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	318	GLU	N-CA-CB	-5.03	102.71	110.16
1	H	17	GLU	CB-CG-CD	5.03	121.14	112.60
1	F	291	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	148	CYS	N-CA-C	-5.00	105.42	112.12
1	C	17	GLU	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	ARG	Sidechain
1	B	133	ARG	Sidechain
1	B	253	ARG	Sidechain
1	B	305	ARG	Sidechain
1	C	253	ARG	Sidechain
1	C	305	ARG	Sidechain
1	C	331	ARG	Sidechain
1	D	331	ARG	Sidechain
1	E	133	ARG	Sidechain
1	E	253	ARG	Sidechain
1	E	305	ARG	Sidechain
1	F	253	ARG	Sidechain
1	G	253	ARG	Sidechain
1	H	133	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	2532	2527	2572	22	0
1	B	2532	2527	2571	18	0
1	C	2532	2527	2572	33	0
1	D	2532	2527	2572	23	0
1	E	2532	2527	2572	16	0
1	F	2532	2527	2572	21	0
1	G	2532	2527	2572	21	0
1	H	2532	2527	2571	29	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0
2	C	2	0	0	1	0
2	D	2	0	0	1	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	1	0
2	H	2	0	0	0	0
3	A	19	0	0	5	0
3	B	14	0	0	7	0
3	C	25	0	0	14	0
3	D	11	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	14	0	0	1	0
3	F	12	0	0	6	0
3	G	11	0	0	5	0
3	H	20	0	0	12	0
All	All	20398	20216	20574	168	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 4.

All (168) 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:H:106:CYS:HB3	3:H:516:HOH:O	1.16	1.31
1:F:95:CYS:HB2	3:F:505:HOH:O	1.00	1.15
1:A:251:ILE:HG21	3:A:513:HOH:O	1.57	1.03
1:C:142:GLU:HG2	3:C:522:HOH:O	1.59	1.01
1:C:106:CYS:SG	3:C:504:HOH:O	2.23	0.97
1:D:43:HIS:NE2	3:D:501:HOH:O	2.01	0.92
1:C:43:HIS:CE1	3:C:501:HOH:O	2.23	0.92
1:C:285:ILE:HA	3:C:510:HOH:O	1.73	0.89
1:C:148:CYS:SG	3:C:525:HOH:O	2.30	0.88
1:C:75:LYS:HA	3:C:507:HOH:O	1.74	0.87
1:H:106:CYS:CB	3:H:516:HOH:O	1.90	0.84
1:E:271:ILE:HD11	1:G:269:ILE:HD11	1.59	0.84
1:F:43:HIS:NE2	3:F:501:HOH:O	1.97	0.82
1:H:91:ALA:HB1	1:H:106:CYS:SG	2.20	0.82
1:F:133:ARG:NE	3:F:502:HOH:O	2.14	0.81
1:C:43:HIS:NE2	3:C:501:HOH:O	2.14	0.80
1:C:95:CYS:SG	3:C:502:HOH:O	2.38	0.79
1:D:148:CYS:SG	2:D:401:ZN:ZN	1.74	0.77
1:D:43:HIS:CE1	3:D:501:HOH:O	2.36	0.76
1:H:43:HIS:NE2	3:H:501:HOH:O	2.17	0.76
1:H:43:HIS:CE1	3:H:501:HOH:O	2.40	0.75
1:F:253:ARG:HD2	3:F:512:HOH:O	1.86	0.75
1:E:91:ALA:HB1	1:E:106:CYS:SG	2.27	0.75
1:C:148:CYS:SG	2:C:401:ZN:ZN	1.76	0.74
1:H:39:HIS:NE2	3:H:501:HOH:O	2.20	0.74
1:E:269:ILE:HD12	1:G:269:ILE:HD12	1.70	0.74
1:G:251:ILE:HD11	1:G:279:ILE:HG23	1.70	0.74
1:B:305:ARG:HD2	3:B:508:HOH:O	1.86	0.73
1:H:251:ILE:HD11	1:H:279:ILE:HG23	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:ILE:HD11	1:F:279:ILE:HG23	1.70	0.71
1:E:251:ILE:HD11	1:E:279:ILE:HG23	1.73	0.71
1:G:101:GLY:HA2	3:G:511:HOH:O	1.90	0.71
1:G:39:HIS:NE2	3:G:501:HOH:O	2.25	0.70
1:H:305:ARG:HD2	3:H:519:HOH:O	1.91	0.69
1:F:239:VAL:HB	1:F:263:PRO:HB3	1.74	0.69
1:B:139:ASP:HB2	3:B:512:HOH:O	1.92	0.69
1:B:251:ILE:HD11	1:B:279:ILE:HG23	1.73	0.69
1:C:251:ILE:HD11	1:C:279:ILE:HG23	1.73	0.69
1:A:148:CYS:SG	2:A:401:ZN:ZN	1.82	0.69
1:G:148:CYS:SG	2:G:401:ZN:ZN	1.80	0.68
1:A:251:ILE:HD11	1:A:279:ILE:HG23	1.76	0.67
1:D:39:HIS:NE2	3:D:501:HOH:O	1.75	0.67
1:B:8:GLN:CG	3:B:513:HOH:O	2.42	0.67
1:B:39:HIS:NE2	3:B:501:HOH:O	2.27	0.66
1:D:251:ILE:HD11	1:D:279:ILE:HG23	1.75	0.66
1:D:17:GLU:HG3	3:D:510:HOH:O	1.95	0.65
1:C:133:ARG:NE	3:C:503:HOH:O	2.19	0.65
1:B:8:GLN:HG2	3:B:513:HOH:O	1.95	0.65
1:D:239:VAL:HB	1:D:263:PRO:HB3	1.79	0.63
1:C:39:HIS:NE2	3:C:501:HOH:O	2.08	0.63
1:B:271:ILE:HD11	1:F:269:ILE:HD11	1.82	0.62
1:E:39:HIS:NE2	3:E:501:HOH:O	2.30	0.60
1:A:39:HIS:NE2	3:A:501:HOH:O	2.31	0.60
1:F:253:ARG:CD	3:F:512:HOH:O	2.46	0.59
1:D:173:ILE:HD11	1:D:193:ALA:HB1	1.86	0.58
1:G:146:ILE:CG1	3:G:507:HOH:O	2.50	0.58
1:G:146:ILE:HG12	3:G:507:HOH:O	2.03	0.57
1:C:173:ILE:HD11	1:C:193:ALA:HB1	1.85	0.57
1:F:286:VAL:HG12	1:F:287:GLY:H	1.69	0.57
1:B:286:VAL:HG13	1:B:287:GLY:H	1.68	0.57
1:D:239:VAL:HG12	1:D:244:PHE:CZ	2.40	0.57
1:F:239:VAL:HG12	1:F:244:PHE:CZ	2.39	0.57
1:E:173:ILE:HD11	1:E:193:ALA:HB1	1.85	0.56
1:A:173:ILE:HD11	1:A:193:ALA:HB1	1.85	0.56
1:A:285:ILE:CD1	1:H:276:LEU:HD12	2.36	0.56
1:A:285:ILE:HD12	1:H:276:LEU:HD12	1.88	0.56
1:A:271:ILE:HD13	1:H:267:LEU:HB3	1.87	0.55
1:F:173:ILE:HD11	1:F:193:ALA:HB1	1.88	0.55
1:A:286:VAL:HG13	1:A:287:GLY:H	1.71	0.54
1:H:173:ILE:HD11	1:H:193:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:VAL:HG13	1:C:287:GLY:H	1.72	0.53
1:H:92:CYS:SG	1:H:93:GLY:N	2.82	0.53
1:A:95:CYS:SG	1:A:98:CYS:HB2	2.48	0.52
1:C:318:GLU:HB2	3:C:516:HOH:O	2.09	0.52
1:A:269:ILE:HG13	1:H:269:ILE:HD12	1.90	0.52
1:F:43:HIS:CE1	3:F:501:HOH:O	2.53	0.52
1:F:70:VAL:HG13	1:F:74:VAL:HB	1.90	0.52
1:G:173:ILE:HD11	1:G:193:ALA:HB1	1.90	0.52
1:E:92:CYS:SG	1:E:93:GLY:N	2.83	0.52
1:B:173:ILE:HD11	1:B:193:ALA:HB1	1.92	0.51
1:G:39:HIS:NE2	1:G:43:HIS:NE2	2.58	0.51
1:H:133:ARG:NE	3:H:502:HOH:O	2.44	0.51
1:C:39:HIS:NE2	1:C:43:HIS:NE2	2.59	0.51
1:F:39:HIS:NE2	1:F:43:HIS:NE2	2.59	0.51
1:F:39:HIS:HE2	1:F:43:HIS:HE2	1.60	0.50
1:H:251:ILE:HD12	1:H:256:CYS:N	2.27	0.50
1:E:39:HIS:NE2	1:E:43:HIS:NE2	2.60	0.50
1:A:271:ILE:CD1	1:H:267:LEU:HB3	2.41	0.49
1:E:275:VAL:HA	1:G:283:GLY:HA3	1.94	0.49
1:G:251:ILE:HD12	1:G:256:CYS:N	2.28	0.49
1:A:251:ILE:CG2	3:A:513:HOH:O	2.31	0.49
1:H:39:HIS:NE2	1:H:43:HIS:NE2	2.60	0.49
1:H:106:CYS:SG	3:H:516:HOH:O	2.56	0.49
1:B:39:HIS:NE2	1:B:43:HIS:NE2	2.60	0.49
1:A:98:CYS:HB3	3:A:516:HOH:O	2.13	0.48
1:A:39:HIS:NE2	1:A:43:HIS:NE2	2.61	0.48
1:D:39:HIS:NE2	1:D:43:HIS:NE2	2.61	0.48
1:C:269:ILE:HD11	1:D:271:ILE:HD11	1.97	0.47
1:H:286:VAL:HG12	1:H:287:GLY:H	1.79	0.47
1:E:251:ILE:HD12	1:E:256:CYS:N	2.30	0.47
1:E:283:GLY:HA3	1:G:275:VAL:HA	1.96	0.47
1:B:251:ILE:HD12	1:B:256:CYS:N	2.29	0.47
1:D:39:HIS:HE2	1:D:43:HIS:HE2	1.61	0.47
1:D:86:PRO:HB2	3:D:505:HOH:O	2.13	0.47
1:D:251:ILE:HD12	1:D:256:CYS:N	2.30	0.47
1:A:251:ILE:HD12	1:A:256:CYS:N	2.30	0.47
1:C:251:ILE:HD12	1:C:256:CYS:N	2.30	0.47
1:G:1:MET:N	3:G:502:HOH:O	2.48	0.46
1:A:244:PHE:CZ	1:A:269:ILE:HD11	2.51	0.46
1:B:70:VAL:HG13	1:B:74:VAL:HB	1.98	0.46
1:E:286:VAL:HG12	1:E:287:GLY:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:PHE:CG	1:F:267:LEU:HD22	2.52	0.45
1:A:43:HIS:NE2	3:A:501:HOH:O	2.22	0.45
1:C:244:PHE:HB2	1:C:267:LEU:HD13	1.97	0.45
1:H:133:ARG:CZ	3:H:502:HOH:O	2.65	0.45
1:C:275:VAL:HA	1:D:283:GLY:HA3	1.99	0.45
1:C:173:ILE:CD1	1:C:193:ALA:HB1	2.47	0.45
1:F:251:ILE:HD12	1:F:256:CYS:N	2.31	0.45
1:D:70:VAL:HG13	1:D:74:VAL:HB	1.99	0.45
1:B:43:HIS:NE2	3:B:501:HOH:O	2.23	0.44
1:C:25:TYR:CE2	1:C:73:GLY:HA3	2.52	0.44
1:E:173:ILE:CD1	1:E:193:ALA:HB1	2.47	0.44
1:C:148:CYS:HA	3:C:525:HOH:O	2.18	0.44
1:C:267:LEU:HB2	3:C:515:HOH:O	2.17	0.44
1:D:173:ILE:CD1	1:D:193:ALA:HB1	2.47	0.44
1:B:171:TYR:CE1	1:B:194:VAL:HG11	2.52	0.44
1:H:87:TRP:O	1:H:111:ASN:HA	2.18	0.44
1:C:269:ILE:HD12	1:D:269:ILE:HD12	1.99	0.43
1:G:8:GLN:OE1	1:G:11:GLN:HG3	2.19	0.43
1:E:269:ILE:HD11	1:G:271:ILE:HD11	2.00	0.43
1:B:244:PHE:HB2	1:B:267:LEU:HD13	2.01	0.43
1:A:87:TRP:O	1:A:111:ASN:HA	2.19	0.43
1:E:87:TRP:O	1:E:111:ASN:HA	2.19	0.42
1:G:87:TRP:O	1:G:111:ASN:HA	2.19	0.42
1:C:87:TRP:O	1:C:111:ASN:HA	2.20	0.42
1:F:173:ILE:CD1	1:F:193:ALA:HB1	2.49	0.42
1:C:171:TYR:CE1	1:C:194:VAL:HG11	2.55	0.42
1:C:285:ILE:O	1:C:286:VAL:C	2.62	0.42
1:D:87:TRP:O	1:D:111:ASN:HA	2.19	0.42
1:D:169:ALA:HB2	1:D:231:VAL:HG11	2.01	0.42
1:A:173:ILE:CD1	1:A:193:ALA:HB1	2.48	0.41
1:C:244:PHE:CB	1:C:267:LEU:HD13	2.50	0.41
1:H:267:LEU:HB2	3:H:512:HOH:O	2.20	0.41
1:B:244:PHE:CB	1:B:267:LEU:HD13	2.50	0.41
1:F:87:TRP:O	1:F:111:ASN:HA	2.20	0.41
1:A:172:GLY:O	1:A:177:GLY:HA3	2.20	0.41
1:E:172:GLY:O	1:E:177:GLY:HA3	2.21	0.41
1:G:286:VAL:HG12	1:G:287:GLY:H	1.84	0.41
1:H:251:ILE:CD1	1:H:279:ILE:HG23	2.45	0.41
1:C:283:GLY:HA3	1:D:275:VAL:HA	2.02	0.41
1:A:285:ILE:O	1:A:286:VAL:C	2.64	0.41
1:H:285:ILE:O	1:H:286:VAL:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TRP:O	1:B:111:ASN:HA	2.20	0.41
1:G:173:ILE:CD1	1:G:193:ALA:HB1	2.49	0.41
1:H:1:MET:N	3:H:504:HOH:O	2.53	0.41
1:H:173:ILE:CD1	1:H:193:ALA:HB1	2.49	0.41
1:H:251:ILE:HD13	1:H:251:ILE:HG21	1.86	0.41
1:C:70:VAL:HG13	1:C:74:VAL:HB	2.02	0.41
1:C:148:CYS:CB	3:C:525:HOH:O	2.65	0.41
1:D:286:VAL:HG12	1:D:287:GLY:H	1.86	0.41
1:H:133:ARG:NH1	3:H:505:HOH:O	2.54	0.41
1:G:171:TYR:CE1	1:G:194:VAL:HG11	2.55	0.41
1:G:172:GLY:O	1:G:177:GLY:HA3	2.21	0.40
1:F:142:GLU:CD	1:F:305:ARG:HH22	2.30	0.40
1:B:164:PRO:HG3	3:B:504:HOH:O	2.20	0.40
1:C:141:VAL:HG12	1:C:308:VAL:HG21	2.03	0.40
1:D:244:PHE:CG	1:D:267:LEU:HD22	2.56	0.40
1:F:171:TYR:CE1	1:F:194:VAL:HG11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/337 (99%)	317 (95%)	15 (4%)	3 (1%)	14	35
1	B	335/337 (99%)	319 (95%)	13 (4%)	3 (1%)	14	35
1	C	335/337 (99%)	316 (94%)	16 (5%)	3 (1%)	14	35
1	D	335/337 (99%)	318 (95%)	14 (4%)	3 (1%)	14	35
1	E	335/337 (99%)	317 (95%)	14 (4%)	4 (1%)	10	27
1	F	335/337 (99%)	316 (94%)	16 (5%)	3 (1%)	14	35
1	G	335/337 (99%)	318 (95%)	14 (4%)	3 (1%)	14	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	335/337 (99%)	317 (95%)	14 (4%)	4 (1%)	10	27
All	All	2680/2696 (99%)	2538 (95%)	116 (4%)	26 (1%)	12	32

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	CYS
1	D	92	CYS
1	E	95	CYS
1	H	92	CYS
1	H	95	CYS
1	A	95	CYS
1	A	286	VAL
1	B	286	VAL
1	C	286	VAL
1	E	92	CYS
1	F	286	VAL
1	G	95	CYS
1	C	92	CYS
1	D	286	VAL
1	E	286	VAL
1	G	286	VAL
1	H	286	VAL
1	F	95	CYS
1	D	86	PRO
1	G	86	PRO
1	H	86	PRO
1	A	86	PRO
1	C	86	PRO
1	E	86	PRO
1	B	86	PRO
1	F	86	PRO

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	268/268 (100%)	246 (92%)	22 (8%)	10	27
1	B	268/268 (100%)	253 (94%)	15 (6%)	19	44
1	C	268/268 (100%)	254 (95%)	14 (5%)	21	47
1	D	268/268 (100%)	249 (93%)	19 (7%)	13	33
1	E	268/268 (100%)	253 (94%)	15 (6%)	19	44
1	F	268/268 (100%)	249 (93%)	19 (7%)	13	33
1	G	268/268 (100%)	247 (92%)	21 (8%)	11	29
1	H	268/268 (100%)	250 (93%)	18 (7%)	15	36
All	All	2144/2144 (100%)	2001 (93%)	143 (7%)	15	36

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	86	PRO
1	A	92	CYS
1	A	95	CYS
1	A	133	ARG
1	A	139	ASP
1	A	142	GLU
1	A	163	LYS
1	A	206	LYS
1	A	236	SER
1	A	237	VAL
1	A	241	LYS
1	A	251	ILE
1	A	267	LEU
1	A	276	LEU
1	A	286	VAL
1	A	305	ARG
1	A	311	VAL
1	A	312	SER
1	A	318	GLU
1	A	325	LYS
1	A	337	GLN
1	B	16	GLU
1	B	54	LYS
1	B	86	PRO
1	B	92	CYS
1	B	139	ASP

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Mol	Chain	Res	Type
1	B	181	LEU
1	B	206	LYS
1	B	236	SER
1	B	237	VAL
1	B	251	ILE
1	B	271	ILE
1	B	286	VAL
1	B	293	GLN
1	B	311	VAL
1	B	312	SER
1	C	8	GLN
1	C	16	GLU
1	C	54	LYS
1	C	86	PRO
1	C	139	ASP
1	C	206	LYS
1	C	236	SER
1	C	237	VAL
1	C	251	ILE
1	C	264	HIS
1	C	276	LEU
1	C	286	VAL
1	C	311	VAL
1	C	312	SER
1	D	24	GLU
1	D	54	LYS
1	D	86	PRO
1	D	92	CYS
1	D	139	ASP
1	D	163	LYS
1	D	181	LEU
1	D	236	SER
1	D	237	VAL
1	D	241	LYS
1	D	242	LYS
1	D	251	ILE
1	D	265	ASP
1	D	266	GLU
1	D	269	ILE
1	D	276	LEU
1	D	311	VAL
1	D	312	SER

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Mol	Chain	Res	Type
1	D	321	GLU
1	E	16	GLU
1	E	54	LYS
1	E	86	PRO
1	E	94	GLU
1	E	95	CYS
1	E	98	CYS
1	E	139	ASP
1	E	236	SER
1	E	237	VAL
1	E	251	ILE
1	E	265	ASP
1	E	266	GLU
1	E	271	ILE
1	E	311	VAL
1	E	312	SER
1	F	2	LYS
1	F	16	GLU
1	F	17	GLU
1	F	54	LYS
1	F	86	PRO
1	F	92	CYS
1	F	95	CYS
1	F	98	CYS
1	F	139	ASP
1	F	181	LEU
1	F	236	SER
1	F	237	VAL
1	F	241	LYS
1	F	251	ILE
1	F	264	HIS
1	F	266	GLU
1	F	276	LEU
1	F	311	VAL
1	F	312	SER
1	G	8	GLN
1	G	16	GLU
1	G	50	PRO
1	G	54	LYS
1	G	76	SER
1	G	86	PRO
1	G	92	CYS

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Mol	Chain	Res	Type
1	G	95	CYS
1	G	98	CYS
1	G	133	ARG
1	G	139	ASP
1	G	163	LYS
1	G	181	LEU
1	G	236	SER
1	G	237	VAL
1	G	251	ILE
1	G	264	HIS
1	G	265	ASP
1	G	271	ILE
1	G	311	VAL
1	G	312	SER
1	H	8	GLN
1	H	16	GLU
1	H	54	LYS
1	H	75	LYS
1	H	86	PRO
1	H	95	CYS
1	H	98	CYS
1	H	106	CYS
1	H	139	ASP
1	H	236	SER
1	H	237	VAL
1	H	251	ILE
1	H	265	ASP
1	H	271	ILE
1	H	276	LEU
1	H	311	VAL
1	H	312	SER
1	H	337	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN
1	B	14	GLN
1	B	264	HIS
1	B	277	ASN
1	C	14	GLN
1	C	301	GLN

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Mol	Chain	Res	Type
1	D	14	GLN
1	D	232	GLN
1	E	327	GLN
1	F	11	GLN
1	F	232	GLN
1	F	277	ASN
1	F	293	GLN
1	F	301	GLN
1	G	190	ASN
1	G	329	ASN
1	H	14	GLN
1	H	46	HIS
1	H	293	GLN
1	H	327	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	337/337 (100%)	-0.26	5 (1%) 72 70	14, 35, 74, 104	0
1	B	337/337 (100%)	0.07	17 (5%) 34 30	22, 44, 96, 141	0
1	C	337/337 (100%)	-0.11	8 (2%) 59 56	17, 36, 81, 140	0
1	D	337/337 (100%)	-0.15	10 (2%) 52 49	17, 36, 85, 117	0
1	E	337/337 (100%)	-0.04	15 (4%) 38 34	19, 41, 92, 146	0
1	F	337/337 (100%)	-0.09	15 (4%) 38 34	19, 37, 84, 131	0
1	G	337/337 (100%)	0.19	16 (4%) 36 33	20, 45, 99, 141	0
1	H	337/337 (100%)	-0.09	11 (3%) 49 45	18, 37, 83, 136	0
All	All	2696/2696 (100%)	-0.06	97 (3%) 46 42	14, 39, 87, 146	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	239	VAL	6.4
1	B	267	LEU	5.7
1	E	267	LEU	5.4
1	F	267	LEU	5.4
1	H	244	PHE	5.3
1	B	239	VAL	5.1
1	C	244	PHE	4.9
1	C	239	VAL	4.9
1	D	239	VAL	4.8
1	H	267	LEU	4.7
1	G	244	PHE	4.6
1	G	328	ILE	4.6
1	D	244	PHE	4.5
1	C	267	LEU	4.5
1	G	267	LEU	4.5
1	C	264	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	244	PHE	4.4
1	D	267	LEU	4.0
1	E	261	GLY	4.0
1	B	244	PHE	4.0
1	F	244	PHE	3.7
1	F	264	HIS	3.6
1	G	329	ASN	3.4
1	G	262	LEU	3.3
1	G	239	VAL	3.3
1	D	262	LEU	3.2
1	H	264	HIS	3.2
1	F	239	VAL	3.2
1	G	332	ILE	3.1
1	F	137	ASN	3.1
1	G	264	HIS	3.0
1	H	329	ASN	3.0
1	A	239	VAL	3.0
1	A	264	HIS	2.9
1	D	337	GLN	2.9
1	E	332	ILE	2.9
1	F	262	LEU	2.9
1	G	261	GLY	2.9
1	G	204	ALA	2.9
1	E	262	LEU	2.9
1	G	263	PRO	2.9
1	F	328	ILE	2.9
1	H	163	LYS	2.8
1	F	75	LYS	2.8
1	C	75	LYS	2.8
1	F	337	GLN	2.7
1	F	329	ASN	2.7
1	D	99	LEU	2.6
1	B	264	HIS	2.6
1	E	163	LYS	2.6
1	B	238	ALA	2.6
1	B	263	PRO	2.6
1	E	323	MET	2.6
1	G	238	ALA	2.6
1	G	195	ASP	2.5
1	A	285	ILE	2.5
1	B	206	LYS	2.5
1	B	262	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	239	VAL	2.5
1	H	263	PRO	2.5
1	B	328	ILE	2.5
1	F	269	ILE	2.5
1	D	261	GLY	2.5
1	H	311	VAL	2.5
1	F	163	LYS	2.4
1	F	285	ILE	2.4
1	D	264	HIS	2.4
1	G	241	LYS	2.4
1	B	337	GLN	2.4
1	H	326	GLY	2.4
1	G	39	HIS	2.3
1	D	328	ILE	2.3
1	F	261	GLY	2.3
1	A	238	ALA	2.3
1	E	44	ALA	2.3
1	E	54	LYS	2.3
1	C	329	ASN	2.3
1	E	285	ILE	2.2
1	H	332	ILE	2.2
1	C	337	GLN	2.2
1	E	328	ILE	2.2
1	B	326	GLY	2.2
1	H	328	ILE	2.2
1	C	142	GLU	2.1
1	E	337	GLN	2.1
1	B	276	LEU	2.1
1	G	236	SER	2.1
1	B	57	LEU	2.1
1	E	264	HIS	2.1
1	B	54	LYS	2.1
1	A	267	LEU	2.1
1	E	333	VAL	2.1
1	D	265	ASP	2.0
1	F	265	ASP	2.0
1	B	75	LYS	2.0
1	B	329	ASN	2.0
1	B	14	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

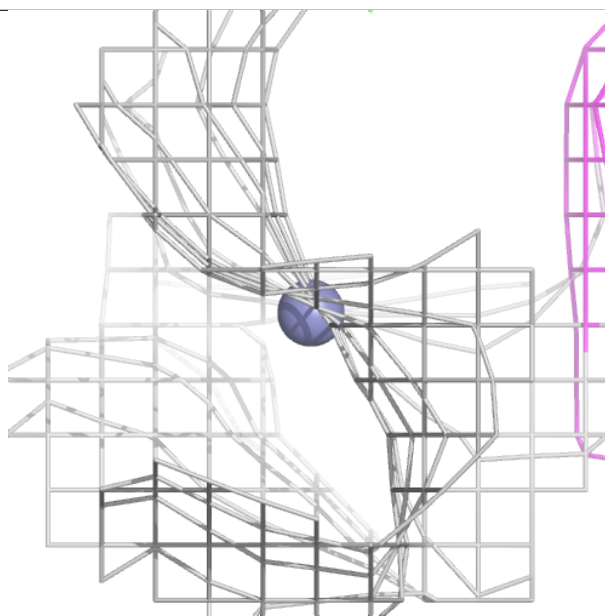
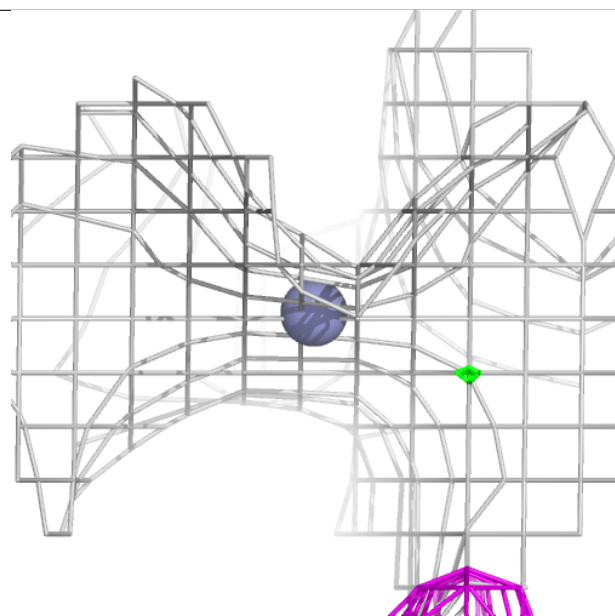
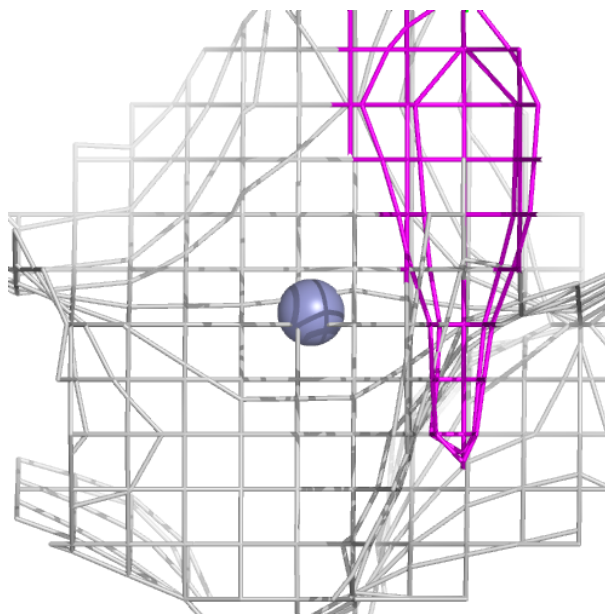
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	402	1/1	0.93	0.16	219,219,219,219	0
2	ZN	A	402	1/1	0.96	0.12	62,62,62,62	0
2	ZN	D	402	1/1	0.97	0.11	102,102,102,102	0
2	ZN	E	402	1/1	0.97	0.04	62,62,62,62	0
2	ZN	G	402	1/1	0.97	0.11	63,63,63,63	0
2	ZN	F	402	1/1	0.98	0.10	61,61,61,61	0
2	ZN	C	402	1/1	0.98	0.10	79,79,79,79	0
2	ZN	H	402	1/1	0.98	0.04	50,50,50,50	0
2	ZN	B	401	1/1	0.99	0.05	44,44,44,44	0
2	ZN	H	401	1/1	0.99	0.03	36,36,36,36	0
2	ZN	G	401	1/1	0.99	0.02	46,46,46,46	0
2	ZN	D	401	1/1	1.00	0.02	43,43,43,43	0
2	ZN	C	401	1/1	1.00	0.05	31,31,31,31	0
2	ZN	E	401	1/1	1.00	0.02	41,41,41,41	0
2	ZN	A	401	1/1	1.00	0.02	37,37,37,37	0
2	ZN	F	401	1/1	1.00	0.02	31,31,31,31	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.

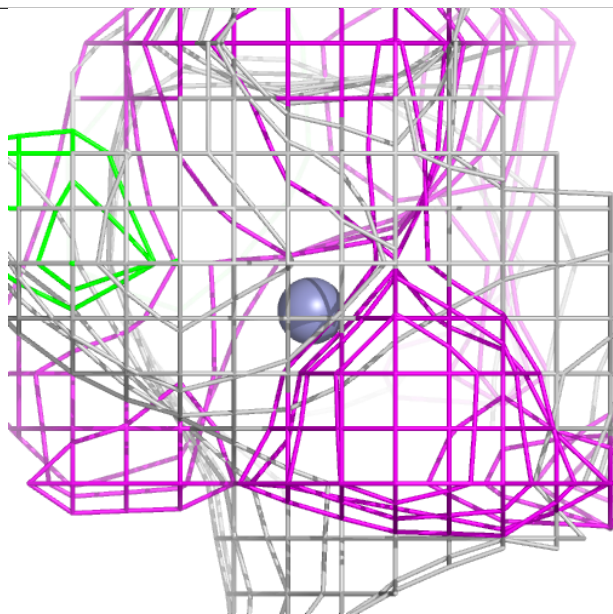
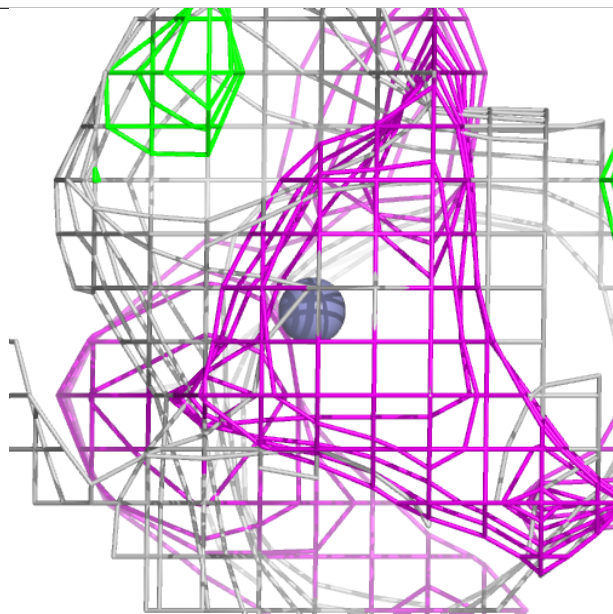
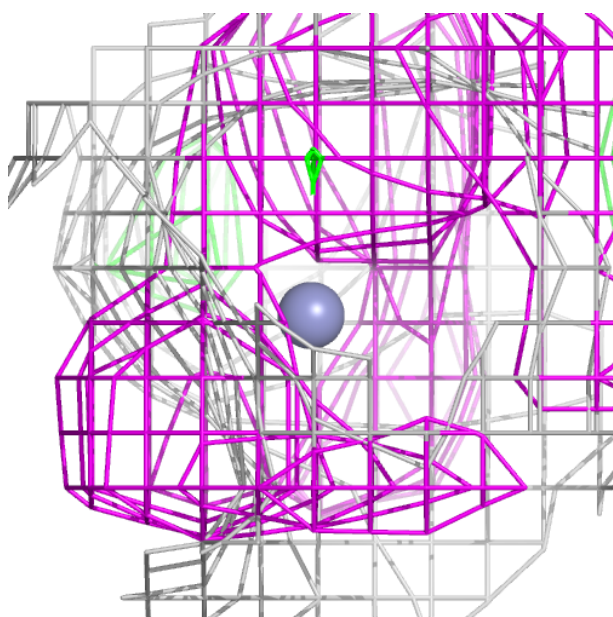
Electron density around ZN B 402:

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



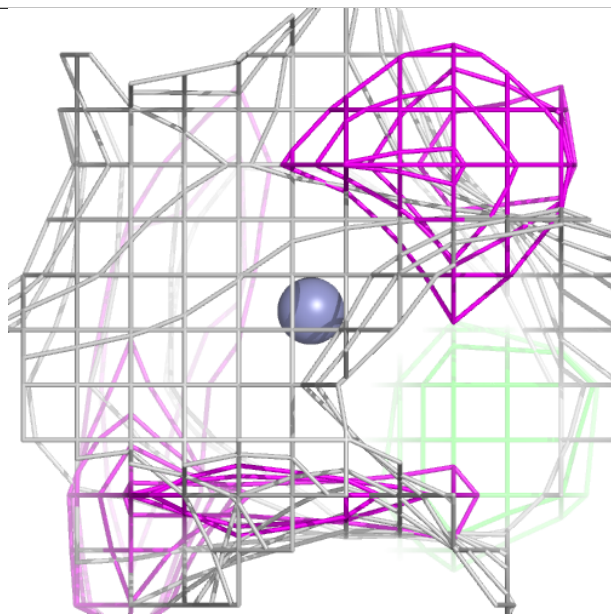
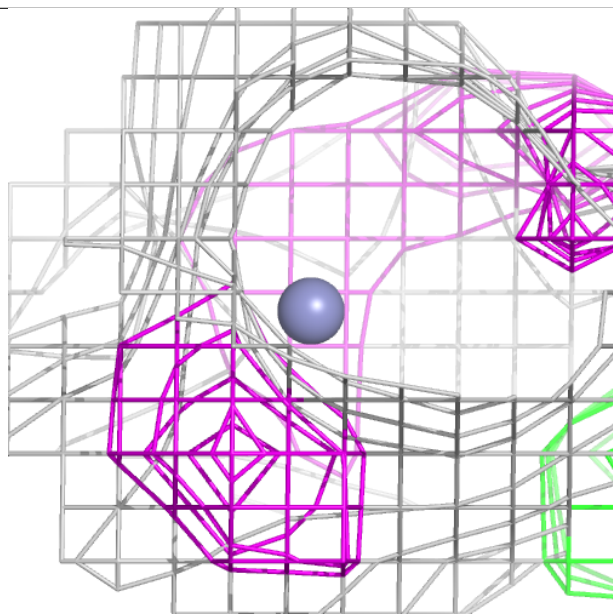
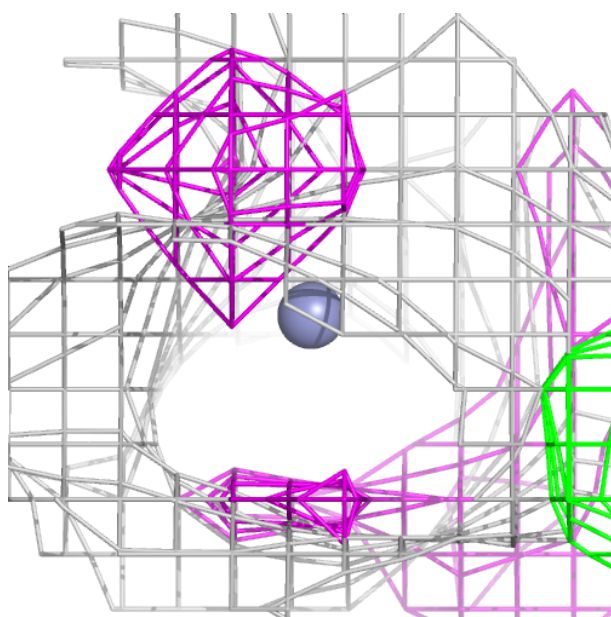
Electron density around ZN A 402:

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



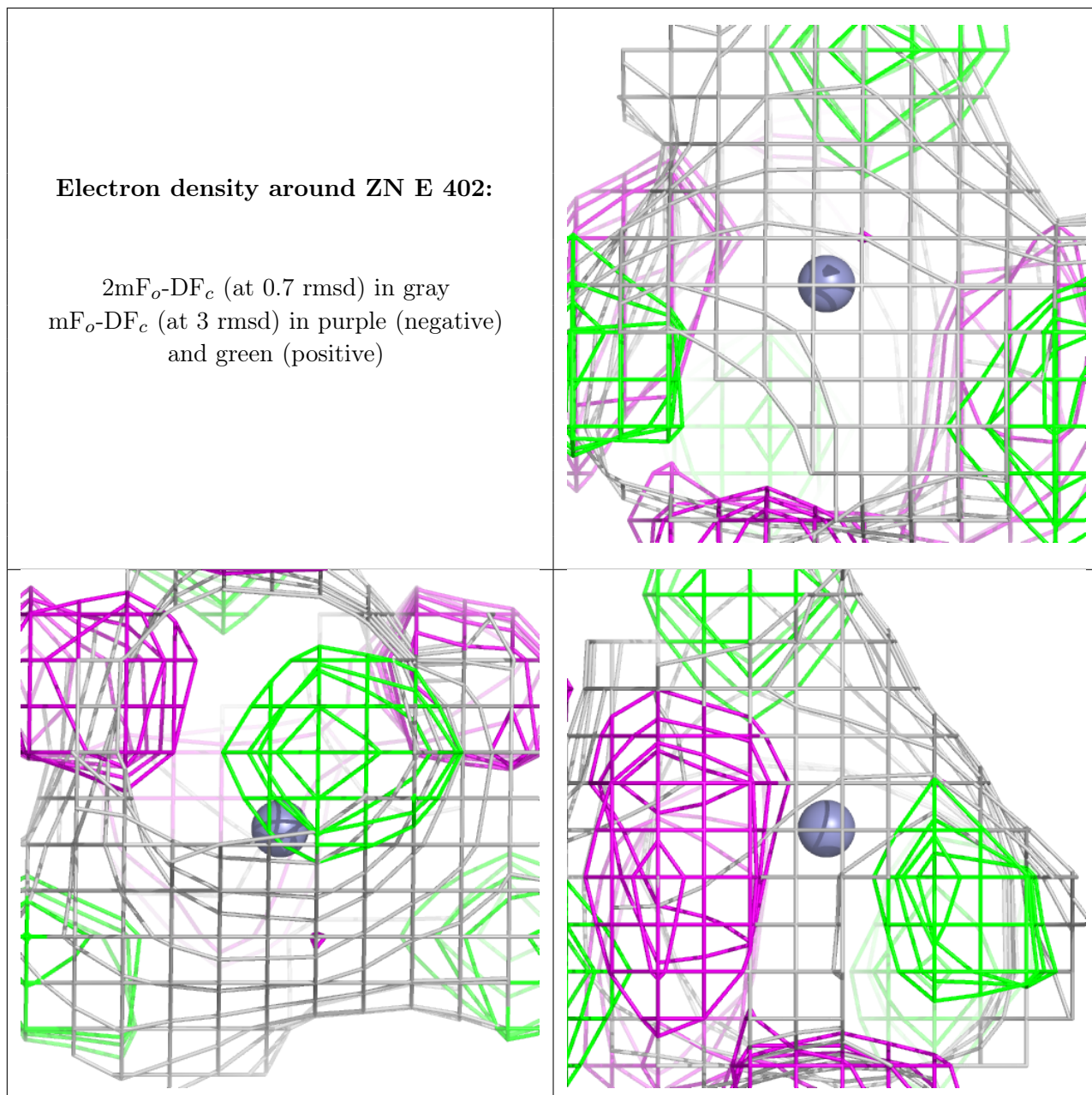
Electron density around ZN D 402:

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



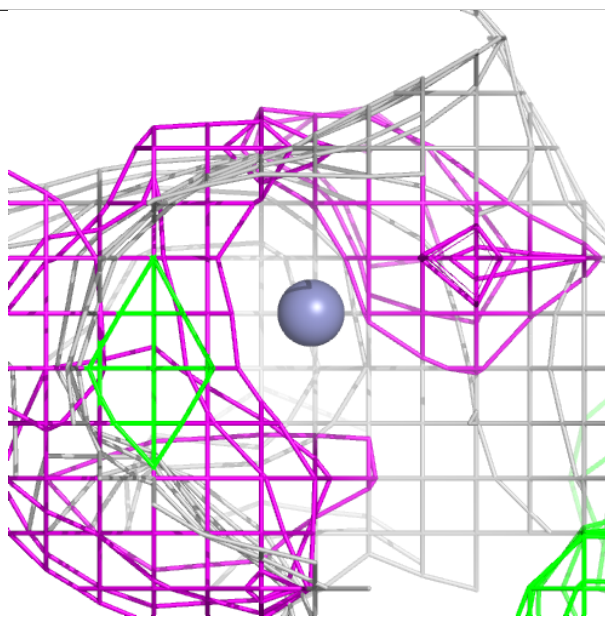
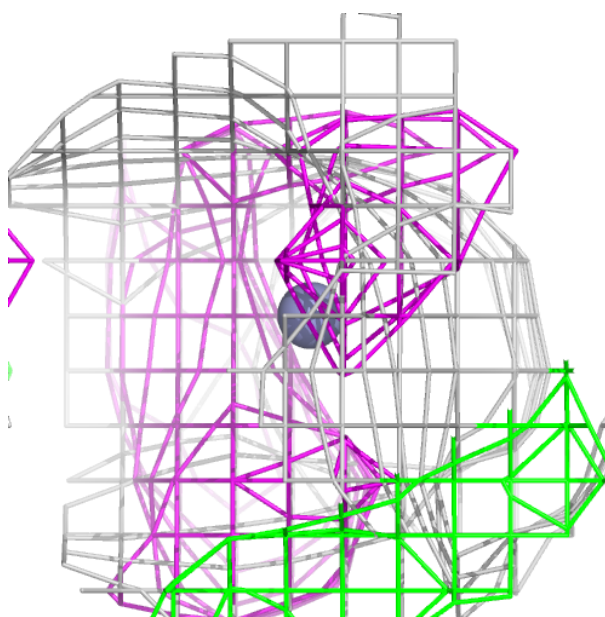
Electron density around ZN E 402:

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



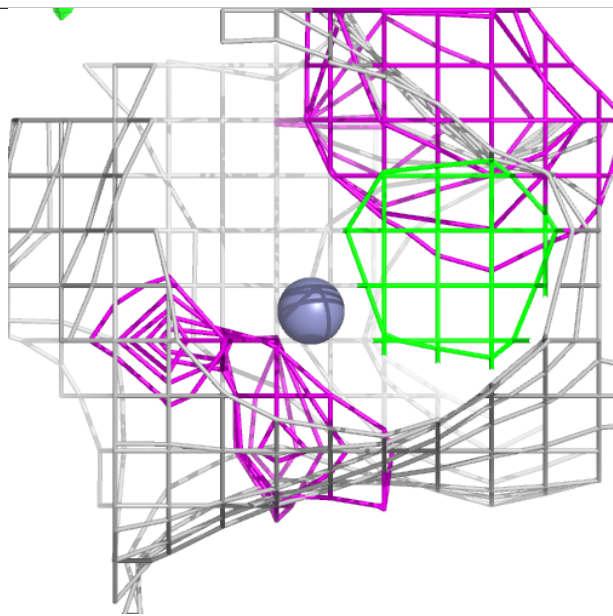
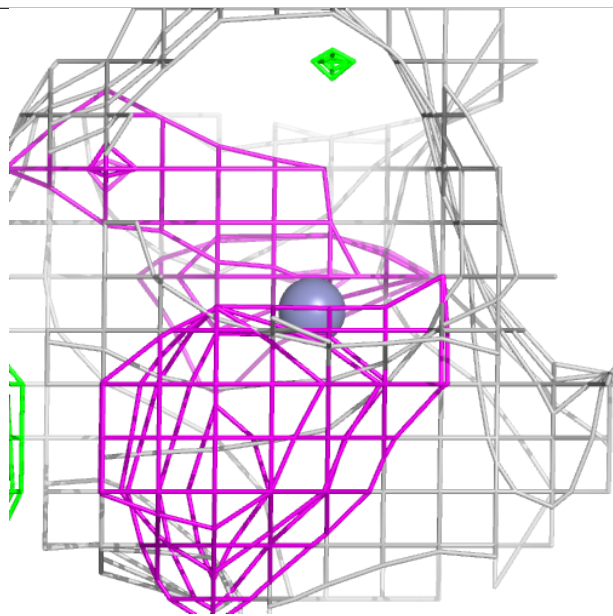
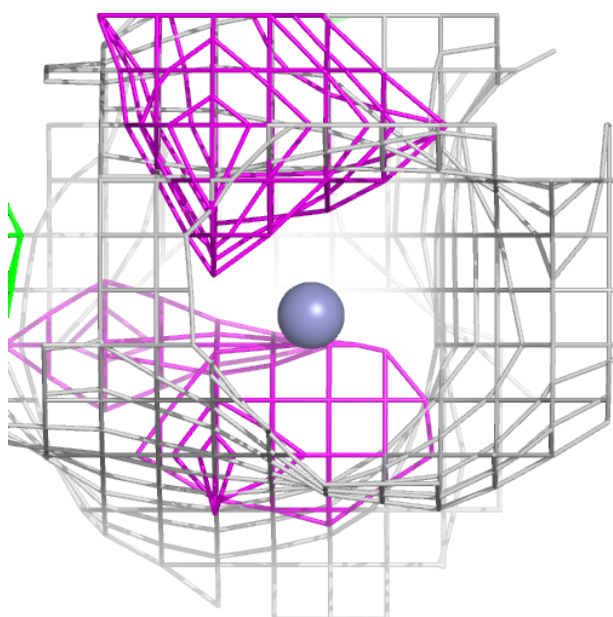
Electron density around ZN G 402:

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



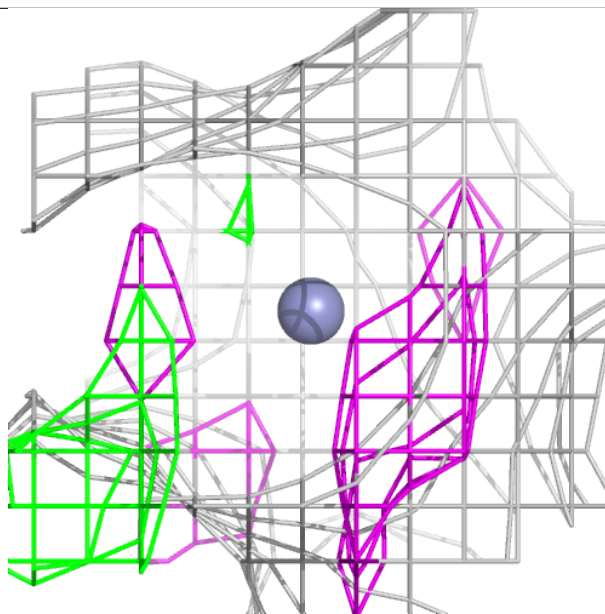
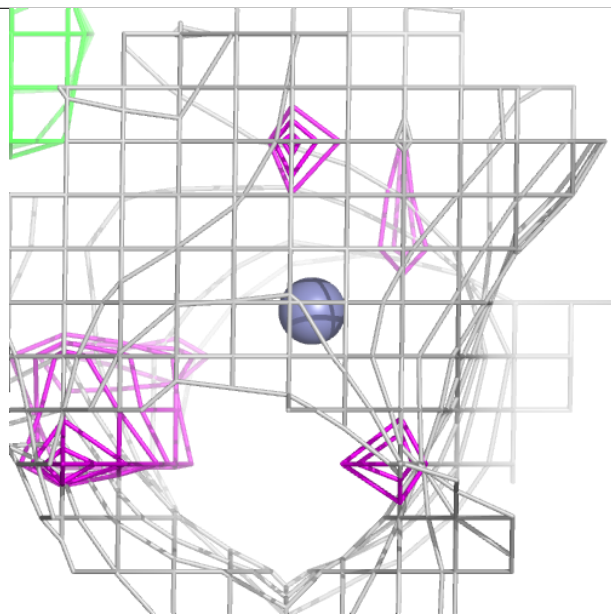
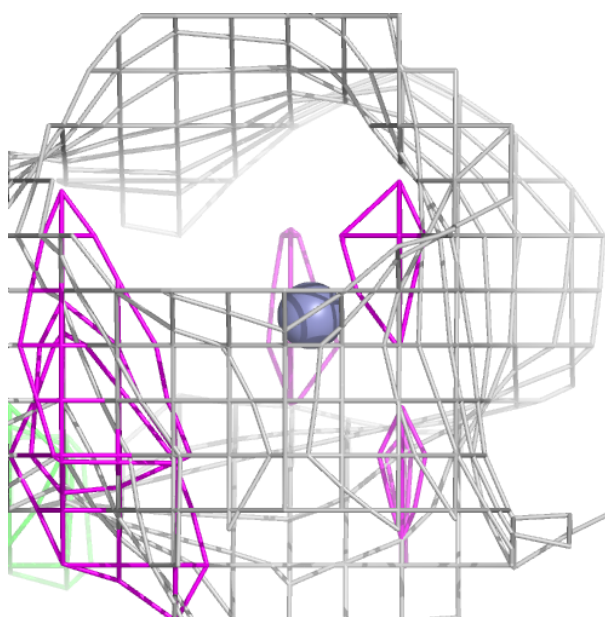
Electron density around ZN F 402:

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



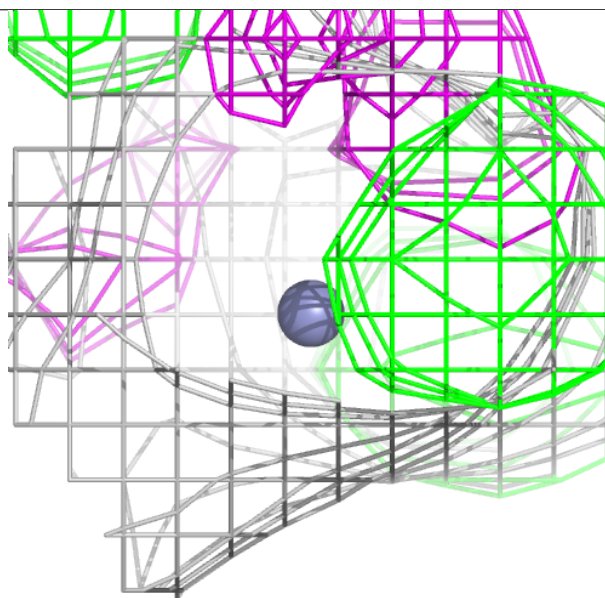
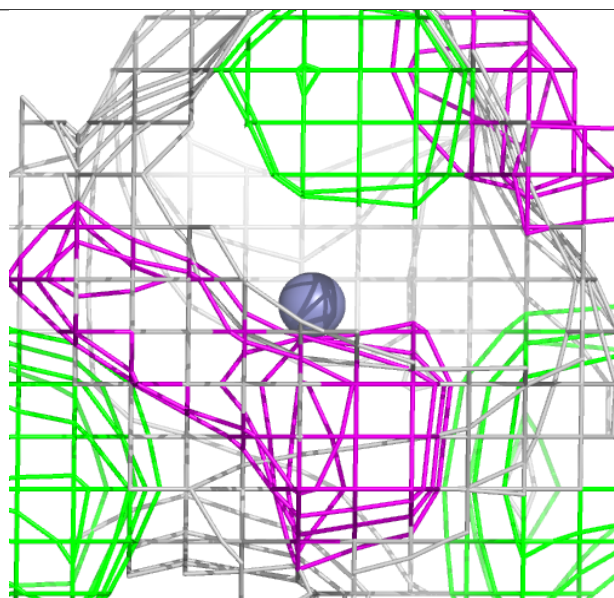
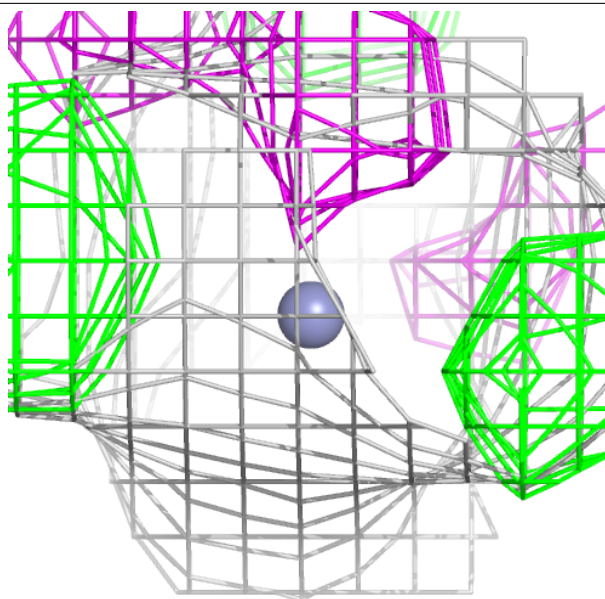
Electron density around ZN C 402:

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



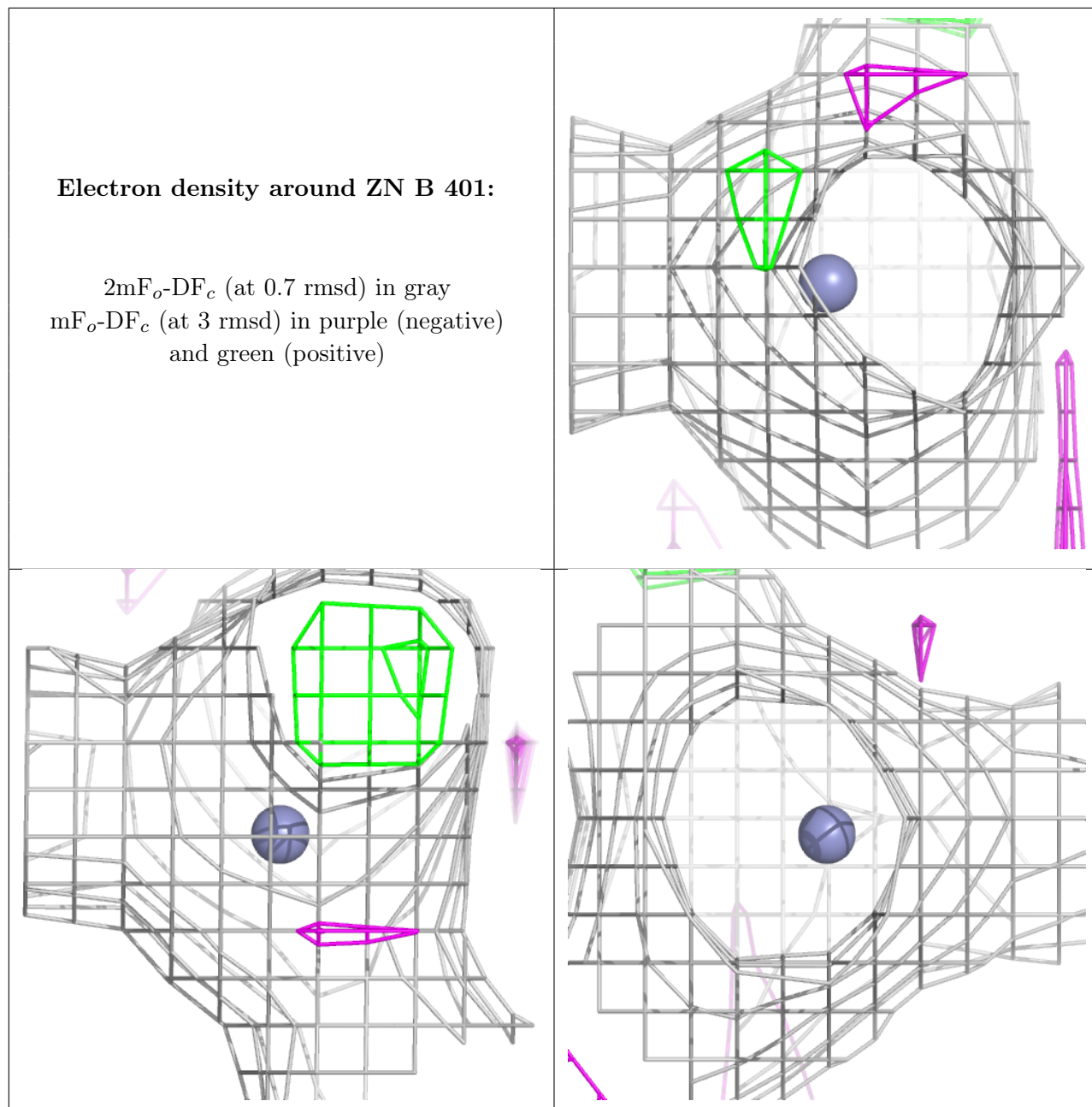
Electron density around ZN H 402:

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



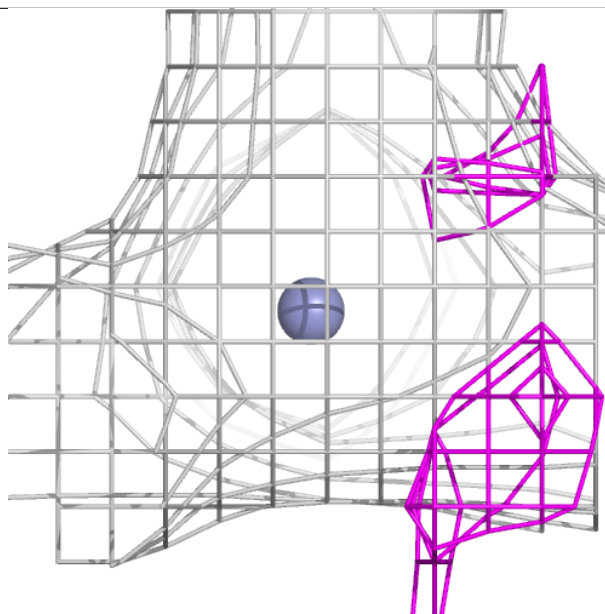
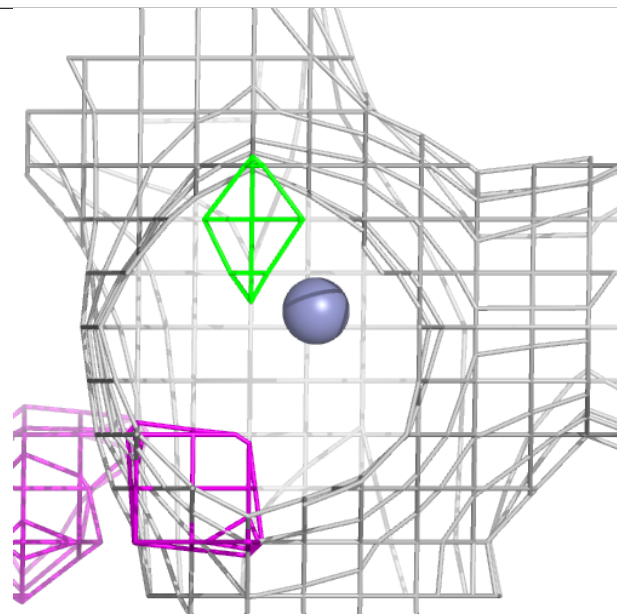
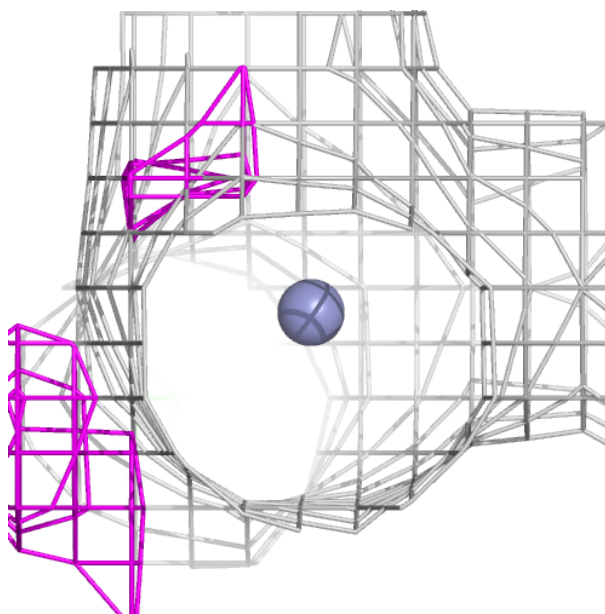
Electron density around ZN B 401:

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



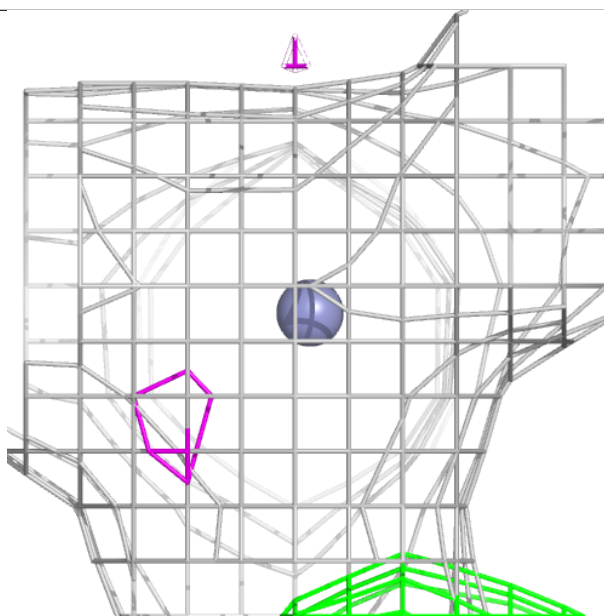
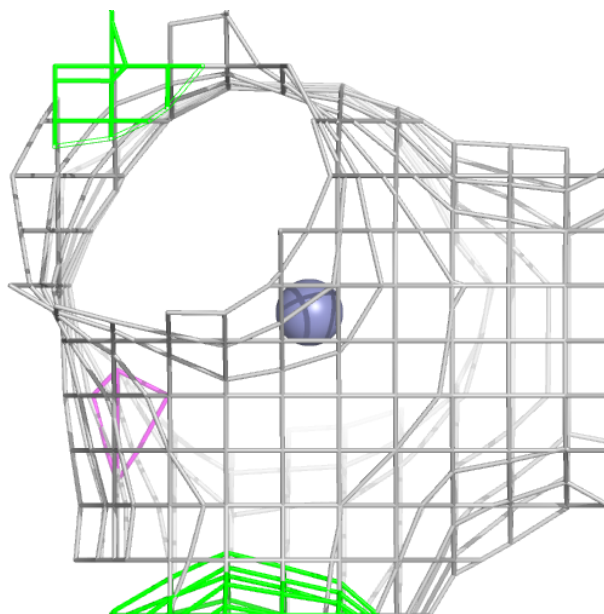
Electron density around ZN H 401:

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



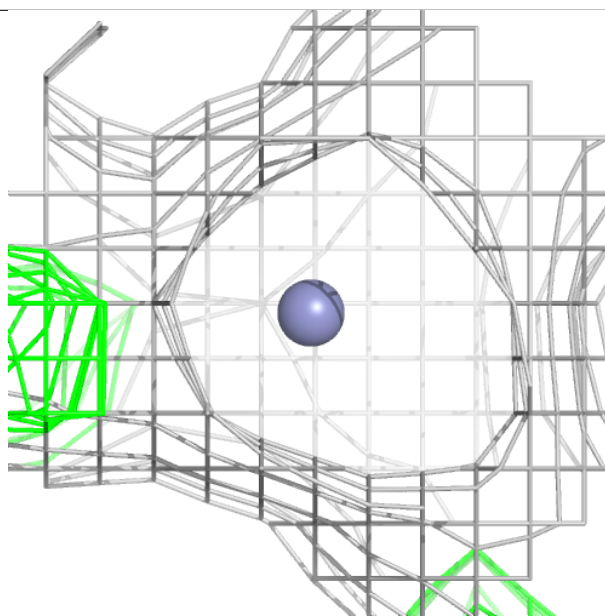
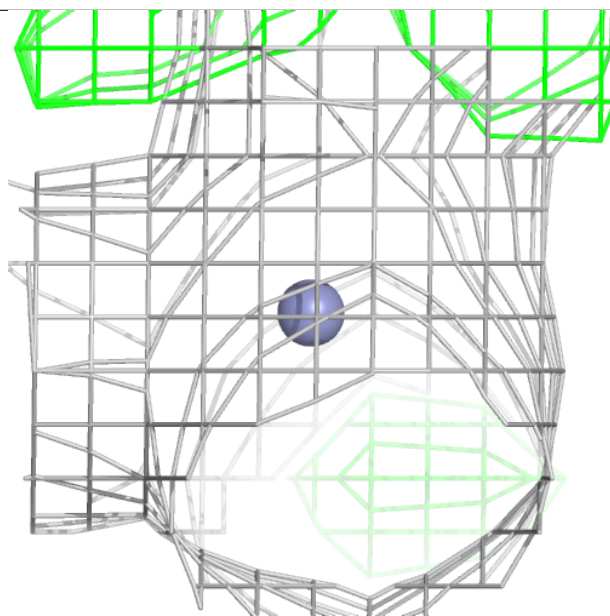
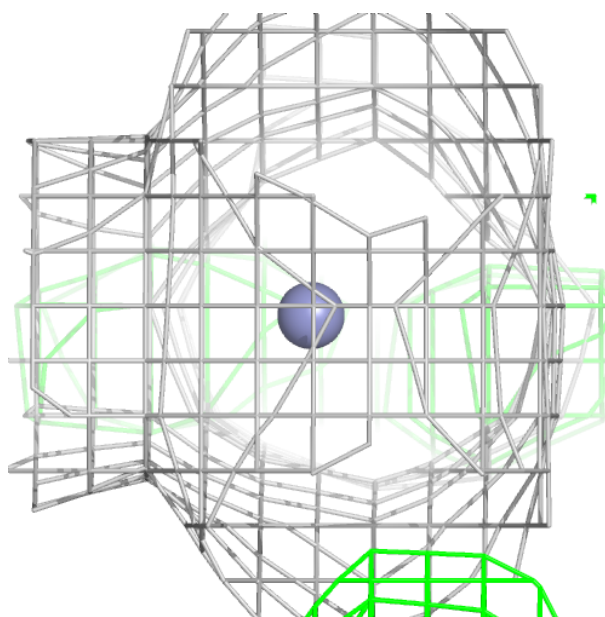
Electron density around ZN G 401:

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



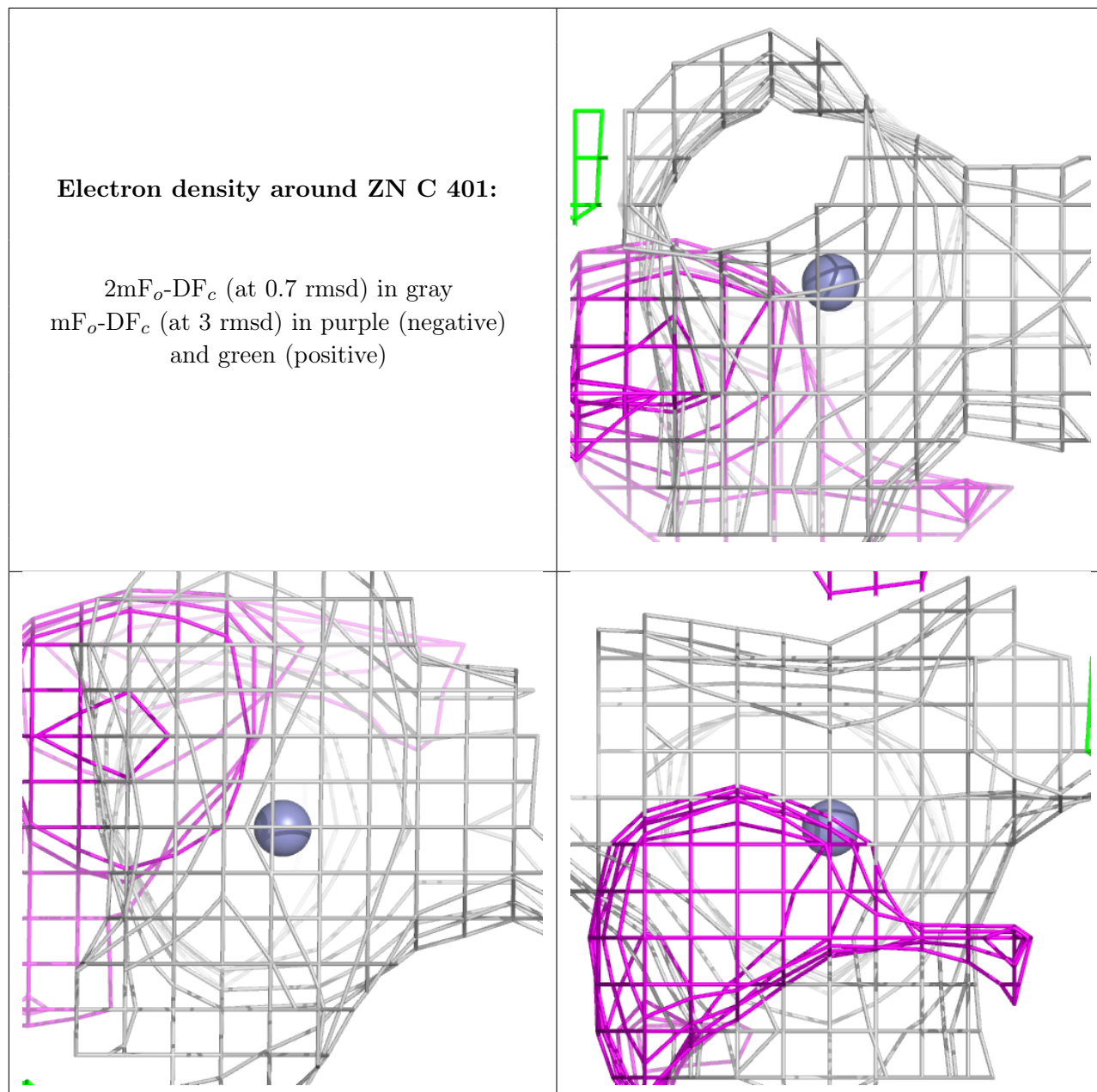
Electron density around ZN D 401:

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



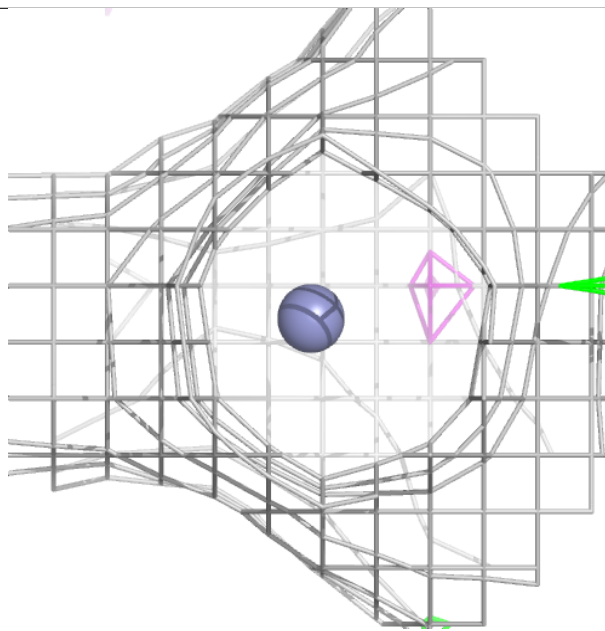
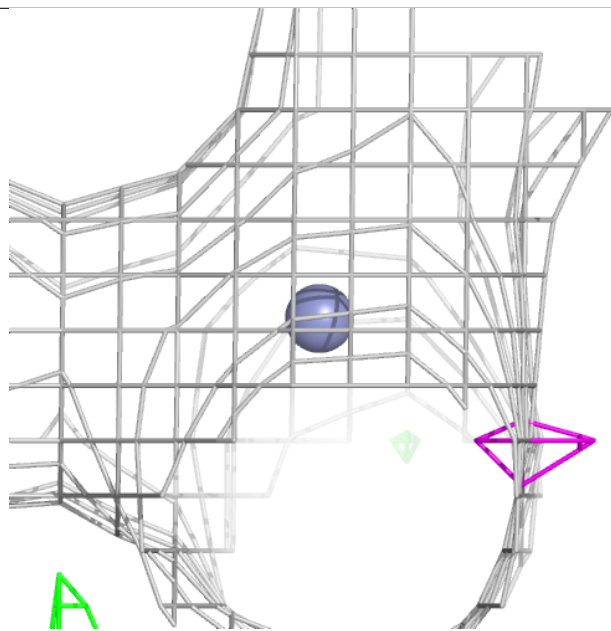
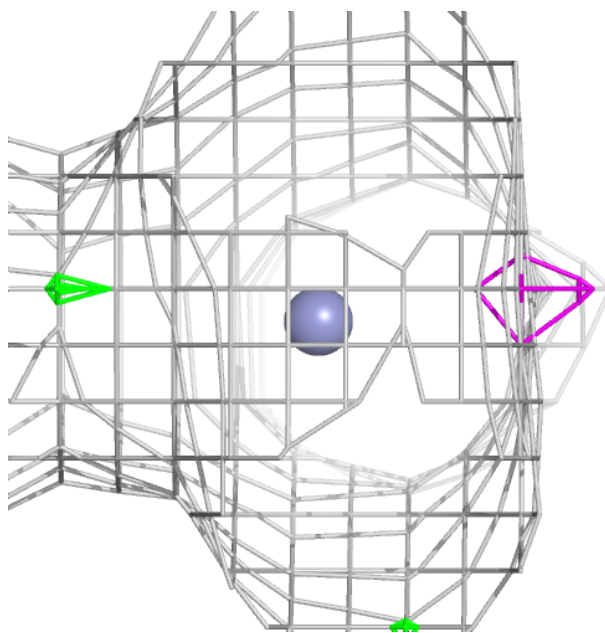
Electron density around ZN C 401:

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



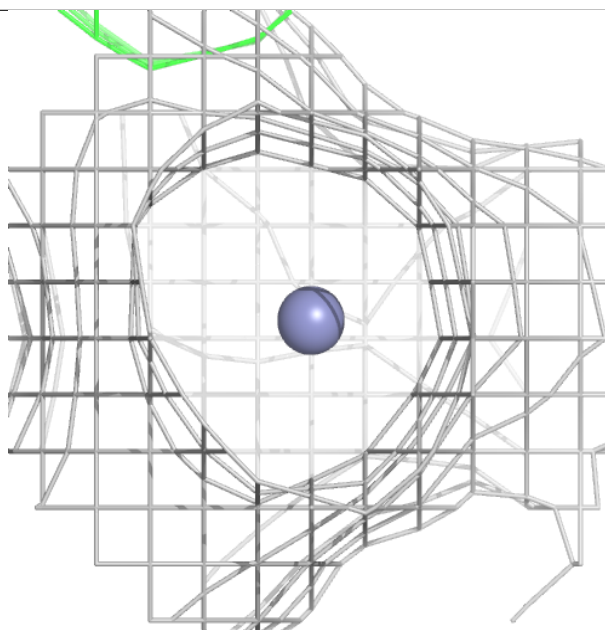
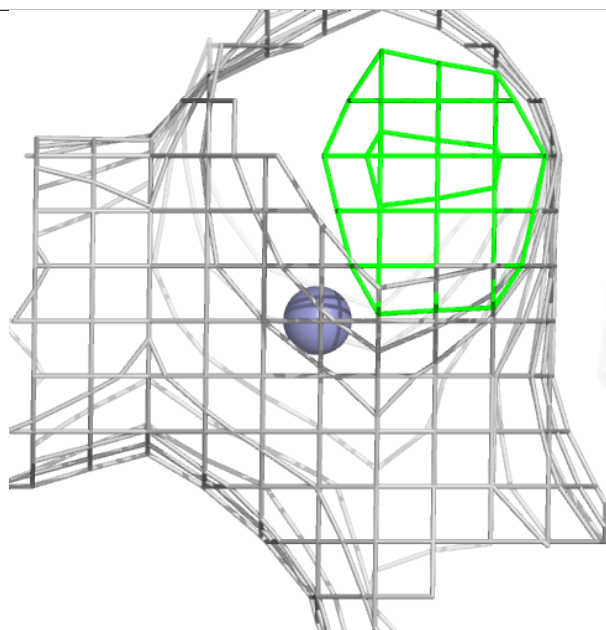
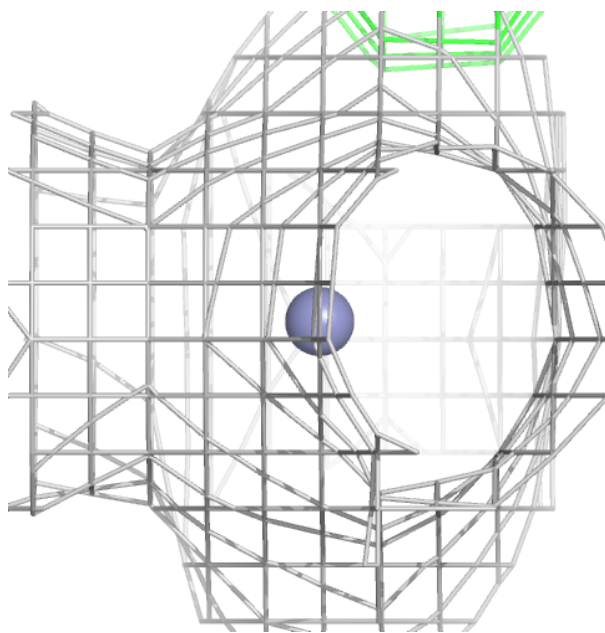
Electron density around ZN E 401:

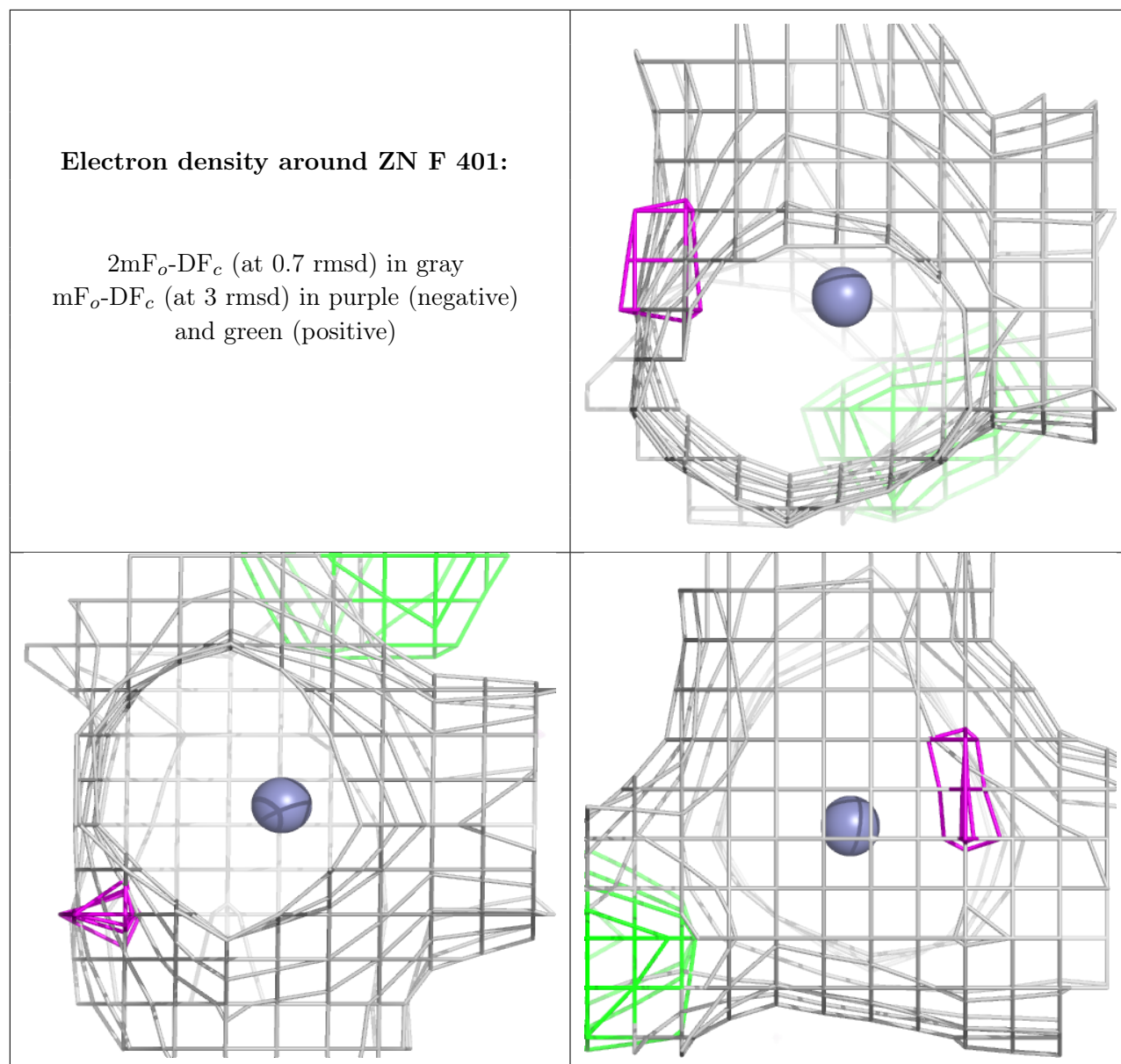
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 401:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.